EBOOK

Michael Andre Franiatte

Excel
Equation of State Resolution for the Study of Fluids

EoSResol.xls

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Before the past nobody had created a tool to calculate the behavior of fluids without the need of using experimental measures. The Excel sheet with VBA macro presented here can correlate all data on fluids with a simple table available with the instructions here. Information about license, EULA and contract for using these following works can be found at https://michaelfraniatte.wordpress.com.

Excel Equation of State Resolution for the Study of Fluids

Michael Franiatte*

Abstract

It's possible with this book and the book "An Equation of State Resolution for the Study of Fluids" by the same author to calculate and verify all the data on fluids at high temperature and high pressure find on all scientific papers talking about the properties *PVTX* and of reactions for fluids from 1 to 8 constituents. Fluids data can be correlated with numerous measurement and fitting studies and the program presented here which use simple parameters with an equation of state (EOS) resolved, corrected and finalized. The book with the VBA macro in a command button put in a Excel sheet, allows resolving *PVTX* and reaction data of fluids combined with only four parameters describing a gas (molar mass and the three critical parameters) without binary interaction coefficient. The readers whom apply the instructions can find and verify the good agreement with the volumes observed by the studies made by the Scientifics in the past. The properties of fluids as well as the properties of the reactions occurring in the fluids are deduced while applying the instructions in this book. The studies of Scientifics whom were working on EOS can be compared by everyone with the Excel sheet made with this book. The equation of state resolution with this easy access by everyone, whom apply the instructions here for calculating volumes, fugacities, pure fugacities functions of pressure, temperature and molar fractions, is important to understand and correlate all the data on the fluids and the reactions acquired until this day.

Keywords: *fluids, PVTX properties, reactions, excel, macro, equation of state*

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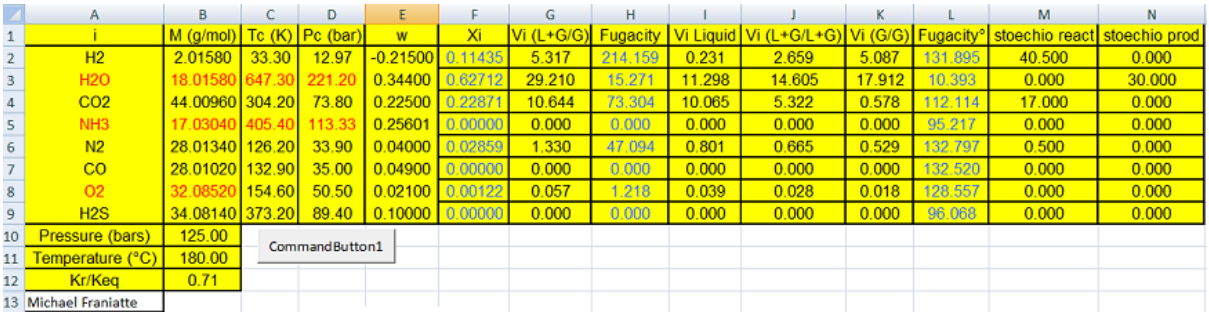
1. Introduction

For more informations on *PVTX* data and reactions, see "An Equation of State Resolution for the Study of Fluids" by the same author.

First, you must download and install Microsoft Office to have Excel access. Create a new empty sheet, named EoSResol. Add a command button, find as a control activeX, and a mode creation tool used to edit the button or enable the macro. Edit the macro of the command button by copying the VBA codes in the chapter 2.

Your excel sheet must looks like this following picture:



	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	i	M (g/mol)	Tc (K)	Pc (bar)	w	Xi	Vi (L+G/G)	Fugacity	Vi Liquid	Vi (L+G/L+G)	Vi (G/G)	Fugacity°	stoechio react	stoechio prod
2	H2	2.01580	33.30	12.97	-0.21500	0.11435	5.317	214.159	0.231	2.659	5.087	131.895	40.500	0.000
3	H2O	18.01580	647.30	221.20	0.34400	0.62712	29.210	15.271	11.298	14.605	17.912	10.393	0.000	30.000
4	CO2	44.00960	304.20	73.80	0.22500	0.22871	10.644	73.304	10.065	5.322	0.578	112.114	17.000	0.000
5	NH3	17.03040	405.40	113.33	0.25601	0.00000	0.000	0.000	0.000	0.000	0.000	95.217	0.000	0.000
6	N2	28.01340	126.20	33.90	0.04000	0.02859	1.330	47.094	0.801	0.665	0.529	132.797	0.500	0.000
7	CO	28.01020	132.90	35.00	0.04900	0.00000	0.000	0.000	0.000	0.000	0.000	132.520	0.000	0.000
8	O2	32.08520	154.60	50.50	0.02100	0.00122	0.057	1.218	0.039	0.028	0.018	128.557	0.000	0.000
9	H2S	34.08140	373.20	89.40	0.10000	0.00000	0.000	0.000	0.000	0.000	0.000	96.068	0.000	0.000
10	Pressure (bars)	125.00												
11	Temperature (°C)	180.00												
12	Kr/Keq	0.71												
13	Michael Franiatte													

CommandButton1

2. Macro codes

```
Private Sub CommandButton1_Click()
XH2Obis = Worksheets(1).Range("F3").Value
XCO2bis = Worksheets(1).Range("F4").Value
XCObis = Worksheets(1).Range("F5").Value
XH2bis = Worksheets(1).Range("F2").Value
XN2bis = Worksheets(1).Range("F8").Value
XCH4bis = Worksheets(1).Range("F6").Value
XNH3bis = Worksheets(1).Range("F9").Value
XMGbis = Worksheets(1).Range("F7").Value

    Pb = Worksheets(1).Range("B10").Value
   P = Pb * 100000 'passage de la pression de bar en Pa
   T = Worksheets(1).Range("B11").Value + 273.15

   TcH2O = Worksheets(1).Range("C3").Value 'température critique de H2O dans la cellule
J8
   PcH2O = Worksheets(1).Range("D3").Value 'pression critique de H2O
   TcCO2 = Worksheets(1).Range("C4").Value
   PcCO2 = Worksheets(1).Range("D4").Value
   TcCO = Worksheets(1).Range("C5").Value
   PcCO = Worksheets(1).Range("D5").Value
```

```
    TcH2 = Worksheets(1).Range("C2").Value
    PcH2 = Worksheets(1).Range("D2").Value
    TcN2 = Worksheets(1).Range("C8").Value
    PcN2 = Worksheets(1).Range("D8").Value
    TcCH4 = Worksheets(1).Range("C6").Value
    PcCH4 = Worksheets(1).Range("D6").Value
    TcNH3 = Worksheets(1).Range("C9").Value
    PcNH3 = Worksheets(1).Range("D9").Value
    TcMG = Worksheets(1).Range("C7").Value
    PcMG = Worksheets(1).Range("D7").Value

    R = 8.314472 'constante des gaz parfaits
    'calcul des facteurs acentriques
    wH2O = Worksheets(1).Range("E3").Value
    nH2O = 0.48508 + 1.55171 * wH2O - 0.15613 * wH2O ^ 2
    alphaH2O = (1 + nH2O * (1 - (T / TcH2O) ^ 0.5)) ^ 2
    wCO2 = Worksheets(1).Range("E4").Value
    nCO2 = 0.48508 + 1.55171 * wCO2 - 0.15613 * wCO2 ^ 2
    alphaCO2 = (1 + nCO2 * (1 - (T / TcCO2) ^ 0.5)) ^ 2
    wCO = Worksheets(1).Range("E5").Value
    nCO = 0.48508 + 1.55171 * wCO - 0.15613 * wCO ^ 2
    alphaCO = (1 + nCO * (1 - (T / TcCO) ^ 0.5)) ^ 2
    wH2 = Worksheets(1).Range("E2").Value
    nH2 = 0.48508 + 1.55171 * wH2 - 0.15613 * wH2 ^ 2
    alphaH2 = (1 + nH2 * (1 - (T / TcH2) ^ 0.5)) ^ 2
    wN2 = Worksheets(1).Range("E8").Value
    nN2 = 0.48508 + 1.55171 * wN2 - 0.15613 * wN2 ^ 2
    alphaN2 = (1 + nN2 * (1 - (T / TcN2) ^ 0.5)) ^ 2
    wCH4 = Worksheets(1).Range("E6").Value
    nCH4 = 0.48508 + 1.55171 * wCH4 - 0.15613 * wCH4 ^ 2
    alphaCH4 = (1 + nCH4 * (1 - (T / TcCH4) ^ 0.5)) ^ 2
    wNH3 = Worksheets(1).Range("E9").Value
    nNH3 = 0.48508 + 1.55171 * wNH3 - 0.15613 * wNH3 ^ 2
    alphaNH3 = (1 + nNH3 * (1 - (T / TcNH3) ^ 0.5)) ^ 2
    wMG = Worksheets(1).Range("E7").Value
    nMG = 0.48508 + 1.55171 * wMG - 0.15613 * wMG ^ 2
    alphaMG = (1 + nMG * (1 - (T / TcMG) ^ 0.5)) ^ 2

    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
```

```
BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

test = 1
ZN = 100.01 'initialisation NR à changer si plantage

While test > 0.000000001
FZ = ZN ^ 3 - ZN ^ 2 + (GRA - GRB ^ 2 - GRB) * ZN - GRA * GRB
FpZ = 3 * ZN ^ 2 - 2 * ZN + (GRA - GRB ^ 2 - GRB)

ZN1 = ZN - FZ / FpZ
test = Abs(ZN1 - ZN)
ZN = ZN1
Wend
VN = (ZN * R * T / P)
V = VN * 1000000
```

```
'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, aialphai et bialphai qui interviennent dans le calcul des coefficients de fugacité
    AH2 = 0.42748 * alphaH2 * (R * TcH2 ^ 2) / (PcH2 * 100000#)
    BH2 = 0.08664 * R * TcH2 / (PcH2 * 100000#)
    BiH2 = BH2 'stockage de bialphai
    ACO2 = 0.42748 * alphaCO2 * (R * TcCO2 ^ 2) / (PcCO2 * 100000#)
    BCO2 = 0.08664 * R * TcCO2 / (PcCO2 * 100000#)
    BiCO2 = BCO2
    AN2 = 0.42748 * alphaN2 * (R * TcN2 ^ 2) / (PcN2 * 100000#)
    BN2 = 0.08664 * R * TcN2 / (PcN2 * 100000#)
    BiN2 = BN2
    AH2O = 0.42748 * alphaH2O * (R * TcH2O ^ 2) / (PcH2O * 100000#)
    BH2O = 0.08664 * R * TcH2O / (PcH2O * 100000#)
    BiH2O = BH2O
    ACO = 0.42748 * alphaCO * (R * TcCO ^ 2) / (PcCO * 100000#)
    BCO = 0.08664 * R * TcCO / (PcCO * 100000#)
    BiCO = BCO
    ACH4 = 0.42748 * alphaCH4 * (R * TcCH4 ^ 2) / (PcCH4 * 100000#)
    BCH4 = 0.08664 * R * TcCH4 / (PcCH4 * 100000#)
    BiCH4 = BCH4
    ANH3 = 0.42748 * alphaNH3 * (R * TcNH3 ^ 2) / (PcNH3 * 100000#)
    BNH3 = 0.08664 * R * TcNH3 / (PcNH3 * 100000#)
    BiNH3 = BNH3
    AMG = 0.42748 * alphaMG * (R * TcMG ^ 2) / (PcMG * 100000#)
    BMG = 0.08664 * R * TcMG / (PcMG * 100000#)
    BiMG = BMG

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, a et b qui n'interviennent pas dans le calcul du coefficient de fugacité
    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG * AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) * XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis * (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4) ^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) * XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis * XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 / 2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 - KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) * XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis * XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3 * ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 * (1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    A = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 /
```

```
2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO +
2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) *
XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO
* AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) +
grAsuite
   B = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis *
BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calcul de dérivés de XiXj(1-Kji)racine(aialphai*akalphak)
   grAbis = (1 - KH2_MG) * (XMGbis) * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * (XCH4bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
(XNH3bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = ((XH2bis)) * AH2 + (1 - KH2O_H2) * (XH2Obis) * (AH2O * AH2) ^ (1 / 2) + (1
- KCO2_H2) * (XCO2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * (XN2bis) * (AN2 *
AH2) ^ (1 / 2) + (1 - KCO_H2) * (XCObis) * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * (XMGbis) * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * (XCH4bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3)
* (XNH3bis) * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = ((XCO2bis)) * ACO2 + (1 - KH2O_HCO2) * (XH2Obis) * (AH2O * ACO2) ^
(1 / 2) + (1 - KCO2_H2) * (XH2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XN2bis)
* (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * (XCObis) * (ACO * ACO2) ^ (1 / 2) +
grAsuite
   grAbis = (1 - KN2_MG) * (XMGbis) * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * (XCH4bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) *
(XNH3bis) * (ANH3 * AN2) ^ (1 / 2) + grAbis
   ArN2 = ((XN2bis)) * AN2 + (1 - KH2O_N2) * (XH2Obis) * (AH2O * AN2) ^ (1 / 2) + (1
- KN2_H2) * (XH2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XCO2bis) * (AN2 *
ACO2) ^ (1 / 2) + (1 - KN2_CO) * (XCObis) * (ACO * AN2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KH2O_MG) * (XMGbis) * (AH2O * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2O_CH4) * (XCH4bis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3)
* (XNH3bis) * (ANH3 * AH2O) ^ (1 / 2) + grAbis
   ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * (XH2bis) * (AH2O * AH2) ^ (1 / 2) +
(1 - KH2O_CO2) * (XCO2bis) * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * (XN2bis) *
(AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * (XCObis) * (ACO * AH2O) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO_MG) * (XMGbis) * (ACO * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO_CH4) * (XCH4bis) * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) *
(XNH3bis) * (ANH3 * ACO) ^ (1 / 2) + grAbis
   ArCO = (XCObis) * ACO + (1 - KH2O_CO) * (XH2Obis) * (AH2O * ACO) ^ (1 / 2) + (1
- KCO_CO2) * (XCO2bis) * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * (XN2bis) * (AN2 *
ACO) ^ (1 / 2) + (1 - KCO_H2) * (XH2bis) * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCH4_MG) * (XMGbis) * (ACH4 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * (XH2bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) *
(XNH3bis) * (ANH3 * ACH4) ^ (1 / 2) + grAbis
   ArCH4 = ((XCH4bis)) * ACH4 + (1 - KH2O_CH4) * (XH2Obis) * (AH2O * ACH4) ^ (1 /
2) + (1 - KCO2_CH4) * (XCO2bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) *
(XN2bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * (XCObis) * (ACO * ACH4) ^ (1 / 2)
+ grAsuite
   grAbis = (1 - KNH3_MG) * (XMGbis) * (ANH3 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCH4_NH3) * (XCH4bis) * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
(XH2bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
```

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    ArNH3 = ((XNH3bis)) * ANH3 + (1 - KH2O_NH3) * (XH2Obis) * (AH2O * ANH3) ^ (1
/ 2) + (1 - KCO2_NH3) * (XCO2bis) * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) *
(XN2bis) * (AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * (XCObis) * (ACO * ANH3) ^ (1 /
2) + grAsuite
    grAbis = (1 - KMG_NH3) * (XNH3bis) * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (1 - KCH4_MG) * (XCH4bis) * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
(XH2bis) * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = ((XMGbis)) * AMG + (1 - KH2O_MG) * (XH2Obis) * (AH2O * AMG) ^ (1 / 2)
+ (1 - KCO2_MG) * (XCO2bis) * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * (XN2bis) *
(AN2 * AMG) ^ (1 / 2) + (1 - KCO_MG) * (XCObis) * (ACO * AMG) ^ (1 / 2) + grAsuite

    SB = BH2O + BH2 + BCO2 + BN2 + BCO + BNH3 + BCH4 + BMG
    DVDXH2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArH2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
    DVDXH2O = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArH2O) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
    DVDXCO2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArCO2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
    DVDXCO = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArCO) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
    DVDXN2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArN2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
    DVDXCH4 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArCH4) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
    DVDXNH3 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArNH3) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
    DVDXMG = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArMG) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)

VCO2M = VN * (XCO2bis) - 1 * (XCO2bis) * 1 / 3 / 8 / 2 * DVDXCO2
VCOM = VN * (XCObis) - 1 * (XCObis) * 1 / 3 / 8 / 2 * DVDXCO
VH2M = VN * (XH2bis) - 1 * (XH2bis) * 1 / 3 / 8 / 2 * DVDXH2
VN2M = VN * (XN2bis) - 1 * (XN2bis) * 1 / 3 / 8 / 2 * DVDXN2
VCH4M = VN * (XCH4bis) - 1 * (XCH4bis) * 1 / 3 / 8 / 2 * DVDXCH4
VNH3M = VN * (XNH3bis) - 1 * (XNH3bis) * 1 / 3 / 8 / 2 * DVDXNH3
VH2OM = VN * (XH2Obis) - 1 * (XH2Obis) * 1 / 3 / 8 / 2 * DVDXH2O
VMGM = VN * (XMGbis) - 1 * (XMGbis) * 1 / 3 / 8 / 2 * DVDXMG

Worksheets(1).Range("G4").Value = VCO2M * 1000000
Worksheets(1).Range("G5").Value = VCOM * 1000000
Worksheets(1).Range("G2").Value = VH2M * 1000000
Worksheets(1).Range("G8").Value = VN2M * 1000000
```

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Worksheets(1).Range("G6").Value = VCH4M * 1000000
Worksheets(1).Range("G9").Value = VNH3M * 1000000
Worksheets(1).Range("G3").Value = VH2OM * 1000000
Worksheets(1).Range("G7").Value = VMGM * 1000000

   'calcul de somme de Xk(1-Kki)racine(aialphai*akalphak)  (avant le 2 dans le calcul du coefficient de fugacité de l'espèce k)
   grAbis = (1 - KH2_MG) * XMGbis * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XCH4bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = (XH2bis) * AH2 + (1 - KH2O_H2) * XH2Obis * (AH2O * AH2) ^ (1 / 2) + (1 - KCO2_H2) * XCO2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * XN2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KCO_H2) * XCObis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * XMGbis * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * XCH4bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) * XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = (XCO2bis) * ACO2 + (1 - KH2O_HCO2) * XH2Obis * (AH2O * ACO2) ^ (1 / 2) + (1 - KCO2_H2) * XH2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XN2bis * (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * XCObis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * XMGbis * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * XCH4bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   ArN2 = (XN2bis) * AN2 + (1 - KH2O_N2) * XH2Obis * (AH2O * AN2) ^ (1 / 2) + (1 - KN2_H2) * XH2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XCO2bis * (AN2 * ACO2) ^ (1 / 2) + (1 - KN2_CO) * XCObis * (ACO * AN2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KH2O_MG) * XMGbis * (AH2O * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2O_CH4) * XCH4bis * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + grAbis
   ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * XH2bis * (AH2O * AH2) ^ (1 / 2) + (1 - KH2O_CO2) * XCO2bis * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * XN2bis * (AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * XCObis * (ACO * AH2O) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO_MG) * XMGbis * (ACO * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO_CH4) * XCH4bis * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) * XNH3bis * (ANH3 * ACO) ^ (1 / 2) + grAbis
   ArCO = (XCObis) * ACO + (1 - KH2O_CO) * XH2Obis * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * XCO2bis * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * XN2bis * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * XH2bis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCH4_MG) * XMGbis * (ACH4 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XH2bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + grAbis
   ArCH4 = (XCH4bis) * ACH4 + (1 - KH2O_CH4) * XH2Obis * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * XN2bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * XCObis * (ACO * ACH4) ^ (1 / 2) + grAsuite
   grAbis = (1 - KNH3_MG) * XMGbis * (ANH3 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCH4_NH3) * XCH4bis * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * XH2bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArNH3 = (XNH3bis) * ANH3 + (1 - KH2O_NH3) * XH2Obis * (AH2O * ANH3) ^ (1 / 2) + (1 - KCO2_NH3) * XCO2bis * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * XN2bis * (AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * XCObis * (ACO * ANH3) ^ (1 / 2) + grAsuite
   grAbis = (1 - KMG_NH3) * XNH3bis * (AMG * ANH3) ^ (1 / 2)
```

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    grAsuite = (1 - KCH4_MG) * XCH4bis * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
XH2bis * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = (XMGbis) * AMG + (1 - KH2O_MG) * XH2Obis * (AH2O * AMG) ^ (1 / 2) +
(1 - KCO2_MG) * XCO2bis * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * XN2bis * (AN2 *
AMG) ^ (1 / 2) + (1 - KCO_MG) * XCObis * (ACO * AMG) ^ (1 / 2) + grAsuite

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, Ai et Bi qui
interviennent dans le calcul du coefficient de fugacité
    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, A et B qui
interviennent dans le calcul du coefficient de fugacité
    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
```

```
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
   GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calculs des coefficients de fugacités
   'logFIH2Osoave = ZN - 1 - Log(ZN - GRB) - GRA / GRB * Log((ZN + GRB) / ZN)
         'FIH2Oincsoave = 10 ^ (logFIH2Osoave / 2.303)
         'Worksheets(1).Range("C31").Value = FIH2Oincsoave

   logFIH2O = BH2O / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2O / GRB - 2
/ A * ArH2O) * Log(1 + GRB / ZN)
         FIH2Oinc = 10 ^ (logFIH2O / 2.303)
         FUH2Oinc = FIH2Oinc * P * XH2Obis
         FUH2Oi = FUH2Oinc * 0.00001
   logFIH2 = BH2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2 / GRB - 2 / A *
ArH2) * Log(1 + GRB / ZN)
         FIH2inc = 10 ^ (logFIH2 / 2.303)
         FUH2inc = FIH2inc * P * XH2bis
         FUH2i = FUH2inc * 0.00001

   logFICO = BCO / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO / GRB - 2 / A
* ArCO) * Log(1 + GRB / ZN)
         FICOinc = 10 ^ (logFICO / 2.303)
         FUCOinc = FICOinc * P * XCObis
         FUCOi = FUCOinc * 0.00001

   logFICO2 = BCO2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO2 / GRB - 2 /
A * ArCO2) * Log(1 + GRB / ZN)
         FICO2inc = 10 ^ (logFICO2 / 2.303)
         FUCO2inc = FICO2inc * P * XCO2bis
         FUCO2i = FUCO2inc * 0.00001 'la même chose mais en bar

   logFIN2 = BN2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BN2 / GRB - 2 / A *
ArN2) * Log(1 + GRB / ZN)
         FIN2inc = 10 ^ (logFIN2 / 2.303)
         FUN2inc = FIN2inc * P * XN2bis
         FUN2i = FUN2inc * 0.00001 'la même chose mais en bar

   logFICH4 = BCH4 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCH4 / GRB - 2 /
A * ArCH4) * Log(1 + GRB / ZN)
         FICH4inc = 10 ^ (logFICH4 / 2.303)
         FUCH4inc = FICH4inc * P * XCH4bis
         FUCH4i = FUCH4inc * 0.00001

   logFINH3 = BNH3 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BNH3 / GRB - 2
/ A * ArNH3) * Log(1 + GRB / ZN)
         FINH3inc = 10 ^ (logFINH3 / 2.303)
```

