Proračuni fazne ravnoteže

Predavanja i upute za
II. numerički zadatak

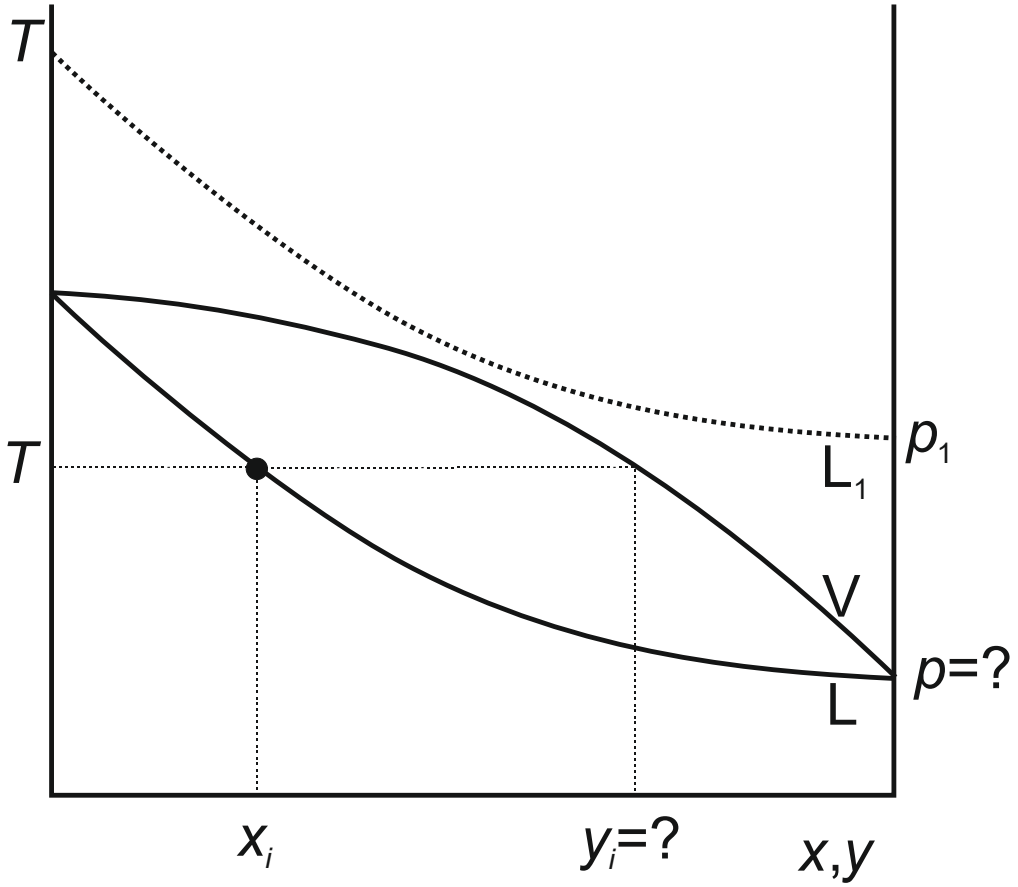
Proračuni fazne ravnoteže

- proračuni vrelišta
- proračuni kapljišta
- proračuni jednokratnog isparavanja

Proračun vrelišta uz stalnu temperaturu

bubble-point problem

npr. pri isparavanju u izoliranom cjevovodu uslijed pada tlaka



Formulacija

$$T, x_i \rightarrow p, y_i$$

Broj nepoznanica: *nk*+1

Proračun vrelišta uz stalnu temperaturu

Jednadžbe

$$f(p) = -1 + \sum_{i=1}^{nk} y_i = -1 + \sum_{i=1}^{nk} K_i x_i = 0$$

Bilanca tvari za parnu fazu

$$K_i = \frac{y_i}{x_i} = f(p, T, x_i, y_i)$$

Ravnotežne jednadžbe

Proračun vrelišta uz stalnu temperaturu

Kombiniranje bilančnih i ravnotežnih jednadžbi

$$\sum_{i=1}^{nk} p y_i = \sum_{i=1}^{nk} x_i \gamma_i^{\mathrm{L}} p_i^{\bullet} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

$$T, x_i \rightarrow p, y_i$$

$$p \sum_{i=1}^{nk} y_i = \sum_{i=1}^{nk} x_i \gamma_i^{\mathrm{L}} p_i^{\bullet} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

$$p = \sum_{i=1}^{nk} x_i \gamma_i^{\mathrm{L}} p_i^{\bullet} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

