Kemijskoinženjerska termodinamika

Numeričke vježbe

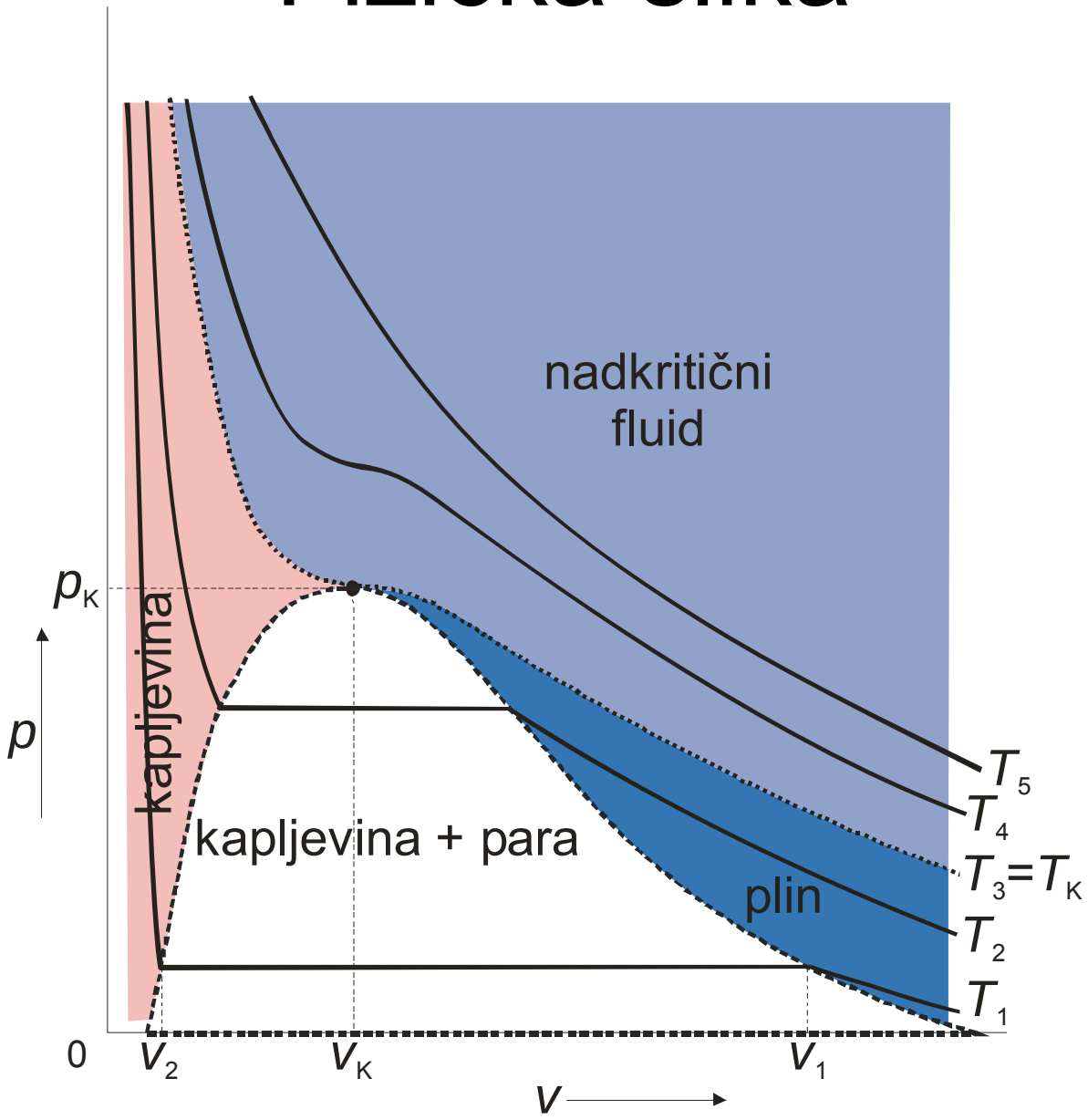
I. zadatak

Umjesto uvoda

"Thermodynamics is a funny subject. The first time you go through it, you don't understand it at all. The second time you go through it, you think you understand it, except for one or two small points. The third time you go through it, you know you don't understand it, but by that time you are so used to it, it doesn't bother you any more."

