

7. ZADATAK

Izračunati koeficijent fugaciteta *n*-pentana pri temperaturi od 273,2 K i tlaku od 1 atm. Pretpostaviti da se pentan pri tim uvjetima vlada prema Soave-Redlich-Kwongovom modelu.

Faktor kompresibilnosti izračunati Newton-Gossetovim postupkom, u skladu sa Soave-Redlich-Kwongovom jednažbom, iskazanom u polinomnom obliku, $z=f(z)$.

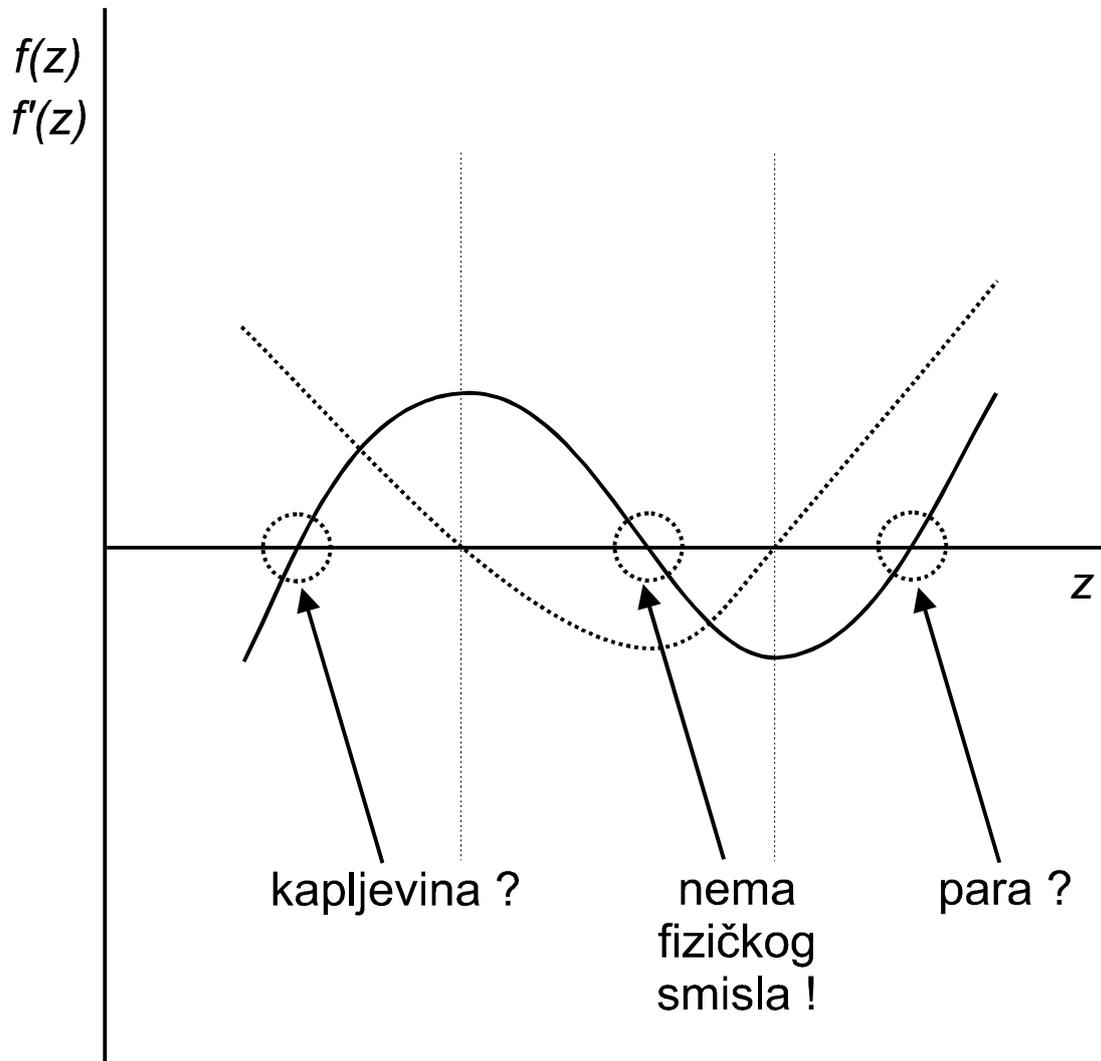
Podaci:

$$T_K=469,7 \text{ K}; \quad p_K=33,7 \text{ bara}; \quad \omega=0,251$$

GOSSET NEWTON METODA (1986)