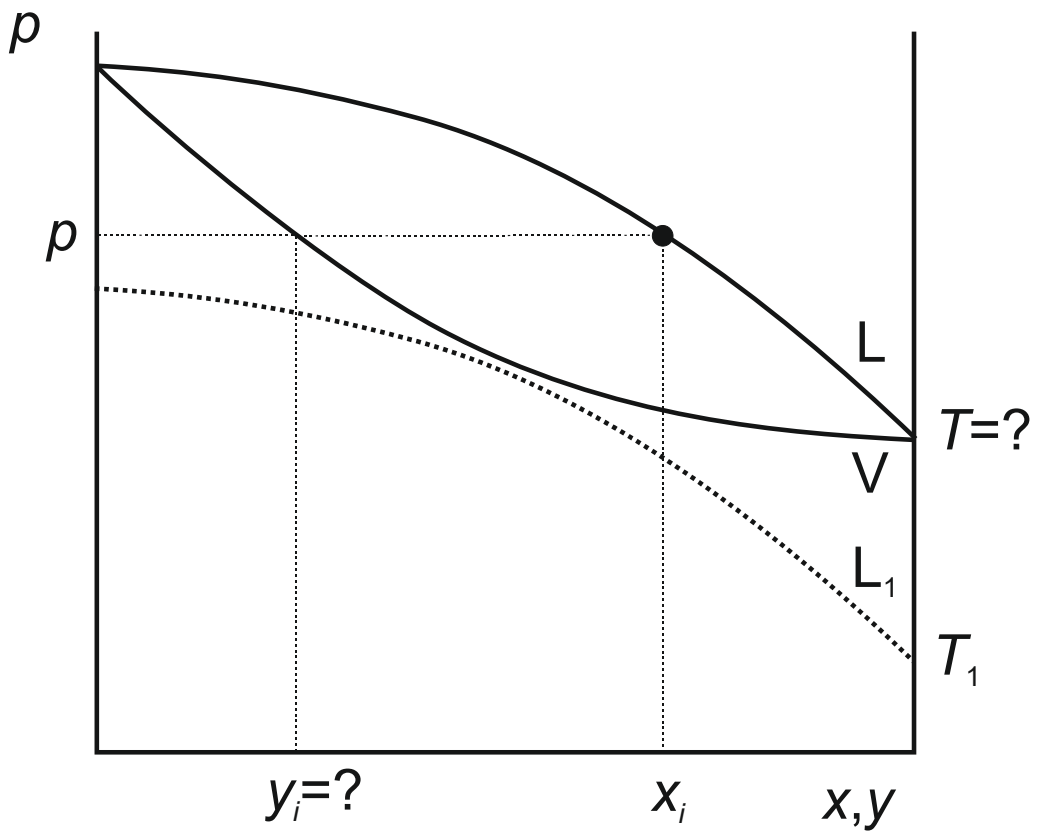
Metoda direktne iteracije

$$y_i = x_i \gamma_i^{\mathrm{L}} p_i^{\bullet} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

Proračun vrelišta uz stalan tlak

bubble-point problem

npr. pri procjeni isparavanja uskladištene kapljevine



Formulacija

$$p, x_i \rightarrow T, y_i$$

Broj nepoznanica: $nk+1$

Proračun vrelišta uz stalan tlak

Jednadžbe

$$f(p) = -1 + \sum_{i=1}^{nk} y_i = -1 + \sum_{i=1}^{nk} K_i x_i = 0$$

Bilanca tvari za parnu fazu

$$K_i = \frac{y_i}{x_i} = f(p, T, x_i, y_i)$$

Ravnotežne jednadžbe

Proračun vrelišta uz stalan tlak

Kombiniranje bilančnih i ravnotežnih jednadžbi $p, x_i \rightarrow T, y_i$

$$p = \sum_{i=1}^{nk} x_i \gamma_i^{\mathrm{L}} p_i^{\bullet} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