```
        FUNH3inc = FINH3inc * P * XNH3bis
        FUNH3i = FUNH3inc * 0.00001

   logFIMG = BMG / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BMG / GRB - 2 /
A * ArMG) * Log(1 + GRB / ZN)
        FIMGinc = 10 ^ (logFIMG / 2.303)
        FUMGinc = FIMGinc * P * XMGbis
        FUMGi = FUMGinc * 0.00001

Worksheets(1).Range("H3").Value = FUH2Oi
Worksheets(1).Range("H4").Value = FUCO2i
Worksheets(1).Range("H5").Value = FUCOi
Worksheets(1).Range("H2").Value = FUH2i
Worksheets(1).Range("H8").Value = FUN2i
Worksheets(1).Range("H6").Value = FUCH4i
Worksheets(1).Range("H9").Value = FUNH3i
Worksheets(1).Range("H7").Value = FUMGi
Call PROPORTION
End Sub

Private Sub PROPORTION()
Worksheets(1).Range("I2").Value = Worksheets(1).Range("F2").Value *
Worksheets(1).Range("B2").Value
Worksheets(1).Range("I3").Value = Worksheets(1).Range("F3").Value *
Worksheets(1).Range("B3").Value
Worksheets(1).Range("I4").Value = Worksheets(1).Range("F4").Value *
Worksheets(1).Range("B4").Value
Worksheets(1).Range("I5").Value = Worksheets(1).Range("F5").Value *
Worksheets(1).Range("B5").Value
Worksheets(1).Range("I6").Value = Worksheets(1).Range("F6").Value *
Worksheets(1).Range("B6").Value
Worksheets(1).Range("I7").Value = Worksheets(1).Range("F7").Value *
Worksheets(1).Range("B7").Value
Worksheets(1).Range("I8").Value = Worksheets(1).Range("F8").Value *
Worksheets(1).Range("B8").Value
Worksheets(1).Range("I9").Value = Worksheets(1).Range("F9").Value *
Worksheets(1).Range("B9").Value

Worksheets(1).Range("J2").Value = Worksheets(1).Range("G2").Value / 2
Worksheets(1).Range("J3").Value = Worksheets(1).Range("G3").Value / 2
Worksheets(1).Range("J4").Value = Worksheets(1).Range("G4").Value / 2
Worksheets(1).Range("J5").Value = Worksheets(1).Range("G5").Value / 2
Worksheets(1).Range("J6").Value = Worksheets(1).Range("G6").Value / 2
Worksheets(1).Range("J7").Value = Worksheets(1).Range("G7").Value / 2
Worksheets(1).Range("J8").Value = Worksheets(1).Range("G8").Value / 2
Worksheets(1).Range("J9").Value = Worksheets(1).Range("G9").Value / 2

Worksheets(1).Range("K2").Value = Worksheets(1).Range("G2").Value -
Worksheets(1).Range("I2").Value
```

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Worksheets(1).Range("K3").Value = Worksheets(1).Range("G3").Value -
Worksheets(1).Range("I3").Value
Worksheets(1).Range("K4").Value = Worksheets(1).Range("G4").Value -
Worksheets(1).Range("I4").Value
Worksheets(1).Range("K5").Value = Worksheets(1).Range("G5").Value -
Worksheets(1).Range("I5").Value
Worksheets(1).Range("K6").Value = Worksheets(1).Range("G6").Value -
Worksheets(1).Range("I6").Value
Worksheets(1).Range("K7").Value = Worksheets(1).Range("G7").Value -
Worksheets(1).Range("I7").Value
Worksheets(1).Range("K8").Value = Worksheets(1).Range("G8").Value -
Worksheets(1).Range("I8").Value
Worksheets(1).Range("K9").Value = Worksheets(1).Range("G9").Value -
Worksheets(1).Range("I9").Value
Call PROPORTION1
End Sub
Private Sub PROPORTION1()

XH2Obis = 0
XCO2bis = 0
XCObis = 0
XH2bis = 1
XN2bis = 0
XCH4bis = 0
XNH3bis = 0
XMGbis = 0

    Pb = Worksheets(1).Range("B10").Value
   P = Pb * 100000 'passage de la pression de bar en Pa
   T = Worksheets(1).Range("B11").Value + 273.15

   TcH2O = Worksheets(1).Range("C3").Value 'température critique de H2O dans la cellule
J8
   PcH2O = Worksheets(1).Range("D3").Value 'pression critique de H2O
   TcCO2 = Worksheets(1).Range("C4").Value
   PcCO2 = Worksheets(1).Range("D4").Value
   TcCO = Worksheets(1).Range("C5").Value
   PcCO = Worksheets(1).Range("D5").Value
   TcH2 = Worksheets(1).Range("C2").Value
   PcH2 = Worksheets(1).Range("D2").Value
   TcN2 = Worksheets(1).Range("C8").Value
   PcN2 = Worksheets(1).Range("D8").Value
   TcCH4 = Worksheets(1).Range("C6").Value
   PcCH4 = Worksheets(1).Range("D6").Value
   TcNH3 = Worksheets(1).Range("C9").Value
   PcNH3 = Worksheets(1).Range("D9").Value
   TcMG = Worksheets(1).Range("C7").Value
   PcMG = Worksheets(1).Range("D7").Value

   R = 8.314472 'constante des gaz parfaits
```

```
    'calcul des facteurs acentriques
    wH2O = Worksheets(1).Range("E3").Value
    nH2O = 0.48508 + 1.55171 * wH2O - 0.15613 * wH2O ^ 2
    alphaH2O = (1 + nH2O * (1 - (T / TcH2O) ^ 0.5)) ^ 2
    wCO2 = Worksheets(1).Range("E4").Value
    nCO2 = 0.48508 + 1.55171 * wCO2 - 0.15613 * wCO2 ^ 2
    alphaCO2 = (1 + nCO2 * (1 - (T / TcCO2) ^ 0.5)) ^ 2
    wCO = Worksheets(1).Range("E5").Value
    nCO = 0.48508 + 1.55171 * wCO - 0.15613 * wCO ^ 2
    alphaCO = (1 + nCO * (1 - (T / TcCO) ^ 0.5)) ^ 2
    wH2 = Worksheets(1).Range("E2").Value
    nH2 = 0.48508 + 1.55171 * wH2 - 0.15613 * wH2 ^ 2
    alphaH2 = (1 + nH2 * (1 - (T / TcH2) ^ 0.5)) ^ 2
    wN2 = Worksheets(1).Range("E8").Value
    nN2 = 0.48508 + 1.55171 * wN2 - 0.15613 * wN2 ^ 2
    alphaN2 = (1 + nN2 * (1 - (T / TcN2) ^ 0.5)) ^ 2
    wCH4 = Worksheets(1).Range("E6").Value
    nCH4 = 0.48508 + 1.55171 * wCH4 - 0.15613 * wCH4 ^ 2
    alphaCH4 = (1 + nCH4 * (1 - (T / TcCH4) ^ 0.5)) ^ 2
    wNH3 = Worksheets(1).Range("E9").Value
    nNH3 = 0.48508 + 1.55171 * wNH3 - 0.15613 * wNH3 ^ 2
    alphaNH3 = (1 + nNH3 * (1 - (T / TcNH3) ^ 0.5)) ^ 2
    wMG = Worksheets(1).Range("E7").Value
    nMG = 0.48508 + 1.55171 * wMG - 0.15613 * wMG ^ 2
    alphaMG = (1 + nMG * (1 - (T / TcMG) ^ 0.5)) ^ 2

    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
```

```
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
    GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

      test = 1
       ZN = 100.01 'initialisation NR à changer si plantage

       While test > 0.000000001
       FZ = ZN ^ 3 - ZN ^ 2 + (GRA - GRB ^ 2 - GRB) * ZN - GRA * GRB
       FpZ = 3 * ZN ^ 2 - 2 * ZN + (GRA - GRB ^ 2 - GRB)

       ZN1 = ZN - FZ / FpZ
       test = Abs(ZN1 - ZN)
       ZN = ZN1
       Wend
       VN = (ZN * R * T / P)
       V = VN * 1000000

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, aialphai et bialphai
qui interviennent dans le calcul des coefficients de fugacité
    AH2 = 0.42748 * alphaH2 * (R * TcH2 ^ 2) / (PcH2 * 100000#)
    BH2 = 0.08664 * R * TcH2 / (PcH2 * 100000#)
    BiH2 = BH2 'stockage de bialphai
    ACO2 = 0.42748 * alphaCO2 * (R * TcCO2 ^ 2) / (PcCO2 * 100000#)
    BCO2 = 0.08664 * R * TcCO2 / (PcCO2 * 100000#)
    BiCO2 = BCO2
    AN2 = 0.42748 * alphaN2 * (R * TcN2 ^ 2) / (PcN2 * 100000#)
    BN2 = 0.08664 * R * TcN2 / (PcN2 * 100000#)
    BiN2 = BN2
    AH2O = 0.42748 * alphaH2O * (R * TcH2O ^ 2) / (PcH2O * 100000#)
    BH2O = 0.08664 * R * TcH2O / (PcH2O * 100000#)
```

```
   BiH2O = BH2O
   ACO = 0.42748 * alphaCO * (R * TcCO ^ 2) / (PcCO * 100000#)
   BCO = 0.08664 * R * TcCO / (PcCO * 100000#)
   BiCO = BCO
   ACH4 = 0.42748 * alphaCH4 * (R * TcCH4 ^ 2) / (PcCH4 * 100000#)
   BCH4 = 0.08664 * R * TcCH4 / (PcCH4 * 100000#)
   BiCH4 = BCH4
   ANH3 = 0.42748 * alphaNH3 * (R * TcNH3 ^ 2) / (PcNH3 * 100000#)
   BNH3 = 0.08664 * R * TcNH3 / (PcNH3 * 100000#)
   BiNH3 = BNH3
   AMG = 0.42748 * alphaMG * (R * TcMG ^ 2) / (PcMG * 100000#)
   BMG = 0.08664 * R * TcMG / (PcMG * 100000#)
   BiMG = BMG

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, a et b qui
n'interviennent pas dans le calcul du coefficient de fugacité
   grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
   grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   A = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis
* XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) *
XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) *
XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis *
(ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 /
2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO +
2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) *
XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO
* AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) +
grAsuite
   B = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis *
BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calcul de dérivés de XiXj(1-Kji)racine(aialphai*akalphak)
   grAbis = (1 - KH2_MG) * (XMGbis) * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * (XCH4bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
(XNH3bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
```

ArH2 = ((XH2bis)) * AH2 + (1 - KH2O_H2) * (XH2Obis) * (AH2O * AH2) ^ (1 / 2) + (1 - KCO2_H2) * (XCO2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * (XN2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KCO_H2) * (XCObis) * (ACO * AH2) ^ (1 / 2) + grAsuite

grAbis = (1 - KCO2_MG) * (XMGbis) * (ACO2 * AMG) ^ (1 / 2)

grAsuite = (1 - KCO2_CH4) * (XCH4bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) * (XNH3bis) * (ANH3 * ACO2) ^ (1 / 2) + grAbis

ArCO2 = ((XCO2bis)) * ACO2 + (1 - KH2O_HCO2) * (XH2Obis) * (AH2O * ACO2) ^ (1 / 2) + (1 - KCO2_H2) * (XH2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XN2bis) * (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * (XCObis) * (ACO * ACO2) ^ (1 / 2) + grAsuite

grAbis = (1 - KN2_MG) * (XMGbis) * (AN2 * AMG) ^ (1 / 2)

grAsuite = (1 - KN2_CH4) * (XCH4bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) * (XNH3bis) * (ANH3 * AN2) ^ (1 / 2) + grAbis

ArN2 = ((XN2bis)) * AN2 + (1 - KH2O_N2) * (XH2Obis) * (AH2O * AN2) ^ (1 / 2) + (1 - KN2_H2) * (XH2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XCO2bis) * (AN2 * ACO2) ^ (1 / 2) + (1 - KN2_CO) * (XCObis) * (ACO * AN2) ^ (1 / 2) + grAsuite

grAbis = (1 - KH2O_MG) * (XMGbis) * (AH2O * AMG) ^ (1 / 2)

grAsuite = (1 - KH2O_CH4) * (XCH4bis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) * (XNH3bis) * (ANH3 * AH2O) ^ (1 / 2) + grAbis

ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * (XH2bis) * (AH2O * AH2) ^ (1 / 2) + (1 - KH2O_CO2) * (XCO2bis) * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * (XN2bis) * (AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * (XCObis) * (ACO * AH2O) ^ (1 / 2) + grAsuite

grAbis = (1 - KCO_MG) * (XMGbis) * (ACO * AMG) ^ (1 / 2)

grAsuite = (1 - KCO_CH4) * (XCH4bis) * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) * (XNH3bis) * (ANH3 * ACO) ^ (1 / 2) + grAbis

ArCO = (XCObis) * ACO + (1 - KH2O_CO) * (XH2Obis) * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * (XCO2bis) * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * (XN2bis) * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * (XH2bis) * (ACO * AH2) ^ (1 / 2) + grAsuite

grAbis = (1 - KCH4_MG) * (XMGbis) * (ACH4 * AMG) ^ (1 / 2)

grAsuite = (1 - KH2_CH4) * (XH2bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * (XNH3bis) * (ANH3 * ACH4) ^ (1 / 2) + grAbis

ArCH4 = ((XCH4bis)) * ACH4 + (1 - KH2O_CH4) * (XH2Obis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * (XCO2bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * (XN2bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * (XCObis) * (ACO * ACH4) ^ (1 / 2) + grAsuite

grAbis = (1 - KNH3_MG) * (XMGbis) * (ANH3 * AMG) ^ (1 / 2)

grAsuite = (1 - KCH4_NH3) * (XCH4bis) * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * (XH2bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis

ArNH3 = ((XNH3bis)) * ANH3 + (1 - KH2O_NH3) * (XH2Obis) * (AH2O * ANH3) ^ (1 / 2) + (1 - KCO2_NH3) * (XCO2bis) * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * (XN2bis) * (AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * (XCObis) * (ACO * ANH3) ^ (1 / 2) + grAsuite

grAbis = (1 - KMG_NH3) * (XNH3bis) * (AMG * ANH3) ^ (1 / 2)

grAsuite = (1 - KCH4_MG) * (XCH4bis) * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) * (XH2bis) * (AMG * AH2) ^ (1 / 2) + grAbis

ArMG = ((XMGbis)) * AMG + (1 - KH2O_MG) * (XH2Obis) * (AH2O * AMG) ^ (1 / 2) + (1 - KCO2_MG) * (XCO2bis) * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * (XN2bis) * (AN2 * AMG) ^ (1 / 2) + (1 - KCO_MG) * (XCObis) * (ACO * AMG) ^ (1 / 2) + grAsuite

SB = BH2O + BH2 + BCO2 + BN2 + BCO + BNH3 + BCH4 + BMG

```
   DVDXH2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArH2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXH2O = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArH2O) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXCO2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArCO2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXCO = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArCO) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXN2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArN2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXCH4 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArCH4) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXNH3 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArNH3) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXMG = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArMG) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)

VCO2M = VN * (XCO2bis) - 1 * (XCO2bis) * 1 / 3 / 8 / 2 * DVDXCO2
VCOM = VN * (XCObis) - 1 * (XCObis) * 1 / 3 / 8 / 2 * DVDXCO
VH2M = VN * (XH2bis) - 1 * (XH2bis) * 1 / 3 / 8 / 2 * DVDXH2
VN2M = VN * (XN2bis) - 1 * (XN2bis) * 1 / 3 / 8 / 2 * DVDXN2
VCH4M = VN * (XCH4bis) - 1 * (XCH4bis) * 1 / 3 / 8 / 2 * DVDXCH4
VNH3M = VN * (XNH3bis) - 1 * (XNH3bis) * 1 / 3 / 8 / 2 * DVDXNH3
VH2OM = VN * (XH2Obis) - 1 * (XH2Obis) * 1 / 3 / 8 / 2 * DVDXH2O
VMGM = VN * (XMGbis) - 1 * (XMGbis) * 1 / 3 / 8 / 2 * DVDXMG

   'calcul de somme de Xk(1-Kki)racine(aialphai*akalphak)  (avant le 2 dans le calcul du
coefficient de fugacité de l'espèce k)
   grAbis = (1 - KH2_MG) * XMGbis * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XCH4bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
XNH3bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = (XH2bis) * AH2 + (1 - KH2O_H2) * XH2Obis * (AH2O * AH2) ^ (1 / 2) + (1 -
KCO2_H2) * XCO2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * XN2bis * (AN2 * AH2)
^ (1 / 2) + (1 - KCO_H2) * XCObis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * XMGbis * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * XCH4bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = (XCO2bis) * ACO2 + (1 - KH2O_HCO2) * XH2Obis * (AH2O * ACO2) ^ (1 /
2) + (1 - KCO2_H2) * XH2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XN2bis * (AN2
* ACO2) ^ (1 / 2) + (1 - KCO_CO2) * XCObis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * XMGbis * (AN2 * AMG) ^ (1 / 2)
```

```
    grAsuite = (1 - KN2_CH4) * XCH4bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) *
XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    ArN2 = (XN2bis) * AN2 + (1 - KH2O_N2) * XH2Obis * (AH2O * AN2) ^ (1 / 2) + (1 -
KN2_H2) * XH2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XCO2bis * (AN2 * ACO2)
^ (1 / 2) + (1 - KN2_CO) * XCObis * (ACO * AN2) ^ (1 / 2) + grAsuite
    grAbis = (1 - KH2O_MG) * XMGbis * (AH2O * AMG) ^ (1 / 2)
    grAsuite = (1 - KH2O_CH4) * XCH4bis * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) *
XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + grAbis
    ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * XH2bis * (AH2O * AH2) ^ (1 / 2) + (1
- KH2O_CO2) * XCO2bis * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * XN2bis * (AN2 *
AH2O) ^ (1 / 2) + (1 - KH2O_CO) * XCObis * (ACO * AH2O) ^ (1 / 2) + grAsuite
    grAbis = (1 - KCO_MG) * XMGbis * (ACO * AMG) ^ (1 / 2)
    grAsuite = (1 - KCO_CH4) * XCH4bis * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) *
XNH3bis * (ANH3 * ACO) ^ (1 / 2) + grAbis
    ArCO = (XCObis) * ACO + (1 - KH2O_CO) * XH2Obis * (AH2O * ACO) ^ (1 / 2) + (1 -
KCO_CO2) * XCO2bis * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * XN2bis * (AN2 *
ACO) ^ (1 / 2) + (1 - KCO_H2) * XH2bis * (ACO * AH2) ^ (1 / 2) + grAsuite
    grAbis = (1 - KCH4_MG) * XMGbis * (ACH4 * AMG) ^ (1 / 2)
    grAsuite = (1 - KH2_CH4) * XH2bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) *
XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + grAbis
    ArCH4 = (XCH4bis) * ACH4 + (1 - KH2O_CH4) * XH2Obis * (AH2O * ACH4) ^ (1 / 2)
+ (1 - KCO2_CH4) * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * XN2bis *
(AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * XCObis * (ACO * ACH4) ^ (1 / 2) + grAsuite
    grAbis = (1 - KNH3_MG) * XMGbis * (ANH3 * AMG) ^ (1 / 2)
    grAsuite = (1 - KCH4_NH3) * XCH4bis * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
XH2bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
    ArNH3 = (XNH3bis) * ANH3 + (1 - KH2O_NH3) * XH2Obis * (AH2O * ANH3) ^ (1 / 2)
+ (1 - KCO2_NH3) * XCO2bis * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * XN2bis *
(AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * XCObis * (ACO * ANH3) ^ (1 / 2) + grAsuite
    grAbis = (1 - KMG_NH3) * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (1 - KCH4_MG) * XCH4bis * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
XH2bis * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = (XMGbis) * AMG + (1 - KH2O_MG) * XH2Obis * (AH2O * AMG) ^ (1 / 2) +
(1 - KCO2_MG) * XCO2bis * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * XN2bis * (AN2 *
AMG) ^ (1 / 2) + (1 - KCO_MG) * XCObis * (ACO * AMG) ^ (1 / 2) + grAsuite

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, Ai et Bi qui
interviennent dans le calcul du coefficient de fugacité
    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
```

```
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, A et B qui
interviennent dans le calcul du coefficient de fugacité
    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
    GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

    'calculs des coefficients de fugacités
    'logFIH2Osoave = ZN - 1 - Log(ZN - GRB) - GRA / GRB * Log((ZN + GRB) / ZN)
        'FIH2Oincsoave = 10 ^ (logFIH2Osoave / 2.303)
        'Worksheets(1).Range("C31").Value = FIH2Oincsoave

    logFIH2O = BH2O / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2O / GRB - 2
/ A * ArH2O) * Log(1 + GRB / ZN)
        FIH2Oinc = 10 ^ (logFIH2O / 2.303)
        FUH2Oinc = FIH2Oinc * P * XH2Obis
        FUH2Oi = FUH2Oinc * 0.00001
    logFIH2 = BH2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2 / GRB - 2 / A *
ArH2) * Log(1 + GRB / ZN)
        FIH2inc = 10 ^ (logFIH2 / 2.303)
```

```
        FUH2inc = FIH2inc * P * XH2bis
        FUH2i = FUH2inc * 0.00001

   logFICO = BCO / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO / GRB - 2 / A
* ArCO) * Log(1 + GRB / ZN)
        FICOinc = 10 ^ (logFICO / 2.303)
        FUCOinc = FICOinc * P * XCObis
        FUCOi = FUCOinc * 0.00001

   logFICO2 = BCO2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO2 / GRB - 2 /
A * ArCO2) * Log(1 + GRB / ZN)
        FICO2inc = 10 ^ (logFICO2 / 2.303)
        FUCO2inc = FICO2inc * P * XCO2bis
        FUCO2i = FUCO2inc * 0.00001 'la même chose mais en bar

   logFIN2 = BN2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BN2 / GRB - 2 / A *
ArN2) * Log(1 + GRB / ZN)
        FIN2inc = 10 ^ (logFIN2 / 2.303)
        FUN2inc = FIN2inc * P * XN2bis
        FUN2i = FUN2inc * 0.00001 'la même chose mais en bar

   logFICH4 = BCH4 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCH4 / GRB - 2 /
A * ArCH4) * Log(1 + GRB / ZN)
        FICH4inc = 10 ^ (logFICH4 / 2.303)
        FUCH4inc = FICH4inc * P * XCH4bis
        FUCH4i = FUCH4inc * 0.00001

   logFINH3 = BNH3 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BNH3 / GRB - 2
/ A * ArNH3) * Log(1 + GRB / ZN)
        FINH3inc = 10 ^ (logFINH3 / 2.303)
        FUNH3inc = FINH3inc * P * XNH3bis
        FUNH3i = FUNH3inc * 0.00001

   logFIMG = BMG / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BMG / GRB - 2 /
A * ArMG) * Log(1 + GRB / ZN)
        FIMGinc = 10 ^ (logFIMG / 2.303)
        FUMGinc = FIMGinc * P * XMGbis
        FUMGi = FUMGinc * 0.00001

Worksheets(1).Range("L2").Value = FUH2i

XH2Obis = 1
XCO2bis = 0
XCObis = 0
XH2bis = 0
XN2bis = 0
XCH4bis = 0
XNH3bis = 0
XMGbis = 0
```

```
 Pb = Worksheets(1).Range("B10").Value
P = Pb * 100000 'passage de la pression de bar en Pa
T = Worksheets(1).Range("B11").Value + 273.15

TcH2O = Worksheets(1).Range("C3").Value 'température critique de H2O dans la cellule J8
PcH2O = Worksheets(1).Range("D3").Value 'pression critique de H2O
TcCO2 = Worksheets(1).Range("C4").Value
PcCO2 = Worksheets(1).Range("D4").Value
TcCO = Worksheets(1).Range("C5").Value
PcCO = Worksheets(1).Range("D5").Value
TcH2 = Worksheets(1).Range("C2").Value
PcH2 = Worksheets(1).Range("D2").Value
TcN2 = Worksheets(1).Range("C8").Value
PcN2 = Worksheets(1).Range("D8").Value
TcCH4 = Worksheets(1).Range("C6").Value
PcCH4 = Worksheets(1).Range("D6").Value
TcNH3 = Worksheets(1).Range("C9").Value
PcNH3 = Worksheets(1).Range("D9").Value
TcMG = Worksheets(1).Range("C7").Value
PcMG = Worksheets(1).Range("D7").Value

R = 8.314472 'constante des gaz parfaits
'calcul des facteurs acentriques
wH2O = Worksheets(1).Range("E3").Value
nH2O = 0.48508 + 1.55171 * wH2O - 0.15613 * wH2O ^ 2
alphaH2O = (1 + nH2O * (1 - (T / TcH2O) ^ 0.5)) ^ 2
wCO2 = Worksheets(1).Range("E4").Value
nCO2 = 0.48508 + 1.55171 * wCO2 - 0.15613 * wCO2 ^ 2
alphaCO2 = (1 + nCO2 * (1 - (T / TcCO2) ^ 0.5)) ^ 2
wCO = Worksheets(1).Range("E5").Value
nCO = 0.48508 + 1.55171 * wCO - 0.15613 * wCO ^ 2
alphaCO = (1 + nCO * (1 - (T / TcCO) ^ 0.5)) ^ 2
wH2 = Worksheets(1).Range("E2").Value
nH2 = 0.48508 + 1.55171 * wH2 - 0.15613 * wH2 ^ 2
alphaH2 = (1 + nH2 * (1 - (T / TcH2) ^ 0.5)) ^ 2
wN2 = Worksheets(1).Range("E8").Value
nN2 = 0.48508 + 1.55171 * wN2 - 0.15613 * wN2 ^ 2
alphaN2 = (1 + nN2 * (1 - (T / TcN2) ^ 0.5)) ^ 2
wCH4 = Worksheets(1).Range("E6").Value
nCH4 = 0.48508 + 1.55171 * wCH4 - 0.15613 * wCH4 ^ 2
alphaCH4 = (1 + nCH4 * (1 - (T / TcCH4) ^ 0.5)) ^ 2
wNH3 = Worksheets(1).Range("E9").Value
nNH3 = 0.48508 + 1.55171 * wNH3 - 0.15613 * wNH3 ^ 2
alphaNH3 = (1 + nNH3 * (1 - (T / TcNH3) ^ 0.5)) ^ 2
wMG = Worksheets(1).Range("E7").Value
nMG = 0.48508 + 1.55171 * wMG - 0.15613 * wMG ^ 2
alphaMG = (1 + nMG * (1 - (T / TcMG) ^ 0.5)) ^ 2
```

```
   AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
   BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
   ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
   BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
   AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
   BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
   AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
   BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
   ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
   BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
   ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
   BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
   ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
   BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
   AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
   BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
   grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
   GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

    test = 1
     ZN = 100.01 'initialisation NR à changer si plantage
```

```
While test > 0.000000001
FZ = ZN ^ 3 - ZN ^ 2 + (GRA - GRB ^ 2 - GRB) * ZN - GRA * GRB
FpZ = 3 * ZN ^ 2 - 2 * ZN + (GRA - GRB ^ 2 - GRB)

ZN1 = ZN - FZ / FpZ
test = Abs(ZN1 - ZN)
ZN = ZN1
Wend
VN = (ZN * R * T / P)
V = VN * 1000000
```

```
'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, aialphai et bialphai qui interviennent dans le calcul des coefficients de fugacité
AH2 = 0.42748 * alphaH2 * (R * TcH2 ^ 2) / (PcH2 * 100000#)
BH2 = 0.08664 * R * TcH2 / (PcH2 * 100000#)
BiH2 = BH2 'stockage de bialphai
ACO2 = 0.42748 * alphaCO2 * (R * TcCO2 ^ 2) / (PcCO2 * 100000#)
BCO2 = 0.08664 * R * TcCO2 / (PcCO2 * 100000#)
BiCO2 = BCO2
AN2 = 0.42748 * alphaN2 * (R * TcN2 ^ 2) / (PcN2 * 100000#)
BN2 = 0.08664 * R * TcN2 / (PcN2 * 100000#)
BiN2 = BN2
AH2O = 0.42748 * alphaH2O * (R * TcH2O ^ 2) / (PcH2O * 100000#)
BH2O = 0.08664 * R * TcH2O / (PcH2O * 100000#)
BiH2O = BH2O
ACO = 0.42748 * alphaCO * (R * TcCO ^ 2) / (PcCO * 100000#)
BCO = 0.08664 * R * TcCO / (PcCO * 100000#)
BiCO = BCO
ACH4 = 0.42748 * alphaCH4 * (R * TcCH4 ^ 2) / (PcCH4 * 100000#)
BCH4 = 0.08664 * R * TcCH4 / (PcCH4 * 100000#)
BiCH4 = BCH4
ANH3 = 0.42748 * alphaNH3 * (R * TcNH3 ^ 2) / (PcNH3 * 100000#)
BNH3 = 0.08664 * R * TcNH3 / (PcNH3 * 100000#)
BiNH3 = BNH3
AMG = 0.42748 * alphaMG * (R * TcMG ^ 2) / (PcMG * 100000#)
BMG = 0.08664 * R * TcMG / (PcMG * 100000#)
BiMG = BMG
```

```
'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, a et b qui n'interviennent pas dans le calcul du coefficient de fugacité
grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG * AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) * XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis * (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4) ^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) * XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis * XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
```

```
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   A = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis
* XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) *
XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) *
XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis *
(ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 /
2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO +
2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) *
XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO
* AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) +
grAsuite
   B = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis *
BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calcul de dérivés de XiXj(1-Kji)racine(aialphai*akalphak)
   grAbis = (1 - KH2_MG) * (XMGbis) * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * (XCH4bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
(XNH3bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = ((XH2bis)) * AH2 + (1 - KH2O_H2) * (XH2Obis) * (AH2O * AH2) ^ (1 / 2) + (1
- KCO2_H2) * (XCO2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * (XN2bis) * (AN2 *
AH2) ^ (1 / 2) + (1 - KCO_H2) * (XCObis) * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * (XMGbis) * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * (XCH4bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3)
* (XNH3bis) * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = ((XCO2bis)) * ACO2 + (1 - KH2O_HCO2) * (XH2Obis) * (AH2O * ACO2) ^
(1 / 2) + (1 - KCO2_H2) * (XH2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XN2bis)
* (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * (XCObis) * (ACO * ACO2) ^ (1 / 2) +
grAsuite
   grAbis = (1 - KN2_MG) * (XMGbis) * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * (XCH4bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) *
(XNH3bis) * (ANH3 * AN2) ^ (1 / 2) + grAbis
   ArN2 = ((XN2bis)) * AN2 + (1 - KH2O_N2) * (XH2Obis) * (AH2O * AN2) ^ (1 / 2) + (1
- KN2_H2) * (XH2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XCO2bis) * (AN2 *
ACO2) ^ (1 / 2) + (1 - KN2_CO) * (XCObis) * (ACO * AN2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KH2O_MG) * (XMGbis) * (AH2O * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2O_CH4) * (XCH4bis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3)
* (XNH3bis) * (ANH3 * AH2O) ^ (1 / 2) + grAbis
   ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * (XH2bis) * (AH2O * AH2) ^ (1 / 2) +
(1 - KH2O_CO2) * (XCO2bis) * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * (XN2bis) *
(AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * (XCObis) * (ACO * AH2O) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO_MG) * (XMGbis) * (ACO * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO_CH4) * (XCH4bis) * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) *
(XNH3bis) * (ANH3 * ACO) ^ (1 / 2) + grAbis
```

