ICS 75.060

# Gas infrastructure - Quality of gas - Group H 

Infrastructure gazière - Qualite du gaz - Groupe it
Gasinfrastruktur - Beschaffenheit von Gas - Gruppe H

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## Annex $A$ (normative)

# Calculation of methane number of gaseous fuels for engines 

## A. 1 Introduction

The methane number of a gaseous fuel can be calculated from its composition according to several different methods, all of which can give different results. For the purposes of compliance with this European standard the methodology described in this Annex shall be employed.
The method is based on the original data of the research program performed by AVL Deutschland GmbH / 1/ for FVV (the Research Association for Combustion Engines) but employs amendments implemented in 2005 and 2011, by MWM GmbH. These amendments have been unpublished until the publication of this European standard.
The method requires input of composition in the form of volume fractions at reference conditions of $0^{\circ} \mathrm{C}$ and $101,325 \mathrm{kPa}$ and expressed as a percentage. Composition is more likely to be available either as mole fraction (e.g. in the natural gas transmission and distribution industry) or as mass fraction (e.g. in the automotive fuel industry) and conversion to volume fraction shall be performed using the methods in ISO 14912.

Numerical examples are provided so as to enable software developers to validate implementations of the methodology described in this annex. As an aid to validation a relatively large number of decimal places has been retained. For expression of the final result rounding to zero decimal points is recommended.

## A. 2 Calculation of methane number

## A.2.1 Applicability

The method described in this European Standard is applicable to gaseous fuels comprising the following gases: carbon monoxide; butadiene; butylene; ethylene; propylene; hydrogen sulphide; hydrogen; propane; ethane; butane; methane; nitrogen and carbon dioxide. The method treats hydrocarbons other than those specified as butane and is therefore applicable to gaseous fuels containing such higher hydrocarbons.
The numerical examples provided in this annex are appropriate to gases of the second family and hence consider mixtures comprising methane, ethane, propane, butane, nitrogen and carbon dioxide. Hydrogen is also included in one example because of the growing interest in injection of hydrogen into gas pipelines. During the preparation of this standard MWM GmbH has confirmed that the method is applicable to both 2 H and 2 L gases.
Oxygen and water vapour shall be ignored and the fuel gas composition shall be calculated on a dry, oxygen-free basis.

## A.2.2 General approach

The methane number of a gaseous fuel is calculated from its composition in five steps. The steps are outlined below and discussed more fully in turn in A.3. Additional examples are discussed in A.4 and A.5. Table A. 10 provides results of calculations for further software validation purposes.
a) The composition of the gaseous fuel is simplified by converting it into an inert-free mixture comprising the combustible compounds carbon monoxide, ethylene, propylene, hydrogen sulphide, hydrogen, propane, ethane, butane and methane.

For gases of the second family conveyed in pipeline systems carbon monoxide, ethylene, propylene, hydrogen sulphide are unlikely to be present at concentrations that would inspact on methane number and can be ignored.
b) The simplified mixture is sub-divided further into a number of partial ternary mixtures. The number and particular partial ternary mixtures chosen is decided by inspection of available ternary systems in a given order, including those systems that contain the relevant combustible compounds. Selection is ceased when all combustible compounds are contained in at least two ternary systems.
c) The composition and fraction of the selected partial mixtures is adjusted iteratively so as to minimize the difference between the methane numbers of each partial mixture.
d) The methane number of the simplified mixture is determined from the weighted average of the methane number of the selected partial mixtures.
e) Finally, the methane number of the gaseous fuel is calculated by correcting the methane number of the simplified mixture to allow for the presence of inerts in the original fuel gas.

## A. 3 Example 1: 2 H -gas

## A.3.1 Simplification of the composition of the gaseous fuel

The description of the calculation is illustrated by reference to a 2 H -gas of composition shown in Table A.1. The composition of the gas (column 1) is simplified by increasing the quantity of butanes to allow for the presence of butadiene, butylene, pentanes and hydrocarbons of carbon number greater than 5 . The adjustment made is as follows:

- Butadiene and butylene are replaced with an equivalent amount of butanes by multiplying their quantities by 1.
- Pentanes are replaced with an equivalent amount of butanes by multiplying the quantity of pentanes by 2,3 .
- Hydrocarbons of carbon number greater than 5 ("hexanest") are replaced with an equivalent amount of butanes by multiplying the quantity of hexanes + by 5,3 .

In the case of example 1 the quantity of butanes

```
\[
=0,2100+0,1900+(0,0400+0,0500) \times 2,3+0,0600 \times 5,3
\]
\[
=0,9250(\text { Column 2) }
\]
```

The simplified mixture is then re-normalized to $100 \%$ (Column 3).

## A.3.2 Selection of the ternary systems

## A.3.2.1 Ternary mixtures

The ternary mixtures are chosen from the following list:

- A1: Methane-Hydrogen - Ethane
- A2: Propane - Ethane - Butane
- A3: Hydrogen - Propane - Propylene
- A4: Methane-Ethane - Propane
- A5: Methane - Hydrogen - Propane
- A6: Methane - Hydrogen - Butane
- A7: Methane - Propane - Butane
- A8: Methane - Ethane - Butane
- A9: Methane-Ethylene - Butane
- A10: Methane - Hydrogen Sulphide - Butane
- Al1: Methane-Ethane-Hydrogen Sulphide
- A12: Methane - Propylene
- A13: Ethane - Propylene
- A14: Carbon Monoxide - Hydrogen
- A15: Ethane - Ethylene
- A16: Propane-Ethylene
- A17: Butadiene
- A18: Butylene

NOTE Mixtures A12-A16 are clearly not ternary systems; however, for ease of mathematical treatment the coefficients have been adjusted so as to allow the expression of the methane number using a single equation.

## A.3.2.2 Range of applicability of ternary mixture data

The range of applicabllity of most ternary systems is wide (each component can vary from 0 to $1.00 \%$ ). However, for some ternary systems there is a reduced range of applicability. This is a major issue when selecting ternary mixtures. The range of applicability of each ternary system is specified in Table A.2, expressed as maximum and minimum content of each component.

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## A.3.2.3 Factors affecting the ternary system selection process

The ternary systems are selected in accordance with three main considerations:
a) The number of gases in the ternary system that are present in the simplified mixture. Priority is always given to ternary systems that have all three of their components present in the simplified mixture. Systems with two of their components present in the simplified mixture are acceptable if insufficient systems with three components present in the simplified mixture are available.
b) Where there is a choice of ternary systems, the system with the highest fitness, $W_{f}$, takes priority.
c) Each component in the simplified mixture shall be represented in at least two ternary systems.