Metoda direktne iteracije

$$p < p \Rightarrow T = T + \Delta T$$

$$p > p \Rightarrow T = T - \Delta T$$

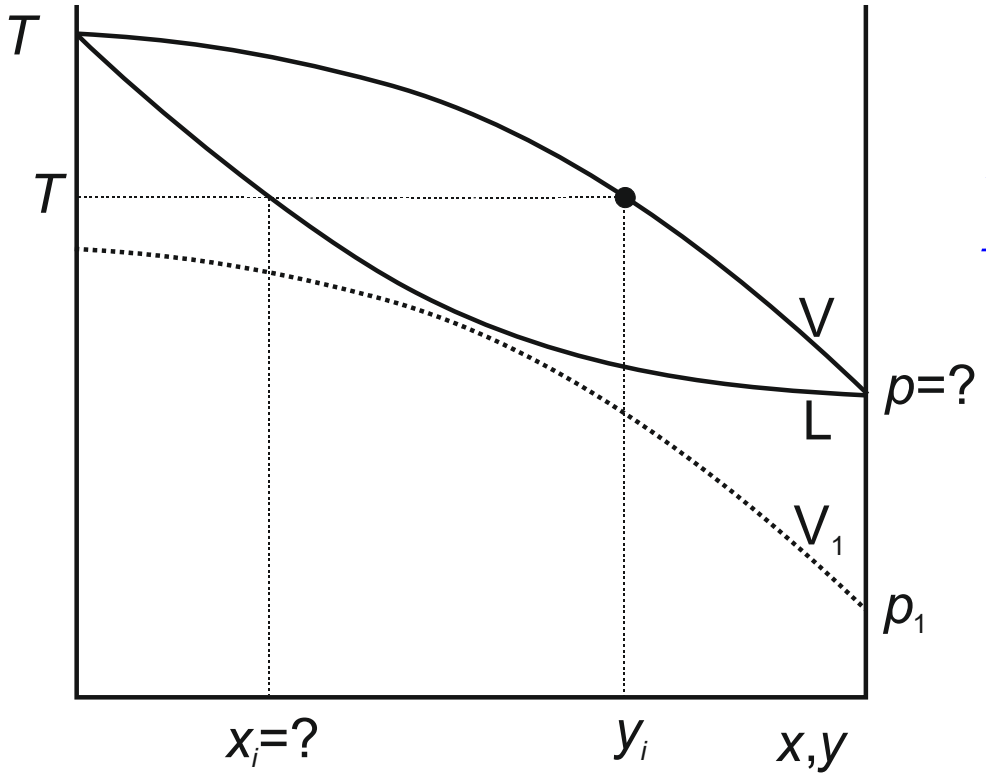
Metoda pokušaja i pogreške

$$y_i = x_i \gamma_i^{\mathrm{L}} p_i^{\bullet} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

Proračun kapljišta uz stalnu temperaturu

dew-point problem

npr. pri ukapljivanju plinovite smjese povećanjem tlaka pri stalnoj temperaturi



Formulacija

$$T, y_i \rightarrow p, x_i$$

Broj nepoznanica: $nk+1$

Proračun kapljišta uz stalnu temperaturu

Jednadžbe

$$f(p) = -1 + \sum_{i=1}^{nk} x_i = -1 + \sum_{i=1}^{nk} \frac{y_i}{K_i} = 0$$

Bilanca tvari za kapljevitu fazu

$$K_i = \frac{y_i}{x_i} = f(p, T, x_i, y_i)$$

Ravnotežne jednadžbe

Proračun kapljišta uz stalnu temperaturu

Kombiniranje bilančnih i ravnotežnih jednadžbi $T, y_i \rightarrow p, x_i$

$$p = \sum_{i=1}^{nk} x_i \gamma_i^{\mathrm{L}} p_i^{\bullet} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