ArCO = (XCObis) * ACO + (1 - KH2O_CO) * (XH2Obis) * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * (XCO2bis) * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * (XN2bis) * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * (XH2bis) * (ACO * AH2) ^ (1 / 2) + grAsuite

grAbis = (1 - KCH4_MG) * (XMGbis) * (ACH4 * AMG) ^ (1 / 2)

grAsuite = (1 - KH2_CH4) * (XH2bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * (XNH3bis) * (ANH3 * ACH4) ^ (1 / 2) + grAbis

ArCH4 = ((XCH4bis)) * ACH4 + (1 - KH2O_CH4) * (XH2Obis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * (XCO2bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * (XN2bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * (XCObis) * (ACO * ACH4) ^ (1 / 2) + grAsuite

grAbis = (1 - KNH3_MG) * (XMGbis) * (ANH3 * AMG) ^ (1 / 2)

grAsuite = (1 - KCH4_NH3) * (XCH4bis) * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * (XH2bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis

ArNH3 = ((XNH3bis)) * ANH3 + (1 - KH2O_NH3) * (XH2Obis) * (AH2O * ANH3) ^ (1 / 2) + (1 - KCO2_NH3) * (XCO2bis) * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * (XN2bis) * (AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * (XCObis) * (ACO * ANH3) ^ (1 / 2) + grAsuite

grAbis = (1 - KMG_NH3) * (XNH3bis) * (AMG * ANH3) ^ (1 / 2)

grAsuite = (1 - KCH4_MG) * (XCH4bis) * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) * (XH2bis) * (AMG * AH2) ^ (1 / 2) + grAbis

ArMG = ((XMGbis)) * AMG + (1 - KH2O_MG) * (XH2Obis) * (AH2O * AMG) ^ (1 / 2) + (1 - KCO2_MG) * (XCO2bis) * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * (XN2bis) * (AN2 * AMG) ^ (1 / 2) + (1 - KCO_MG) * (XCObis) * (ACO * AMG) ^ (1 / 2) + grAsuite

SB = BH2O + BH2 + BCO2 + BN2 + BCO + BNH3 + BCH4 + BMG

DVDXH2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArH2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXH2O = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArH2O) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCO2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCO2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCO = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCO) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXN2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArN2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCH4 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCH4) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXNH3 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArNH3) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXMG = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArMG) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

```
VCO2M = VN * (XCO2bis) - 1 * (XCO2bis) * 1 / 3 / 8 / 2 * DVDXCO2
VCOM = VN * (XCObis) - 1 * (XCObis) * 1 / 3 / 8 / 2 * DVDXCO
VH2M = VN * (XH2bis) - 1 * (XH2bis) * 1 / 3 / 8 / 2 * DVDXH2
VN2M = VN * (XN2bis) - 1 * (XN2bis) * 1 / 3 / 8 / 2 * DVDXN2
VCH4M = VN * (XCH4bis) - 1 * (XCH4bis) * 1 / 3 / 8 / 2 * DVDXCH4
VNH3M = VN * (XNH3bis) - 1 * (XNH3bis) * 1 / 3 / 8 / 2 * DVDXNH3
VH2OM = VN * (XH2Obis) - 1 * (XH2Obis) * 1 / 3 / 8 / 2 * DVDXH2O
VMGM = VN * (XMGbis) - 1 * (XMGbis) * 1 / 3 / 8 / 2 * DVDXMG

   'calcul de somme de Xk(1-Kki)racine(aialphai*akalphak)  (avant le 2 dans le calcul du coefficient de fugacité de l'espèce k)
   grAbis = (1 - KH2_MG) * XMGbis * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XCH4bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = (XH2bis) * AH2 + (1 - KH2O_H2) * XH2Obis * (AH2O * AH2) ^ (1 / 2) + (1 - KCO2_H2) * XCO2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * XN2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KCO_H2) * XCObis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * XMGbis * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * XCH4bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) * XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = (XCO2bis) * ACO2 + (1 - KH2O_HCO2) * XH2Obis * (AH2O * ACO2) ^ (1 / 2) + (1 - KCO2_H2) * XH2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XN2bis * (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * XCObis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * XMGbis * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * XCH4bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   ArN2 = (XN2bis) * AN2 + (1 - KH2O_N2) * XH2Obis * (AH2O * AN2) ^ (1 / 2) + (1 - KN2_H2) * XH2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XCO2bis * (AN2 * ACO2) ^ (1 / 2) + (1 - KN2_CO) * XCObis * (ACO * AN2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KH2O_MG) * XMGbis * (AH2O * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2O_CH4) * XCH4bis * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + grAbis
   ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * XH2bis * (AH2O * AH2) ^ (1 / 2) + (1 - KH2O_CO2) * XCO2bis * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * XN2bis * (AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * XCObis * (ACO * AH2O) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO_MG) * XMGbis * (ACO * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO_CH4) * XCH4bis * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) * XNH3bis * (ANH3 * ACO) ^ (1 / 2) + grAbis
   ArCO = (XCObis) * ACO + (1 - KH2O_CO) * XH2Obis * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * XCO2bis * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * XN2bis * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * XH2bis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCH4_MG) * XMGbis * (ACH4 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XH2bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + grAbis
   ArCH4 = (XCH4bis) * ACH4 + (1 - KH2O_CH4) * XH2Obis * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * XN2bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * XCObis * (ACO * ACH4) ^ (1 / 2) + grAsuite
   grAbis = (1 - KNH3_MG) * XMGbis * (ANH3 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCH4_NH3) * XCH4bis * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * XH2bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
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    ArNH3 = (XNH3bis) * ANH3 + (1 - KH2O_NH3) * XH2Obis * (AH2O * ANH3) ^ (1 / 2)
+ (1 - KCO2_NH3) * XCO2bis * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * XN2bis *
(AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * XCObis * (ACO * ANH3) ^ (1 / 2) + grAsuite
    grAbis = (1 - KMG_NH3) * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (1 - KCH4_MG) * XCH4bis * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
XH2bis * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = (XMGbis) * AMG + (1 - KH2O_MG) * XH2Obis * (AH2O * AMG) ^ (1 / 2) +
(1 - KCO2_MG) * XCO2bis * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * XN2bis * (AN2 *
AMG) ^ (1 / 2) + (1 - KCO_MG) * XCObis * (ACO * AMG) ^ (1 / 2) + grAsuite

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, Ai et Bi qui
interviennent dans le calcul du coefficient de fugacité
    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, A et B qui
interviennent dans le calcul du coefficient de fugacité
    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
```

```
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
   GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calculs des coefficients de fugacités
   'logFIH2Osoave = ZN - 1 - Log(ZN - GRB) - GRA / GRB * Log((ZN + GRB) / ZN)
         'FIH2Oincsoave = 10 ^ (logFIH2Osoave / 2.303)
         'Worksheets(1).Range("C31").Value = FIH2Oincsoave

   logFIH2O = BH2O / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2O / GRB - 2
/ A * ArH2O) * Log(1 + GRB / ZN)
         FIH2Oinc = 10 ^ (logFIH2O / 2.303)
         FUH2Oinc = FIH2Oinc * P * XH2Obis
         FUH2Oi = FUH2Oinc * 0.00001
   logFIH2 = BH2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2 / GRB - 2 / A *
ArH2) * Log(1 + GRB / ZN)
         FIH2inc = 10 ^ (logFIH2 / 2.303)
         FUH2inc = FIH2inc * P * XH2bis
         FUH2i = FUH2inc * 0.00001

   logFICO = BCO / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO / GRB - 2 / A
* ArCO) * Log(1 + GRB / ZN)
         FICOinc = 10 ^ (logFICO / 2.303)
         FUCOinc = FICOinc * P * XCObis
         FUCOi = FUCOinc * 0.00001

   logFICO2 = BCO2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO2 / GRB - 2 /
A * ArCO2) * Log(1 + GRB / ZN)
         FICO2inc = 10 ^ (logFICO2 / 2.303)
         FUCO2inc = FICO2inc * P * XCO2bis
         FUCO2i = FUCO2inc * 0.00001 'la même chose mais en bar

   logFIN2 = BN2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BN2 / GRB - 2 / A *
ArN2) * Log(1 + GRB / ZN)
         FIN2inc = 10 ^ (logFIN2 / 2.303)
         FUN2inc = FIN2inc * P * XN2bis
         FUN2i = FUN2inc * 0.00001 'la même chose mais en bar

   logFICH4 = BCH4 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCH4 / GRB - 2 /
A * ArCH4) * Log(1 + GRB / ZN)
         FICH4inc = 10 ^ (logFICH4 / 2.303)
         FUCH4inc = FICH4inc * P * XCH4bis
         FUCH4i = FUCH4inc * 0.00001
```

```
   logFINH3 = BNH3 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BNH3 / GRB - 2
/ A * ArNH3) * Log(1 + GRB / ZN)
          FINH3inc = 10 ^ (logFINH3 / 2.303)
          FUNH3inc = FINH3inc * P * XNH3bis
          FUNH3i = FUNH3inc * 0.00001

   logFIMG = BMG / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BMG / GRB - 2 /
A * ArMG) * Log(1 + GRB / ZN)
          FIMGinc = 10 ^ (logFIMG / 2.303)
          FUMGinc = FIMGinc * P * XMGbis
          FUMGi = FUMGinc * 0.00001

Worksheets(1).Range("L3").Value = FUH2Oi
Call PROPORTION2
End Sub
Private Sub PROPORTION2()
XH2Obis = 0
XCO2bis = 1
XCObis = 0
XH2bis = 0
XN2bis = 0
XCH4bis = 0
XNH3bis = 0
XMGbis = 0

    Pb = Worksheets(1).Range("B10").Value
   P = Pb * 100000 'passage de la pression de bar en Pa
   T = Worksheets(1).Range("B11").Value + 273.15

   TcH2O = Worksheets(1).Range("C3").Value 'température critique de H2O dans la cellule
J8
   PcH2O = Worksheets(1).Range("D3").Value 'pression critique de H2O
   TcCO2 = Worksheets(1).Range("C4").Value
   PcCO2 = Worksheets(1).Range("D4").Value
   TcCO = Worksheets(1).Range("C5").Value
   PcCO = Worksheets(1).Range("D5").Value
   TcH2 = Worksheets(1).Range("C2").Value
   PcH2 = Worksheets(1).Range("D2").Value
   TcN2 = Worksheets(1).Range("C8").Value
   PcN2 = Worksheets(1).Range("D8").Value
   TcCH4 = Worksheets(1).Range("C6").Value
   PcCH4 = Worksheets(1).Range("D6").Value
   TcNH3 = Worksheets(1).Range("C9").Value
   PcNH3 = Worksheets(1).Range("D9").Value
   TcMG = Worksheets(1).Range("C7").Value
   PcMG = Worksheets(1).Range("D7").Value

   R = 8.314472 'constante des gaz parfaits
   'calcul des facteurs acentriques
```

```
    wH2O = Worksheets(1).Range("E3").Value
    nH2O = 0.48508 + 1.55171 * wH2O - 0.15613 * wH2O ^ 2
    alphaH2O = (1 + nH2O * (1 - (T / TcH2O) ^ 0.5)) ^ 2
    wCO2 = Worksheets(1).Range("E4").Value
    nCO2 = 0.48508 + 1.55171 * wCO2 - 0.15613 * wCO2 ^ 2
    alphaCO2 = (1 + nCO2 * (1 - (T / TcCO2) ^ 0.5)) ^ 2
    wCO = Worksheets(1).Range("E5").Value
    nCO = 0.48508 + 1.55171 * wCO - 0.15613 * wCO ^ 2
    alphaCO = (1 + nCO * (1 - (T / TcCO) ^ 0.5)) ^ 2
    wH2 = Worksheets(1).Range("E2").Value
    nH2 = 0.48508 + 1.55171 * wH2 - 0.15613 * wH2 ^ 2
    alphaH2 = (1 + nH2 * (1 - (T / TcH2) ^ 0.5)) ^ 2
    wN2 = Worksheets(1).Range("E8").Value
    nN2 = 0.48508 + 1.55171 * wN2 - 0.15613 * wN2 ^ 2
    alphaN2 = (1 + nN2 * (1 - (T / TcN2) ^ 0.5)) ^ 2
    wCH4 = Worksheets(1).Range("E6").Value
    nCH4 = 0.48508 + 1.55171 * wCH4 - 0.15613 * wCH4 ^ 2
    alphaCH4 = (1 + nCH4 * (1 - (T / TcCH4) ^ 0.5)) ^ 2
    wNH3 = Worksheets(1).Range("E9").Value
    nNH3 = 0.48508 + 1.55171 * wNH3 - 0.15613 * wNH3 ^ 2
    alphaNH3 = (1 + nNH3 * (1 - (T / TcNH3) ^ 0.5)) ^ 2
    wMG = Worksheets(1).Range("E7").Value
    nMG = 0.48508 + 1.55171 * wMG - 0.15613 * wMG ^ 2
    alphaMG = (1 + nMG * (1 - (T / TcMG) ^ 0.5)) ^ 2

    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
```

```
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
    GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

      test = 1
       ZN = 100.01 'initialisation NR à changer si plantage

       While test > 0.000000001
       FZ = ZN ^ 3 - ZN ^ 2 + (GRA - GRB ^ 2 - GRB) * ZN - GRA * GRB
       FpZ = 3 * ZN ^ 2 - 2 * ZN + (GRA - GRB ^ 2 - GRB)

       ZN1 = ZN - FZ / FpZ
       test = Abs(ZN1 - ZN)
       ZN = ZN1
       Wend
       VN = (ZN * R * T / P)
       V = VN * 1000000

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, aialphai et bialphai
qui interviennent dans le calcul des coefficients de fugacité
    AH2 = 0.42748 * alphaH2 * (R * TcH2 ^ 2) / (PcH2 * 100000#)
    BH2 = 0.08664 * R * TcH2 / (PcH2 * 100000#)
    BiH2 = BH2 'stockage de bialphai
    ACO2 = 0.42748 * alphaCO2 * (R * TcCO2 ^ 2) / (PcCO2 * 100000#)
    BCO2 = 0.08664 * R * TcCO2 / (PcCO2 * 100000#)
    BiCO2 = BCO2
    AN2 = 0.42748 * alphaN2 * (R * TcN2 ^ 2) / (PcN2 * 100000#)
    BN2 = 0.08664 * R * TcN2 / (PcN2 * 100000#)
    BiN2 = BN2
    AH2O = 0.42748 * alphaH2O * (R * TcH2O ^ 2) / (PcH2O * 100000#)
    BH2O = 0.08664 * R * TcH2O / (PcH2O * 100000#)
```

```
   BiH2O = BH2O
   ACO = 0.42748 * alphaCO * (R * TcCO ^ 2) / (PcCO * 100000#)
   BCO = 0.08664 * R * TcCO / (PcCO * 100000#)
   BiCO = BCO
   ACH4 = 0.42748 * alphaCH4 * (R * TcCH4 ^ 2) / (PcCH4 * 100000#)
   BCH4 = 0.08664 * R * TcCH4 / (PcCH4 * 100000#)
   BiCH4 = BCH4
   ANH3 = 0.42748 * alphaNH3 * (R * TcNH3 ^ 2) / (PcNH3 * 100000#)
   BNH3 = 0.08664 * R * TcNH3 / (PcNH3 * 100000#)
   BiNH3 = BNH3
   AMG = 0.42748 * alphaMG * (R * TcMG ^ 2) / (PcMG * 100000#)
   BMG = 0.08664 * R * TcMG / (PcMG * 100000#)
   BiMG = BMG

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, a et b qui
n'interviennent pas dans le calcul du coefficient de fugacité
   grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
   grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   A = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis
* XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) *
XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) *
XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis *
(ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 /
2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO +
2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) *
XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO
* AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) +
grAsuite
   B = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis *
BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calcul de dérivés de XiXj(1-Kji)racine(aialphai*akalphak)
   grAbis = (1 - KH2_MG) * (XMGbis) * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * (XCH4bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
(XNH3bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
```