Fitness of a system is calculated from the following formula:

$$
\begin{equation*}
W_{j}=\sum_{i=1}^{i=n} \frac{V_{i}, \min \left(100,\left(\operatorname{Vmax}_{i, j}+15\right)\right)}{V s u m_{i}} \tag{A.1}
\end{equation*}
$$

where
$n$ is the number of components in the simplified mixture
$V_{i} \quad$ is the volume fraction of component $i$ in the simplified mixture
Vmax ${ }_{i j} \quad$ is the maximum content of component $i$ for the range of applicability of system $j$
Vsum $\quad$ is the sum of all maximum contents of component $i$ for the range of applicability of all systems, i.e.

$$
\begin{equation*}
V \operatorname{sum}_{i}=\sum_{i=1}^{j=18} \min \left(100,\left(V \max _{i, j}+15\right)\right) \tag{A.2}
\end{equation*}
$$

Values of Vsum, are independent of the composition of the simplified mixture. However, $W_{J}$ is dependent upon the composition of the simplifled mixture and so shall be calculated prior to selection. Note that this also means that the choice of ternary mixtures may be different for mixtures containing the same components, but in different proportions.
In the case of example 1, the calculation of Vsum and $W_{j}$ is shown in Tables A. 3 and A.4.

## A.3.2.4 Description of the ternary system selection process

The aim is to identify the optimum number of ternary systems that meet the three criteria described in A.3.2.3 and this is achleved by consideration of each component present in the simplifled mixture in the following sequence:

1) Carbon Monoxide
2) Butadiene
3) Butylene
4) Ethylene
5) Propylene
6) Hydrogen Sulphide
7) Hydrogen

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8) Propane
9) Ethane
10) Butane

## 11) Methane

Step 1: For the first component in the simplified mixture, one ternary system that contains that component is selected. The priority of selection is as follows:
a) Ternary systems with all three components present in the simplified mixture have priority over systems having one or two components present.
b) The ternary mixture with the highest fitness has priority.

Step 2: Consideration is then given to the second component in the simplified mixture. If this component is not present in the ternary system selected for the first component, then a ternary system is selected for this component using the same priority of selection as in step 1. If, however, the ternary system selected for the first component contains the second component, then the selection proceeds for the third component (step 3).
Step 3: Consideration is then given to third, fourth, fifth, etc. components in the same manner as Steps 1-2.
Step 4: When all components in the simplified mixture have been examined once, steps 1.3 are repeated in the same component order. If any component is represented in only one selected ternary mixture, then an additional ternary mixture is selected, again using the same priority of selection as in step 1.
The selection process ends when all components in the simplified mixture are represented in at least two ternary systems.

## In the case of example 1:

- The first component in the simplified mixture is propane and this is present in four ternary systems that have all their components present in the simplified mixture $-A 2, A 4, A 7$ and $A 8$. In this case, $A 4$ is selected because it has the largest value of fitness (ie. 10,3138).
- The second component in the simplified mixture is ethane and this is already represented in system A4, so no ternary mixture is selected.
- The third component of the simplified mixture, butane, is not represented in system A4, so system selection continues and system $A 8$ is selected because it has the highest value of fitness (10,2859).
- The fourth component in the simplified mixture is methane and this is already represented in systems A4 and A8, so no ternary mixture is selected.
- Selection is repeated with the first component in the simplified mixture, propane, and ternary system A7 is selected because it has the next highest value of fitness (9,6263; system A4 has already been selected).

All components in the simplified mixture are now represented in at least two of the ternary systems selected and the selection process ends. The systems selected are cherefore: A4, A7 and A8,

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## A.3.3 Sub-division of the inert-free mixture into the selected partial mixtures

The simplified mixture is dividec into the selected partial ternary mixtures, A preliminary division of the simplified mixture is made by assigning each component equally between the ternary systems in which it is represented.
In the case of example 1, three ternary systems $-A 4, A 7$ and $A 8 \cdots$ are selected. The prellminary division is made by assigning: methane equally between A4, A7 and A8; ethane equally between A4 and A8; propane equally between A4 and A\%; and butanes equally between A7 and A8 (Columns 4, 6 and 8).

## A.3.4 Calculation of the methane number of the partial mixtures

The methane number of each partial mixture is calculated from the general formula

$$
\begin{equation*}
M N_{i}=\sum_{i=0}^{i=7} \sum_{j=0}^{j=6}\left(a_{i, j} x^{i} y^{j}\right) \tag{A.3}
\end{equation*}
$$

Where $x$ and $y$ are the volume fractions of the first and second components in each partial ternary mixture, expressed as a percentage. In order to calculate the methane number of each partial mixture, therefore, the composition of each is normalized to $100 \%$.

In the case of example 1 the composition of each partial mixture is calculated by renormalizing to $100 \%$ (Columns 5, 7 and 9).
'Table A. 2 lists the values of coefficients $a_{i j}$ for the partial ternary systems A1-A18.
In the case of example 1 application of Formula $(A, 3)$ for each preliminary composition of partial mixture results in calculated methane numbers of $76,2489,77,3777$ and 71,9706 for A4, A7 and A8 respectively (Columns 5, 7 and 9).

## A.3.5 Adjustment of the composition and fraction of the partial mixtures

The composition and fraction $\left(F_{t}\right)$ of each partial mixture is adjusted iteratively by varying the quantity of each component in each partial mixture so as to minimize the difference between the methane numbers of each partial mixture.

The value to be minimised is therefore:

$$
\left(M N_{\max }-M N_{\min }\right)
$$

where $M N_{\max }$ and $M N_{\text {min }}$ are the maximum and minimum methane numbers for the selected partial mixtures.

In the case of example 1, three tarnary partial mixtures are selected and hence there are nine quantities to be determined, however four of these may be obtained by material balance considerations.
$N_{\text {A8, methane }}=N_{\text {methane }}-N_{\text {A4, methane }}-N_{\text {A7, methane }}$
$N_{\text {A8, ethane }}=N_{\text {ethane }}-N_{\text {A4 }}$, ethane
$N_{\text {A7, propane }}=N_{\text {propane }}-N_{\text {A4 }}$, propane
$N_{\text {A8, butane }}=N_{\text {butane }}-N_{\text {A7, butane }}$
Where $\mathrm{N}_{t, c o m p}$ is the quantity of the respective component in partial mixture $t$.

The composition and fraction of each partial mixture is therefore performed by adjustment of five quantities: the quantities of methane, ethane and propane in A4, and the quantity of methane and butane in $A 7$.
During adjustment the volume fraction of any component in any partial mixture shall be within the range for which the coefficients of Formula ( $\mathrm{A}, 3$ ) are valid. Table A .2 lists the ranges of validity.