Metoda direktne iteracije

$$y_i = x_i \gamma_i^{\mathrm{L}} p_i^{\bullet} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

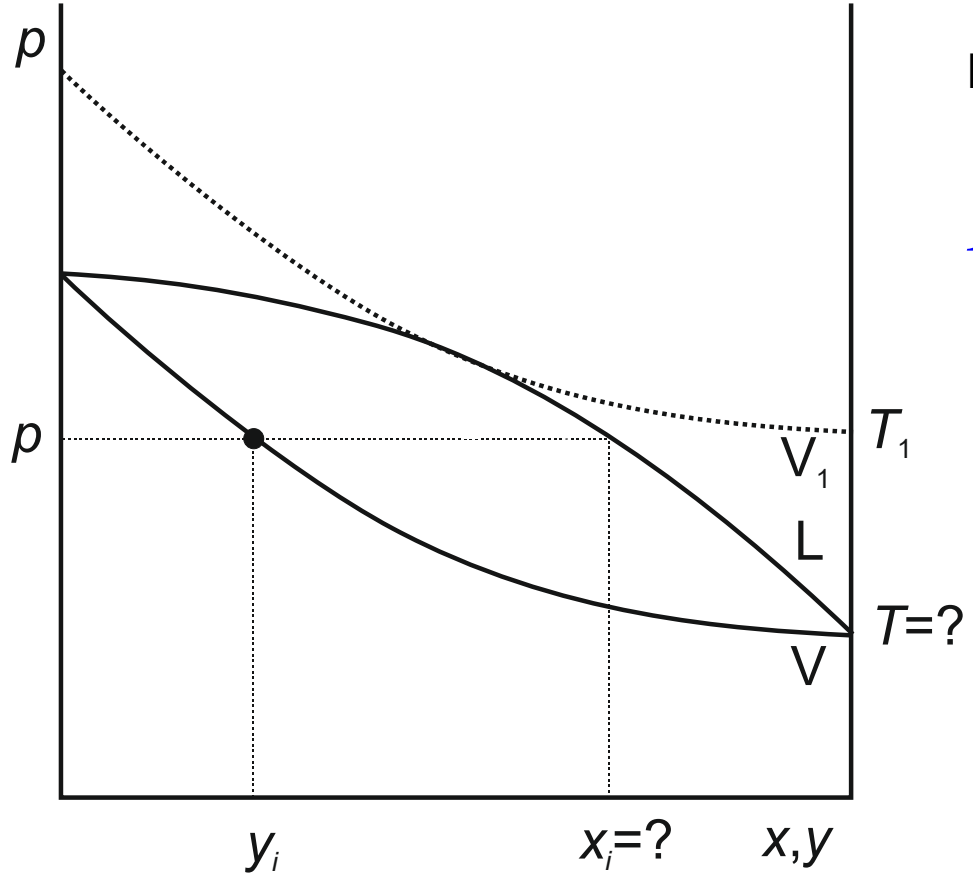
$$y_i = y_i \qquad x_{\mathrm{i}} = \frac{y_{\mathrm{i}}}{\frac{\gamma_{\mathrm{i}}^{\mathrm{L}} p_{\mathrm{i}}^{\bullet}}{p} \exp\left[\frac{v_{\mathrm{i}}^{\mathrm{L}}(p - p_{\mathrm{i}}^{\bullet})}{RT}\right]}$$

Metoda pokušaja i pogreške

Proračun kapljišta uz stalan tlak

dew-point problem

npr. skladištenju ili strujanju plinovite smjese u uvjetima niskih, zimskih temperatura