ArH2 = ((XH2bis)) * AH2 + (1 - KH2O_H2) * (XH2Obis) * (AH2O * AH2) ^ (1 / 2) + (1 - KCO2_H2) * (XCO2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * (XN2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KCO_H2) * (XCObis) * (ACO * AH2) ^ (1 / 2) + grAsuite

grAbis = (1 - KCO2_MG) * (XMGbis) * (ACO2 * AMG) ^ (1 / 2)

grAsuite = (1 - KCO2_CH4) * (XCH4bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) * (XNH3bis) * (ANH3 * ACO2) ^ (1 / 2) + grAbis

ArCO2 = ((XCO2bis)) * ACO2 + (1 - KH2O_HCO2) * (XH2Obis) * (AH2O * ACO2) ^ (1 / 2) + (1 - KCO2_H2) * (XH2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XN2bis) * (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * (XCObis) * (ACO * ACO2) ^ (1 / 2) + grAsuite

grAbis = (1 - KN2_MG) * (XMGbis) * (AN2 * AMG) ^ (1 / 2)

grAsuite = (1 - KN2_CH4) * (XCH4bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) * (XNH3bis) * (ANH3 * AN2) ^ (1 / 2) + grAbis

ArN2 = ((XN2bis)) * AN2 + (1 - KH2O_N2) * (XH2Obis) * (AH2O * AN2) ^ (1 / 2) + (1 - KN2_H2) * (XH2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XCO2bis) * (AN2 * ACO2) ^ (1 / 2) + (1 - KN2_CO) * (XCObis) * (ACO * AN2) ^ (1 / 2) + grAsuite

grAbis = (1 - KH2O_MG) * (XMGbis) * (AH2O * AMG) ^ (1 / 2)

grAsuite = (1 - KH2O_CH4) * (XCH4bis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) * (XNH3bis) * (ANH3 * AH2O) ^ (1 / 2) + grAbis

ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * (XH2bis) * (AH2O * AH2) ^ (1 / 2) + (1 - KH2O_CO2) * (XCO2bis) * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * (XN2bis) * (AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * (XCObis) * (ACO * AH2O) ^ (1 / 2) + grAsuite

grAbis = (1 - KCO_MG) * (XMGbis) * (ACO * AMG) ^ (1 / 2)

grAsuite = (1 - KCO_CH4) * (XCH4bis) * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) * (XNH3bis) * (ANH3 * ACO) ^ (1 / 2) + grAbis

ArCO = (XCObis) * ACO + (1 - KH2O_CO) * (XH2Obis) * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * (XCO2bis) * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * (XN2bis) * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * (XH2bis) * (ACO * AH2) ^ (1 / 2) + grAsuite

grAbis = (1 - KCH4_MG) * (XMGbis) * (ACH4 * AMG) ^ (1 / 2)

grAsuite = (1 - KH2_CH4) * (XH2bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * (XNH3bis) * (ANH3 * ACH4) ^ (1 / 2) + grAbis

ArCH4 = ((XCH4bis)) * ACH4 + (1 - KH2O_CH4) * (XH2Obis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * (XCO2bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * (XN2bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * (XCObis) * (ACO * ACH4) ^ (1 / 2) + grAsuite

grAbis = (1 - KNH3_MG) * (XMGbis) * (ANH3 * AMG) ^ (1 / 2)

grAsuite = (1 - KCH4_NH3) * (XCH4bis) * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * (XH2bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis

ArNH3 = ((XNH3bis)) * ANH3 + (1 - KH2O_NH3) * (XH2Obis) * (AH2O * ANH3) ^ (1 / 2) + (1 - KCO2_NH3) * (XCO2bis) * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * (XN2bis) * (AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * (XCObis) * (ACO * ANH3) ^ (1 / 2) + grAsuite

grAbis = (1 - KMG_NH3) * (XNH3bis) * (AMG * ANH3) ^ (1 / 2)

grAsuite = (1 - KCH4_MG) * (XCH4bis) * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) * (XH2bis) * (AMG * AH2) ^ (1 / 2) + grAbis

ArMG = ((XMGbis)) * AMG + (1 - KH2O_MG) * (XH2Obis) * (AH2O * AMG) ^ (1 / 2) + (1 - KCO2_MG) * (XCO2bis) * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * (XN2bis) * (AN2 * AMG) ^ (1 / 2) + (1 - KCO_MG) * (XCObis) * (ACO * AMG) ^ (1 / 2) + grAsuite

SB = BH2O + BH2 + BCO2 + BN2 + BCO + BNH3 + BCH4 + BMG

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   DVDXH2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArH2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXH2O = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArH2O) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXCO2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArCO2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXCO = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArCO) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXN2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArN2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXCH4 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArCH4) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXNH3 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArNH3) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXMG = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArMG) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)

VCO2M = VN * (XCO2bis) - 1 * (XCO2bis) * 1 / 3 / 8 / 2 * DVDXCO2
VCOM = VN * (XCObis) - 1 * (XCObis) * 1 / 3 / 8 / 2 * DVDXCO
VH2M = VN * (XH2bis) - 1 * (XH2bis) * 1 / 3 / 8 / 2 * DVDXH2
VN2M = VN * (XN2bis) - 1 * (XN2bis) * 1 / 3 / 8 / 2 * DVDXN2
VCH4M = VN * (XCH4bis) - 1 * (XCH4bis) * 1 / 3 / 8 / 2 * DVDXCH4
VNH3M = VN * (XNH3bis) - 1 * (XNH3bis) * 1 / 3 / 8 / 2 * DVDXNH3
VH2OM = VN * (XH2Obis) - 1 * (XH2Obis) * 1 / 3 / 8 / 2 * DVDXH2O
VMGM = VN * (XMGbis) - 1 * (XMGbis) * 1 / 3 / 8 / 2 * DVDXMG

   'calcul de somme de Xk(1-Kki)racine(aialphai*akalphak)  (avant le 2 dans le calcul du
coefficient de fugacité de l'espèce k)
   grAbis = (1 - KH2_MG) * XMGbis * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XCH4bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
XNH3bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = (XH2bis) * AH2 + (1 - KH2O_H2) * XH2Obis * (AH2O * AH2) ^ (1 / 2) + (1 -
KCO2_H2) * XCO2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * XN2bis * (AN2 * AH2)
^ (1 / 2) + (1 - KCO_H2) * XCObis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * XMGbis * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * XCH4bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = (XCO2bis) * ACO2 + (1 - KH2O_HCO2) * XH2Obis * (AH2O * ACO2) ^ (1 /
2) + (1 - KCO2_H2) * XH2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XN2bis * (AN2
* ACO2) ^ (1 / 2) + (1 - KCO_CO2) * XCObis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * XMGbis * (AN2 * AMG) ^ (1 / 2)
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    grAsuite = (1 - KN2_CH4) * XCH4bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) *
XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    ArN2 = (XN2bis) * AN2 + (1 - KH2O_N2) * XH2Obis * (AH2O * AN2) ^ (1 / 2) + (1 -
KN2_H2) * XH2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XCO2bis * (AN2 * ACO2)
^ (1 / 2) + (1 - KN2_CO) * XCObis * (ACO * AN2) ^ (1 / 2) + grAsuite
    grAbis = (1 - KH2O_MG) * XMGbis * (AH2O * AMG) ^ (1 / 2)
    grAsuite = (1 - KH2O_CH4) * XCH4bis * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) *
XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + grAbis
    ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * XH2bis * (AH2O * AH2) ^ (1 / 2) + (1
- KH2O_CO2) * XCO2bis * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * XN2bis * (AN2 *
AH2O) ^ (1 / 2) + (1 - KH2O_CO) * XCObis * (ACO * AH2O) ^ (1 / 2) + grAsuite
    grAbis = (1 - KCO_MG) * XMGbis * (ACO * AMG) ^ (1 / 2)
    grAsuite = (1 - KCO_CH4) * XCH4bis * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) *
XNH3bis * (ANH3 * ACO) ^ (1 / 2) + grAbis
    ArCO = (XCObis) * ACO + (1 - KH2O_CO) * XH2Obis * (AH2O * ACO) ^ (1 / 2) + (1 -
KCO_CO2) * XCO2bis * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * XN2bis * (AN2 *
ACO) ^ (1 / 2) + (1 - KCO_H2) * XH2bis * (ACO * AH2) ^ (1 / 2) + grAsuite
    grAbis = (1 - KCH4_MG) * XMGbis * (ACH4 * AMG) ^ (1 / 2)
    grAsuite = (1 - KH2_CH4) * XH2bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) *
XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + grAbis
    ArCH4 = (XCH4bis) * ACH4 + (1 - KH2O_CH4) * XH2Obis * (AH2O * ACH4) ^ (1 / 2)
+ (1 - KCO2_CH4) * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * XN2bis *
(AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * XCObis * (ACO * ACH4) ^ (1 / 2) + grAsuite
    grAbis = (1 - KNH3_MG) * XMGbis * (ANH3 * AMG) ^ (1 / 2)
    grAsuite = (1 - KCH4_NH3) * XCH4bis * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
XH2bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
    ArNH3 = (XNH3bis) * ANH3 + (1 - KH2O_NH3) * XH2Obis * (AH2O * ANH3) ^ (1 / 2)
+ (1 - KCO2_NH3) * XCO2bis * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * XN2bis *
(AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * XCObis * (ACO * ANH3) ^ (1 / 2) + grAsuite
    grAbis = (1 - KMG_NH3) * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (1 - KCH4_MG) * XCH4bis * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
XH2bis * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = (XMGbis) * AMG + (1 - KH2O_MG) * XH2Obis * (AH2O * AMG) ^ (1 / 2) +
(1 - KCO2_MG) * XCO2bis * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * XN2bis * (AN2 *
AMG) ^ (1 / 2) + (1 - KCO_MG) * XCObis * (ACO * AMG) ^ (1 / 2) + grAsuite

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, Ai et Bi qui
interviennent dans le calcul du coefficient de fugacité
    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
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    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, A et B qui
interviennent dans le calcul du coefficient de fugacité
    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
    GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

    'calculs des coefficients de fugacités
    'logFIH2Osoave = ZN - 1 - Log(ZN - GRB) - GRA / GRB * Log((ZN + GRB) / ZN)
        'FIH2Oincsoave = 10 ^ (logFIH2Osoave / 2.303)
        'Worksheets(1).Range("C31").Value = FIH2Oincsoave

    logFIH2O = BH2O / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2O / GRB - 2
/ A * ArH2O) * Log(1 + GRB / ZN)
        FIH2Oinc = 10 ^ (logFIH2O / 2.303)
        FUH2Oinc = FIH2Oinc * P * XH2Obis
        FUH2Oi = FUH2Oinc * 0.00001
    logFIH2 = BH2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2 / GRB - 2 / A *
ArH2) * Log(1 + GRB / ZN)
        FIH2inc = 10 ^ (logFIH2 / 2.303)
```

```
        FUH2inc = FIH2inc * P * XH2bis
        FUH2i = FUH2inc * 0.00001

   logFICO = BCO / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO / GRB - 2 / A
* ArCO) * Log(1 + GRB / ZN)
        FICOinc = 10 ^ (logFICO / 2.303)
        FUCOinc = FICOinc * P * XCObis
        FUCOi = FUCOinc * 0.00001

   logFICO2 = BCO2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO2 / GRB - 2 /
A * ArCO2) * Log(1 + GRB / ZN)
        FICO2inc = 10 ^ (logFICO2 / 2.303)
        FUCO2inc = FICO2inc * P * XCO2bis
        FUCO2i = FUCO2inc * 0.00001 'la même chose mais en bar

   logFIN2 = BN2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BN2 / GRB - 2 / A *
ArN2) * Log(1 + GRB / ZN)
        FIN2inc = 10 ^ (logFIN2 / 2.303)
        FUN2inc = FIN2inc * P * XN2bis
        FUN2i = FUN2inc * 0.00001 'la même chose mais en bar

   logFICH4 = BCH4 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCH4 / GRB - 2 /
A * ArCH4) * Log(1 + GRB / ZN)
        FICH4inc = 10 ^ (logFICH4 / 2.303)
        FUCH4inc = FICH4inc * P * XCH4bis
        FUCH4i = FUCH4inc * 0.00001

   logFINH3 = BNH3 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BNH3 / GRB - 2
/ A * ArNH3) * Log(1 + GRB / ZN)
        FINH3inc = 10 ^ (logFINH3 / 2.303)
        FUNH3inc = FINH3inc * P * XNH3bis
        FUNH3i = FUNH3inc * 0.00001

   logFIMG = BMG / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BMG / GRB - 2 /
A * ArMG) * Log(1 + GRB / ZN)
        FIMGinc = 10 ^ (logFIMG / 2.303)
        FUMGinc = FIMGinc * P * XMGbis
        FUMGi = FUMGinc * 0.00001

Worksheets(1).Range("L4").Value = FUCO2i
Call PROPORTION3
End Sub
Private Sub PROPORTION3()
XH2Obis = 0
XCO2bis = 0
XCObis = 1
XH2bis = 0
XN2bis = 0
XCH4bis = 0
XNH3bis = 0
```

```
XMGbis = 0

    Pb = Worksheets(1).Range("B10").Value
   P = Pb * 100000 'passage de la pression de bar en Pa
   T = Worksheets(1).Range("B11").Value + 273.15

   TcH2O = Worksheets(1).Range("C3").Value 'température critique de H2O dans la cellule
J8
   PcH2O = Worksheets(1).Range("D3").Value 'pression critique de H2O
   TcCO2 = Worksheets(1).Range("C4").Value
   PcCO2 = Worksheets(1).Range("D4").Value
   TcCO = Worksheets(1).Range("C5").Value
   PcCO = Worksheets(1).Range("D5").Value
   TcH2 = Worksheets(1).Range("C2").Value
   PcH2 = Worksheets(1).Range("D2").Value
   TcN2 = Worksheets(1).Range("C8").Value
   PcN2 = Worksheets(1).Range("D8").Value
   TcCH4 = Worksheets(1).Range("C6").Value
   PcCH4 = Worksheets(1).Range("D6").Value
   TcNH3 = Worksheets(1).Range("C9").Value
   PcNH3 = Worksheets(1).Range("D9").Value
   TcMG = Worksheets(1).Range("C7").Value
   PcMG = Worksheets(1).Range("D7").Value

   R = 8.314472 'constante des gaz parfaits
   'calcul des facteurs acentriques
   wH2O = Worksheets(1).Range("E3").Value
   nH2O = 0.48508 + 1.55171 * wH2O - 0.15613 * wH2O ^ 2
   alphaH2O = (1 + nH2O * (1 - (T / TcH2O) ^ 0.5)) ^ 2
   wCO2 = Worksheets(1).Range("E4").Value
   nCO2 = 0.48508 + 1.55171 * wCO2 - 0.15613 * wCO2 ^ 2
   alphaCO2 = (1 + nCO2 * (1 - (T / TcCO2) ^ 0.5)) ^ 2
   wCO = Worksheets(1).Range("E5").Value
   nCO = 0.48508 + 1.55171 * wCO - 0.15613 * wCO ^ 2
   alphaCO = (1 + nCO * (1 - (T / TcCO) ^ 0.5)) ^ 2
   wH2 = Worksheets(1).Range("E2").Value
   nH2 = 0.48508 + 1.55171 * wH2 - 0.15613 * wH2 ^ 2
   alphaH2 = (1 + nH2 * (1 - (T / TcH2) ^ 0.5)) ^ 2
   wN2 = Worksheets(1).Range("E8").Value
   nN2 = 0.48508 + 1.55171 * wN2 - 0.15613 * wN2 ^ 2
   alphaN2 = (1 + nN2 * (1 - (T / TcN2) ^ 0.5)) ^ 2
   wCH4 = Worksheets(1).Range("E6").Value
   nCH4 = 0.48508 + 1.55171 * wCH4 - 0.15613 * wCH4 ^ 2
   alphaCH4 = (1 + nCH4 * (1 - (T / TcCH4) ^ 0.5)) ^ 2
   wNH3 = Worksheets(1).Range("E9").Value
   nNH3 = 0.48508 + 1.55171 * wNH3 - 0.15613 * wNH3 ^ 2
   alphaNH3 = (1 + nNH3 * (1 - (T / TcNH3) ^ 0.5)) ^ 2
   wMG = Worksheets(1).Range("E7").Value
   nMG = 0.48508 + 1.55171 * wMG - 0.15613 * wMG ^ 2
   alphaMG = (1 + nMG * (1 - (T / TcMG) ^ 0.5)) ^ 2
```

```
   AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
   BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
   ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
   BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
   AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
   BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
   AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
   BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
   ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
   BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
   ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
   BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
   ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
   BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
   AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
   BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
   grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
   GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

    test = 1
     ZN = 100.01 'initialisation NR à changer si plantage
```

```
While test > 0.000000001
FZ = ZN ^ 3 - ZN ^ 2 + (GRA - GRB ^ 2 - GRB) * ZN - GRA * GRB
FpZ = 3 * ZN ^ 2 - 2 * ZN + (GRA - GRB ^ 2 - GRB)

ZN1 = ZN - FZ / FpZ
test = Abs(ZN1 - ZN)
ZN = ZN1
Wend
VN = (ZN * R * T / P)
V = VN * 1000000

'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, aialphai et bialphai qui interviennent dans le calcul des coefficients de fugacité
AH2 = 0.42748 * alphaH2 * (R * TcH2 ^ 2) / (PcH2 * 100000#)
BH2 = 0.08664 * R * TcH2 / (PcH2 * 100000#)
BiH2 = BH2 'stockage de bialphai
ACO2 = 0.42748 * alphaCO2 * (R * TcCO2 ^ 2) / (PcCO2 * 100000#)
BCO2 = 0.08664 * R * TcCO2 / (PcCO2 * 100000#)
BiCO2 = BCO2
AN2 = 0.42748 * alphaN2 * (R * TcN2 ^ 2) / (PcN2 * 100000#)
BN2 = 0.08664 * R * TcN2 / (PcN2 * 100000#)
BiN2 = BN2
AH2O = 0.42748 * alphaH2O * (R * TcH2O ^ 2) / (PcH2O * 100000#)
BH2O = 0.08664 * R * TcH2O / (PcH2O * 100000#)
BiH2O = BH2O
ACO = 0.42748 * alphaCO * (R * TcCO ^ 2) / (PcCO * 100000#)
BCO = 0.08664 * R * TcCO / (PcCO * 100000#)
BiCO = BCO
ACH4 = 0.42748 * alphaCH4 * (R * TcCH4 ^ 2) / (PcCH4 * 100000#)
BCH4 = 0.08664 * R * TcCH4 / (PcCH4 * 100000#)
BiCH4 = BCH4
ANH3 = 0.42748 * alphaNH3 * (R * TcNH3 ^ 2) / (PcNH3 * 100000#)
BNH3 = 0.08664 * R * TcNH3 / (PcNH3 * 100000#)
BiNH3 = BNH3
AMG = 0.42748 * alphaMG * (R * TcMG ^ 2) / (PcMG * 100000#)
BMG = 0.08664 * R * TcMG / (PcMG * 100000#)
BiMG = BMG

'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, a et b qui n'interviennent pas dans le calcul du coefficient de fugacité
grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG * AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) * XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis * (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4) ^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) * XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis * XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
```

```
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 / 2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 - KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) * XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis * XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3 * ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 * (1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   A = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   B = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calcul de dérivés de XiXj(1-Kji)racine(aialphai*akalphak)
   grAbis = (1 - KH2_MG) * (XMGbis) * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * (XCH4bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * (XNH3bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = ((XH2bis)) * AH2 + (1 - KH2O_H2) * (XH2Obis) * (AH2O * AH2) ^ (1 / 2) + (1 - KCO2_H2) * (XCO2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * (XN2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KCO_H2) * (XCObis) * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * (XMGbis) * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * (XCH4bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) * (XNH3bis) * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = ((XCO2bis)) * ACO2 + (1 - KH2O_HCO2) * (XH2Obis) * (AH2O * ACO2) ^ (1 / 2) + (1 - KCO2_H2) * (XH2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XN2bis) * (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * (XCObis) * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * (XMGbis) * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * (XCH4bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) * (XNH3bis) * (ANH3 * AN2) ^ (1 / 2) + grAbis
   ArN2 = ((XN2bis)) * AN2 + (1 - KH2O_N2) * (XH2Obis) * (AH2O * AN2) ^ (1 / 2) + (1 - KN2_H2) * (XH2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XCO2bis) * (AN2 * ACO2) ^ (1 / 2) + (1 - KN2_CO) * (XCObis) * (ACO * AN2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KH2O_MG) * (XMGbis) * (AH2O * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2O_CH4) * (XCH4bis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) * (XNH3bis) * (ANH3 * AH2O) ^ (1 / 2) + grAbis
   ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * (XH2bis) * (AH2O * AH2) ^ (1 / 2) + (1 - KH2O_CO2) * (XCO2bis) * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * (XN2bis) * (AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * (XCObis) * (ACO * AH2O) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO_MG) * (XMGbis) * (ACO * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO_CH4) * (XCH4bis) * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) * (XNH3bis) * (ANH3 * ACO) ^ (1 / 2) + grAbis
```

ArCO = (XCObis) * ACO + (1 - KH2O_CO) * (XH2Obis) * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * (XCO2bis) * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * (XN2bis) * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * (XH2bis) * (ACO * AH2) ^ (1 / 2) + grAsuite

grAbis = (1 - KCH4_MG) * (XMGbis) * (ACH4 * AMG) ^ (1 / 2)

grAsuite = (1 - KH2_CH4) * (XH2bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * (XNH3bis) * (ANH3 * ACH4) ^ (1 / 2) + grAbis

ArCH4 = ((XCH4bis)) * ACH4 + (1 - KH2O_CH4) * (XH2Obis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * (XCO2bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * (XN2bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * (XCObis) * (ACO * ACH4) ^ (1 / 2) + grAsuite

grAbis = (1 - KNH3_MG) * (XMGbis) * (ANH3 * AMG) ^ (1 / 2)

grAsuite = (1 - KCH4_NH3) * (XCH4bis) * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * (XH2bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis

ArNH3 = ((XNH3bis)) * ANH3 + (1 - KH2O_NH3) * (XH2Obis) * (AH2O * ANH3) ^ (1 / 2) + (1 - KCO2_NH3) * (XCO2bis) * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * (XN2bis) * (AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * (XCObis) * (ACO * ANH3) ^ (1 / 2) + grAsuite

grAbis = (1 - KMG_NH3) * (XNH3bis) * (AMG * ANH3) ^ (1 / 2)

grAsuite = (1 - KCH4_MG) * (XCH4bis) * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) * (XH2bis) * (AMG * AH2) ^ (1 / 2) + grAbis

ArMG = ((XMGbis)) * AMG + (1 - KH2O_MG) * (XH2Obis) * (AH2O * AMG) ^ (1 / 2) + (1 - KCO2_MG) * (XCO2bis) * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * (XN2bis) * (AN2 * AMG) ^ (1 / 2) + (1 - KCO_MG) * (XCObis) * (ACO * AMG) ^ (1 / 2) + grAsuite

SB = BH2O + BH2 + BCO2 + BN2 + BCO + BNH3 + BCH4 + BMG

DVDXH2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArH2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXH2O = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArH2O) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCO2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCO2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCO = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCO) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXN2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArN2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCH4 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCH4) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXNH3 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArNH3) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXMG = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArMG) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