The problem of adjusting the composition and fraction of each partial mixture is therefore a constrained minimization one and in principal any appropriate numerical procedure may be employed, For the examples described in this Annex, the Solver supplied with Microsoft Excel (using default settings) produces an acceptable solution.
Depending upon the ending criterion of the numerical method employed, slight differences in the value of ( $M N_{\max }-M N_{\min }$ ) will result in slightly different values of methane number of the simplified mixture. In addition, the use of different starting values for the composition and fraction of each partial mixture will result in slightly different values of methane number of the simplified mixture. These differences are within the uncertainties of this method and it is recommended that the final value of methane number is rounded to zero decimal places before reporting.
In the case of example 1, the composition and fraction of partial mixtures is provided in Table A. 5 (Columns 4-9). For clarity, the five adjusted quantities are shown in underlined text.

## A.3.6 Calculation of the methane number of the simplified mixture

The methane number of the simplified mixture is determined from the weighted average of the methane number of the relevant partial ternary mixtures:

$$
\begin{equation*}
M N^{\prime}=\sum_{t=1}^{t=N_{\text {sys }}}\left(M N_{t} \cdot F_{t}\right) \tag{A.4}
\end{equation*}
$$

Where
$M N^{\prime}$ is the methane number of the simplified mixture
$M N_{t} \quad$ is the methame number of partial mixture $t$
$F_{t} \quad$ is the fraction of the partial mixture $t$
$N_{\text {sys }}$ is the number of ternary systems selected
In the case of example 1 , this results in a methane number of the simplified mixture of $M N^{\prime}=74,9018$.

## A.3.7 Calculation of the methane number of the gaseous fuel

The methane number of the gaseous fuel is calculated by correcting the methane number of the simplified mixture to allow for the presence of inerts in the original fuel gas:

$$
\begin{equation*}
M N=M N^{\prime}+M N_{\text {inerts }}-M N_{\text {methane }} \tag{A.5}
\end{equation*}
$$

In the original work of AVL/ $1 / M N_{\text {inerts }}$ is the methane number of a methane-carbon dioxide-nitrogen mixture having the same inerts content as that of the original mixture. However in the amendment of MWM the $M N_{\text {inerts }}$ is calculated for a methane-carbon dioxide-nitrogen mixture containing only carbon dioxide and methane. $M N_{\text {methane }}$ is calculated for a methane-carbon dioxide-nitrogen mixture containing pure methane and is equal to 100,0003 .
The methane number of the methane-carbon dioxide-nitrogen mixture is calculated using Formula (A.3). T'able A. 2 lists the appropriate coefficients (system A20).

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In the case of example 1, the methane-carbon dioxide-nitrogen mixture comprises methane (97,8750 volumes, the sum of the volumes of combustible components in the simplified mixture), nitrogen $\{1,0400$ volumes) and carbon dioxide (1,4600 volumes) (Table A.5, column 10), which is normalized to a nitrogenfree mixture comprising methane ( $98,5302 \%$ vol/vol) and carbon dioxide ( $1,4698 \%$ vol/vol) (Table A.5, column 11). Application of Formula (A.3) results in a methane number of $M N_{\text {inerts }}=101,4201$.

Application of Formula (A.5) results th a methane number of the gaseous fuel of

$$
74,9018+101,4201-100,0003=76,33217
$$

The value of methane number is reported as 76.

## A. 4 Example 2: enriched biomethane

## A.4. 1 Simplification of the composition of the gaseous fuel

This example illustrates the calculation for a biomethane derived from anaerobic digestion that has been enriched by addition of propane. The composition is shown in Table A.6.

In the case of example 2 the quantity of butanes

$$
\begin{aligned}
& =0,1461+0,0292 \times 2,3+0,0000 \times 5,3 \\
& =0,2133(\text { Column 2 })
\end{aligned}
$$

The simplified mixture is then re-normalized to $100 \%$ (Column 3).

## A.4.2 Calculation of fitness of the ternary systems

Application of FormuIa (A.1) to example 2 results in the values of $W_{i}$ shown in Table A.7.

## A.4.3 Selection of ternary mixtures

The first component in the simplified mixture is propane and this is present in ternary systems that have all their components present in the simplified mixture $-A 2, A 4, A 7$ and $A 8$. In this case,$A 7$ is selected because it has the largest value of fitness (10,6652).
The second component in the simplified mixture is ethane and this is not represented in system A7, so system selection continues and system A4 is selected because it has the highest value of fitness $(10,6380)$.
The third and fourth components of the simplified mixture are represented in system A7 (butane and methane) and A4 (methane) so the selection process restarts.
The selection process is repeated with the first component in the simplified mixture (propane), which is already represented in selected systems A4 and A7.

Selection continues with the second component in the simplified mixture (ethane), which is represented in only one selected system (A4), so system A8 is selected because it has the next highest value of fitness ( 9,0508 ).
All components of the simplified mixture are represented in at least two systems and so selection ends. The systems selected are therefore: A4, A7 and A8.

## A.4.4 Calculation of the methane number

After preliminary division of the simplified mixture the calculation of methane number according to the methods in A.3.3 to A.3.7 the methane number of the gaseous fuel of example 2 is shown in Table A.5. Again, for clarity, the five adjusted quantities are shown in underlined text. The value of methane number obtained $(69,0336)$ is reported as 69.

## A. 5 Example 3: 2H-gas with hydrogen addition

## A.5.1 Simplification of the composition of the gaseous fuel

This example illustrates the calculation for the 2 H -gas of composition of example 1 to which hydrogen has been added. The composition is shown in Table A.8.
In the case of example 3 the quantity of butanes

$$
\begin{aligned}
& =0,1909+0,1727+(0,0364+0,0455) \times 2,3+0,0545 \times 5,3 \\
& =0,8408(\text { Column } 2)
\end{aligned}
$$

The simplified mixture is then re-normalized to $100 \%$ (Column 3).

## A.5.2 Calculation of fitness of the ternary systems

Application of Formula (A.1) to example 3 results in the values of $W_{1}$ shown in Table A.9.

## A.5.3 Selection of ternary mixtures

The first component in the simplified mixture is hydrogen and this is present in ternary systems that have all their components present in the simplified mixture - A1, A5 and A6. In this case, A1 is selected because it has the largest value of fitness $(10,5906)$.

The second component in the simplified mixture is propane and this is not represented in system A1, so system selection continues and system A5 is selected because it has the largest value of fitness (9,9921),
The third component in the simplified mixture is ethane and this is aiready represented in system A1, so no additional system is selected.
The fourth component in the simplified mixture is butane and this is not represented in the systems already selected. System A6 is selected because it has the largest value of fitness $(9,9668)$.
The fitth component of the simplified mixture (methane) is represented in all three of the systems already selected, so no additional system is required.
Selection is repeated with the first component in the simplified mixture (hydrogen) and thls is already represented in systems $A 1, A 5$ and $A 6$, so no ceddlitional system is required.
Selection is continued with the second component in the simplified mixture (propane) and ternary system A4 is selected because it has the largest value of fitness $(9,7749)$.
The third component in the simplified mixture (ethane) is represented in systems A1 and A4, so no additional system is required.
The fourth component in the simplified mixture (butane) is represented in one system (A6) and so system A8 is selected because it has the next largest value offitness $(7,9495)$.
All components in the simplified mixture are now represented in at least two of the ternary systems selected and the selection process ends. The systems selected are therefore: $A 1, A 4, A 5, A 6$ and $A 8$.