Formulacija

$$p, y_i \rightarrow T, x_i$$

Broj nepoznanica: *nk*+1

Proračun kapljišta uz stalan tlak

Jednadžbe

$$f(T) = -1 + \sum_{i=1}^{nk} x_i = -1 + \sum_{i=1}^{nk} \frac{y_i}{K_i} = 0$$

Bilanca tvari za kapljevitu fazu

$$K_i = \frac{y_i}{x_i} = f(p, T, x_i, y_i)$$

Ravnotežne jednadžbe

Proračun kapljišta uz stalan tlak

Kombiniranje bilančnih i ravnotežnih jednadžbi

$$p, y_i \rightarrow T, x_i$$

$$p = \sum_{i=1}^{nk} x_i \gamma_i^{\mathrm{L}} p_i^{\bullet} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

Metoda direktne iteracije

$$y_i = x_i \gamma_i^{\mathrm{L}} p_i^{\bullet} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

$$y_i = y_i \qquad x_{\mathrm{i}} = \frac{y_{\mathrm{i}}}{\frac{\gamma_{\mathrm{i}}^{\mathrm{L}} p_{\mathrm{i}}^{\bullet}}{p} \exp\left[\frac{v_{\mathrm{i}}^{\mathrm{L}}(p - p_{\mathrm{i}}^{\bullet})}{RT}\right]}$$

Metoda pokušaja i pogreške

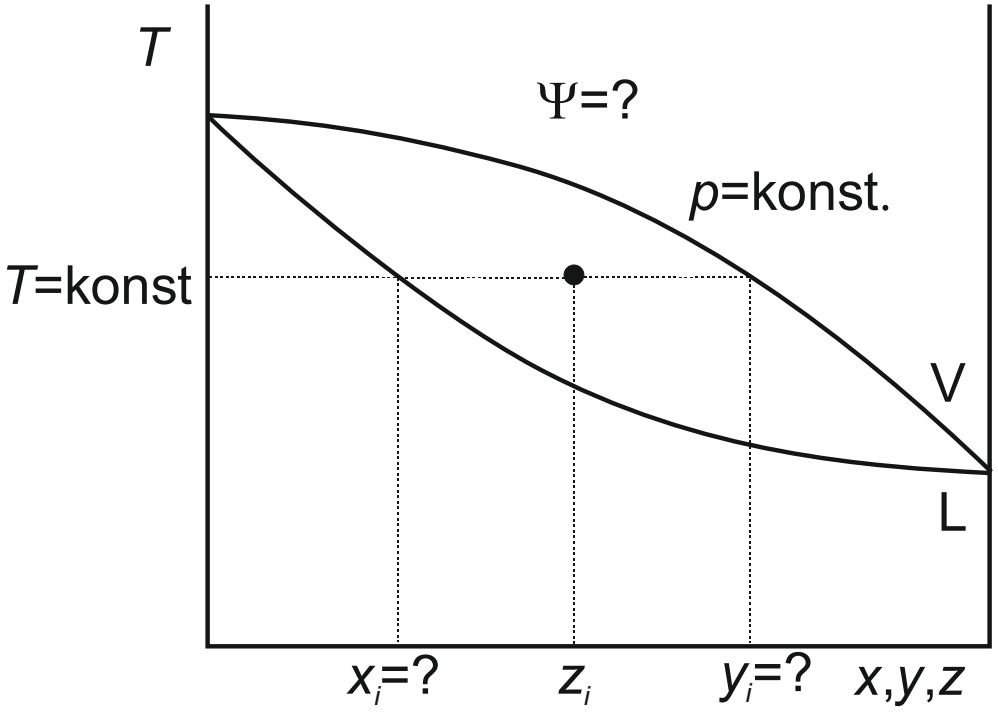
$$p < p \Rightarrow T = T + \Delta T$$
$$p < p \Rightarrow T = T - \Delta T$$