```
VCO2M = VN * (XCO2bis) - 1 * (XCO2bis) * 1 / 3 / 8 / 2 * DVDXCO2
VCOM = VN * (XCObis) - 1 * (XCObis) * 1 / 3 / 8 / 2 * DVDXCO
VH2M = VN * (XH2bis) - 1 * (XH2bis) * 1 / 3 / 8 / 2 * DVDXH2
VN2M = VN * (XN2bis) - 1 * (XN2bis) * 1 / 3 / 8 / 2 * DVDXN2
VCH4M = VN * (XCH4bis) - 1 * (XCH4bis) * 1 / 3 / 8 / 2 * DVDXCH4
VNH3M = VN * (XNH3bis) - 1 * (XNH3bis) * 1 / 3 / 8 / 2 * DVDXNH3
VH2OM = VN * (XH2Obis) - 1 * (XH2Obis) * 1 / 3 / 8 / 2 * DVDXH2O
VMGM = VN * (XMGbis) - 1 * (XMGbis) * 1 / 3 / 8 / 2 * DVDXMG

   'calcul de somme de Xk(1-Kki)racine(aialphai*akalphak)  (avant le 2 dans le calcul du coefficient de fugacité de l'espèce k)
   grAbis = (1 - KH2_MG) * XMGbis * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XCH4bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = (XH2bis) * AH2 + (1 - KH2O_H2) * XH2Obis * (AH2O * AH2) ^ (1 / 2) + (1 - KCO2_H2) * XCO2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * XN2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KCO_H2) * XCObis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * XMGbis * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * XCH4bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) * XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = (XCO2bis) * ACO2 + (1 - KH2O_HCO2) * XH2Obis * (AH2O * ACO2) ^ (1 / 2) + (1 - KCO2_H2) * XH2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XN2bis * (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * XCObis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * XMGbis * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * XCH4bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   ArN2 = (XN2bis) * AN2 + (1 - KH2O_N2) * XH2Obis * (AH2O * AN2) ^ (1 / 2) + (1 - KN2_H2) * XH2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XCO2bis * (AN2 * ACO2) ^ (1 / 2) + (1 - KN2_CO) * XCObis * (ACO * AN2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KH2O_MG) * XMGbis * (AH2O * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2O_CH4) * XCH4bis * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + grAbis
   ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * XH2bis * (AH2O * AH2) ^ (1 / 2) + (1 - KH2O_CO2) * XCO2bis * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * XN2bis * (AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * XCObis * (ACO * AH2O) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO_MG) * XMGbis * (ACO * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO_CH4) * XCH4bis * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) * XNH3bis * (ANH3 * ACO) ^ (1 / 2) + grAbis
   ArCO = (XCObis) * ACO + (1 - KH2O_CO) * XH2Obis * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * XCO2bis * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * XN2bis * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * XH2bis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCH4_MG) * XMGbis * (ACH4 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XH2bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + grAbis
   ArCH4 = (XCH4bis) * ACH4 + (1 - KH2O_CH4) * XH2Obis * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * XN2bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * XCObis * (ACO * ACH4) ^ (1 / 2) + grAsuite
   grAbis = (1 - KNH3_MG) * XMGbis * (ANH3 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCH4_NH3) * XCH4bis * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * XH2bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
```

```
    ArNH3 = (XNH3bis) * ANH3 + (1 - KH2O_NH3) * XH2Obis * (AH2O * ANH3) ^ (1 / 2)
+ (1 - KCO2_NH3) * XCO2bis * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * XN2bis *
(AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * XCObis * (ACO * ANH3) ^ (1 / 2) + grAsuite
    grAbis = (1 - KMG_NH3) * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (1 - KCH4_MG) * XCH4bis * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
XH2bis * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = (XMGbis) * AMG + (1 - KH2O_MG) * XH2Obis * (AH2O * AMG) ^ (1 / 2) +
(1 - KCO2_MG) * XCO2bis * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * XN2bis * (AN2 *
AMG) ^ (1 / 2) + (1 - KCO_MG) * XCObis * (ACO * AMG) ^ (1 / 2) + grAsuite

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, Ai et Bi qui
interviennent dans le calcul du coefficient de fugacité
    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, A et B qui
interviennent dans le calcul du coefficient de fugacité
    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
```

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KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
   GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calculs des coefficients de fugacités
   'logFIH2Osoave = ZN - 1 - Log(ZN - GRB) - GRA / GRB * Log((ZN + GRB) / ZN)
         'FIH2Oincsoave = 10 ^ (logFIH2Osoave / 2.303)
         'Worksheets(1).Range("C31").Value = FIH2Oincsoave

   logFIH2O = BH2O / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2O / GRB - 2
/ A * ArH2O) * Log(1 + GRB / ZN)
         FIH2Oinc = 10 ^ (logFIH2O / 2.303)
         FUH2Oinc = FIH2Oinc * P * XH2Obis
         FUH2Oi = FUH2Oinc * 0.00001
   logFIH2 = BH2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2 / GRB - 2 / A *
ArH2) * Log(1 + GRB / ZN)
         FIH2inc = 10 ^ (logFIH2 / 2.303)
         FUH2inc = FIH2inc * P * XH2bis
         FUH2i = FUH2inc * 0.00001

   logFICO = BCO / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO / GRB - 2 / A
* ArCO) * Log(1 + GRB / ZN)
         FICOinc = 10 ^ (logFICO / 2.303)
         FUCOinc = FICOinc * P * XCObis
         FUCOi = FUCOinc * 0.00001

   logFICO2 = BCO2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO2 / GRB - 2 /
A * ArCO2) * Log(1 + GRB / ZN)
         FICO2inc = 10 ^ (logFICO2 / 2.303)
         FUCO2inc = FICO2inc * P * XCO2bis
         FUCO2i = FUCO2inc * 0.00001 'la même chose mais en bar

   logFIN2 = BN2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BN2 / GRB - 2 / A *
ArN2) * Log(1 + GRB / ZN)
         FIN2inc = 10 ^ (logFIN2 / 2.303)
         FUN2inc = FIN2inc * P * XN2bis
         FUN2i = FUN2inc * 0.00001 'la même chose mais en bar

   logFICH4 = BCH4 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCH4 / GRB - 2 /
A * ArCH4) * Log(1 + GRB / ZN)
         FICH4inc = 10 ^ (logFICH4 / 2.303)
         FUCH4inc = FICH4inc * P * XCH4bis
         FUCH4i = FUCH4inc * 0.00001
```

```
   logFINH3 = BNH3 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BNH3 / GRB - 2
/ A * ArNH3) * Log(1 + GRB / ZN)
          FINH3inc = 10 ^ (logFINH3 / 2.303)
          FUNH3inc = FINH3inc * P * XNH3bis
          FUNH3i = FUNH3inc * 0.00001

   logFIMG = BMG / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BMG / GRB - 2 /
A * ArMG) * Log(1 + GRB / ZN)
          FIMGinc = 10 ^ (logFIMG / 2.303)
          FUMGinc = FIMGinc * P * XMGbis
          FUMGi = FUMGinc * 0.00001

Worksheets(1).Range("L5").Value = FUCOi

XH2Obis = 0
XCO2bis = 0
XCObis = 0
XH2bis = 0
XN2bis = 0
XCH4bis = 1
XNH3bis = 0
XMGbis = 0

    Pb = Worksheets(1).Range("B10").Value
   P = Pb * 100000 'passage de la pression de bar en Pa
   T = Worksheets(1).Range("B11").Value + 273.15

   TcH2O = Worksheets(1).Range("C3").Value 'température critique de H2O dans la cellule
J8
   PcH2O = Worksheets(1).Range("D3").Value 'pression critique de H2O
   TcCO2 = Worksheets(1).Range("C4").Value
   PcCO2 = Worksheets(1).Range("D4").Value
   TcCO = Worksheets(1).Range("C5").Value
   PcCO = Worksheets(1).Range("D5").Value
   TcH2 = Worksheets(1).Range("C2").Value
   PcH2 = Worksheets(1).Range("D2").Value
   TcN2 = Worksheets(1).Range("C8").Value
   PcN2 = Worksheets(1).Range("D8").Value
   TcCH4 = Worksheets(1).Range("C6").Value
   PcCH4 = Worksheets(1).Range("D6").Value
   TcNH3 = Worksheets(1).Range("C9").Value
   PcNH3 = Worksheets(1).Range("D9").Value
   TcMG = Worksheets(1).Range("C7").Value
   PcMG = Worksheets(1).Range("D7").Value

   R = 8.314472 'constante des gaz parfaits
   'calcul des facteurs acentriques
   wH2O = Worksheets(1).Range("E3").Value
   nH2O = 0.48508 + 1.55171 * wH2O - 0.15613 * wH2O ^ 2
```

```
    alphaH2O = (1 + nH2O * (1 - (T / TcH2O) ^ 0.5)) ^ 2
    wCO2 = Worksheets(1).Range("E4").Value
    nCO2 = 0.48508 + 1.55171 * wCO2 - 0.15613 * wCO2 ^ 2
    alphaCO2 = (1 + nCO2 * (1 - (T / TcCO2) ^ 0.5)) ^ 2
    wCO = Worksheets(1).Range("E5").Value
    nCO = 0.48508 + 1.55171 * wCO - 0.15613 * wCO ^ 2
    alphaCO = (1 + nCO * (1 - (T / TcCO) ^ 0.5)) ^ 2
    wH2 = Worksheets(1).Range("E2").Value
    nH2 = 0.48508 + 1.55171 * wH2 - 0.15613 * wH2 ^ 2
    alphaH2 = (1 + nH2 * (1 - (T / TcH2) ^ 0.5)) ^ 2
    wN2 = Worksheets(1).Range("E8").Value
    nN2 = 0.48508 + 1.55171 * wN2 - 0.15613 * wN2 ^ 2
    alphaN2 = (1 + nN2 * (1 - (T / TcN2) ^ 0.5)) ^ 2
    wCH4 = Worksheets(1).Range("E6").Value
    nCH4 = 0.48508 + 1.55171 * wCH4 - 0.15613 * wCH4 ^ 2
    alphaCH4 = (1 + nCH4 * (1 - (T / TcCH4) ^ 0.5)) ^ 2
    wNH3 = Worksheets(1).Range("E9").Value
    nNH3 = 0.48508 + 1.55171 * wNH3 - 0.15613 * wNH3 ^ 2
    alphaNH3 = (1 + nNH3 * (1 - (T / TcNH3) ^ 0.5)) ^ 2
    wMG = Worksheets(1).Range("E7").Value
    nMG = 0.48508 + 1.55171 * wMG - 0.15613 * wMG ^ 2
    alphaMG = (1 + nMG * (1 - (T / TcMG) ^ 0.5)) ^ 2

    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
```

```
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 / 2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 - KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) * XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis * XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3 * ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 * (1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

      test = 1
       ZN = 100.01 'initialisation NR à changer si plantage

       While test > 0.000000001
       FZ = ZN ^ 3 - ZN ^ 2 + (GRA - GRB ^ 2 - GRB) * ZN - GRA * GRB
       FpZ = 3 * ZN ^ 2 - 2 * ZN + (GRA - GRB ^ 2 - GRB)

       ZN1 = ZN - FZ / FpZ
       test = Abs(ZN1 - ZN)
       ZN = ZN1
       Wend
       VN = (ZN * R * T / P)
       V = VN * 1000000

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, aialphai et bialphai qui interviennent dans le calcul des coefficients de fugacité
   AH2 = 0.42748 * alphaH2 * (R * TcH2 ^ 2) / (PcH2 * 100000#)
   BH2 = 0.08664 * R * TcH2 / (PcH2 * 100000#)
   BiH2 = BH2 'stockage de bialphai
   ACO2 = 0.42748 * alphaCO2 * (R * TcCO2 ^ 2) / (PcCO2 * 100000#)
   BCO2 = 0.08664 * R * TcCO2 / (PcCO2 * 100000#)
   BiCO2 = BCO2
   AN2 = 0.42748 * alphaN2 * (R * TcN2 ^ 2) / (PcN2 * 100000#)
   BN2 = 0.08664 * R * TcN2 / (PcN2 * 100000#)
   BiN2 = BN2
   AH2O = 0.42748 * alphaH2O * (R * TcH2O ^ 2) / (PcH2O * 100000#)
   BH2O = 0.08664 * R * TcH2O / (PcH2O * 100000#)
   BiH2O = BH2O
   ACO = 0.42748 * alphaCO * (R * TcCO ^ 2) / (PcCO * 100000#)
   BCO = 0.08664 * R * TcCO / (PcCO * 100000#)
```

```
   BiCO = BCO
   ACH4 = 0.42748 * alphaCH4 * (R * TcCH4 ^ 2) / (PcCH4 * 100000#)
   BCH4 = 0.08664 * R * TcCH4 / (PcCH4 * 100000#)
   BiCH4 = BCH4
   ANH3 = 0.42748 * alphaNH3 * (R * TcNH3 ^ 2) / (PcNH3 * 100000#)
   BNH3 = 0.08664 * R * TcNH3 / (PcNH3 * 100000#)
   BiNH3 = BNH3
   AMG = 0.42748 * alphaMG * (R * TcMG ^ 2) / (PcMG * 100000#)
   BMG = 0.08664 * R * TcMG / (PcMG * 100000#)
   BiMG = BMG

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, a et b qui
n'interviennent pas dans le calcul du coefficient de fugacité
   grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
   grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   A = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis
* XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) *
XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) *
XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis *
(ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 /
2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO +
2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) *
XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO
* AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) +
grAsuite
   B = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis *
BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calcul de dérivés de XiXj(1-Kji)racine(aialphai*akalphak)
   grAbis = (1 - KH2_MG) * (XMGbis) * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * (XCH4bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
(XNH3bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = ((XH2bis)) * AH2 + (1 - KH2O_H2) * (XH2Obis) * (AH2O * AH2) ^ (1 / 2) + (1
- KCO2_H2) * (XCO2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * (XN2bis) * (AN2 *
AH2) ^ (1 / 2) + (1 - KCO_H2) * (XCObis) * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * (XMGbis) * (ACO2 * AMG) ^ (1 / 2)
```

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    grAsuite = (1 - KCO2_CH4) * (XCH4bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3)
* (XNH3bis) * (ANH3 * ACO2) ^ (1 / 2) + grAbis
    ArCO2 = ((XCO2bis)) * ACO2 + (1 - KH2O_HCO2) * (XH2Obis) * (AH2O * ACO2) ^
(1 / 2) + (1 - KCO2_H2) * (XH2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XN2bis)
* (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * (XCObis) * (ACO * ACO2) ^ (1 / 2) +
grAsuite
    grAbis = (1 - KN2_MG) * (XMGbis) * (AN2 * AMG) ^ (1 / 2)
    grAsuite = (1 - KN2_CH4) * (XCH4bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) *
(XNH3bis) * (ANH3 * AN2) ^ (1 / 2) + grAbis
    ArN2 = ((XN2bis)) * AN2 + (1 - KH2O_N2) * (XH2Obis) * (AH2O * AN2) ^ (1 / 2) + (1
- KN2_H2) * (XH2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XCO2bis) * (AN2 *
ACO2) ^ (1 / 2) + (1 - KN2_CO) * (XCObis) * (ACO * AN2) ^ (1 / 2) + grAsuite
    grAbis = (1 - KH2O_MG) * (XMGbis) * (AH2O * AMG) ^ (1 / 2)
    grAsuite = (1 - KH2O_CH4) * (XCH4bis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3)
* (XNH3bis) * (ANH3 * AH2O) ^ (1 / 2) + grAbis
    ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * (XH2bis) * (AH2O * AH2) ^ (1 / 2) +
(1 - KH2O_CO2) * (XCO2bis) * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * (XN2bis) *
(AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * (XCObis) * (ACO * AH2O) ^ (1 / 2) + grAsuite
    grAbis = (1 - KCO_MG) * (XMGbis) * (ACO * AMG) ^ (1 / 2)
    grAsuite = (1 - KCO_CH4) * (XCH4bis) * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) *
(XNH3bis) * (ANH3 * ACO) ^ (1 / 2) + grAbis
    ArCO = (XCObis) * ACO + (1 - KH2O_CO) * (XH2Obis) * (AH2O * ACO) ^ (1 / 2) + (1
- KCO_CO2) * (XCO2bis) * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * (XN2bis) * (AN2 *
ACO) ^ (1 / 2) + (1 - KCO_H2) * (XH2bis) * (ACO * AH2) ^ (1 / 2) + grAsuite
    grAbis = (1 - KCH4_MG) * (XMGbis) * (ACH4 * AMG) ^ (1 / 2)
    grAsuite = (1 - KH2_CH4) * (XH2bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) *
(XNH3bis) * (ANH3 * ACH4) ^ (1 / 2) + grAbis
    ArCH4 = ((XCH4bis)) * ACH4 + (1 - KH2O_CH4) * (XH2Obis) * (AH2O * ACH4) ^ (1 /
2) + (1 - KCO2_CH4) * (XCO2bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) *
(XN2bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * (XCObis) * (ACO * ACH4) ^ (1 / 2)
+ grAsuite
    grAbis = (1 - KNH3_MG) * (XMGbis) * (ANH3 * AMG) ^ (1 / 2)
    grAsuite = (1 - KCH4_NH3) * (XCH4bis) * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
(XH2bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
    ArNH3 = ((XNH3bis)) * ANH3 + (1 - KH2O_NH3) * (XH2Obis) * (AH2O * ANH3) ^ (1
/ 2) + (1 - KCO2_NH3) * (XCO2bis) * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) *
(XN2bis) * (AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * (XCObis) * (ACO * ANH3) ^ (1 /
2) + grAsuite
    grAbis = (1 - KMG_NH3) * (XNH3bis) * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (1 - KCH4_MG) * (XCH4bis) * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
(XH2bis) * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = ((XMGbis)) * AMG + (1 - KH2O_MG) * (XH2Obis) * (AH2O * AMG) ^ (1 / 2)
+ (1 - KCO2_MG) * (XCO2bis) * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * (XN2bis) *
(AN2 * AMG) ^ (1 / 2) + (1 - KCO_MG) * (XCObis) * (ACO * AMG) ^ (1 / 2) + grAsuite

    SB = BH2O + BH2 + BCO2 + BN2 + BCO + BNH3 + BCH4 + BMG
    DVDXH2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArH2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
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   DVDXH2O = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArH2O) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXCO2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArCO2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXCO = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArCO) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXN2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArN2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXCH4 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArCH4) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXNH3 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArNH3) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXMG = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArMG) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)

VCO2M = VN * (XCO2bis) - 1 * (XCO2bis) * 1 / 3 / 8 / 2 * DVDXCO2
VCOM = VN * (XCObis) - 1 * (XCObis) * 1 / 3 / 8 / 2 * DVDXCO
VH2M = VN * (XH2bis) - 1 * (XH2bis) * 1 / 3 / 8 / 2 * DVDXH2
VN2M = VN * (XN2bis) - 1 * (XN2bis) * 1 / 3 / 8 / 2 * DVDXN2
VCH4M = VN * (XCH4bis) - 1 * (XCH4bis) * 1 / 3 / 8 / 2 * DVDXCH4
VNH3M = VN * (XNH3bis) - 1 * (XNH3bis) * 1 / 3 / 8 / 2 * DVDXNH3
VH2OM = VN * (XH2Obis) - 1 * (XH2Obis) * 1 / 3 / 8 / 2 * DVDXH2O
VMGM = VN * (XMGbis) - 1 * (XMGbis) * 1 / 3 / 8 / 2 * DVDXMG

   'calcul de somme de Xk(1-Kki)racine(aialphai*akalphak)  (avant le 2 dans le calcul du
coefficient de fugacité de l'espèce k)
   grAbis = (1 - KH2_MG) * XMGbis * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XCH4bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
XNH3bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = (XH2bis) * AH2 + (1 - KH2O_H2) * XH2Obis * (AH2O * AH2) ^ (1 / 2) + (1 -
KCO2_H2) * XCO2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * XN2bis * (AN2 * AH2)
^ (1 / 2) + (1 - KCO_H2) * XCObis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * XMGbis * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * XCH4bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = (XCO2bis) * ACO2 + (1 - KH2O_HCO2) * XH2Obis * (AH2O * ACO2) ^ (1 /
2) + (1 - KCO2_H2) * XH2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XN2bis * (AN2
* ACO2) ^ (1 / 2) + (1 - KCO_CO2) * XCObis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * XMGbis * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * XCH4bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) *
XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
```

```
    ArN2 = (XN2bis) * AN2 + (1 - KH2O_N2) * XH2Obis * (AH2O * AN2) ^ (1 / 2) + (1 -
KN2_H2) * XH2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XCO2bis * (AN2 * ACO2)
^ (1 / 2) + (1 - KN2_CO) * XCObis * (ACO * AN2) ^ (1 / 2) + grAsuite
    grAbis = (1 - KH2O_MG) * XMGbis * (AH2O * AMG) ^ (1 / 2)
    grAsuite = (1 - KH2O_CH4) * XCH4bis * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) *
XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + grAbis
    ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * XH2bis * (AH2O * AH2) ^ (1 / 2) + (1
- KH2O_CO2) * XCO2bis * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * XN2bis * (AN2 *
AH2O) ^ (1 / 2) + (1 - KH2O_CO) * XCObis * (ACO * AH2O) ^ (1 / 2) + grAsuite
    grAbis = (1 - KCO_MG) * XMGbis * (ACO * AMG) ^ (1 / 2)
    grAsuite = (1 - KCO_CH4) * XCH4bis * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) *
XNH3bis * (ANH3 * ACO) ^ (1 / 2) + grAbis
    ArCO = (XCObis) * ACO + (1 - KH2O_CO) * XH2Obis * (AH2O * ACO) ^ (1 / 2) + (1 -
KCO_CO2) * XCO2bis * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * XN2bis * (AN2 *
ACO) ^ (1 / 2) + (1 - KCO_H2) * XH2bis * (ACO * AH2) ^ (1 / 2) + grAsuite
    grAbis = (1 - KCH4_MG) * XMGbis * (ACH4 * AMG) ^ (1 / 2)
    grAsuite = (1 - KH2_CH4) * XH2bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) *
XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + grAbis
    ArCH4 = (XCH4bis) * ACH4 + (1 - KH2O_CH4) * XH2Obis * (AH2O * ACH4) ^ (1 / 2)
+ (1 - KCO2_CH4) * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * XN2bis *
(AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * XCObis * (ACO * ACH4) ^ (1 / 2) + grAsuite
    grAbis = (1 - KNH3_MG) * XMGbis * (ANH3 * AMG) ^ (1 / 2)
    grAsuite = (1 - KCH4_NH3) * XCH4bis * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
XH2bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
    ArNH3 = (XNH3bis) * ANH3 + (1 - KH2O_NH3) * XH2Obis * (AH2O * ANH3) ^ (1 / 2)
+ (1 - KCO2_NH3) * XCO2bis * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * XN2bis *
(AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * XCObis * (ACO * ANH3) ^ (1 / 2) + grAsuite
    grAbis = (1 - KMG_NH3) * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (1 - KCH4_MG) * XCH4bis * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
XH2bis * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = (XMGbis) * AMG + (1 - KH2O_MG) * XH2Obis * (AH2O * AMG) ^ (1 / 2) +
(1 - KCO2_MG) * XCO2bis * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * XN2bis * (AN2 *
AMG) ^ (1 / 2) + (1 - KCO_MG) * XCObis * (ACO * AMG) ^ (1 / 2) + grAsuite