## A.5.4 Calculation of the methane number

In the case of example 3, five ternary partial mixtures are selected and hence there are 15 quantities to be determined, however five of these may be obtained by material balance considerations.

$$
\begin{aligned}
& N_{\text {A8, methane }}=N_{\text {methane }}-N_{\text {A } 1, \text { methane }}-N_{\text {A4 }} \text { methane }-N_{\text {A }, \text { methane }}-N_{\text {A6 }} \text {, methane } \\
& N_{\text {A8, ethane }}=N_{\text {ethane }}-N_{\text {A1 }} \text { ethane }-N_{\text {A4 }} \text { ethane }
\end{aligned}
$$

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$N_{\text {A5 }}$, propane $=N_{\text {propane }}-N_{\text {A4 }}$, propane
$N_{\text {A8 }}$, butane $=N_{\text {butane }}-N_{\text {A6 }}$, butane
$N_{\text {A6, hydrogen }}=N_{\text {hydrogen }}-N_{\text {A5 }}$, hydrogen $-N_{\text {A1 }}$, hydrogen
The composition and fraction of each partial mixture is therefore determined by adjustment of 10 quantities: the quantities of methane, ethane and hydrogen in A1, the quantities of methane, ethane and propane in A4, the quantities of methane and hydrogen in $A .5$ and the quantities of methane and butane in A6.
After preliminary division of the simplified mixture and calculation of methane number according to the methods in A.3.3 to A.3.7 the methone number of the gaseous fuel of example 3 is shown in Table A.8. For clarity, the 10 adjusted quantities are shown in underlined text. The value of methane number obtained $(75,695)$ is reported as 76.

## A.5.5 Additional numerical examples

Table A. 10 provides the results of calculations for a variety of compositions for additional software validation purposes.

Table A. 1 - Worked example of methane number calculation (example 1) - preliminary assignment of partial mixtures

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  | mix A4 |  | mix A7 |  | mixA8 |  |
|  |  |  |  | $N_{A 4, i}$ | $V_{A S, 1}$ | $N_{A 7, i}$ | $V_{A 7,1}$ | $N_{A E, 1}$ | $V_{A 8, i}$ |
| $\because$ - | \% \% vol/vol? | \% | \% voli\% vol | - | \% vorvoir | W | V/vol/vol | 40 | \% voi/vol |
| methane | 90,0900 | 90,0900 | 92,0460 | 30.6820 | 89,7490 | 30,6820 | 96,3968 | 30,6820 | 90,2818 |
| ethane | 5,5400 | 5,5400 | - 5,6603 | $\underline{2.8301}$ | 8,2785 |  |  | 2,8301 | 8,3277 |
| propane | 1,3200 | 1,3200 | 1,3487 | 0.6743 | 1,9725 | 0,6743 | 2,1186 |  |  |
| butanes |  | 0,9250 | 0,9451 |  |  | 0.4725 | 1,4846 | 0,4725 | 1,3905 |
| i-butane | 0,2100 |  |  |  |  |  |  |  |  |
| n -butane | 0,1900 |  |  |  |  |  |  |  |  |
| i-pentane | 0,0400 |  |  |  |  |  |  |  |  |
| n -pentane | 0,0500 |  |  |  |  |  |  |  |  |
| hexanes+ | 0,0600 |  |  |  |  |  |  |  |  |
| nitrogen | 1,0400 |  |  |  |  |  |  |  |  |
| carbon dioxide | 1,4600 |  |  |  |  |  |  |  |  |
| hydrogen | 0,0000 |  |  |  |  |  |  |  |  |
| total | $\cdots 100,0000$ | 997,8750 | - 100,0000 | 34,4865 | 1000000 | 31.8289 | 1000000 | W 3 3,9847 | . 100.0000 |
| Fraction, $F_{t}$ |  |  |  |  | 0,3419 |  | 0,3183 |  | 0,3398 |
| MN: |  |  |  |  | 75,2489 |  | 77,3777 |  | 71,9706 |

Table A. 2 - Components, coefficients and their ranges of validity of Formula (A.1) for the ternary partial mixtures