Metoda pokušaja i pogreške

Proračun jednokratnog isparavanja uz stalan tlak i temperaturu

npr. pri proračunu teorijske plitice destilacijske kolone

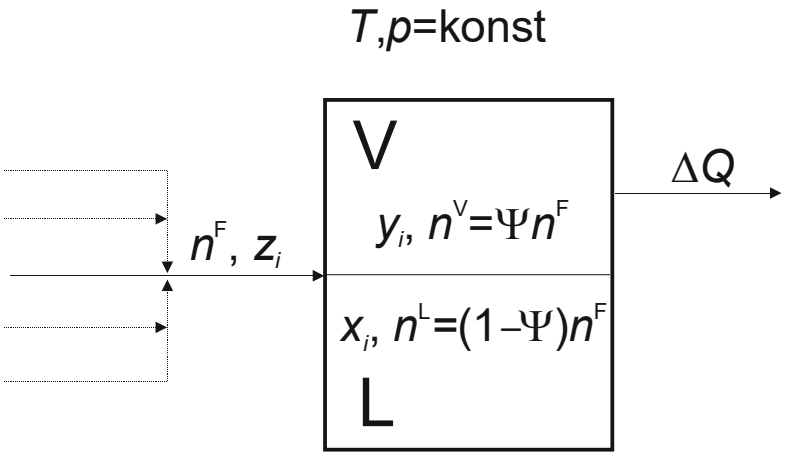
Isothermal flash problem



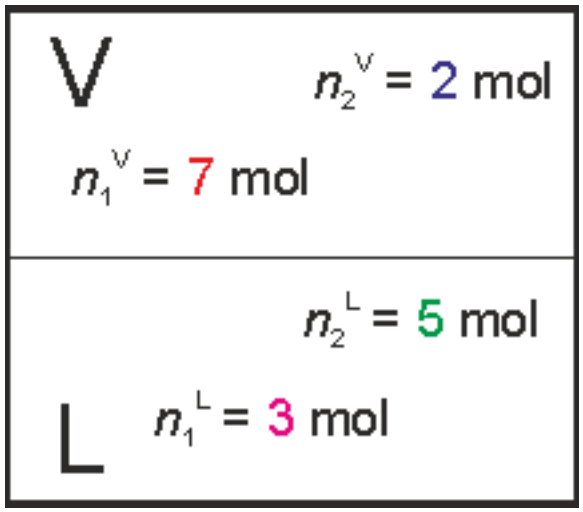
Formulacija

$$p, T, z_i \rightarrow x_i, y_i, \Psi$$

Broj nepoznanica: 2**nk*+1



Proračun jednokratnog isparavanja uz stalan tlak i temperaturu



$$x_1 = \frac{3}{3+5} \qquad x_2 = \frac{5}{3+5}$$

$$y_1 = \frac{7}{7+2} \qquad y_2 = \frac{2}{7+2}$$

$$z_1 = \frac{3+7}{3+5+7+2} \qquad z_2 = \frac{5+2}{3+5+7+2}$$

$$\Psi = \frac{7+2}{3+5+7+2}$$

$$K_1 = \frac{\frac{7}{7+2}}{\frac{3}{3+5}} = \frac{56}{27}$$

$$K_2 = \frac{\frac{2}{7+2}}{\frac{5}{3+5}} = \frac{16}{45}$$

Proračun jednokratnog isparavanja uz stalan tlak i temperaturu

Jednadžbe $K_i = \frac{y_i}{x_i} = f\left(p, T, x_i, y_i\right)$ Ravnotežne jednadžbe

$$n_i^{\mathrm{F}} = n_i^{\mathrm{L}} + n_i^{\mathrm{V}}$$
$$z_i n^{\mathrm{F}} = x_i n^{\mathrm{L}} + y_i n^{\mathrm{V}}$$

Bilančne jednadžbe za komponente

$$z_i = \left(1 - \Psi\right) x_i + \Psi y_i$$

Jedna od tri bilančne jednadžbe za faze

$$\sum_{i=1}^{nk} x_i = 1 \qquad \sum_{i=1}^{nk} y_i = 1 \qquad \sum_{i=1}^{nk} y_i - \sum_{i=1}^{nk} x_i = 0$$

