

> restart

> $\Delta H_{mix} := -25000$; $\Delta H_{el} := -109300$; $\gamma_A := 0.636$; $\gamma_B := 0.805$; $\sigma := 31217$; $z := 8$; $R := 8.31$; $\alpha := \frac{5}{6}$; $v := \frac{1}{2}$; $t := 0.4$; $X_0 := 0.04$; $T := 900 + 273$

$$\Delta H_{mix} := -25000$$

$$\Delta H_{el} := -109300$$

$$\gamma_A := 0.636$$

$$\gamma_B := 0.805$$

$$\sigma := 31217$$

$$z := 8$$

$$R := 8.31$$

$$\alpha := \frac{5}{6}$$

$$v := \frac{1}{2}$$

$$t := 0.4$$

$$X_0 := 0.04$$

$$T := 1173$$

(1)

> $\omega := \frac{4 \cdot \Delta H_{mix}}{z}$

$$\omega := -12500$$

(2)

> $eq1 := \omega \cdot z \cdot (1 - 2 \cdot X_b) \cdot (1 - fig) + \alpha \cdot \omega \cdot v \cdot z \cdot (1 - 2 \cdot X_{ig}) \cdot fig + v \cdot \sigma \cdot (\gamma_A - \gamma_B) \cdot fig + R \cdot T \cdot (\ln(X_b) - \ln(1 - X_b)) \cdot (1 - fig) - \lambda \cdot (1 - fig)$

$$eq1 := -100000 (1 - 2 X_b) (1 - fig) - \frac{125000}{3} (1 - 2 X_{ig}) fig - 2637.836500 fig + 9747.63 (\ln(X_b) - \ln(1 - X_b)) (1 - fig) - \lambda (1 - fig) \quad (3)$$

> $eq2 := \alpha \cdot \omega \cdot v \cdot z \cdot (1 - 2 \cdot X_b) \cdot fig + v \cdot \sigma \cdot (\gamma_A - \gamma_B) \cdot fig + \alpha \cdot \omega \cdot (1 - 2 \cdot v) \cdot z \cdot (1 - 2 \cdot X_{ig}) \cdot fig + (1 - 2 \cdot v) \cdot \sigma \cdot (\gamma_A - \gamma_B) \cdot fig + \Delta H_{el} \cdot fig + R \cdot T \cdot (\ln(X_{ig}) - \ln(1 - X_{ig})) \cdot fig - \lambda \cdot fig$

$$eq2 := -\frac{125000}{3} (1 - 2 X_b) fig - 1.119378365 \cdot 10^5 fig + 9747.63 (\ln(X_{ig}) - \ln(1 - X_{ig})) fig - \lambda fig \quad (4)$$

> $eq3 := -\omega \cdot z \cdot X_b \cdot (1 - X_b) + \alpha \cdot \omega \cdot v \cdot z \cdot (X_b \cdot (1 - X_{ig}) + X_{ig} \cdot (1 - X_b)) + v \cdot \sigma \cdot (X_b + X_{ig}) \cdot \gamma_A + (1 - X_b + 1 - X_{ig}) \cdot \gamma_B + \alpha \cdot \omega \cdot (1 - 2 \cdot v) \cdot z \cdot X_{ig} \cdot (1 - X_{ig}) + (1 - 2 \cdot v) \cdot \sigma \cdot (X_{ig} \cdot \gamma_A + (1 - X_{ig}) \cdot \gamma_B) + X_{ig} \cdot \Delta H_{el} - R \cdot T \cdot (X_b \cdot \ln(X_b) + (1 - X_b) \cdot \ln(1 - X_b)) + R \cdot T \cdot (X_{ig} \cdot \ln(X_{ig}) + (1 - X_{ig}) \cdot \ln(1 - X_{ig})) - \lambda \cdot (X_{ig} - X_b)$