Jednadžbe stanja trećeg stupnja po z
(Soave Redlich Kwong)

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



Zadatak:

$$p = 1 \text{ atm} = 101325 \text{ Pa}$$

$$T = 273,2 \text{ K}$$

Jednadžba stanja trećeg stupnja

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

Parametri:

$$a = \frac{\Omega_a R^2 T_K^2}{p_K} = \frac{0,427480 \cdot 8,314^2 \cdot 469,7^2}{33,7 \cdot 100000} = 1,9344$$

$$b = \frac{\Omega_b R T_K}{p_K} = \frac{0,086640 \cdot 8,314 \cdot 469,7}{33,7 \cdot 100000} = 1,004 \cdot 10^{-4}$$

$$T_r = T/T_K = 273,2/469,7 = 0,581861$$

$$\begin{aligned} \kappa &= 0,48508 + 1,55171\omega - 0,1561\omega^2 = \\ &= 0,48508 + 1,55171 \cdot 0,251 - 0,1561 \cdot 0,251^2 = \\ &= 0,8647 \end{aligned}$$

$$\begin{aligned} \alpha &= \left[1 + \kappa \left(1 - \sqrt{T_r} \right) \right]^2 = \\ &= \left[1 + 0,8647 \left(1 - \sqrt{0,581861} \right) \right]^2 = 1,4526 \end{aligned}$$

$$A = \frac{a\alpha p}{R^2 T^2} = \frac{1,9344 \cdot 1,4526 \cdot 101325}{8,314^2 \cdot 273,2^2} = 0,0552$$

$$B = \frac{bp}{RT} = \frac{1,004 \cdot 10^{-4} \cdot 101325}{8,314 \cdot 273,2} = 4,4788 \cdot 10^{-3}$$

Proračun parne faze:

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

$$f'(z) = 3z^2 - 2z + (A - B^2 - B)$$

$$f(z) = 0$$

$$z^{(i+1)} = z^{(i)} - \frac{f(z^{(i)})}{f'(z^{(i)})}$$

Prva aproksimacija – idealni plin:

$$z^{(0)} = \frac{pv}{RT} = 1$$

$$f(z^{(0)}) = 1^3 - 1^2 + (0,0552 - (4,4788 \cdot 10^{-3})^2 - 4,4788 \cdot 10^{-3})1 - 0,0552 \cdot 4,4788 \cdot 10^{-3} = 0,0504$$

$$f'(z^{(0)}) = 3 \cdot 1^2 - 2 \cdot 1 + (0,0552 - (4,4788 \cdot 10^{-3})^2 - 4,4788 \cdot 10^{-3}) = 1,0507$$

$$z^{(1)} = z^{(0)} - \frac{f(z^{(0)})}{f'(z^{(0)})} = 1 - \frac{0,0504}{1,0507} = 0,9520$$

$$f(z^{(1)}) = 0,9520^3 - 0,9520^2 + (0,0507)0,9520 - 2,472 \cdot 10^{-4} = 4,516 \cdot 10^{-4}$$

$$f'(z^{(1)}) = 3 \cdot 0,9520^2 - 2 \cdot 0,9520 + (0,0507) = 0,7351$$

$$z^{(2)} = z^{(1)} - \frac{f(z^{(1)})}{f'(z^{(1)})} = 0,9520 - \frac{4,516 \cdot 10^{-4}}{0,7351} = 0,9514$$

$$z^{(5)} = 0,9467$$

$$v^v = \frac{z^v RT}{p} = \frac{0,9467 \cdot 8,314 \cdot 273,2}{101325} = 2,1222 \cdot 10^{-2} \text{ m}^3 \text{ mol}^{-1}$$