Rachford-Rice

Proračun jednokratnog isparavanja uz stalan tlak i temperaturu

Kombiniranje bilančnih jednadžbi s ravnotežnim

$$z_i = (1-\Psi)\frac{y_i}{K_i} + \Psi y_i \qquad z_i = (1-\Psi)x_i + \Psi K_i x_i$$

$$y_i = \frac{K_i z_i}{1+\Psi(K_i-1)} \qquad x_i = \frac{z_i}{1+\Psi(K_i-1)}$$

Kombiniranje s bilančnim uvjetom za faze

$$f(\Psi) = -1 + \sum_{i=1}^{nk} \frac{z_i}{1+\Psi(K_i-1)} = 0 \qquad f(\Psi) = \sum_{i=1}^{nk} \frac{z_i(K_i-1)}{1+\Psi(K_i-1)} = 0$$

Proračun jednokratnog isparavanja uz stalan tlak i temperaturu

$$p, T, z_i \rightarrow x_i, y_i, \Psi$$

$$K_i = \frac{\gamma_i^{\mathrm{L}} p_i^{\bullet}}{p} \exp\left[\frac{v_i^{\mathrm{L}}\left(p - p_i^{\bullet}\right)}{RT}\right]$$

$$\sum_{i=1}^{nk} \frac{z_i\left(K_i - 1\right)}{1 + \Psi\left(K_i - 1\right)} = 0$$

Newtonova metoda tangente

$$x_i = \frac{z_i}{1 + \Psi\left(K_i - 1\right)}$$

Metoda pokušaja i pogreške

$$y_i = \frac{K_i z_i}{1 + \Psi\left(K_i - 1\right)}$$

Proračun jednokratnog isparavanja uz stalan tlak i entalpiju

npr. pri proračunu teorijske plitice destilacijske kolone u adijabatskim uvjetima

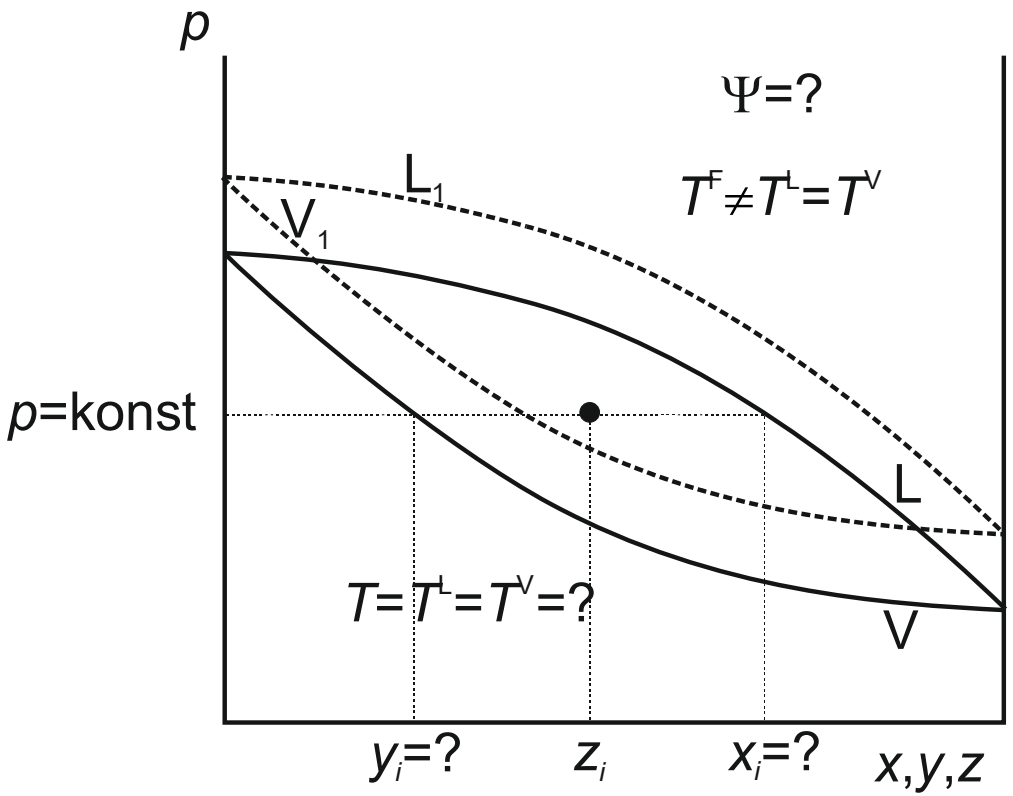
- brza isparavanja
- isparavanja u izoliranim posudama

