

Para cada punto

$T_{calc} = 301.442 \text{ K}$

$x\gamma :=$   
 $x_2 \leftarrow 0.50$   
 $x_1 \leftarrow 0.50$   
 $\gamma_2 \leftarrow 1.0$   
 $\gamma_1 \leftarrow 1.0$

$$x2UN \leftarrow \frac{\exp\left[\frac{\Delta Hf_2}{R \cdot Tm_2} \cdot PM_2 \cdot \left(\frac{T_{calc} - Tm_2}{T_{calc}}\right)\right] \cdot \gamma_2}{\gamma_1}$$

for  $i \in 1..nc$

$f_i \leftarrow 0$   
 $q_i \leftarrow 0$

for  $k \in 1..ng$

$f_i \leftarrow f_i + v_{k,i} \cdot Ru_k$   
 $q_i \leftarrow q_i + v_{k,i} \cdot Qu_k$

for  $kc \in 1..20$

for  $i \in 1..nc$

$$Ji_i \leftarrow \frac{f_i}{nc \sum_{j=1}^{nc} (f_j \cdot x_j)}$$

$$Li_i \leftarrow \frac{q_i}{nc \sum_{j=1}^{nc} (q_j \cdot x_j)}$$

for  $k \in 1..ng$

$G_{k,i} \leftarrow v_{k,i} \cdot Qu_k$

for  $k \in 1..ng$

$\theta_k \leftarrow 0$

for  $i \in 1..nc$

$\theta_k \leftarrow \theta_k + G_{k,i} \cdot x_i$

for  $l \in 1..ng$

$$\Gamma_{k,l} \leftarrow \exp\left(\frac{-\theta_{k,l}}{T_{calc}}\right)$$

for  $i \in 1..nc$

for  $k \in 1..ng$

$s_{k,i} \leftarrow 0$

for  $l \in 1..ng$

$s_{k,i} \leftarrow s_{k,i} + G_{l,i} \cdot \Gamma_{l,i,k}$

for  $k \in 1..ng$

$\eta_k \leftarrow 0$

for  $i \in 1..nc$

$\eta_k \leftarrow \eta_k + s_{k,i} \cdot x_i$

for  $i \in 1..nc$

$\ln\gamma R1_i \leftarrow q_i \cdot (1 - \ln(L_i))$

$\ln\gamma R2_i \leftarrow 0$

for  $k \in 1..ng$

$$\ln\gamma R2_i \leftarrow \ln\gamma R2_i + \left( \theta_k \cdot \frac{s_{k,i}}{\eta_k} - G_{k,i} \cdot \ln\left(\frac{s_{k,i}}{\eta_k}\right) \right)$$

$\ln\gamma R_i \leftarrow \ln\gamma R1_i - \ln\gamma R2_i$

$$\ln\gamma C_i \leftarrow 1 - Ji_i + \ln(Ji_i) - 5 \cdot q_i \cdot \left( 1 - \frac{Ji_i}{Li_i} + \ln\left(\frac{Ji_i}{Li_i}\right) \right)$$

$\ln\gamma_i \leftarrow \ln\gamma C_i + \ln\gamma R_i$

$\gamma_i \leftarrow \exp(\ln\gamma_i)$

$$x2UN \leftarrow \frac{\exp\left[\frac{\Delta Hf_2}{R \cdot Tm_2} \cdot PM_2 \cdot \left(\frac{T_{calc} - Tm_2}{T_{calc}}\right)\right] \cdot \gamma_2}{\gamma_1}$$

$x_2 \leftarrow x2UN$  if  $|x_2 - x2UN| > 0.0001$

$x_1 \leftarrow 1 - x_2$

$x\gamma_1 := x$

$x\gamma_2 := \gamma$

$x\gamma$

$T_{calc} = 301.442 \text{ K}$

$x := x\gamma_1 = \begin{pmatrix} 0.16 \\ 0.84 \end{pmatrix}$

$\gamma := x\gamma_2 = \begin{pmatrix} 1.916 \\ 1.01 \end{pmatrix}$

$i = 1..9$

$xA_i :=$

0
0.079
0.16
0.241
0.324
0.408
0.492
0.576
0.66

$\gamma_1 :=$

2.135
2.025
1.916
1.81
1.705
1.603
1.505
1.41
1.32

$\gamma_2 :=$

1
1.002
1.01
1.026
1.051
1.091
1.152
1.244
1.391

$TA_i :=$

314.0
307.721
301.442
295.163
288.884
282.605
276.326
270.047
263.768

$vsA :=$

$regress(xA, TA, 4) =$

3
3
4
313.999
-79.973
8.398
-0.673
-4.834

$TxA_i := TA_i \cdot K$