|  | A1 | A2 | A3 | A4 | A5 | A6 | A7 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $x$ $y$ : $z$ $z$. | methane <br> hydrogen <br> ethane | propane <br> ethane <br> butane | hydrogen <br> propane <br> propyiene | methane ethane propaze | methane <br> hydrogen <br> propane | methane <br> hydrogen <br> butane | methane propane butane |
| $a(0,0)$ | 4,3628190E+01 | 1,0245130E+01 | 1,8627940E+01 | 3,3539090E+01 | 3,4758040E+01 | 1,2299020E -01 | 1,0169140E+01 |
| $a(1,0)$ | -9,2508870E-02 | 8,5906610E-02 | -1,2035810E-01 | -1,0282240E-01 | -5,1949050E-01 | -7,5182070E-01 | 4,3666120E-01 |
| $\mathrm{a}(0,1)$ | -1,0488580E-02 | 1,4982130E-01 | 1,0871090E-01 | 2,0683750E-01 | 5,4737050E-02 | -4,5103700E-01 | 3,8170960E-02 |
| $\mathrm{a}(2,0)$ | 1,6449270E-02 | 7,3843960E-03 | 1,9298010E-02 | 2,3981410E-02 | 4,4054490E-02 | 5,1433330E-02 | -8,7264540E-02 |
| $a\{1,1\}$ | $-2,5007730 \mathrm{E}-03$ | \$,5705040E-03 | -1,3050630E-03 | 3,3161370E-03 | 2,64253108-02 | 5,1261470]-02 | -7,9478640E-03 |
| $a(0,2)$ | -4,3202740E-03 | 5,1369710E-03 | 1,7985000E-03 | -3,5536890E-03 | $-1,0567810 \mathrm{E}-02$ | 1,7866300E-02 | 1,0365010E-02 |
| $a(3,0)$ | -3,1191690E-04. | -1,0036620E-04 | -1,3018080E-03 | -9,5847460E-04 | -8,7433290E-04 | -1,0241590E-03 | 5,9397950E-03 |
| $a(2,1)$ | $-6,0486960 \mathrm{E}-05$ | -2,0203270E-04 | 2,9904470E-05 | -2,4096040E-06 | -1,0846450E-03 | -1,6406520E-03 | 3,2678860E-04 |
| a $(1,2)$ | -5,3528010 ${ }^{\text {- }}$-05 | -4,5802770E-05 | 8,5613760E-05 | 3,9418400E-05 | -3,5553270E-04 | -1,0022400E-03 | 2,3714910E-04 |
| a $(0,3)$ | 6,8507420E-05 | -5,6856150E-05 | -2,5836670E-05 | 5,0018560E-05 | 2,2897690E-04 | -1,4279120E-04 | -1,6152150E-04 |
| a $(4,0)$ | 2,1223340E-06 | 4,1273050E-07 | 4,1692950E-05 | 2,0052880E-05 | 5,4767420E-06 | 6,6995630E-06 | -1,8541270E-04 |
| a $(3,1)$ | 2,1993700E-06 | 1,2511380E-06 | 2,0011240E-07 | 3,4585100E-06 | 1,1309800E-05 | 1,5661210E-05 | -3,3085860E-07 |
| $a(2,2)$ | 1,2109690E-06 | 3,1147030E-07 | -6,8546460E-07 | 8,0364540E-07 | 7,9874880E-06 | 1,5763060E-05 | -4,9758630E-06 |
| 2(1,3) | 2,9706580E-07 | -3,1401570E-07 | -6,2626130E-07 | -4,3338760E-07 | 7,4860850E-07 | 5,2498880E-06 | -8,7822910E-07 |
| 2(0,4) | -6,7138020E-07 | 2,4039480E-07 | 1,1987890E-07 | -2,5042560E-07 | -1,6340240E-06 | 0,0000000E +00 | 7,7408400E-07 |
| $a(5,0)$ | 0,0000000E +00 | $0,0000000 \mathrm{E}+00$ | -6,9526380E-07 | -2,1154170E-07 | 0,0000000E+00 | 0,0000000E $\div 00$ | 2,9565980E-06 |
| $a(6,0)$ | $0,0000000 \mathrm{E}+00$ | $0,0000000 \mathrm{E}+00$ | 5,7989840E-09 | 9,0540200E-10 | $0,0000000 \mathrm{E}+00$ | 0,0000000E+00 | $-2,33707<0 \mathrm{E}-08$ |
| $a(7,0)$ | $0,0000000 \mathrm{E}+00$ | 0,0000000E +00 | -1,9133740E-11 | 0,0000000E -00 | 0,0000000E -00 | 0,0000000E+00 | 7,3223480E-11 |
| a 00.5 ) | 0,0000000E+00 | 0,0000000E +00 | 0,0000000E+00 | 0,0000000E+00 | 0,0000000E +00 | 0,0000000E+00 | 0,0000000E $\div 00$ |
| a 00,6 ] | 0,0000000E +00 | 0,0000000E +00 | 0,0000000E +00 | 0,0000000E +00 | 0,0000000E +00 | $0,0000000 \mathrm{E}+00$ | 0,0000000 $\div 00$ |
| $x$ (max), \% vol/vol | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 |
| $x$ (min), \% vol/ rol | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 |
| $y$ (max), \% vol/vol | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 |
| $\nu$ (min), \% vol/vol | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 |
| $z$ (max), \% vol/ vol | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 |
| $z$ (min), \% vol/vol | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 |

Table A. 2 (continued)

|  | A8 | A9 | A10 | A. 11 | A12 | A13 | A14 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $x$ $y:$ $z$ $z$ | methane <br> ethane <br> butane | methane <br> ethylene <br> butane | methane hydrogen sulphide butane | methane ethane hydrogen sulphide | methane <br> propylene | ethane propylene | carbon monoxide bydrogen |
| $2(0,0)$ | 1,0777610E+01 | $-2,2408570 \mathrm{E}+05$ | 1,8388506E+05 | $-1,1788466 \mathrm{E} \div 05$ | 5,9095515E*01 | 3,1550700E+01 | 0,0000000E +00 |
| $a(1,0)$ | 1,6474900E-01 | $1,1938458 \mathrm{E}+04$ | $-1,5396773 \mathrm{~F} \div 04$ | 1,1251043E+04 | 1,0602705E-01 | 7,9749400E-02 | $1,5000000 \mathrm{~F}+00$ |
| $2(0,1)$ | -1,4050070E-01 | $-1,9962282 \mathrm{E} \div 02$ | $-1,4160386 \mathrm{E} \div 01$ | $-2,67125 \pm 9 \mathrm{E}+02$ | $-3,4069240 \mathrm{E}+00$ | -1,7706875E-01 | 0,0000000E +00 |
| $a(2,0)$ | -5,1987300E-02 | $-4,8574811 \mathrm{E}+02$ | $5,4158924 \mathrm{E}+02$ | $-4,5492745 \mathrm{E} \div 02$ | -3,1884830E-03 | 4,8659675E-04 | $-7,5000000 \mathrm{E}-03$ |
| $2(1,1)$ | -7,0448690E-03 | 7,8748002E+00 | 5,6775484E-01 | 1,0645736E+01 | 0,0000000E $\div 00$ | 0,0000000E +00 | $-7,5000000 \mathrm{E}-03$ |
| $a(0,2)$ | 1,6154370E-02 | 2,5929804E $\div 00$ | 1,1942148E -00 | 3,6669 $21 \mathrm{E}+00$ | 1,5370325E-01 | 4,8659675E-04 | $0,0000000 \mathrm{E}+00$ |
| a(3,0) | 3,9913150E-03 | 1,0855881E+01 | $-1,0358971 \mathrm{E}+01$ | 1,0120505E+01 | -1,0801210E-04 | 0,0000000E+00 | 0,0000000E+00 |
| $a(2,1)$ | 1,4794820E-04 | -1,0256703E-01 | -7,7071033E-03 | -1,3986048E-01 | $0,0000000 \mathrm{E}+00$ | 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 $\div 00$ |
| $a(0,3)$ | -1,7545700E-04 | -1,4,504600E-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 | 1,1503083E-01 | -1,3401172E-01 | 8,4599300E-06 | 0,0000000E+00 | $0,0000000 \mathrm{E}+00$ |
| $a(3,1)$ | 2,7564440E-06 | 4,4431373E-04 | 3,3083382E-05 | 6,0764355E-04 | $0,0000000 \mathrm{E}+00$ | $0,0000000 \mathrm{E}+00$ | 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 $\div 00$ |
| $a(1,3)$ | -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-0¢ | 1,0579750E-03 | -1,3928745E-07 | 0,0000000E+00 | 0,0000000E +00 |
| $a(6,0)$ | -1,5580170E-08 | -4,9703336E-06 | 2,6162473E-06 | -4,6175613E-06 | 7,1638300E-10 | $0,0000000 \mathrm{E}+00$ | 0,0000000E+00 |
| $a(7,0)$ | 4,7976930E-11 | 9,2406348E-09 | -3,7606039E-09 | 8,6063163E-09 | $0,0000000 \mathrm{E}+00$ | $0,0000000 \mathrm{E}+00$ | $0,0000000 \mathrm{E} \div 00$ |
| $2\{0,5)$ | $0,0000000 \mathrm{E}+00$ | 0,0000000E +00 | $-3,5650030 \mathrm{E}-05$ | 0,0000000E +00 | -2,9054230E-07 | 0,0000000E+00 | 0,0000000E $\div 00$ |
| $\mathrm{a}(0,6)$ | 0,0000000E +00 | 0,0000000E +00 | 3,0668448E-07 | 0,0000000E+00 | 7,1638300E-10 | 0,0000000E+00 | $0,0000000 \mathrm{E}+00$ |
| $x$ (max), \% vol/vol | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 | 100,0 |
| $x(\mathrm{~min}), \% \mathrm{vol} / \mathrm{vol}$ | 0,0 | 75,0 | 75,0 | 75,0 | 0,0, | 0,0 | 0,0 |
| $y$ (max), \% vol/vol | 200,0 | 25,0 | 25,0 | 25,0 | 100,0 | 200,0 | 100,0 |
| $y$ (min $), \% \mathrm{vol} / \mathrm{vol}$ | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 |
| $z$ (max), \% vol/vol | 100,0 | 25,0 | 25,0 | 25,0 |  |  |  |
| $z($ min $), \% \mathrm{vol} / \mathrm{vol}$ | 0,0 | 0,0 | 0,0 | 0,0 |  |  |  |