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, Ai et Bi qui
interviennent dans le calcul du coefficient de fugacité
    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
```

```
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, A et B qui interviennent dans le calcul du coefficient de fugacité
    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG * AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) * XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis * (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4) ^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) * XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis * XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 / 2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 - KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) * XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis * XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3 * ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 * (1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) + grAsuite
    GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

    'calculs des coefficients de fugacités
    'logFIH2Osoave = ZN - 1 - Log(ZN - GRB) - GRA / GRB * Log((ZN + GRB) / ZN)
        'FIH2Oincsoave = 10 ^ (logFIH2Osoave / 2.303)
        'Worksheets(1).Range("C31").Value = FIH2Oincsoave

    logFIH2O = BH2O / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2O / GRB - 2 / A * ArH2O) * Log(1 + GRB / ZN)
        FIH2Oinc = 10 ^ (logFIH2O / 2.303)
        FUH2Oinc = FIH2Oinc * P * XH2Obis
        FUH2Oi = FUH2Oinc * 0.00001
    logFIH2 = BH2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2 / GRB - 2 / A * ArH2) * Log(1 + GRB / ZN)
        FIH2inc = 10 ^ (logFIH2 / 2.303)
        FUH2inc = FIH2inc * P * XH2bis
        FUH2i = FUH2inc * 0.00001
```

```
   logFICO = BCO / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO / GRB - 2 / A
* ArCO) * Log(1 + GRB / ZN)
         FICOinc = 10 ^ (logFICO / 2.303)
         FUCOinc = FICOinc * P * XCObis
         FUCOi = FUCOinc * 0.00001

   logFICO2 = BCO2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO2 / GRB - 2 /
A * ArCO2) * Log(1 + GRB / ZN)
         FICO2inc = 10 ^ (logFICO2 / 2.303)
         FUCO2inc = FICO2inc * P * XCO2bis
         FUCO2i = FUCO2inc * 0.00001 'la même chose mais en bar

   logFIN2 = BN2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BN2 / GRB - 2 / A *
ArN2) * Log(1 + GRB / ZN)
         FIN2inc = 10 ^ (logFIN2 / 2.303)
         FUN2inc = FIN2inc * P * XN2bis
         FUN2i = FUN2inc * 0.00001 'la même chose mais en bar

   logFICH4 = BCH4 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCH4 / GRB - 2 /
A * ArCH4) * Log(1 + GRB / ZN)
         FICH4inc = 10 ^ (logFICH4 / 2.303)
         FUCH4inc = FICH4inc * P * XCH4bis
         FUCH4i = FUCH4inc * 0.00001

   logFINH3 = BNH3 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BNH3 / GRB - 2
/ A * ArNH3) * Log(1 + GRB / ZN)
         FINH3inc = 10 ^ (logFINH3 / 2.303)
         FUNH3inc = FINH3inc * P * XNH3bis
         FUNH3i = FUNH3inc * 0.00001

   logFIMG = BMG / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BMG / GRB - 2 /
A * ArMG) * Log(1 + GRB / ZN)
         FIMGinc = 10 ^ (logFIMG / 2.303)
         FUMGinc = FIMGinc * P * XMGbis
         FUMGi = FUMGinc * 0.00001

Worksheets(1).Range("L6").Value = FUCH4i
Call PROPORTION4
End Sub
Private Sub PROPORTION4()
XH2Obis = 0
XCO2bis = 0
XCObis = 0
XH2bis = 0
XN2bis = 0
XCH4bis = 0
XNH3bis = 0
XMGbis = 1
```

```
 Pb = Worksheets(1).Range("B10").Value
P = Pb * 100000 'passage de la pression de bar en Pa
T = Worksheets(1).Range("B11").Value + 273.15

TcH2O = Worksheets(1).Range("C3").Value 'température critique de H2O dans la cellule
J8
PcH2O = Worksheets(1).Range("D3").Value 'pression critique de H2O
TcCO2 = Worksheets(1).Range("C4").Value
PcCO2 = Worksheets(1).Range("D4").Value
TcCO = Worksheets(1).Range("C5").Value
PcCO = Worksheets(1).Range("D5").Value
TcH2 = Worksheets(1).Range("C2").Value
PcH2 = Worksheets(1).Range("D2").Value
TcN2 = Worksheets(1).Range("C8").Value
PcN2 = Worksheets(1).Range("D8").Value
TcCH4 = Worksheets(1).Range("C6").Value
PcCH4 = Worksheets(1).Range("D6").Value
TcNH3 = Worksheets(1).Range("C9").Value
PcNH3 = Worksheets(1).Range("D9").Value
TcMG = Worksheets(1).Range("C7").Value
PcMG = Worksheets(1).Range("D7").Value

R = 8.314472 'constante des gaz parfaits
'calcul des facteurs acentriques
wH2O = Worksheets(1).Range("E3").Value
nH2O = 0.48508 + 1.55171 * wH2O - 0.15613 * wH2O ^ 2
alphaH2O = (1 + nH2O * (1 - (T / TcH2O) ^ 0.5)) ^ 2
wCO2 = Worksheets(1).Range("E4").Value
nCO2 = 0.48508 + 1.55171 * wCO2 - 0.15613 * wCO2 ^ 2
alphaCO2 = (1 + nCO2 * (1 - (T / TcCO2) ^ 0.5)) ^ 2
wCO = Worksheets(1).Range("E5").Value
nCO = 0.48508 + 1.55171 * wCO - 0.15613 * wCO ^ 2
alphaCO = (1 + nCO * (1 - (T / TcCO) ^ 0.5)) ^ 2
wH2 = Worksheets(1).Range("E2").Value
nH2 = 0.48508 + 1.55171 * wH2 - 0.15613 * wH2 ^ 2
alphaH2 = (1 + nH2 * (1 - (T / TcH2) ^ 0.5)) ^ 2
wN2 = Worksheets(1).Range("E8").Value
nN2 = 0.48508 + 1.55171 * wN2 - 0.15613 * wN2 ^ 2
alphaN2 = (1 + nN2 * (1 - (T / TcN2) ^ 0.5)) ^ 2
wCH4 = Worksheets(1).Range("E6").Value
nCH4 = 0.48508 + 1.55171 * wCH4 - 0.15613 * wCH4 ^ 2
alphaCH4 = (1 + nCH4 * (1 - (T / TcCH4) ^ 0.5)) ^ 2
wNH3 = Worksheets(1).Range("E9").Value
nNH3 = 0.48508 + 1.55171 * wNH3 - 0.15613 * wNH3 ^ 2
alphaNH3 = (1 + nNH3 * (1 - (T / TcNH3) ^ 0.5)) ^ 2
wMG = Worksheets(1).Range("E7").Value
nMG = 0.48508 + 1.55171 * wMG - 0.15613 * wMG ^ 2
alphaMG = (1 + nMG * (1 - (T / TcMG) ^ 0.5)) ^ 2
```

```
   AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
   BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
   ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
   BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
   AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
   BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
   AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
   BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
   ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
   BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
   ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
   BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
   ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
   BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
   AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
   BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
   grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
   GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

    test = 1
     ZN = 100.01 'initialisation NR à changer si plantage
```

```
While test > 0.000000001
FZ = ZN ^ 3 - ZN ^ 2 + (GRA - GRB ^ 2 - GRB) * ZN - GRA * GRB
FpZ = 3 * ZN ^ 2 - 2 * ZN + (GRA - GRB ^ 2 - GRB)

ZN1 = ZN - FZ / FpZ
test = Abs(ZN1 - ZN)
ZN = ZN1
Wend
VN = (ZN * R * T / P)
V = VN * 1000000
```

'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, aialphai et bialphai qui interviennent dans le calcul des coefficients de fugacité

```
AH2 = 0.42748 * alphaH2 * (R * TcH2 ^ 2) / (PcH2 * 100000#)
BH2 = 0.08664 * R * TcH2 / (PcH2 * 100000#)
BiH2 = BH2 'stockage de bialphai
ACO2 = 0.42748 * alphaCO2 * (R * TcCO2 ^ 2) / (PcCO2 * 100000#)
BCO2 = 0.08664 * R * TcCO2 / (PcCO2 * 100000#)
BiCO2 = BCO2
AN2 = 0.42748 * alphaN2 * (R * TcN2 ^ 2) / (PcN2 * 100000#)
BN2 = 0.08664 * R * TcN2 / (PcN2 * 100000#)
BiN2 = BN2
AH2O = 0.42748 * alphaH2O * (R * TcH2O ^ 2) / (PcH2O * 100000#)
BH2O = 0.08664 * R * TcH2O / (PcH2O * 100000#)
BiH2O = BH2O
ACO = 0.42748 * alphaCO * (R * TcCO ^ 2) / (PcCO * 100000#)
BCO = 0.08664 * R * TcCO / (PcCO * 100000#)
BiCO = BCO
ACH4 = 0.42748 * alphaCH4 * (R * TcCH4 ^ 2) / (PcCH4 * 100000#)
BCH4 = 0.08664 * R * TcCH4 / (PcCH4 * 100000#)
BiCH4 = BCH4
ANH3 = 0.42748 * alphaNH3 * (R * TcNH3 ^ 2) / (PcNH3 * 100000#)
BNH3 = 0.08664 * R * TcNH3 / (PcNH3 * 100000#)
BiNH3 = BNH3
AMG = 0.42748 * alphaMG * (R * TcMG ^ 2) / (PcMG * 100000#)
BMG = 0.08664 * R * TcMG / (PcMG * 100000#)
BiMG = BMG
```

'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, a et b qui n'interviennent pas dans le calcul du coefficient de fugacité

```
grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG * AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) * XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis * (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4) ^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) * XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis * XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
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```
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   A = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis
* XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) *
XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) *
XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis *
(ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 /
2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO +
2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) *
XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO
* AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) +
grAsuite
   B = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis *
BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calcul de dérivés de XiXj(1-Kji)racine(aialphai*akalphak)
   grAbis = (1 - KH2_MG) * (XMGbis) * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * (XCH4bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
(XNH3bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = ((XH2bis)) * AH2 + (1 - KH2O_H2) * (XH2Obis) * (AH2O * AH2) ^ (1 / 2) + (1
- KCO2_H2) * (XCO2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * (XN2bis) * (AN2 *
AH2) ^ (1 / 2) + (1 - KCO_H2) * (XCObis) * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * (XMGbis) * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * (XCH4bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3)
* (XNH3bis) * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = ((XCO2bis)) * ACO2 + (1 - KH2O_HCO2) * (XH2Obis) * (AH2O * ACO2) ^
(1 / 2) + (1 - KCO2_H2) * (XH2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XN2bis)
* (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * (XCObis) * (ACO * ACO2) ^ (1 / 2) +
grAsuite
   grAbis = (1 - KN2_MG) * (XMGbis) * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * (XCH4bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) *
(XNH3bis) * (ANH3 * AN2) ^ (1 / 2) + grAbis
   ArN2 = ((XN2bis)) * AN2 + (1 - KH2O_N2) * (XH2Obis) * (AH2O * AN2) ^ (1 / 2) + (1
- KN2_H2) * (XH2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XCO2bis) * (AN2 *
ACO2) ^ (1 / 2) + (1 - KN2_CO) * (XCObis) * (ACO * AN2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KH2O_MG) * (XMGbis) * (AH2O * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2O_CH4) * (XCH4bis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3)
* (XNH3bis) * (ANH3 * AH2O) ^ (1 / 2) + grAbis
   ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * (XH2bis) * (AH2O * AH2) ^ (1 / 2) +
(1 - KH2O_CO2) * (XCO2bis) * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * (XN2bis) *
(AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * (XCObis) * (ACO * AH2O) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO_MG) * (XMGbis) * (ACO * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO_CH4) * (XCH4bis) * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) *
(XNH3bis) * (ANH3 * ACO) ^ (1 / 2) + grAbis
```

ArCO = (XCObis) * ACO + (1 - KH2O_CO) * (XH2Obis) * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * (XCO2bis) * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * (XN2bis) * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * (XH2bis) * (ACO * AH2) ^ (1 / 2) + grAsuite

grAbis = (1 - KCH4_MG) * (XMGbis) * (ACH4 * AMG) ^ (1 / 2)

grAsuite = (1 - KH2_CH4) * (XH2bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * (XNH3bis) * (ANH3 * ACH4) ^ (1 / 2) + grAbis

ArCH4 = ((XCH4bis)) * ACH4 + (1 - KH2O_CH4) * (XH2Obis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * (XCO2bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * (XN2bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * (XCObis) * (ACO * ACH4) ^ (1 / 2) + grAsuite

grAbis = (1 - KNH3_MG) * (XMGbis) * (ANH3 * AMG) ^ (1 / 2)

grAsuite = (1 - KCH4_NH3) * (XCH4bis) * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * (XH2bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis

ArNH3 = ((XNH3bis)) * ANH3 + (1 - KH2O_NH3) * (XH2Obis) * (AH2O * ANH3) ^ (1 / 2) + (1 - KCO2_NH3) * (XCO2bis) * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * (XN2bis) * (AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * (XCObis) * (ACO * ANH3) ^ (1 / 2) + grAsuite

grAbis = (1 - KMG_NH3) * (XNH3bis) * (AMG * ANH3) ^ (1 / 2)

grAsuite = (1 - KCH4_MG) * (XCH4bis) * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) * (XH2bis) * (AMG * AH2) ^ (1 / 2) + grAbis

ArMG = ((XMGbis)) * AMG + (1 - KH2O_MG) * (XH2Obis) * (AH2O * AMG) ^ (1 / 2) + (1 - KCO2_MG) * (XCO2bis) * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * (XN2bis) * (AN2 * AMG) ^ (1 / 2) + (1 - KCO_MG) * (XCObis) * (ACO * AMG) ^ (1 / 2) + grAsuite

SB = BH2O + BH2 + BCO2 + BN2 + BCO + BNH3 + BCH4 + BMG

DVDXH2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArH2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXH2O = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArH2O) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCO2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCO2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCO = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCO) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXN2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArN2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCH4 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCH4) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXNH3 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArNH3) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXMG = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArMG) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

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VCO2M = VN * (XCO2bis) - 1 * (XCO2bis) * 1 / 3 / 8 / 2 * DVDXCO2
VCOM = VN * (XCObis) - 1 * (XCObis) * 1 / 3 / 8 / 2 * DVDXCO
VH2M = VN * (XH2bis) - 1 * (XH2bis) * 1 / 3 / 8 / 2 * DVDXH2
VN2M = VN * (XN2bis) - 1 * (XN2bis) * 1 / 3 / 8 / 2 * DVDXN2
VCH4M = VN * (XCH4bis) - 1 * (XCH4bis) * 1 / 3 / 8 / 2 * DVDXCH4
VNH3M = VN * (XNH3bis) - 1 * (XNH3bis) * 1 / 3 / 8 / 2 * DVDXNH3
VH2OM = VN * (XH2Obis) - 1 * (XH2Obis) * 1 / 3 / 8 / 2 * DVDXH2O
VMGM = VN * (XMGbis) - 1 * (XMGbis) * 1 / 3 / 8 / 2 * DVDXMG

   'calcul de somme de Xk(1-Kki)racine(aialphai*akalphak)  (avant le 2 dans le calcul du coefficient de fugacité de l'espèce k)
   grAbis = (1 - KH2_MG) * XMGbis * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XCH4bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = (XH2bis) * AH2 + (1 - KH2O_H2) * XH2Obis * (AH2O * AH2) ^ (1 / 2) + (1 - KCO2_H2) * XCO2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * XN2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KCO_H2) * XCObis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * XMGbis * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * XCH4bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) * XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = (XCO2bis) * ACO2 + (1 - KH2O_HCO2) * XH2Obis * (AH2O * ACO2) ^ (1 / 2) + (1 - KCO2_H2) * XH2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XN2bis * (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * XCObis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * XMGbis * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * XCH4bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   ArN2 = (XN2bis) * AN2 + (1 - KH2O_N2) * XH2Obis * (AH2O * AN2) ^ (1 / 2) + (1 - KN2_H2) * XH2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XCO2bis * (AN2 * ACO2) ^ (1 / 2) + (1 - KN2_CO) * XCObis * (ACO * AN2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KH2O_MG) * XMGbis * (AH2O * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2O_CH4) * XCH4bis * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + grAbis
   ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * XH2bis * (AH2O * AH2) ^ (1 / 2) + (1 - KH2O_CO2) * XCO2bis * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * XN2bis * (AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * XCObis * (ACO * AH2O) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO_MG) * XMGbis * (ACO * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO_CH4) * XCH4bis * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) * XNH3bis * (ANH3 * ACO) ^ (1 / 2) + grAbis
   ArCO = (XCObis) * ACO + (1 - KH2O_CO) * XH2Obis * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * XCO2bis * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * XN2bis * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * XH2bis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCH4_MG) * XMGbis * (ACH4 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XH2bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + grAbis
   ArCH4 = (XCH4bis) * ACH4 + (1 - KH2O_CH4) * XH2Obis * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * XN2bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * XCObis * (ACO * ACH4) ^ (1 / 2) + grAsuite
   grAbis = (1 - KNH3_MG) * XMGbis * (ANH3 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCH4_NH3) * XCH4bis * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * XH2bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
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    ArNH3 = (XNH3bis) * ANH3 + (1 - KH2O_NH3) * XH2Obis * (AH2O * ANH3) ^ (1 / 2)
+ (1 - KCO2_NH3) * XCO2bis * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * XN2bis *
(AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * XCObis * (ACO * ANH3) ^ (1 / 2) + grAsuite
    grAbis = (1 - KMG_NH3) * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (1 - KCH4_MG) * XCH4bis * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
XH2bis * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = (XMGbis) * AMG + (1 - KH2O_MG) * XH2Obis * (AH2O * AMG) ^ (1 / 2) +
(1 - KCO2_MG) * XCO2bis * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * XN2bis * (AN2 *
AMG) ^ (1 / 2) + (1 - KCO_MG) * XCObis * (ACO * AMG) ^ (1 / 2) + grAsuite

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, Ai et Bi qui
interviennent dans le calcul du coefficient de fugacité
    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, A et B qui
interviennent dans le calcul du coefficient de fugacité
    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
```

```
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
   GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calculs des coefficients de fugacités
   'logFIH2Osoave = ZN - 1 - Log(ZN - GRB) - GRA / GRB * Log((ZN + GRB) / ZN)
         'FIH2Oincsoave = 10 ^ (logFIH2Osoave / 2.303)
         'Worksheets(1).Range("C31").Value = FIH2Oincsoave

   logFIH2O = BH2O / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2O / GRB - 2
/ A * ArH2O) * Log(1 + GRB / ZN)
         FIH2Oinc = 10 ^ (logFIH2O / 2.303)
         FUH2Oinc = FIH2Oinc * P * XH2Obis
         FUH2Oi = FUH2Oinc * 0.00001
   logFIH2 = BH2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2 / GRB - 2 / A *
ArH2) * Log(1 + GRB / ZN)
         FIH2inc = 10 ^ (logFIH2 / 2.303)
         FUH2inc = FIH2inc * P * XH2bis
         FUH2i = FUH2inc * 0.00001

   logFICO = BCO / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO / GRB - 2 / A
* ArCO) * Log(1 + GRB / ZN)
         FICOinc = 10 ^ (logFICO / 2.303)
         FUCOinc = FICOinc * P * XCObis
         FUCOi = FUCOinc * 0.00001

   logFICO2 = BCO2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO2 / GRB - 2 /
A * ArCO2) * Log(1 + GRB / ZN)
         FICO2inc = 10 ^ (logFICO2 / 2.303)
         FUCO2inc = FICO2inc * P * XCO2bis
         FUCO2i = FUCO2inc * 0.00001 'la même chose mais en bar

   logFIN2 = BN2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BN2 / GRB - 2 / A *
ArN2) * Log(1 + GRB / ZN)
         FIN2inc = 10 ^ (logFIN2 / 2.303)
         FUN2inc = FIN2inc * P * XN2bis
         FUN2i = FUN2inc * 0.00001 'la même chose mais en bar

   logFICH4 = BCH4 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCH4 / GRB - 2 /
A * ArCH4) * Log(1 + GRB / ZN)
         FICH4inc = 10 ^ (logFICH4 / 2.303)
         FUCH4inc = FICH4inc * P * XCH4bis
         FUCH4i = FUCH4inc * 0.00001
```

```
   logFINH3 = BNH3 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BNH3 / GRB - 2
/ A * ArNH3) * Log(1 + GRB / ZN)
          FINH3inc = 10 ^ (logFINH3 / 2.303)
          FUNH3inc = FINH3inc * P * XNH3bis
          FUNH3i = FUNH3inc * 0.00001

   logFIMG = BMG / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BMG / GRB - 2 /
A * ArMG) * Log(1 + GRB / ZN)
          FIMGinc = 10 ^ (logFIMG / 2.303)
          FUMGinc = FIMGinc * P * XMGbis
          FUMGi = FUMGinc * 0.00001

Worksheets(1).Range("L7").Value = FUMGi
Call PROPORTION5
End Sub
Private Sub PROPORTION5()
XH2Obis = 0
XCO2bis = 0
XCObis = 0
XH2bis = 0
XN2bis = 1
XCH4bis = 0
XNH3bis = 0
XMGbis = 0

    Pb = Worksheets(1).Range("B10").Value
   P = Pb * 100000 'passage de la pression de bar en Pa
   T = Worksheets(1).Range("B11").Value + 273.15

   TcH2O = Worksheets(1).Range("C3").Value 'température critique de H2O dans la cellule
J8
   PcH2O = Worksheets(1).Range("D3").Value 'pression critique de H2O
   TcCO2 = Worksheets(1).Range("C4").Value
   PcCO2 = Worksheets(1).Range("D4").Value
   TcCO = Worksheets(1).Range("C5").Value
   PcCO = Worksheets(1).Range("D5").Value
   TcH2 = Worksheets(1).Range("C2").Value
   PcH2 = Worksheets(1).Range("D2").Value
   TcN2 = Worksheets(1).Range("C8").Value
   PcN2 = Worksheets(1).Range("D8").Value
   TcCH4 = Worksheets(1).Range("C6").Value
   PcCH4 = Worksheets(1).Range("D6").Value
   TcNH3 = Worksheets(1).Range("C9").Value
   PcNH3 = Worksheets(1).Range("D9").Value
   TcMG = Worksheets(1).Range("C7").Value
   PcMG = Worksheets(1).Range("D7").Value

   R = 8.314472 'constante des gaz parfaits
   'calcul des facteurs acentriques
```

```
    wH2O = Worksheets(1).Range("E3").Value
    nH2O = 0.48508 + 1.55171 * wH2O - 0.15613 * wH2O ^ 2
    alphaH2O = (1 + nH2O * (1 - (T / TcH2O) ^ 0.5)) ^ 2
    wCO2 = Worksheets(1).Range("E4").Value
    nCO2 = 0.48508 + 1.55171 * wCO2 - 0.15613 * wCO2 ^ 2
    alphaCO2 = (1 + nCO2 * (1 - (T / TcCO2) ^ 0.5)) ^ 2
    wCO = Worksheets(1).Range("E5").Value
    nCO = 0.48508 + 1.55171 * wCO - 0.15613 * wCO ^ 2
    alphaCO = (1 + nCO * (1 - (T / TcCO) ^ 0.5)) ^ 2
    wH2 = Worksheets(1).Range("E2").Value
    nH2 = 0.48508 + 1.55171 * wH2 - 0.15613 * wH2 ^ 2
    alphaH2 = (1 + nH2 * (1 - (T / TcH2) ^ 0.5)) ^ 2
    wN2 = Worksheets(1).Range("E8").Value
    nN2 = 0.48508 + 1.55171 * wN2 - 0.15613 * wN2 ^ 2
    alphaN2 = (1 + nN2 * (1 - (T / TcN2) ^ 0.5)) ^ 2
    wCH4 = Worksheets(1).Range("E6").Value
    nCH4 = 0.48508 + 1.55171 * wCH4 - 0.15613 * wCH4 ^ 2
    alphaCH4 = (1 + nCH4 * (1 - (T / TcCH4) ^ 0.5)) ^ 2
    wNH3 = Worksheets(1).Range("E9").Value
    nNH3 = 0.48508 + 1.55171 * wNH3 - 0.15613 * wNH3 ^ 2
    alphaNH3 = (1 + nNH3 * (1 - (T / TcNH3) ^ 0.5)) ^ 2
    wMG = Worksheets(1).Range("E7").Value
    nMG = 0.48508 + 1.55171 * wMG - 0.15613 * wMG ^ 2
    alphaMG = (1 + nMG * (1 - (T / TcMG) ^ 0.5)) ^ 2

    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
```

```
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
    GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

       test = 1
       ZN = 100.01 'initialisation NR à changer si plantage

       While test > 0.000000001
       FZ = ZN ^ 3 - ZN ^ 2 + (GRA - GRB ^ 2 - GRB) * ZN - GRA * GRB
       FpZ = 3 * ZN ^ 2 - 2 * ZN + (GRA - GRB ^ 2 - GRB)

       ZN1 = ZN - FZ / FpZ
       test = Abs(ZN1 - ZN)
       ZN = ZN1
       Wend
       VN = (ZN * R * T / P)
       V = VN * 1000000

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, aialphai et bialphai
qui interviennent dans le calcul des coefficients de fugacité
    AH2 = 0.42748 * alphaH2 * (R * TcH2 ^ 2) / (PcH2 * 100000#)
    BH2 = 0.08664 * R * TcH2 / (PcH2 * 100000#)
    BiH2 = BH2 'stockage de bialphai
    ACO2 = 0.42748 * alphaCO2 * (R * TcCO2 ^ 2) / (PcCO2 * 100000#)
    BCO2 = 0.08664 * R * TcCO2 / (PcCO2 * 100000#)
    BiCO2 = BCO2
    AN2 = 0.42748 * alphaN2 * (R * TcN2 ^ 2) / (PcN2 * 100000#)
    BN2 = 0.08664 * R * TcN2 / (PcN2 * 100000#)
    BiN2 = BN2
    AH2O = 0.42748 * alphaH2O * (R * TcH2O ^ 2) / (PcH2O * 100000#)
    BH2O = 0.08664 * R * TcH2O / (PcH2O * 100000#)
```

```
   BiH2O = BH2O
   ACO = 0.42748 * alphaCO * (R * TcCO ^ 2) / (PcCO * 100000#)
   BCO = 0.08664 * R * TcCO / (PcCO * 100000#)
   BiCO = BCO
   ACH4 = 0.42748 * alphaCH4 * (R * TcCH4 ^ 2) / (PcCH4 * 100000#)
   BCH4 = 0.08664 * R * TcCH4 / (PcCH4 * 100000#)
   BiCH4 = BCH4
   ANH3 = 0.42748 * alphaNH3 * (R * TcNH3 ^ 2) / (PcNH3 * 100000#)
   BNH3 = 0.08664 * R * TcNH3 / (PcNH3 * 100000#)
   BiNH3 = BNH3
   AMG = 0.42748 * alphaMG * (R * TcMG ^ 2) / (PcMG * 100000#)
   BMG = 0.08664 * R * TcMG / (PcMG * 100000#)
   BiMG = BMG

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, a et b qui
n'interviennent pas dans le calcul du coefficient de fugacité
   grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
   grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   A = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis
* XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) *
XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) *
XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis *
(ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 /
2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO +
2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) *
XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO
* AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) +
grAsuite
   B = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis *
BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calcul de dérivés de XiXj(1-Kji)racine(aialphai*akalphak)
   grAbis = (1 - KH2_MG) * (XMGbis) * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * (XCH4bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
(XNH3bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
```