- Arnold Sommerfield

Fizička slika



Jednadžbe stanja III. stupnja

Virijalna $$v^3 - \frac{RT}{p}v^2 - \frac{B(T)RT}{p}v - \frac{C(T)RT}{p} = 0$$

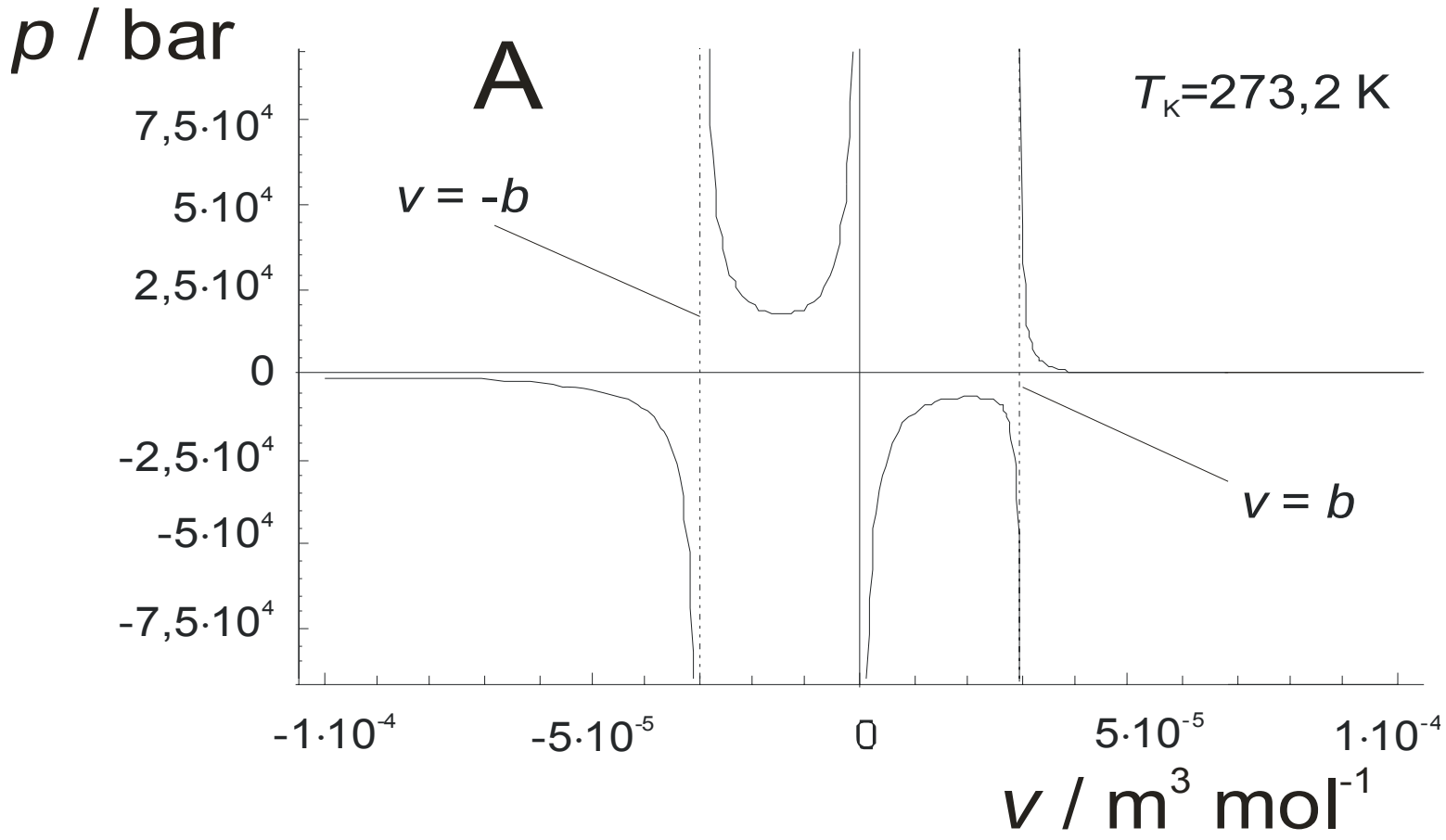
van der Waals $$v^3 - v^2\left(b + \frac{RT}{p}\right) + v\left(\frac{a}{p}\right) - \frac{ab}{p} = 0$$