|  | A15 | A16 | A17 | A18 | A20 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| x: | ethane <br> ethylene | propane <br> ethylene | butadiene | butylene | methane carbon dioxide nitrogen |
| a $(0,0)$ | 2,9655595E+01 | 2,4494755E -01 | 1,2000000E+01 | 2,0000000E+01 | 2,99174308+02 |
| a( 1,0 ] | 1,7064685E-01 | 1,3676575E-01 | 0,0000000E+00 | 0,0000000E+00 | $-1,5119580 \mathrm{E}+01$ |
| $2(0,1)$ | -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 -0.0 | 7,6359480E-01 |
| a $1,1,1)$ | 0,0000000E -00 | 0,0000000E+00 | 0,0000000E+00 | 0,0000000E +00 | 4,5489690E-02 |
| $2(0,2)$ | -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 |
| $\mathrm{a}(2,1)$ | 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 24,0$)$ | 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 | $0,0000000 \mathrm{E}+00$ | 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 $\div 00$ | 0,0000000푸0 | 6,6993640E-05 |
| a $(5,0)$ | 0,0000000E+00 | 0,0000000E -00 | 0,0000000E $\div 0$ | 0,0000000E +00 | -4,6077260E-06 |
| a $(6,0)$ | 0,0000000E+00 | 0,0000000E+00 | 0,0000000E+00 | 0,0000000E+00 | 2,61057008-08 |
| a $2(7,0)$ | 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 $), \% \mathrm{vol} / \mathrm{vol}$ | 0,0 | 0,0 | 100,0 | 100,0 | 50,0 |
| $y$ (max), \% vol/vol | 100,0 | 100,0 |  |  | 30,0 |
| $y$ (min), \% vol/vol | 0,0 | 0,0 |  |  | 0,0 |
| $z$ (max), \% vol/vol |  |  |  |  | 50,0 |
| $z(\mathrm{~min}), \% \mathrm{vol} / \mathrm{vol}$ |  |  |  |  | 0,0 |

Table A. 3 - Calculation of Vsumi

|  | $\min \left\{100,\left(\operatorname{Tmax} x_{i j}+15\right)\right)$ |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| System | CO | Butadiene | Butylene | Ethylene | Propylene | $\mathrm{H}_{2} \mathrm{~S}$ | Hydrogen | Propane | Ethane | Butane | Methane |
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 100 | 0 | 100 |
| 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 100 | 100 | 0 |
| 3 | 0 | 0 | 0 | 0 | 100 | 0 | 100 | 100 | 0 | 0 | 0 |
| 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 100 | 0 | 100 |
| 5 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 100 | 0 | 0 | 100 |
| 6 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 100 | 100 |
| 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 100 | 100 |
| 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 100 | 100 |
| 9 | 0 | 0 | 0 | 40 | 0 | 0 | 0 | 0 | 0 | 40 | 100 |
| 10 | 0 | 0 | 0 | 0 | 0 | 40 | 0 | 0 | 0 | 40 | 100 |
| 11 | 0 | 0 | 0 | 0 | 0 | 40 | 0 | 0 | 40 | 0 | 100 |
| 12 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 100 |
| 13 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 100 | 0 | 0 |
| 14 | 100 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 |
| 15 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 100 | 0 | 0 |
| 16 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 100 | 0 | 0 | 0 |
| 17 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 18 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Vsumit | 100 | 100 | 100 | 240 | 300 | 80 | 500 | 600 | 640 | 480 | 1000 |

Table A. 4 - Calculation of fitness, $W_{j}$ (example 1)

|  | $V_{i}$ |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | co | Butadiene | Butylexe | Ethylene | Propylene | $\mathrm{H}_{2} \mathrm{~S}$ | Hyărogen | Propane | Ethane | Butane | Methane |  |
|  | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 1,3487 | 5,6603 | 0,9451 | 92,0460 |  |
|  | $\mathrm{V}_{\text {sum }_{i}}$ |  |  |  |  |  |  |  |  |  |  |  |
| System | co | Butadiene | Butylene | Ethylere | Propylene | $\mathrm{H}_{2} \mathrm{~S}$ | Hydrogen | Propane | Ethane | Butane | Methane | Wi |
| 1 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,8844 | 0,0000 | 9,2046 | 10,0890 |
| 2 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,2248 | 0,8844 | 0,7969 | 0,0000 | 1,3061 |
| 3 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,2248 | 0,0000 | 0,0000 | 0,0000 | 0,2248 |
| 4 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,2248 | 0,8844 | 0,0000 | 9,2046 | 10,3138 |
| 5 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,2248 | 0,0000 | 0,0000 | 9,2046 | 9,4294 |
| 6 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,1969 | 9,2046 | 9,4015 |
| 7 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,2248 | 0,0000 | 0,1969 | 9,2046 | 9,5263 |
| 8 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,8844 | 0,1969 | 9,2046 | 10,2859 |
| 9 | 0.0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0788 | 9,2046 | 9,2834 |
| 10 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0788 | 9,2045 | 9,2834 |
| 11 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,3538 | 0,0000 | 9,2046 | 9,5584 |
| 12 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 9,2046 | 9,2046 |
| 13 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,8844 | 0,0000 | 0,0000 | 0,8844 |
| 14 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 |
| 15 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,8844 | 0,0000 | 0,0000 | 0,884.4 |
| 16 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,2248 | 0,0000 | 0,0000 | 0,0000 | 0,2248 |
| 17 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 |
| 18 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 |

Table A. 5 - Worked example of methane number calcalation (composition 1) - final calculation

