

12. ZADATAK

Izračunati temperaturu smjese kisika (1) i etena (2) sastava $y_1=0,75$ pri tlaku od 100 atm, uz pretpostavku da se plinska smjesa vlada prema Redlich-Kwongovu modelu. Molarni volumen smjese pri tim uvjetima iznosi $v=2,54 \cdot 10^{-4} \text{ m}^3\text{mol}^{-1}$.

Pseudokritične parametre smjese izračunati prema Prausnitz-Gunnovu pravilu. Temperaturu računati postupkom direktne iteracije.

Termodinamički parametri čistih tvari:

	T_K/K	$v_k/\text{cm}^3\text{mol}^{-1}$	z_k
kisik (1)	154,8	73,4	0,288
eten (2)	282,4	130,4	0,280

REDLICH KWONG (1949)

Prva moderna jednačba stanja trećeg stupnja

Jednačba

$$p = \frac{RT}{v-b} - \frac{a}{\sqrt{T}v(v+b)}$$

$$v^3 - \frac{RT}{p}v^2 - \left(b^2 + \frac{RTb}{p} - \frac{a}{p\sqrt{T}} \right)v - \frac{ab}{p\sqrt{T}} = 0$$

$$z^3 - z^2 - \left(\frac{b^2 p^2}{R^2 T^2} + \frac{pb}{RT} - \frac{ap}{R^2 T^2 \sqrt{T}} \right)z - \frac{abp^2}{R^3 T^3 \sqrt{T}} = 0$$

$$z^3 - z^2 + (A - B^2 - B)z - AB = 0$$

Parametri

$$a = \frac{\Omega_a R^2 T_K^{5/2}}{p_K} \qquad b = \frac{\Omega_b R T_K}{p_K}$$

$$\Omega_a = \frac{1}{9(2^{1/3} - 1)} = 0,427480$$

$$\Omega_b = \frac{(2^{1/3} - 1)}{3} = 0,086640$$

$$A = \frac{ap}{R^2 T^{5/2}} = \frac{\Omega_a p_r}{T_r^{5/2}} \qquad B = \frac{bp}{RT} = \frac{\Omega_b p_r}{T_r}$$

Pseudokritični parametri

Prausnitz i Gunn

$$v_{pk} = \sum y_i v_{ki}$$

$$T_{pk} = \sum y_i T_{ki}$$

$$z_{pk} = \sum y_i z_{ki}$$

$$p_{pk} = \frac{z_{pk} R T_{pk}}{v_{pk}}$$

Izravna (direktna) iteracija

RK Jednadžba stanja trećeg stupnja

$$p = \frac{RT}{v-b} - \frac{a}{\sqrt{T}v(v+b)}$$

Nije eksplicitna po temperaturi!

$$T = f(T)$$

$$T^{(i+1)} = f(T^{(i)})$$

$$T^{(i+1)} = \frac{v-b}{R} \left[p + \frac{a}{\sqrt{T^{(i)}}v(v+b)} \right]$$

Prva aproksimacija – idealni plin

Zadatak:

KISIĆ (1) – ETEN (2)

$$v = 2,54 \cdot 10^{-4} \text{ m}^3 \text{ mol}^{-1}$$

$$p = 100 \text{ atm} = 10,013250 \text{ MPa}$$

$$y_1 = 0,75$$

Pseudokritični parametri

$$v_{\text{KM}} = 0,75 \cdot 73,4 + (1 - 0,75) \cdot 130,4 = 87,65 \text{ cm}^3 \text{ mol}^{-1}$$

$$T_{\text{KM}} = 0,75 \cdot 154,8 + (1 - 0,75) \cdot 282,4 = 186,7 \text{ K}$$

$$z_{\text{KM}} = 0,75 \cdot 0,288 + (1 - 0,75) \cdot 0,280 = 0,286$$

$$p_{\text{KM}} = \frac{0,286 \cdot 8,314 \cdot 186,7}{87,65 \cdot 10^{-6}} = 5,064917 \text{ MPa}$$

Parametri a i b za smjesu

$$a_{\text{M}} = \frac{\Omega_a R^2 T_{\text{KM}}^{2,5}}{p_{\text{KM}}} = \frac{0,42748 \cdot 8,314^2 \cdot 186,7^{2,5}}{5,064917 \cdot 10^6} = 2,7786$$

$$b_{\text{M}} = \frac{\Omega_b R T_{\text{KM}}}{p_{\text{KM}}} = \frac{0,08664 \cdot 8,314 \cdot 186,7}{5,064917 \cdot 10^6} = 2,655 \cdot 10^{-5}$$

Iteracija po temperaturi

$$T^{(i+1)} = \frac{v - b_M}{R} \left[p + \frac{a_M}{\sqrt{T^{(i)}} v (v + b_M)} \right]$$

Idealni plin:

$$T_0 = \frac{pv}{R} = \frac{100 \cdot 101325 \cdot 2,54 \cdot 10^{-4}}{8,314} = 309,56 \text{ K}$$

$$T^{(i+1)} = \frac{v - b_M}{R} \left[p + \frac{a_M}{\sqrt{T^{(i)}} v (v + b_M)} \right]$$

$$T_1 = \frac{2,54 \cdot 10^{-4} - 2,655 \cdot 10^{-5}}{8,314} \left[100 \cdot 101325 + \frac{2,7786}{\sqrt{309,56} \cdot 2,54 \cdot 10^{-4} (2,54 \cdot 10^{-4} + 2,655 \cdot 10^{-5})} \right]$$

$$T_1 = 2,73575 \cdot 10^{-5} \left[100 \cdot 101325 + \frac{3,89926 \cdot 10^7}{\sqrt{309,56}} \right]$$