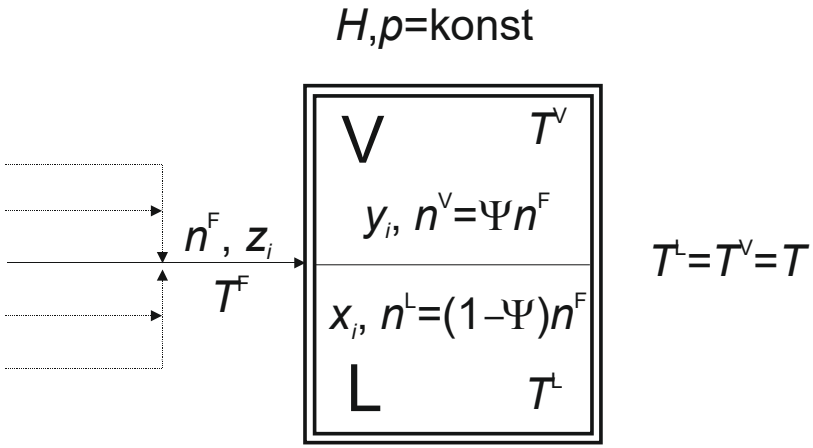
Adiabatic flash problem

Formulacija

$$p, T^F, z_i \rightarrow x_i, y_i, \Psi, T$$

Broj nepoznanica: 2**nk*+2





Proračun jednokratnog isparavanja uz stalan tlak i entalpiju

Jednadžbe $K_i = \frac{y_i}{x_i} = f\left(p, T, x_i, y_i\right)$ Ravnotežne jednadžbe

$$n_i^{\mathrm{F}} = n_i^{\mathrm{L}} + n_i^{\mathrm{V}}$$

$$z_i n^{\mathrm{F}} = x_i n^{\mathrm{L}} + y_i n^{\mathrm{V}}$$ Bilančne jednadžbe za komponente

$$z_i = \left(1 - \Psi\right) x_i + \Psi y_i$$

Rachford-Rice

$$\sum_{i=1}^{nk} x_i = 1 \qquad \sum_{i=1}^{nk} y_i = 1 \qquad \sum_{i=1}^{nk} y_i - \sum_{i=1}^{nk} x_i = 0$$

Jedna od tri bilančne jednadžbe za faze

$$H^{\mathrm{F}}\left(p, T, z_i\right) = H^{\mathrm{L}}\left(p, T, x_i\right) + H^{\mathrm{V}}\left(p, T, y_i\right)$$

Bilančna jednadžba za entalpiju

Proračun jednokratnog isparavanja uz stalan tlak i entalpiju

Formalizam rješavanja

$$f(\Psi,T)=\sum_{i=1}^{nk}\frac{z_i(K_i-1)}{1+\Psi(K_i-1)}=0$$

$$K_i=f(T)$$

$$h_i^{\bullet L}=f(T)$$

$$h_i^{\bullet V}=f(T)$$

$$h_i^{\bullet F}=f(T^F)$$

$$g(\Psi,T)=$$

$$=\left(\sum_{i=1}^{nk}z_i h_i^{\bullet F}+h^{ex,F}\right)-\left[(1-\Psi)\left(\sum_{i=1}^{nk}x_i h_i^{\bullet L}+h^{ex,L}\right)+\Psi\left(\sum_{i=1}^{nk}y_i h_i^{\bullet V}+h^{ex,V}\right)\right]=0$$

Sustav dviju jednadžbi s dvjema nepoznanicama