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  | mix $\mathrm{A}_{4}$ |  | mix A7 |  | mix A8 |  | mix A 20 |  |
|  |  |  |  | $N_{A 4, i}$ | $V_{A 4, i}$ | ${ }^{N_{A 7, i}}$ | $V_{A Z, i}$ | $N_{A 8, i}$ | $V_{A B, i}$ | $N_{A 20, i}$ | $\nabla_{A 20, i}$ |
|  | \% vol/vol | $\because$ | \%\% vol/vol | 疗 | \%\%vi/vol | \% | \% \% \% \% vol | 26 | \% vol/fol | \% | \% vol/vol |
| metane | 90,0900 | 90,0900 | 92,0460 | $\underline{27.9390}$ | 88,7108 | $\underline{27.3417}$ | 95,8205 | 36,7653 | 91,9793 | 97,8750 | 98,5302 |
| ethane | 5,5400 | 5,5400 | 5,6603 | 2.9012 | 9,2119 |  |  | 2,7590 | 6,9025 |  |  |
| propane | 1,3200 | 1,3200 | 1,3487 | 0.6542 | 2,0773 | 0,6944 | 2,4337 |  |  |  |  |
| butanes |  | 0,9250 | 0,9451 |  |  | 0.4982 | 1,7458 | 0,4469 | 1,1181 |  |  |
| i-butane | 0,2100 |  |  |  |  |  |  |  |  |  |  |
| n-butane | 0,1900 |  |  |  |  |  |  |  |  |  |  |
| i-pentane | 0,0400 |  |  |  |  |  |  |  |  |  |  |
| n-pentane | 0,0500 |  |  |  |  |  |  |  |  |  |  |
| hexanes+ | 0,0600 |  |  |  |  |  |  |  |  |  |  |
| nitrogen | 1,0400 |  |  |  |  |  |  |  |  | 1,0400 | 0,0000 |
| carbon dioxide | 1,4600 |  |  |  |  |  |  |  |  | 1,4600 | 1,4698 |
| hydrogen | 0,0000 | 0,0000 | 0,0000 |  |  |  |  |  |  |  |  |
| total | 100,0000 | \% 97, ${ }^{\text {8it }}$ | 100,0000 |  | 100,0000 | - 28,5343 | 1000000 |  | 1000000 | 10033750 | 100,0000 |
| Fraction, $F_{t}$ |  |  |  |  | 0,3149 |  | 0,2853 |  | 0,3997 |  |  |
| M ${ }_{\text {c }}$ |  |  | - |  | 74,9017 |  | 74,9019 |  | 74,9019 |  | 101,4201 |
|  |  |  |  |  |  |  |  |  |  |  |  |
| $\triangle M N$ | 0,000 | 262 |  |  |  |  |  |  |  |  |  |
| $3 N^{\prime}$ | 74,9 | 018 |  |  |  |  |  |  |  |  |  |
| $M N$ | 76,3 | 217 |  |  |  |  |  |  |  |  |  |

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Table A. 6 - Worked example of methane number calcutation (example 2) - final calculation

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  | mixa4 |  | mix A7 |  | mix 48 |  | mix A20 |  |
|  |  |  |  | $N_{A 4,1}$ | $V_{A 4, i}$ | $N_{A 7, i}$ | $V_{A 7, i}$ | $N_{A 8, i}$ | $V_{A 8, i}$ | $N_{\text {A20, }}$ | $V_{A 20, i}$ |
| \% vol/vol |  |  | \% vol/vol | \% vol/vol |  |  | \% vol/vol | \% vol/vol |  | \% vol/vol |  |
| methane | 86,6475 | 86,6475 | 89,8575 | 41.1188 | 88,8181 | 46.3797 | 90,6616 | 2,3590 | 92,5995 | 96,4277 | 96,3911 |
| ethane | 0,1169 | 0,1169 | 0,1212 | 0.0585 | 0,1263 |  |  | 0,0628 | 2,4632 |  |  |
| propane | 9,4500 | 9,4500 | 9,8001 | 5.1182 | 11,0556 | 4,6819 | 9,1520 |  |  |  |  |
| butanes |  | 0,2133 | 0,2212 |  |  | $\underline{0,0954}$ | 0,1854 | 0,1258 | 4,9373 |  |  |
| i-butane | 0,0000 |  |  |  |  |  |  |  |  |  |  |
| n-butane | 0,1461 |  |  |  |  |  |  |  |  |  |  |
| i-pentane | 0,0000 |  |  |  |  |  |  |  |  |  |  |
| n-pentane | 0,0292 |  |  |  |  |  |  |  |  |  |  |
| hexanes+ | 0,0000 |  |  |  |  |  |  |  |  |  |  |
| nitrogen | 0,0000 |  |  |  |  |  |  |  |  | 0,0000 | 0,0000 |
| carbon dioxide | 3,6103 |  |  |  |  |  |  |  |  | 3,6103 | 3,6089 |
| hydrogen | 0,0000 | 0,0000 | 0,0000 |  |  |  |  |  |  |  |  |
| total | 100,0000 | 96,4277 | 100,0000 | 46,2955 | 100,0000 | 51,1569 | 100,0000 | 2,5476 | 100,0000 | 100,0380 | 100,0000 |
| Fraction, $F_{t}$ |  |  |  |  | 0,4630 |  | 0,5116 |  | 0,0255 |  |  |
| $M N_{t}$ |  |  |  |  | 65,3039 |  | 65,3059 |  | 65,3039 |  | 103,7290 |


| $\triangle M N$ | 0,002016 |
| :--- | ---: |
| $M N^{\prime}$ | 65,3049 |
| $M N$ | 69,0336 |

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Table A. 7 - Calculation of fituess, $W_{j}$ (example 2)


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Table A. 8 - Worked example of methane number calculation (example 3) - final calculation