$$eq3 := 100000 X_b (1 - X_b) - \frac{125000}{3} X_b (1 - X_{ig}) - \frac{125000}{3} X_{ig} (1 - X_b) - 2637.836500 X_b - 1.119378365 \cdot 10^5 X_{ig} + 25129.68500 - 9747.63 X_b \ln(X_b) - 9747.63 (1 - X_b) \ln(1 - X_b) + 9747.63 X_{ig} \ln(X_{ig}) + 9747.63 (1 - X_{ig}) \ln(1 - X_{ig}) - \lambda (X_{ig} - X_b) \quad (5)$$

$$\begin{aligned} &> eq4 := Xb \cdot (1 - fig) + Xig \cdot fig - X0 \\ &eq4 := Xb (1 - fig) + Xig fig - 0.04 \end{aligned} \quad (6)$$

$$\begin{aligned} &> \lambda_s := solve(eq2=0, \lambda) \\ \lambda_s &:= -1.536045032 \cdot 10^5 + 83333.33333 Xb + 9747.630000 \ln(Xig) - 9747.630000 \ln(1. \\ &\quad - 1. Xig) \end{aligned} \quad (7)$$

$$\begin{aligned} &> eq1 := subs(\lambda = \lambda_s, eq1) \\ eq1 &:= -100000 (1 - 2 Xb) (1 - fig) - \frac{125000}{3} (1 - 2 Xig) fig - 2637.836500 fig \\ &\quad + 9747.63 (\ln(Xb) - \ln(1 - Xb)) (1 - fig) - (-1.536045032 \cdot 10^5 + 83333.33333 Xb \\ &\quad + 9747.630000 \ln(Xig) - 9747.630000 \ln(1. - 1. Xig)) (1 - fig) \end{aligned} \quad (8)$$

$$\begin{aligned} &> eq3 := subs(\lambda = \lambda_s, eq3) \\ eq3 &:= 100000 Xb (1 - Xb) - \frac{125000}{3} Xb (1 - Xig) - \frac{125000}{3} Xig (1 - Xb) \\ &\quad - 2637.836500 Xb - 1.119378365 \cdot 10^5 Xig + 25129.68500 - 9747.63 Xb \ln(Xb) \\ &\quad - 9747.63 (1 - Xb) \ln(1 - Xb) + 9747.63 Xig \ln(Xig) + 9747.63 (1 - Xig) \ln(1 - Xig) \\ &\quad - (-1.536045032 \cdot 10^5 + 83333.33333 Xb + 9747.630000 \ln(Xig) - 9747.630000 \ln(1. \\ &\quad - 1. Xig)) (Xig - Xb) \end{aligned} \quad (9)$$

$$\begin{aligned} &> sol := fsolve(\{eq1=0, eq3=0, eq4=0\}, \{Xb=0..1, Xig=0..1, fig=0..1\}) \\ sol &:= \{Xb=0.02946935418, Xig=0.9165972538, fig=0.01187049334\} \end{aligned} \quad (10)$$

$$\begin{aligned} &> Xb := subs(sol[1], Xb) \\ Xb &:= 0.02946935418 \end{aligned} \quad (11)$$

$$\begin{aligned} &> Xig := subs(sol[2], Xig) \\ Xig &:= 0.9165972538 \end{aligned} \quad (12)$$

$$\begin{aligned} &> fig := subs(sol[3], fig) \\ fig &:= 0.01187049334 \end{aligned} \quad (13)$$

$$\begin{aligned} &> eq5 := fig - 1 + \left(\frac{d-t}{d} \right)^3 \\ eq5 &:= -0.9881295067 + \frac{(d-0.4)^3}{d^3} \end{aligned} \quad (14)$$

$$\begin{aligned} &> d := fsolve(eq5=0, d) \\ d &:= 100.6899353 \end{aligned} \quad (15)$$

$$\begin{aligned} &> Gamma := \frac{(Xig - Xb)}{\sigma \cdot (1 - Xb)} \\ \Gamma &:= 0.00002928099429 \end{aligned} \quad (16)$$

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