ArH2 = ((XH2bis)) * AH2 + (1 - KH2O_H2) * (XH2Obis) * (AH2O * AH2) ^ (1 / 2) + (1 - KCO2_H2) * (XCO2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * (XN2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KCO_H2) * (XCObis) * (ACO * AH2) ^ (1 / 2) + grAsuite

grAbis = (1 - KCO2_MG) * (XMGbis) * (ACO2 * AMG) ^ (1 / 2)

grAsuite = (1 - KCO2_CH4) * (XCH4bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) * (XNH3bis) * (ANH3 * ACO2) ^ (1 / 2) + grAbis

ArCO2 = ((XCO2bis)) * ACO2 + (1 - KH2O_HCO2) * (XH2Obis) * (AH2O * ACO2) ^ (1 / 2) + (1 - KCO2_H2) * (XH2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XN2bis) * (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * (XCObis) * (ACO * ACO2) ^ (1 / 2) + grAsuite

grAbis = (1 - KN2_MG) * (XMGbis) * (AN2 * AMG) ^ (1 / 2)

grAsuite = (1 - KN2_CH4) * (XCH4bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) * (XNH3bis) * (ANH3 * AN2) ^ (1 / 2) + grAbis

ArN2 = ((XN2bis)) * AN2 + (1 - KH2O_N2) * (XH2Obis) * (AH2O * AN2) ^ (1 / 2) + (1 - KN2_H2) * (XH2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XCO2bis) * (AN2 * ACO2) ^ (1 / 2) + (1 - KN2_CO) * (XCObis) * (ACO * AN2) ^ (1 / 2) + grAsuite

grAbis = (1 - KH2O_MG) * (XMGbis) * (AH2O * AMG) ^ (1 / 2)

grAsuite = (1 - KH2O_CH4) * (XCH4bis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) * (XNH3bis) * (ANH3 * AH2O) ^ (1 / 2) + grAbis

ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * (XH2bis) * (AH2O * AH2) ^ (1 / 2) + (1 - KH2O_CO2) * (XCO2bis) * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * (XN2bis) * (AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * (XCObis) * (ACO * AH2O) ^ (1 / 2) + grAsuite

grAbis = (1 - KCO_MG) * (XMGbis) * (ACO * AMG) ^ (1 / 2)

grAsuite = (1 - KCO_CH4) * (XCH4bis) * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) * (XNH3bis) * (ANH3 * ACO) ^ (1 / 2) + grAbis

ArCO = (XCObis) * ACO + (1 - KH2O_CO) * (XH2Obis) * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * (XCO2bis) * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * (XN2bis) * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * (XH2bis) * (ACO * AH2) ^ (1 / 2) + grAsuite

grAbis = (1 - KCH4_MG) * (XMGbis) * (ACH4 * AMG) ^ (1 / 2)

grAsuite = (1 - KH2_CH4) * (XH2bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * (XNH3bis) * (ANH3 * ACH4) ^ (1 / 2) + grAbis

ArCH4 = ((XCH4bis)) * ACH4 + (1 - KH2O_CH4) * (XH2Obis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * (XCO2bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * (XN2bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * (XCObis) * (ACO * ACH4) ^ (1 / 2) + grAsuite

grAbis = (1 - KNH3_MG) * (XMGbis) * (ANH3 * AMG) ^ (1 / 2)

grAsuite = (1 - KCH4_NH3) * (XCH4bis) * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * (XH2bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis

ArNH3 = ((XNH3bis)) * ANH3 + (1 - KH2O_NH3) * (XH2Obis) * (AH2O * ANH3) ^ (1 / 2) + (1 - KCO2_NH3) * (XCO2bis) * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * (XN2bis) * (AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * (XCObis) * (ACO * ANH3) ^ (1 / 2) + grAsuite

grAbis = (1 - KMG_NH3) * (XNH3bis) * (AMG * ANH3) ^ (1 / 2)

grAsuite = (1 - KCH4_MG) * (XCH4bis) * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) * (XH2bis) * (AMG * AH2) ^ (1 / 2) + grAbis

ArMG = ((XMGbis)) * AMG + (1 - KH2O_MG) * (XH2Obis) * (AH2O * AMG) ^ (1 / 2) + (1 - KCO2_MG) * (XCO2bis) * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * (XN2bis) * (AN2 * AMG) ^ (1 / 2) + (1 - KCO_MG) * (XCObis) * (ACO * AMG) ^ (1 / 2) + grAsuite

SB = BH2O + BH2 + BCO2 + BN2 + BCO + BNH3 + BCH4 + BMG

```
   DVDXH2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArH2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXH2O = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArH2O) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXCO2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArCO2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXCO = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArCO) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXN2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArN2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)
   DVDXCH4 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArCH4) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXNH3 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN -
B) * VN * (VN ^ 2 - B ^ 2) * ArNH3) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B)
* (VN - B) ^ 2)
   DVDXMG = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B)
* VN * (VN ^ 2 - B ^ 2) * ArMG) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) *
(VN - B) ^ 2)

VCO2M = VN * (XCO2bis) - 1 * (XCO2bis) * 1 / 3 / 8 / 2 * DVDXCO2
VCOM = VN * (XCObis) - 1 * (XCObis) * 1 / 3 / 8 / 2 * DVDXCO
VH2M = VN * (XH2bis) - 1 * (XH2bis) * 1 / 3 / 8 / 2 * DVDXH2
VN2M = VN * (XN2bis) - 1 * (XN2bis) * 1 / 3 / 8 / 2 * DVDXN2
VCH4M = VN * (XCH4bis) - 1 * (XCH4bis) * 1 / 3 / 8 / 2 * DVDXCH4
VNH3M = VN * (XNH3bis) - 1 * (XNH3bis) * 1 / 3 / 8 / 2 * DVDXNH3
VH2OM = VN * (XH2Obis) - 1 * (XH2Obis) * 1 / 3 / 8 / 2 * DVDXH2O
VMGM = VN * (XMGbis) - 1 * (XMGbis) * 1 / 3 / 8 / 2 * DVDXMG

   'calcul de somme de Xk(1-Kki)racine(aialphai*akalphak)  (avant le 2 dans le calcul du
coefficient de fugacité de l'espèce k)
   grAbis = (1 - KH2_MG) * XMGbis * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XCH4bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
XNH3bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = (XH2bis) * AH2 + (1 - KH2O_H2) * XH2Obis * (AH2O * AH2) ^ (1 / 2) + (1 -
KCO2_H2) * XCO2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * XN2bis * (AN2 * AH2)
^ (1 / 2) + (1 - KCO_H2) * XCObis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * XMGbis * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * XCH4bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = (XCO2bis) * ACO2 + (1 - KH2O_HCO2) * XH2Obis * (AH2O * ACO2) ^ (1 /
2) + (1 - KCO2_H2) * XH2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XN2bis * (AN2
* ACO2) ^ (1 / 2) + (1 - KCO_CO2) * XCObis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * XMGbis * (AN2 * AMG) ^ (1 / 2)
```

```
    grAsuite = (1 - KN2_CH4) * XCH4bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) *
XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    ArN2 = (XN2bis) * AN2 + (1 - KH2O_N2) * XH2Obis * (AH2O * AN2) ^ (1 / 2) + (1 -
KN2_H2) * XH2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XCO2bis * (AN2 * ACO2)
^ (1 / 2) + (1 - KN2_CO) * XCObis * (ACO * AN2) ^ (1 / 2) + grAsuite
    grAbis = (1 - KH2O_MG) * XMGbis * (AH2O * AMG) ^ (1 / 2)
    grAsuite = (1 - KH2O_CH4) * XCH4bis * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) *
XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + grAbis
    ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * XH2bis * (AH2O * AH2) ^ (1 / 2) + (1
- KH2O_CO2) * XCO2bis * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * XN2bis * (AN2 *
AH2O) ^ (1 / 2) + (1 - KH2O_CO) * XCObis * (ACO * AH2O) ^ (1 / 2) + grAsuite
    grAbis = (1 - KCO_MG) * XMGbis * (ACO * AMG) ^ (1 / 2)
    grAsuite = (1 - KCO_CH4) * XCH4bis * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) *
XNH3bis * (ANH3 * ACO) ^ (1 / 2) + grAbis
    ArCO = (XCObis) * ACO + (1 - KH2O_CO) * XH2Obis * (AH2O * ACO) ^ (1 / 2) + (1 -
KCO_CO2) * XCO2bis * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * XN2bis * (AN2 *
ACO) ^ (1 / 2) + (1 - KCO_H2) * XH2bis * (ACO * AH2) ^ (1 / 2) + grAsuite
    grAbis = (1 - KCH4_MG) * XMGbis * (ACH4 * AMG) ^ (1 / 2)
    grAsuite = (1 - KH2_CH4) * XH2bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) *
XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + grAbis
    ArCH4 = (XCH4bis) * ACH4 + (1 - KH2O_CH4) * XH2Obis * (AH2O * ACH4) ^ (1 / 2)
+ (1 - KCO2_CH4) * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * XN2bis *
(AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * XCObis * (ACO * ACH4) ^ (1 / 2) + grAsuite
    grAbis = (1 - KNH3_MG) * XMGbis * (ANH3 * AMG) ^ (1 / 2)
    grAsuite = (1 - KCH4_NH3) * XCH4bis * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) *
XH2bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
    ArNH3 = (XNH3bis) * ANH3 + (1 - KH2O_NH3) * XH2Obis * (AH2O * ANH3) ^ (1 / 2)
+ (1 - KCO2_NH3) * XCO2bis * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * XN2bis *
(AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * XCObis * (ACO * ANH3) ^ (1 / 2) + grAsuite
    grAbis = (1 - KMG_NH3) * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (1 - KCH4_MG) * XCH4bis * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
XH2bis * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = (XMGbis) * AMG + (1 - KH2O_MG) * XH2Obis * (AH2O * AMG) ^ (1 / 2) +
(1 - KCO2_MG) * XCO2bis * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * XN2bis * (AN2 *
AMG) ^ (1 / 2) + (1 - KCO_MG) * XCObis * (ACO * AMG) ^ (1 / 2) + grAsuite

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, Ai et Bi qui
interviennent dans le calcul du coefficient de fugacité
    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
```

```
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, A et B qui
interviennent dans le calcul du coefficient de fugacité
    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
    GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

    'calculs des coefficients de fugacités
    'logFIH2Osoave = ZN - 1 - Log(ZN - GRB) - GRA / GRB * Log((ZN + GRB) / ZN)
        'FIH2Oincsoave = 10 ^ (logFIH2Osoave / 2.303)
        'Worksheets(1).Range("C31").Value = FIH2Oincsoave

    logFIH2O = BH2O / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2O / GRB - 2
/ A * ArH2O) * Log(1 + GRB / ZN)
        FIH2Oinc = 10 ^ (logFIH2O / 2.303)
        FUH2Oinc = FIH2Oinc * P * XH2Obis
        FUH2Oi = FUH2Oinc * 0.00001
    logFIH2 = BH2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2 / GRB - 2 / A *
ArH2) * Log(1 + GRB / ZN)
        FIH2inc = 10 ^ (logFIH2 / 2.303)
```

```
        FUH2inc = FIH2inc * P * XH2bis
        FUH2i = FUH2inc * 0.00001

   logFICO = BCO / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO / GRB - 2 / A
* ArCO) * Log(1 + GRB / ZN)
        FICOinc = 10 ^ (logFICO / 2.303)
        FUCOinc = FICOinc * P * XCObis
        FUCOi = FUCOinc * 0.00001

   logFICO2 = BCO2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO2 / GRB - 2 /
A * ArCO2) * Log(1 + GRB / ZN)
        FICO2inc = 10 ^ (logFICO2 / 2.303)
        FUCO2inc = FICO2inc * P * XCO2bis
        FUCO2i = FUCO2inc * 0.00001 'la même chose mais en bar

   logFIN2 = BN2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BN2 / GRB - 2 / A *
ArN2) * Log(1 + GRB / ZN)
        FIN2inc = 10 ^ (logFIN2 / 2.303)
        FUN2inc = FIN2inc * P * XN2bis
        FUN2i = FUN2inc * 0.00001 'la même chose mais en bar

   logFICH4 = BCH4 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCH4 / GRB - 2 /
A * ArCH4) * Log(1 + GRB / ZN)
        FICH4inc = 10 ^ (logFICH4 / 2.303)
        FUCH4inc = FICH4inc * P * XCH4bis
        FUCH4i = FUCH4inc * 0.00001

   logFINH3 = BNH3 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BNH3 / GRB - 2
/ A * ArNH3) * Log(1 + GRB / ZN)
        FINH3inc = 10 ^ (logFINH3 / 2.303)
        FUNH3inc = FINH3inc * P * XNH3bis
        FUNH3i = FUNH3inc * 0.00001

   logFIMG = BMG / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BMG / GRB - 2 /
A * ArMG) * Log(1 + GRB / ZN)
        FIMGinc = 10 ^ (logFIMG / 2.303)
        FUMGinc = FIMGinc * P * XMGbis
        FUMGi = FUMGinc * 0.00001

Worksheets(1).Range("L8").Value = FUN2i
Call PROPORTION6
End Sub
Private Sub PROPORTION6()
XH2Obis = 0
XCO2bis = 0
XCObis = 0
XH2bis = 0
XN2bis = 0
XCH4bis = 0
XNH3bis = 1
```

```
XMGbis = 0

    Pb = Worksheets(1).Range("B10").Value
   P = Pb * 100000 'passage de la pression de bar en Pa
   T = Worksheets(1).Range("B11").Value + 273.15

   TcH2O = Worksheets(1).Range("C3").Value 'température critique de H2O dans la cellule
J8
   PcH2O = Worksheets(1).Range("D3").Value 'pression critique de H2O
   TcCO2 = Worksheets(1).Range("C4").Value
   PcCO2 = Worksheets(1).Range("D4").Value
   TcCO = Worksheets(1).Range("C5").Value
   PcCO = Worksheets(1).Range("D5").Value
   TcH2 = Worksheets(1).Range("C2").Value
   PcH2 = Worksheets(1).Range("D2").Value
   TcN2 = Worksheets(1).Range("C8").Value
   PcN2 = Worksheets(1).Range("D8").Value
   TcCH4 = Worksheets(1).Range("C6").Value
   PcCH4 = Worksheets(1).Range("D6").Value
   TcNH3 = Worksheets(1).Range("C9").Value
   PcNH3 = Worksheets(1).Range("D9").Value
   TcMG = Worksheets(1).Range("C7").Value
   PcMG = Worksheets(1).Range("D7").Value

   R = 8.314472 'constante des gaz parfaits
   'calcul des facteurs acentriques
   wH2O = Worksheets(1).Range("E3").Value
   nH2O = 0.48508 + 1.55171 * wH2O - 0.15613 * wH2O ^ 2
   alphaH2O = (1 + nH2O * (1 - (T / TcH2O) ^ 0.5)) ^ 2
   wCO2 = Worksheets(1).Range("E4").Value
   nCO2 = 0.48508 + 1.55171 * wCO2 - 0.15613 * wCO2 ^ 2
   alphaCO2 = (1 + nCO2 * (1 - (T / TcCO2) ^ 0.5)) ^ 2
   wCO = Worksheets(1).Range("E5").Value
   nCO = 0.48508 + 1.55171 * wCO - 0.15613 * wCO ^ 2
   alphaCO = (1 + nCO * (1 - (T / TcCO) ^ 0.5)) ^ 2
   wH2 = Worksheets(1).Range("E2").Value
   nH2 = 0.48508 + 1.55171 * wH2 - 0.15613 * wH2 ^ 2
   alphaH2 = (1 + nH2 * (1 - (T / TcH2) ^ 0.5)) ^ 2
   wN2 = Worksheets(1).Range("E8").Value
   nN2 = 0.48508 + 1.55171 * wN2 - 0.15613 * wN2 ^ 2
   alphaN2 = (1 + nN2 * (1 - (T / TcN2) ^ 0.5)) ^ 2
   wCH4 = Worksheets(1).Range("E6").Value
   nCH4 = 0.48508 + 1.55171 * wCH4 - 0.15613 * wCH4 ^ 2
   alphaCH4 = (1 + nCH4 * (1 - (T / TcCH4) ^ 0.5)) ^ 2
   wNH3 = Worksheets(1).Range("E9").Value
   nNH3 = 0.48508 + 1.55171 * wNH3 - 0.15613 * wNH3 ^ 2
   alphaNH3 = (1 + nNH3 * (1 - (T / TcNH3) ^ 0.5)) ^ 2
   wMG = Worksheets(1).Range("E7").Value
   nMG = 0.48508 + 1.55171 * wMG - 0.15613 * wMG ^ 2
   alphaMG = (1 + nMG * (1 - (T / TcMG) ^ 0.5)) ^ 2
```

```
   AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
   BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
   ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
   BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
   AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
   BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
   AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
   BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
   ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
   BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
   ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
   BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
   ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
   BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
   AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
   BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
   grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
   GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

    test = 1
     ZN = 100.01 'initialisation NR à changer si plantage
```

```
While test > 0.000000001
FZ = ZN ^ 3 - ZN ^ 2 + (GRA - GRB ^ 2 - GRB) * ZN - GRA * GRB
FpZ = 3 * ZN ^ 2 - 2 * ZN + (GRA - GRB ^ 2 - GRB)

ZN1 = ZN - FZ / FpZ
test = Abs(ZN1 - ZN)
ZN = ZN1
Wend
VN = (ZN * R * T / P)
V = VN * 1000000

'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, aialphai et bialphai
qui interviennent dans le calcul des coefficients de fugacité
AH2 = 0.42748 * alphaH2 * (R * TcH2 ^ 2) / (PcH2 * 100000#)
BH2 = 0.08664 * R * TcH2 / (PcH2 * 100000#)
BiH2 = BH2 'stockage de bialphai
ACO2 = 0.42748 * alphaCO2 * (R * TcCO2 ^ 2) / (PcCO2 * 100000#)
BCO2 = 0.08664 * R * TcCO2 / (PcCO2 * 100000#)
BiCO2 = BCO2
AN2 = 0.42748 * alphaN2 * (R * TcN2 ^ 2) / (PcN2 * 100000#)
BN2 = 0.08664 * R * TcN2 / (PcN2 * 100000#)
BiN2 = BN2
AH2O = 0.42748 * alphaH2O * (R * TcH2O ^ 2) / (PcH2O * 100000#)
BH2O = 0.08664 * R * TcH2O / (PcH2O * 100000#)
BiH2O = BH2O
ACO = 0.42748 * alphaCO * (R * TcCO ^ 2) / (PcCO * 100000#)
BCO = 0.08664 * R * TcCO / (PcCO * 100000#)
BiCO = BCO
ACH4 = 0.42748 * alphaCH4 * (R * TcCH4 ^ 2) / (PcCH4 * 100000#)
BCH4 = 0.08664 * R * TcCH4 / (PcCH4 * 100000#)
BiCH4 = BCH4
ANH3 = 0.42748 * alphaNH3 * (R * TcNH3 ^ 2) / (PcNH3 * 100000#)
BNH3 = 0.08664 * R * TcNH3 / (PcNH3 * 100000#)
BiNH3 = BNH3
AMG = 0.42748 * alphaMG * (R * TcMG ^ 2) / (PcMG * 100000#)
BMG = 0.08664 * R * TcMG / (PcMG * 100000#)
BiMG = BMG

'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, a et b qui
n'interviennent pas dans le calcul du coefficient de fugacité
grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
```

```
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 / 2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 - KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) * XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis * XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3 * ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 * (1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   A = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) * XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 - KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 - KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) * XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis * (ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) + (XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2) + 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) * XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   B = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 + XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calcul de dérivés de XiXj(1-Kji)racine(aialphai*akalphak)
   grAbis = (1 - KH2_MG) * (XMGbis) * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * (XCH4bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * (XNH3bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = ((XH2bis)) * AH2 + (1 - KH2O_H2) * (XH2Obis) * (AH2O * AH2) ^ (1 / 2) + (1 - KCO2_H2) * (XCO2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * (XN2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KCO_H2) * (XCObis) * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * (XMGbis) * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * (XCH4bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) * (XNH3bis) * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = ((XCO2bis)) * ACO2 + (1 - KH2O_HCO2) * (XH2Obis) * (AH2O * ACO2) ^ (1 / 2) + (1 - KCO2_H2) * (XH2bis) * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XN2bis) * (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * (XCObis) * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * (XMGbis) * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * (XCH4bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) * (XNH3bis) * (ANH3 * AN2) ^ (1 / 2) + grAbis
   ArN2 = ((XN2bis)) * AN2 + (1 - KH2O_N2) * (XH2Obis) * (AH2O * AN2) ^ (1 / 2) + (1 - KN2_H2) * (XH2bis) * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * (XCO2bis) * (AN2 * ACO2) ^ (1 / 2) + (1 - KN2_CO) * (XCObis) * (ACO * AN2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KH2O_MG) * (XMGbis) * (AH2O * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2O_CH4) * (XCH4bis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) * (XNH3bis) * (ANH3 * AH2O) ^ (1 / 2) + grAbis
   ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * (XH2bis) * (AH2O * AH2) ^ (1 / 2) + (1 - KH2O_CO2) * (XCO2bis) * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * (XN2bis) * (AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * (XCObis) * (ACO * AH2O) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO_MG) * (XMGbis) * (ACO * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO_CH4) * (XCH4bis) * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) * (XNH3bis) * (ANH3 * ACO) ^ (1 / 2) + grAbis
```