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 理 | 12 | 13 | 14 | 15 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  | mix A1 |  | mix A4 |  | mixa5 |  | mixas |  | mixa8 |  | mix A20 |  |
|  |  |  |  | $N_{A 1,1}$ | $V_{A 1, i}$ | $N_{A 4, i}$ | $V_{A 4, i}$ | ${ }^{N_{A 5, i}}$ | $v_{A 5, i}$ | $N_{A 6, i}$ | ${ }^{\text {V }}$ A6, | $N_{A B, \text { i }}$ | $\nabla_{A 8, i}$ | $N_{\text {A2O,i }}$ | $V_{4} 20, i$ |
|  | \% vol/vol | $\therefore$ : | \% vol/vol | $\bigcirc$ | \% vol/vol | < | \% vol/vol | 8, | \% voi/vol | \% \% | \% vol\% \%ol | ¢ $\quad 1$ | \% vol/wol | \% | \% yol/vol |
| methane | 85,991 | 85,991 | 87,685 | 14.001 | 80,221 | 16.424 | 88,778 | 14.270 | 84,092 | 15.601 | 89,710 | 27,389 | 92,258 | 98,068 | 98,665 |
| ethane | 5,036 | 5,036 | 5,136 | 1667 | 9,549 | 1.509 | 8,645 |  |  |  |  | 1,870 | 6,298 |  |  |
| propane | 1,200 | 1,200 | 1,224 |  |  | $\underline{0.477}$ | 2,577 | 0,747 | 4,402 |  |  |  |  |  |  |
| butanes |  | 0,841 | 0,857 |  |  |  |  |  |  | 0.429 | 2,465 | 0,429 | 1,444 |  |  |
| i-butane | 0,191 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| n-butane | 0,173 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| i-pentane | 0,036 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| n-pentane | 0,046 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| hexanest | 0,055 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| nitrogen | 0,946 |  |  |  |  |  |  |  |  |  |  |  |  | 0,946 | 0,000 |
| carbon dioxide | 1,327 |  |  |  |  |  |  |  |  |  |  |  |  | 1,327 | 1,335 |
| hydrogen | 5,000 | 5,000 | 5,099 | 1,785 | 10,229 |  |  | 1,952 | 11,506 | 1,361 | 7,824 |  |  |  |  |
| Eotat | 100,000 | 98,068 | 100,000 | 17,453 | 100,000 | : 18,500 | 100000 | 16,969 | 100,000 | 173,91 | - -1000000 | 29,687 | -100,000 | 100;341 | 100,000 |
| Fraction, $F_{5}$ |  |  |  |  | 0,175 |  | 0,185 |  | 0,170 |  | 0,174 |  | 0,297 |  |  |
| $M N_{5}$ |  |  |  |  | 74,411 |  | 74,411 |  | 74,411 |  | 74,411 |  | 74,411 |  | 101,284 |


| $\triangle M N$ | 0,00012 |
| :--- | ---: |
| $M N^{\prime}$ | 74,411 |
| $M N$ | 75,695 |

Table A. 9 - Calculation of fitness, $W_{j}$ (example 3)

|  | $V_{i}$ |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | co | Butadiene | Butylene | Ethylene | Propylene | $\mathrm{H}_{2} \mathrm{~S}$ | Hydrogen | Propane | Ethane | Butane | Methane |  |
|  | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 5,0985 | 1,2236 | 5,1356 | 0,8574 | 87,6849 |  |
|  | $V_{i} \cdot V_{\text {max }}{ }_{\text {i, }}$ |  |  |  |  |  |  |  |  |  |  |  |
| System | CO | Butadiene | Butylene | Ethylene | Propylene | $\mathrm{H}_{2} \mathrm{~S}$ | Hydrogen | Propane | Ethane | Butane | Methane | $W_{f}$ |
| 1 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 1,0197 | 0,0000 | 0,8024 | 0,0000 | 8,7685 | 10,5906 |
| 2 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,2039 | 0,8024 | 0,1786 | 0,0000 | 1,1850 |
| 3 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 1,0197 | 0,2039 | 0,0000 | 0,0000 | 0,0000 | 1,2236 |
| 4 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,2039 | 0,8024 | 0,0000 | 8,7685 | 9,7749 |
| 5 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 1,0197 | 0,2039 | 0,0000 | 0,0000 | 8,7685 | 9,9921 |
| 6 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 1,0197 | 0,0000 | 0,0000 | 0,1786 | 8,7685 | 9,9668 |
| 7 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,2039 | 0,0000 | 0,1786 | 8,7685 | 9,1510 |
| 8 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,8024 | 0,1786 | 8,7685 | 9,7495 |
| 9 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0714 | 8,7685 | 8,8399 |
| 10 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0714 | 8,7685 | 8,8399 |
| 11 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,3210 | 0,0000 | 8,7685 | 9,0895 |
| 12 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 8,7685 | 8,7685 |
| 13 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,8024 | 0,0000 | 0,0000 | 0,8024 |
| 14 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 1,0197 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 1,0197 |
| 15 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,8024 | 0,0000 | 0,0000 | 0,8024 |
| 16 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,2039 | 0,0000 | 0,0000 | 0,0000 | 0,2039 |
| 17 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 |
| 18 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 | 0,0000 |

Table A. 10 - 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 |  |  |  |
| ethame | 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 |
| pertane |  | 0,10 | 0,20 |  | 0,11 | 0,51 | 0,82 |  |  |  |  |  |  |  |  |  |
| hexanes+ |  |  |  |  | 0,20 |  | 0,60 |  |  |  |  |  |  |  |  |  |
| hydrogen sulphide |  |  |  |  |  |  |  |  |  |  |  | 5 |  | 5 | 10 |  |
| total | 100,00 | 100,00 | 100,00 | 100,00 | 100,00 | 100,00 | 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 | 21,55 | 53,20 | 41,25 | 19,59 | 35,01 | 23,89 | 44,15 | 30,45 | 10,04 |
| Ternary mixtures selected | $\begin{aligned} & \mathrm{A} 1 \\ & \mathrm{~A} 4 \end{aligned}$ | A4 <br> A7 <br> A8 | $\begin{aligned} & \text { A4 } \\ & \text { A7 } \\ & \text { A8 } \end{aligned}$ | $\begin{aligned} & \text { A4 } \\ & \text { A7 } \\ & \text { A8 } \end{aligned}$ | $\begin{aligned} & \text { A4 } \\ & \text { A7 } \\ & \text { A8 } \end{aligned}$ | A4 <br> A.7 <br> A8 | $\begin{aligned} & \text { A4 } \\ & \text { A7 } \\ & \text { A8 } \end{aligned}$ | $\begin{aligned} & \text { A1 } \\ & \text { A3 } \\ & \text { A5 } \\ & \text { A6 } \\ & \text { A8 } \end{aligned}$ | $\begin{aligned} & \text { AI } \\ & \text { A5 } \\ & \text { A6 } \\ & \text { A7 } \\ & \text { A8 } \end{aligned}$ | $\begin{gathered} \text { A1 } \\ \text { A6 } \\ \text { A7 } \\ \text { A8 } \\ \text { A9 } \\ \text { A12 } \end{gathered}$ | AI | A6 | A1 | A5 | A1 | A1 |
|  |  |  |  |  |  |  |  |  |  |  | A3 | $A^{7}$ | A2 | A6 | A 5 | A3 |
|  |  |  |  |  |  |  |  |  |  |  | A6 | A8 | A 3 | A7 | A6 | A5 |
|  |  |  |  |  |  |  |  |  |  |  | A7 | A9 | A6 | A8 | AT | A6 |
|  |  |  |  |  |  |  |  |  |  |  | A12 | A10 | A13 | A10 | A10 | A8 |
|  |  |  |  |  |  |  |  |  |  |  | A15 | A11 | A14 | A11 | A11 |  |
|  |  |  |  |  |  |  |  |  |  |  | A16 | A12 | A15 |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  | A16 |  |  |  |

