pTM 2020-04-17 Thermo Calc Epi

Constants $Rpg := 8.314$ J/K/mol $\quad cal2J := 4.184\ J$

Process $Tg := 600 + 273.15$ K

Thermo $KAs := 1.62 \cdot 10^{22} \cdot (Rpg \cdot Tg)^{-5} \quad KSb := 4.824 \cdot 10^{21} \cdot (Rpg \cdot Tg)^{-5}$

$\Omega i := 3843 \cdot cal2J$ J/mol $\quad KAs = 803.5643 \quad KSb = 239.2836$

$\boxed{VoIII := 3} \quad \boxed{PzAl := 1}$

Partial Pressures $PzAs(PzSb) := \frac{VoIII}{4} \cdot PzAl - PzSb \quad \frac{VoIII}{4} \cdot PzAl = 0.75$

$Pal(Pas, Psb, PzSb) := PzAl - 4 \cdot (PzAs(PzSb) - Pas) - 4 \cdot (PzSb - Psb)$

Solid Mole Fraction $x(Pas, Psb, PzSb) := \frac{PzSb - Psb}{PzAs(PzSb) - Pas + PzSb - Psb}$

Activities $aAs(Pas, Psb, PzSb) := (1 - x(Pas, Psb, PzSb)) \cdot e^{\frac{\Omega i}{Rpg \cdot Tg} \cdot x(Pas, Psb, PzSb)^2}$

$aSb(Pas, Psb, PzSb) := x(Pas, Psb, PzSb) \cdot e^{\frac{\Omega i}{Rpg \cdot Tg} \cdot (1 - x(Pas, Psb, PzSb))^2}$

Equilibrium Constants $KAlAs(Pas, Psb, PzSb) := \frac{aAs(Pas, Psb, PzSb)}{Pal(Pas, Psb, PzSb) \cdot Pas^{\frac{1}{4}}}$

$KAlSb(Pas, Psb, PzSb) := \frac{aSb(Pas, Psb, PzSb)}{Pal(Pas, Psb, PzSb) \cdot Psb^{\frac{1}{4}}}$

Given $target(x) := \left| \begin{array}{l} [Pas \ \ Psb] := [x_1 \ \ x_2] \\ \begin{bmatrix} KAlAs(Pas, Psb, PzSb) - KAs \\ KAlSb(Pas, Psb, PzSb) - KSb \end{bmatrix} \end{array} \right.$

$Jx := \text{Jacob}\left(target(x), \overrightarrow{x_{[1..2]}}\right)$

$J(x) := \text{eval}(Jx)$

Solve $\varepsilon := 10^{-12}$

$f(PzSb, guess) := \left| \begin{array}{l} sol := \text{al\_nleqsolve}(guess, 0, \varepsilon, target, J) \\ \text{if } \text{normi}(target(sol)) < \sqrt{\varepsilon} \\ \quad sol \\ \text{else} \\ \quad \text{stack}(0, 0) \end{array} \right.$

Check function $guess := \begin{bmatrix} 1 \\ 0.51 \end{bmatrix} \quad f(0.5, guess) = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad f(1.5, guess) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

$\boxed{PzSb := 0.1102} \quad \boxed{\begin{bmatrix} Pas \\ Psb \end{bmatrix} := f(PzSb, guess) = \begin{bmatrix} 0.3965 \\ 0.1039 \end{bmatrix}} \quad target\left(\begin{bmatrix} Pas \\ Psb \end{bmatrix}\right) = \begin{bmatrix} 6.2711 \cdot 10^{-10} \\ 1.8797 \cdot 10^{-10} \end{bmatrix}$

Output $PzAs(PzSb) = 0.6398 \quad 4 \cdot \frac{PzAs(PzSb) + PzSb}{PzAl} = 3$

Review

$$\frac{PzSb}{PzAs\left(PzSb\right)+PzSb}=0.1469 \qquad x\left(Pas,\ Psb,\ PzSb\right)=0.0254$$

$$Pal\left(Pas,\ Psb,\ PzSb\right)=0.0015$$

$$aAs\left(Pas,\ Psb,\ PzSb\right)=0.976 \qquad aSb\left(Pas,\ Psb,\ PzSb\right)=0.2079$$

Program

$N := 100$ $\qquad ko := 0$ $\qquad IP\left(k\right) := \frac{M6_{k}-M6_{k-1}}{M7_{k}-M7_{k-1}} < \frac{M6_{k-1}-M6_{k-2}}{M7_{k-1}-M7_{k-2}}$

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for k ∈ [1..(N − 1)]
    PzAs := (VoIII/4)·(1 − k/N)
    PzSb := (VoIII/4)·(k/N)
    [Pas; Psb] := f(PzSb, [Pas; Psb])
    M1_k := k
    M2_k := PzAs
    M3_k := PzSb
    M4_k := Pas
    M5_k := Psb
    M6_k := Pal(Pas, Psb, PzSb)
    M7_k := PzSb/(PzAs + PzSb)
    M8_k := x(Pas, Psb, PzSb)
    if ((ko = 0) ∧ (k > 2)) ∧ IP(k)
        ko := k − 2
    else
        continue
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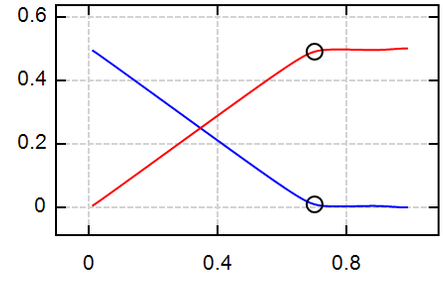
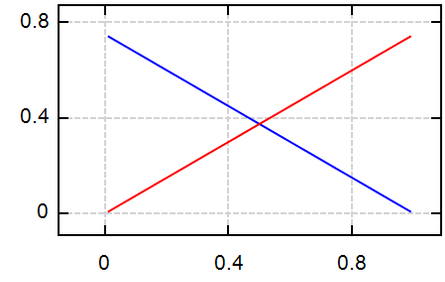
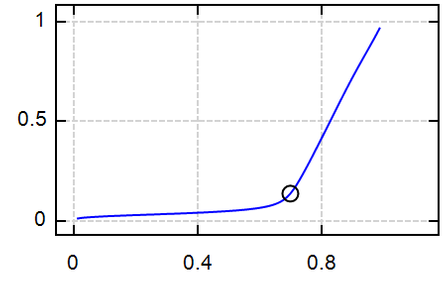


augment(M7, M4)
augment(M7, M5)
augment(M7_ko, M4_ko, "○")
augment(M7_ko, M5_ko, "○")

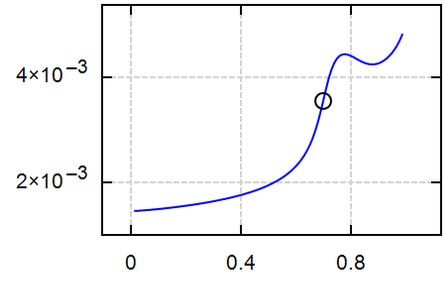


augment(M7, M2)
augment(M7, M3)



augment(M7, M8)
augment(M7_ko, M8_ko, "○")

Inflexion point of the Partial pressure



augment(M7, M6)
augment(M7_ko, M6_ko, "○")

Alvaro