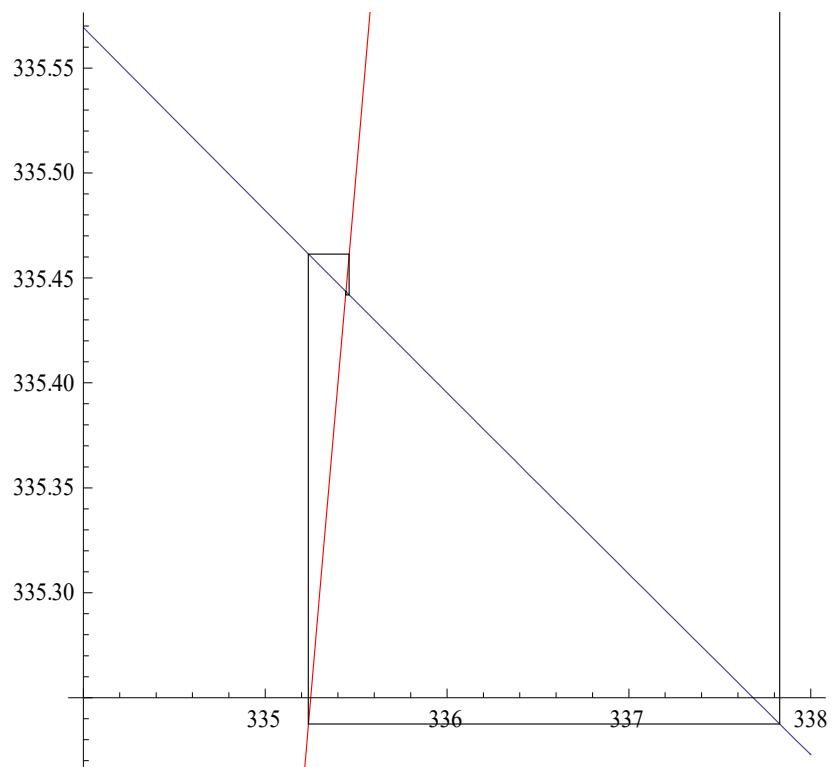
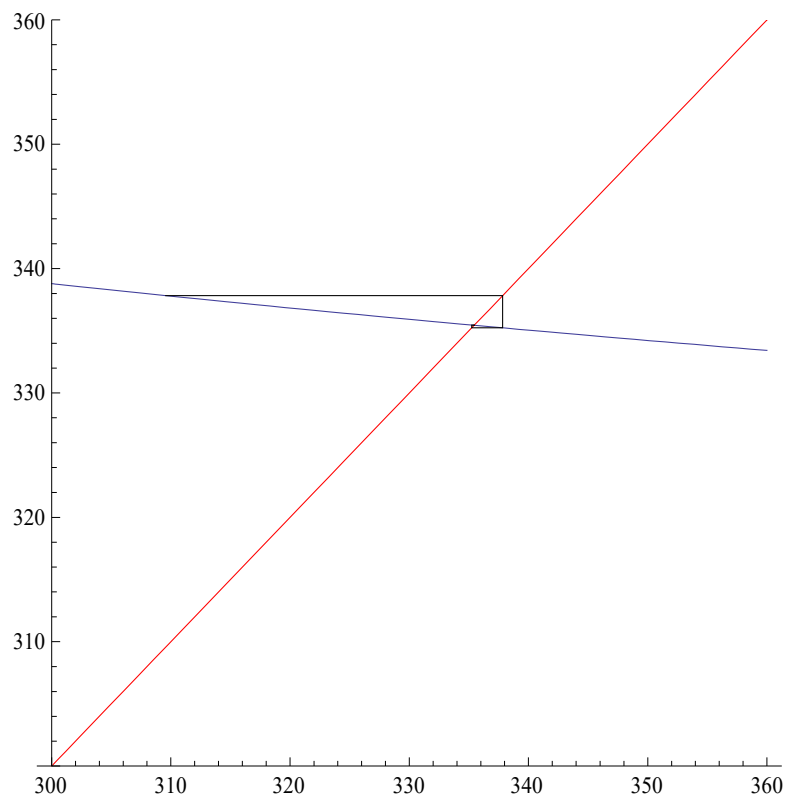
$$T_1 = 337,82 \text{ K}$$

$$T_2 = 2,73575 \cdot 10^{-5} \left[100 \cdot 101325 + \frac{3,89926 \cdot 10^7}{\sqrt{337,82}} \right]$$

$$T_2 = 335,23 \text{ K}$$

$$T_3 = 335,45 \text{ K}$$

$$T_4 = 335,44 \text{ K}$$



Iteracijska formula za SRK

$$\kappa = 0,48508 + 1,55171\omega - 0,15613\omega^2$$

$$\alpha = \left[1 + \kappa \left(1 - \sqrt{\frac{T^{(i)}}{T_K}} \right) \right]^2$$

$$T^{(i+1)} = \frac{v-b}{R} \left[p + \frac{a\alpha}{v(v+b)} \right]$$

Iteracijska formula za PR

$$\kappa = 0,37464 + 1,54226\omega - 0,26992\omega^2$$

$$\alpha = \left[1 + \kappa \left(1 - \sqrt{\frac{T^{(i)}}{T_K}} \right) \right]^2$$

$$T^{(i+1)} = \frac{v-b}{R} \left[p + \frac{a\alpha}{v^2 + 2bv - b^2} \right]$$