# 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-Kwongovom modelu. Molarni volumen smjese pri tim uvjetima iznosi $v$=2,54·10$^{-4}$ m$^3$mol$^{-1}$.

Pseudokritične parametre smjese izračunati prema Kayevom i Prausnitz-Gunnovom pravilu. Temperaturu računati postupkom direktne iteracije.

Termodinamički parametri čistih tvari:

| | $T_K$/K | $v_k$/cm$^3$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 jednadžba stanja trećeg stupnja

Prva moderna jednadžba stanja trećeg stupnja

Jednadžba

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

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

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

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

Parametri

$$a = \frac{\Omega_a R^2 T_{\mathrm{K}}^{5/2}}{p_{\mathrm{K}}} \qquad b = \frac{\Omega_b R T_{\mathrm{K}}}{p_{\mathrm{K}}}$$

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

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

$$A = \frac{ap}{R^2T^{5/2}} = \frac{\Omega_a p_{\mathrm{r}}}{T_{\mathrm{r}}^{5/2}} \qquad B = \frac{bp}{RT} = \frac{\Omega_b p_{\mathrm{r}}}{T_{\mathrm{r}}}$$

## Pseudokritični parametri

**Kay**

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

**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!

$$T = f(T)$$

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

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

Prva aproksimacija – idealni plin

Zadatak:

KISIK(1) – ETEN(2)

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

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

$y_1 = 0,75$

Pseudokritični parametri

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

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

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

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

Parametri *a* i *b* za smjesu

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

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

Iteracija po temperaturi

$$T^{(i+1)} = \frac{v - b_{\mathrm{M}}}{R}\left[p + \frac{a_{\mathrm{M}}}{\sqrt{T^{(i)}}\,v\left(v + b_{\mathrm{M}}\right)}\right]$$

Idealni plin:

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

$$T^{(i+1)} = \frac{v - b_{\mathrm{M}}}{R}\left[p + \frac{a_{\mathrm{M}}}{\sqrt{T^{(i)}}\,v\left(v + b_{\mathrm{M}}\right)}\right]$$

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

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

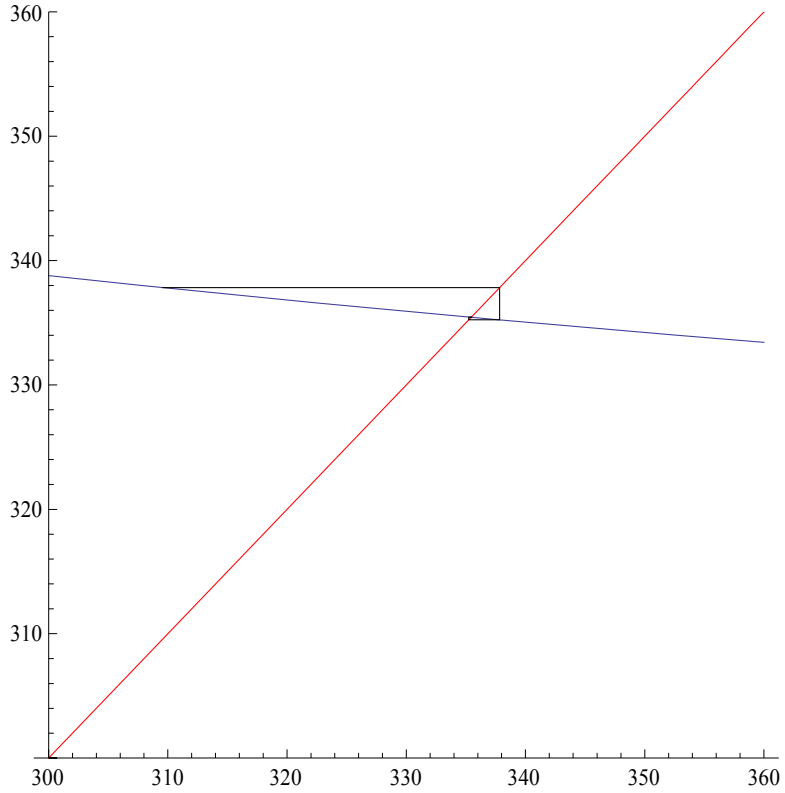
$$T_1 = 337{,}82\ \mathrm{K}$$

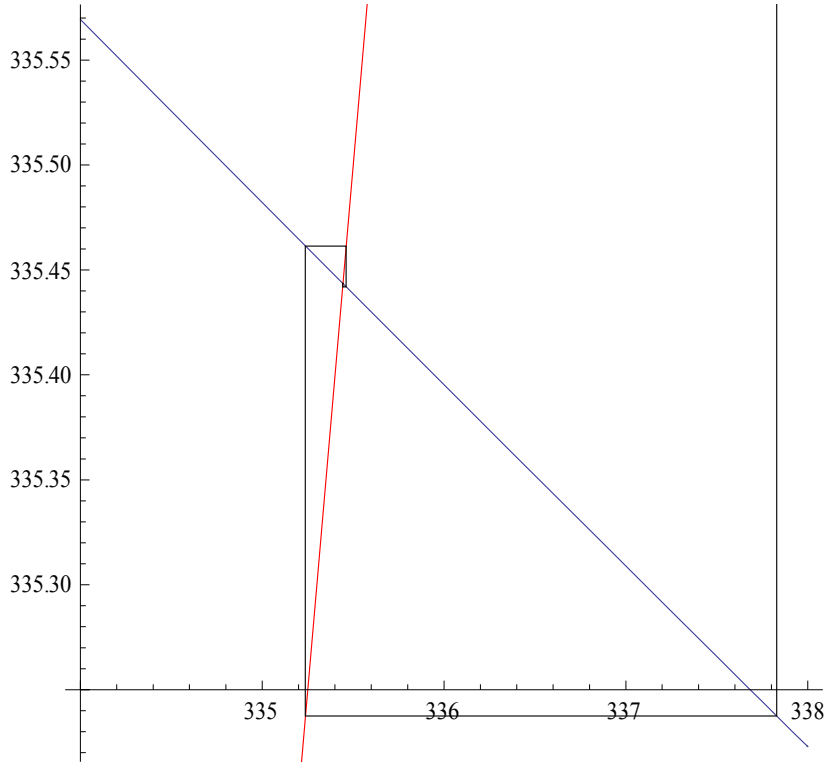
$$T_2 = 2{,}73575 \cdot 10^{-5}\left[100 \cdot 101325 + \frac{3{,}89926 \cdot 10^{7}}{\sqrt{337{,}82}}\right]$$

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

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

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


360
350
340
330
320
310
300
310
320
330
340
350
360


335.55
335.50
335.45
335.40
335.35
335.30
335
336
337
338

Iteracijska formula za SRK

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

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

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

Iteracijska formula za PR

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

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

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