ArCO = (XCObis) * ACO + (1 - KH2O_CO) * (XH2Obis) * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * (XCO2bis) * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * (XN2bis) * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * (XH2bis) * (ACO * AH2) ^ (1 / 2) + grAsuite

grAbis = (1 - KCH4_MG) * (XMGbis) * (ACH4 * AMG) ^ (1 / 2)

grAsuite = (1 - KH2_CH4) * (XH2bis) * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * (XNH3bis) * (ANH3 * ACH4) ^ (1 / 2) + grAbis

ArCH4 = ((XCH4bis)) * ACH4 + (1 - KH2O_CH4) * (XH2Obis) * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * (XCO2bis) * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * (XN2bis) * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * (XCObis) * (ACO * ACH4) ^ (1 / 2) + grAsuite

grAbis = (1 - KNH3_MG) * (XMGbis) * (ANH3 * AMG) ^ (1 / 2)

grAsuite = (1 - KCH4_NH3) * (XCH4bis) * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * (XH2bis) * (ANH3 * AH2) ^ (1 / 2) + grAbis

ArNH3 = ((XNH3bis)) * ANH3 + (1 - KH2O_NH3) * (XH2Obis) * (AH2O * ANH3) ^ (1 / 2) + (1 - KCO2_NH3) * (XCO2bis) * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * (XN2bis) * (AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * (XCObis) * (ACO * ANH3) ^ (1 / 2) + grAsuite

grAbis = (1 - KMG_NH3) * (XNH3bis) * (AMG * ANH3) ^ (1 / 2)

grAsuite = (1 - KCH4_MG) * (XCH4bis) * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) * (XH2bis) * (AMG * AH2) ^ (1 / 2) + grAbis

ArMG = ((XMGbis)) * AMG + (1 - KH2O_MG) * (XH2Obis) * (AH2O * AMG) ^ (1 / 2) + (1 - KCO2_MG) * (XCO2bis) * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * (XN2bis) * (AN2 * AMG) ^ (1 / 2) + (1 - KCO_MG) * (XCObis) * (ACO * AMG) ^ (1 / 2) + grAsuite

SB = BH2O + BH2 + BCO2 + BN2 + BCO + BNH3 + BCH4 + BMG

DVDXH2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArH2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXH2O = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArH2O) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCO2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCO2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCO = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCO) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXN2 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArN2) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXCH4 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArCH4) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXNH3 = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArNH3) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

DVDXMG = (-(R * T * VN ^ 2 * (VN + B) ^ 2 + A * VN * (VN - B) ^ 2) * SB + (VN - B) * VN * (VN ^ 2 - B ^ 2) * ArMG) / (-R * T * VN ^ 2 * (VN + B) ^ 2 + A * (2 * VN + B) * (VN - B) ^ 2)

```
VCO2M = VN * (XCO2bis) - 1 * (XCO2bis) * 1 / 3 / 8 / 2 * DVDXCO2
VCOM = VN * (XCObis) - 1 * (XCObis) * 1 / 3 / 8 / 2 * DVDXCO
VH2M = VN * (XH2bis) - 1 * (XH2bis) * 1 / 3 / 8 / 2 * DVDXH2
VN2M = VN * (XN2bis) - 1 * (XN2bis) * 1 / 3 / 8 / 2 * DVDXN2
VCH4M = VN * (XCH4bis) - 1 * (XCH4bis) * 1 / 3 / 8 / 2 * DVDXCH4
VNH3M = VN * (XNH3bis) - 1 * (XNH3bis) * 1 / 3 / 8 / 2 * DVDXNH3
VH2OM = VN * (XH2Obis) - 1 * (XH2Obis) * 1 / 3 / 8 / 2 * DVDXH2O
VMGM = VN * (XMGbis) - 1 * (XMGbis) * 1 / 3 / 8 / 2 * DVDXMG

   'calcul de somme de Xk(1-Kki)racine(aialphai*akalphak)  (avant le 2 dans le calcul du coefficient de fugacité de l'espèce k)
   grAbis = (1 - KH2_MG) * XMGbis * (AH2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XCH4bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
   ArH2 = (XH2bis) * AH2 + (1 - KH2O_H2) * XH2Obis * (AH2O * AH2) ^ (1 / 2) + (1 - KCO2_H2) * XCO2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_H2) * XN2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KCO_H2) * XCObis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO2_MG) * XMGbis * (ACO2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO2_CH4) * XCH4bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KCO2_NH3) * XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + grAbis
   ArCO2 = (XCO2bis) * ACO2 + (1 - KH2O_HCO2) * XH2Obis * (AH2O * ACO2) ^ (1 / 2) + (1 - KCO2_H2) * XH2bis * (ACO2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XN2bis * (AN2 * ACO2) ^ (1 / 2) + (1 - KCO_CO2) * XCObis * (ACO * ACO2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KN2_MG) * XMGbis * (AN2 * AMG) ^ (1 / 2)
   grAsuite = (1 - KN2_CH4) * XCH4bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KN2_NH3) * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
   ArN2 = (XN2bis) * AN2 + (1 - KH2O_N2) * XH2Obis * (AH2O * AN2) ^ (1 / 2) + (1 - KN2_H2) * XH2bis * (AN2 * AH2) ^ (1 / 2) + (1 - KN2_CO2) * XCO2bis * (AN2 * ACO2) ^ (1 / 2) + (1 - KN2_CO) * XCObis * (ACO * AN2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KH2O_MG) * XMGbis * (AH2O * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2O_CH4) * XCH4bis * (AH2O * ACH4) ^ (1 / 2) + (1 - KH2O_NH3) * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + grAbis
   ArH2O = (XH2Obis) * AH2O + (1 - KH2O_H2) * XH2bis * (AH2O * AH2) ^ (1 / 2) + (1 - KH2O_CO2) * XCO2bis * (ACO2 * AH2O) ^ (1 / 2) + (1 - KH2O_N2) * XN2bis * (AN2 * AH2O) ^ (1 / 2) + (1 - KH2O_CO) * XCObis * (ACO * AH2O) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCO_MG) * XMGbis * (ACO * AMG) ^ (1 / 2)
   grAsuite = (1 - KCO_CH4) * XCH4bis * (ACO * ACH4) ^ (1 / 2) + (1 - KCO_NH3) * XNH3bis * (ANH3 * ACO) ^ (1 / 2) + grAbis
   ArCO = (XCObis) * ACO + (1 - KH2O_CO) * XH2Obis * (AH2O * ACO) ^ (1 / 2) + (1 - KCO_CO2) * XCO2bis * (ACO2 * ACO) ^ (1 / 2) + (1 - KN2_CO) * XN2bis * (AN2 * ACO) ^ (1 / 2) + (1 - KCO_H2) * XH2bis * (ACO * AH2) ^ (1 / 2) + grAsuite
   grAbis = (1 - KCH4_MG) * XMGbis * (ACH4 * AMG) ^ (1 / 2)
   grAsuite = (1 - KH2_CH4) * XH2bis * (AH2 * ACH4) ^ (1 / 2) + (1 - KCH4_NH3) * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + grAbis
   ArCH4 = (XCH4bis) * ACH4 + (1 - KH2O_CH4) * XH2Obis * (AH2O * ACH4) ^ (1 / 2) + (1 - KCO2_CH4) * XCO2bis * (ACO2 * ACH4) ^ (1 / 2) + (1 - KN2_CH4) * XN2bis * (AN2 * ACH4) ^ (1 / 2) + (1 - KCO_CH4) * XCObis * (ACO * ACH4) ^ (1 / 2) + grAsuite
   grAbis = (1 - KNH3_MG) * XMGbis * (ANH3 * AMG) ^ (1 / 2)
   grAsuite = (1 - KCH4_NH3) * XCH4bis * (ANH3 * ACH4) ^ (1 / 2) + (1 - KH2_NH3) * XH2bis * (ANH3 * AH2) ^ (1 / 2) + grAbis
```

```
    ArNH3 = (XNH3bis) * ANH3 + (1 - KH2O_NH3) * XH2Obis * (AH2O * ANH3) ^ (1 / 2)
+ (1 - KCO2_NH3) * XCO2bis * (ACO2 * ANH3) ^ (1 / 2) + (1 - KN2_NH3) * XN2bis *
(AN2 * ANH3) ^ (1 / 2) + (1 - KCO_NH3) * XCObis * (ACO * ANH3) ^ (1 / 2) + grAsuite
    grAbis = (1 - KMG_NH3) * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (1 - KCH4_MG) * XCH4bis * (AMG * ACH4) ^ (1 / 2) + (1 - KH2_MG) *
XH2bis * (AMG * AH2) ^ (1 / 2) + grAbis
    ArMG = (XMGbis) * AMG + (1 - KH2O_MG) * XH2Obis * (AH2O * AMG) ^ (1 / 2) +
(1 - KCO2_MG) * XCO2bis * (ACO2 * AMG) ^ (1 / 2) + (1 - KN2_MG) * XN2bis * (AN2 *
AMG) ^ (1 / 2) + (1 - KCO_MG) * XCObis * (ACO * AMG) ^ (1 / 2) + grAsuite

    'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, Ai et Bi qui
interviennent dans le calcul du coefficient de fugacité
    AH2 = 0.42748 * alphaH2 * (TcH2 ^ 2) / (PcH2 * 100000#) * P / (T ^ 2) 'avec Tr=T/Tc et
Pr=P/Pc
    BH2 = 0.08664 * TcH2 / (PcH2 * 100000#) * P / (T)
    ACO2 = 0.42748 * alphaCO2 * (TcCO2 ^ 2) / (PcCO2 * 100000#) * P / (T ^ 2)
    BCO2 = 0.08664 * TcCO2 / (PcCO2 * 100000#) * P / (T)
    AN2 = 0.42748 * alphaN2 * (TcN2 ^ 2) / (PcN2 * 100000#) * P / (T ^ 2)
    BN2 = 0.08664 * TcN2 / (PcN2 * 100000#) * P / (T)
    AH2O = 0.42748 * alphaH2O * (TcH2O ^ 2) / (PcH2O * 100000#) * P / (T ^ 2)
    BH2O = 0.08664 * TcH2O / (PcH2O * 100000#) * P / (T)
    ACO = 0.42748 * alphaCO * (TcCO ^ 2) / (PcCO * 100000#) * P / (T ^ 2)
    BCO = 0.08664 * TcCO / (PcCO * 100000#) * P / (T)
    ACH4 = 0.42748 * alphaCH4 * (TcCH4 ^ 2) / (PcCH4 * 100000#) * P / (T ^ 2)
    BCH4 = 0.08664 * TcCH4 / (PcCH4 * 100000#) * P / (T)
    ANH3 = 0.42748 * alphaNH3 * (TcNH3 ^ 2) / (PcNH3 * 100000#) * P / (T ^ 2)
    BNH3 = 0.08664 * TcNH3 / (PcNH3 * 100000#) * P / (T)
    AMG = 0.42748 * alphaMG * (TcMG ^ 2) / (PcMG * 100000#) * P / (T ^ 2)
    BMG = 0.08664 * TcMG / (PcMG * 100000#) * P / (T)

   'calculs des paramètres de repulsion et d'attraction de l'equation d'etat, A et B qui
interviennent dans le calcul du coefficient de fugacité
    grAbis = (XMGbis ^ 2) * AMG + 2 * (1 - KMG_KH2) * XMGbis * XH2bis * (AMG *
AH2) ^ (1 / 2) + 2 * (1 - KMG_KCO2) * XMGbis * XCO2bis * (AMG * ACO2) ^ (1 / 2) + 2
* (1 - KMG_KN2) * XMGbis * XN2bis * (AMG * AN2) ^ (1 / 2) + 2 * (1 - KMG_KH2O) *
XMGbis * XH2Obis * (AMG * AH2O) ^ (1 / 2) + 2 * (1 - KMG_KCO) * XMGbis * XCObis
* (AMG * ACO2) ^ (1 / 2) + 2 * (1 - KMG_KCH4) * XMGbis * XCH4bis * (AMG * ACH4)
^ (1 / 2) + 2 * (1 - KMG_KNH3) * XMGbis * XNH3bis * (AMG * ANH3) ^ (1 / 2)
    grAsuite = (XCH4bis ^ 2) * ACH4 + (XNH3bis ^ 2) * ANH3 + 2 * (1 - KCO_CH4) *
XCH4bis * XCObis * (ACO * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_CH4) * XCH4bis *
XH2Obis * (AH2O * ACH4) ^ (1 / 2) + 2 * (1 - KCO2_CH4) * XCH4bis * XCO2bis *
(ACO2 * ACH4) ^ (1 / 2) + 2 * (1 - KH2_CH4) * XCH4bis * XH2bis * (AH2 * ACH4) ^ (1 /
2) + 2 * (1 - KN2_CH4) * XCH4bis * XN2bis * (AN2 * ACH4) ^ (1 / 2) + 2 * (1 -
KCH4_NH3) * XCH4bis * XNH3bis * (ANH3 * ACH4) ^ (1 / 2) + 2 * (1 - KH2O_NH3) *
XH2Obis * XNH3bis * (ANH3 * AH2O) ^ (1 / 2) + 2 * (1 - KCO2_NH3) * XCO2bis *
XNH3bis * (ANH3 * ACO2) ^ (1 / 2) + 2 * (1 - KCO_NH3) * XCObis * XNH3bis * (ANH3
* ACO) ^ (1 / 2) + 2 * (1 - KH2_NH3) * XH2bis * XNH3bis * (ANH3 * AH2) ^ (1 / 2) + 2 *
(1 - KN2_NH3) * XN2bis * XNH3bis * (ANH3 * AN2) ^ (1 / 2) + grAbis
    GRA = (XH2Obis ^ 2) * AH2O + (XCO2bis ^ 2) * ACO2 + 2 * (1 - KH2O_CO2) *
XH2Obis * XCO2bis * (AH2O * ACO2) ^ (1 / 2) + (XH2bis ^ 2) * AH2 + 2 * (1 -
```

```
KH2O_H2) * XH2Obis * XH2bis * (AH2O * AH2) ^ (1 / 2) + (XN2bis ^ 2) * AN2 + 2 * (1 -
KH2O_N2) * XH2Obis * XN2bis * (AH2O * AN2) ^ (1 / 2) + 2 * (1 - KCO2_H2) *
XCO2bis * XH2bis * (ACO2 * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO2) * XCO2bis * XN2bis *
(ACO2 * AN2) ^ (1 / 2) + 2 * (1 - KN2_H2) * XN2bis * XH2bis * (AN2 * AH2) ^ (1 / 2) +
(XCObis ^ 2) * ACO + 2 * (1 - KH2O_CO) * XH2Obis * XCObis * (AH2O * ACO) ^ (1 / 2)
+ 2 * (1 - KCO_H2) * XCObis * XH2bis * (ACO * AH2) ^ (1 / 2) + 2 * (1 - KN2_CO) *
XCObis * XN2bis * (ACO * AN2) ^ (1 / 2) + 2 * (1 - KCO_CO2) * XCObis * XCO2bis *
(ACO * ACO2) ^ (1 / 2) + grAsuite
   GRB = XH2Obis * BH2O + XH2bis * BH2 + XCO2bis * BCO2 + XN2bis * BN2 +
XCObis * BCO + XNH3bis * BNH3 + XCH4bis * BCH4 + XMGbis * BMG

   'calculs des coefficients de fugacités
   'logFIH2Osoave = ZN - 1 - Log(ZN - GRB) - GRA / GRB * Log((ZN + GRB) / ZN)
         'FIH2Oincsoave = 10 ^ (logFIH2Osoave / 2.303)
         'Worksheets(1).Range("C31").Value = FIH2Oincsoave

   logFIH2O = BH2O / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2O / GRB - 2
/ A * ArH2O) * Log(1 + GRB / ZN)
         FIH2Oinc = 10 ^ (logFIH2O / 2.303)
         FUH2Oinc = FIH2Oinc * P * XH2Obis
         FUH2Oi = FUH2Oinc * 0.00001
   logFIH2 = BH2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BH2 / GRB - 2 / A *
ArH2) * Log(1 + GRB / ZN)
         FIH2inc = 10 ^ (logFIH2 / 2.303)
         FUH2inc = FIH2inc * P * XH2bis
         FUH2i = FUH2inc * 0.00001

   logFICO = BCO / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO / GRB - 2 / A
* ArCO) * Log(1 + GRB / ZN)
         FICOinc = 10 ^ (logFICO / 2.303)
         FUCOinc = FICOinc * P * XCObis
         FUCOi = FUCOinc * 0.00001

   logFICO2 = BCO2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCO2 / GRB - 2 /
A * ArCO2) * Log(1 + GRB / ZN)
         FICO2inc = 10 ^ (logFICO2 / 2.303)
         FUCO2inc = FICO2inc * P * XCO2bis
         FUCO2i = FUCO2inc * 0.00001 'la même chose mais en bar

   logFIN2 = BN2 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BN2 / GRB - 2 / A *
ArN2) * Log(1 + GRB / ZN)
         FIN2inc = 10 ^ (logFIN2 / 2.303)
         FUN2inc = FIN2inc * P * XN2bis
         FUN2i = FUN2inc * 0.00001 'la même chose mais en bar

   logFICH4 = BCH4 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BCH4 / GRB - 2 /
A * ArCH4) * Log(1 + GRB / ZN)
         FICH4inc = 10 ^ (logFICH4 / 2.303)
         FUCH4inc = FICH4inc * P * XCH4bis
         FUCH4i = FUCH4inc * 0.00001
```

```
   logFINH3 = BNH3 / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BNH3 / GRB - 2
/ A * ArNH3) * Log(1 + GRB / ZN)
        FINH3inc = 10 ^ (logFINH3 / 2.303)
        FUNH3inc = FINH3inc * P * XNH3bis
        FUNH3i = FUNH3inc * 0.00001

   logFIMG = BMG / GRB * (ZN - 1) - Log(ZN - GRB) + GRA / GRB * (BMG / GRB - 2 /
A * ArMG) * Log(1 + GRB / ZN)
        FIMGinc = 10 ^ (logFIMG / 2.303)
        FUMGinc = FIMGinc * P * XMGbis
        FUMGi = FUMGinc * 0.00001

Worksheets(1).Range("L9").Value = FUNH3i
End Sub
B12 =
((H2^N2*H3^N3*H4^N4*H5^N5*H6^N6*H7^N7*H8^N8*H9^N9)/(H2^M2*H3^M3*H4^
M4*H5^M5*H6^M6*H7^M7*H8^M8*H9^M9))/((L2^N2*L3^N3*L4^N4*L5^N5*L6^N6*
L7^N7*L8^N8*L9^N9)/(L2^M2*L3^M3*L4^M4*L5^M5*L6^M6*L7^M7*L8^M8*L9^M9
))
```

3. Conclusion

To calculate PT traject with homogenisation temperature (Th) and composition of a fluid inclusion, do as following: Put the Th and change pressure until there is a hole for a bar of the volume. Take the pressure minimum under the hole, or the gap of the volume (the low volume). This volume correspond of the fluid inclusion volume. It must be the same volume for the PT traject.

To view macro: In the upper right, near the buttons save and redo, click on the down arrow, it open Ecxel options, on personnalize the task bar tag, choose currently commands, then choose the tag of display macros then add creation mode. After it you can click on it, in the upper right, and double click on the commands button, it display the macro.

To use buttons: Calculate with the command button each time you change the fluid composition, temperature and pressure.

To add a constituent: Change the molar mass (M), the critical parameters (Tc, Pc), and the acentric factor (wc). See the thermochemistry of fluid on NIST for these parameters.

4. Use and Agreement Contract

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Contact: michael.franiatte@gmail.com.

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