$$\ln \varphi^V = \ln \frac{v^V}{v^V - b} + \frac{a\alpha(T)}{bRT} \ln \frac{v^V}{v^V + b} + (z^V - 1) - \ln z^V$$

$$\begin{aligned} \ln \varphi^V = & \ln \frac{2,1222 \cdot 10^{-2}}{2,1222 \cdot 10^{-2} - 1,004 \cdot 10^{-4}} + \\ & + \frac{1,9344 \cdot 1,4526}{1,004 \cdot 10^{-4} \cdot 8,314 \cdot 273,2} \ln \frac{2,1222 \cdot 10^{-2}}{2,1222 \cdot 10^{-2} + 1,004 \cdot 10^{-4}} + \\ & + (0,9467 - 1) - \ln 0,9467 \end{aligned}$$

$$\begin{aligned} \ln \varphi^V = & 0,00474217 + \\ & + 12,3216 \cdot (-0,00471978) + \\ & + (0,9467 - 1) - \ln 0,9467 \end{aligned}$$

$$\ln \varphi^V = -0,05194$$

$$\varphi^V = 0,949386$$

Proračun kapljevite faze:

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

$$f'(z) = 3z^2 - 2z + (A - B^2 - B)$$

$$f(z) = 0$$

$$z^{(i+1)} = z^{(i)} - \frac{f(z^{(i)})}{f'(z^{(i)})}$$

Prva aproksimacija – reducirani volumen čestica:

$$z^{(0)} = B = \frac{b}{v^{\text{id}}} = \frac{bp}{RT} = 4,4788 \cdot 10^{-3}$$

$$f(z^{(0)}) = (4,4788 \cdot 10^{-3})^3 - (4,4788 \cdot 10^{-3})^2 + (0,0507)4,4788 \cdot 10^{-3} - 2,472 \cdot 10^{-4} = -4,0095 \cdot 10^{-5}$$

$$f'(z^{(0)}) = (3 \cdot 4,4788 \cdot 10^{-3})^2 - 2 \cdot 4,4788 \cdot 10^{-3} + (0,0507) = 0,0418$$

$$z^{(1)} = z^{(0)} - \frac{f(z^{(0)})}{f'(z^{(0)})} = 4,4788 \cdot 10^{-3} - \frac{-4,0095 \cdot 10^{-5}}{0,0418} = 5,438 \cdot 10^{-3}$$

$$z^{(5)} = 5,46066 \cdot 10^{-3}$$

$$v^{\text{L}} = \frac{z^{\text{L}} RT}{p} = \frac{5,46066 \cdot 10^{-3} \cdot 8,314 \cdot 273,2}{101325} = 1,22411 \cdot 10^{-4} \text{ m}^3 \text{ mol}^{-1}$$

$$\ln \varphi^L = \ln \frac{v^L}{v^L - b} + \frac{a\alpha(T)}{bRT} \ln \frac{v^L}{v^L + b} + (z^L - 1) - \ln z^L$$

$$\begin{aligned} \ln \varphi^L &= \ln \frac{1,22411 \cdot 10^{-4}}{1,22411 \cdot 10^{-4} - 1,004 \cdot 10^{-4}} + \\ &+ \frac{1,9344 \cdot 1,4526}{1,004 \cdot 10^{-4} \cdot 8,314 \cdot 273,2} \ln \frac{1,22411 \cdot 10^{-4}}{1,22411 \cdot 10^{-4} + 1,004 \cdot 10^{-4}} + \\ &+ (5,46066 \cdot 10^{-3} - 1) - \ln 5,46066 \cdot 10^{-3} \end{aligned}$$

$$\begin{aligned} \ln \varphi^L &= 1,71584 + \\ &+ 12,3216 \cdot (-0,59894) + \\ &+ (5,46066 \cdot 10^{-3} - 1) - \ln 5,46066 \cdot 10^{-3} \end{aligned}$$

$$\ln \varphi^L = -1,44841$$

$$\varphi^L = 0,234943$$

$$\varphi^V \geq \varphi^L$$

Stabilna faza je kapljevina!!

Normalno vrelišče pentana: 36,1 °C