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

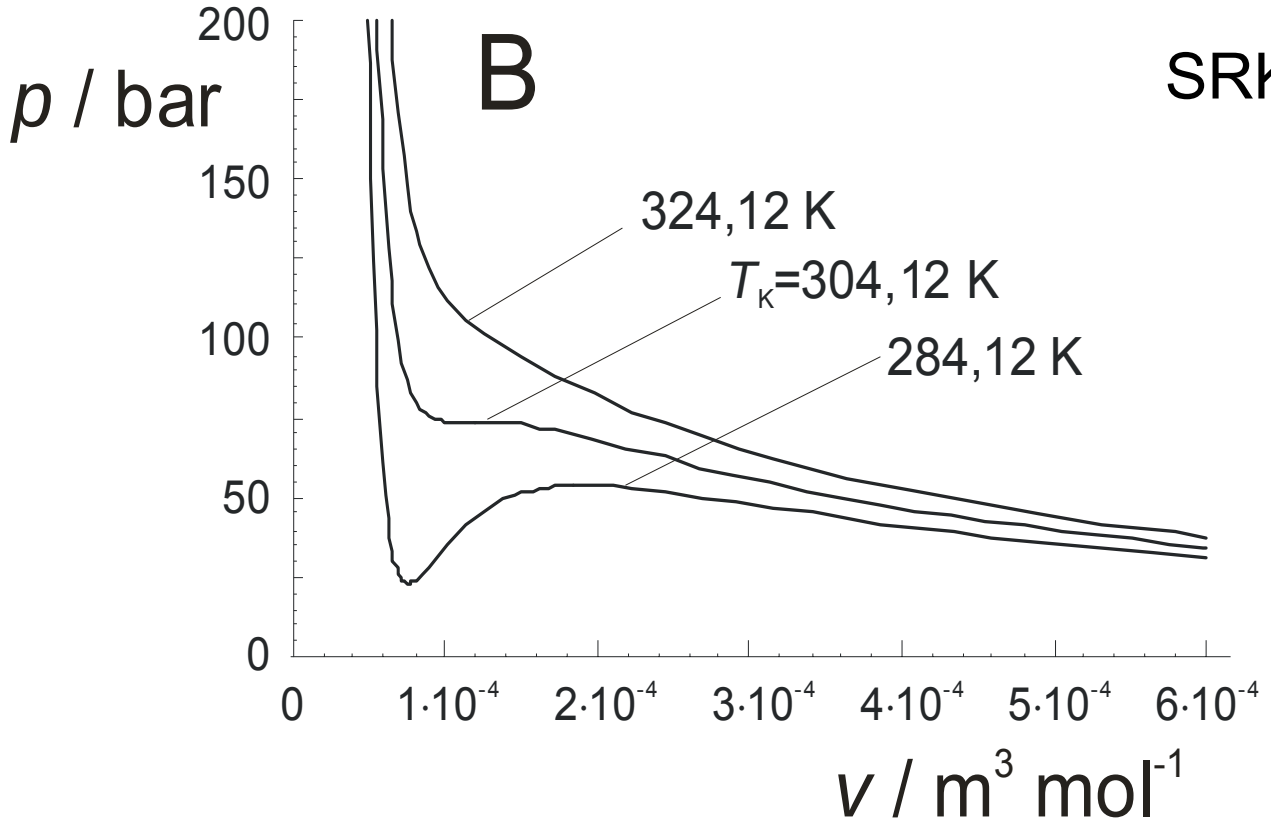
SRK $$v^3 - \frac{RT}{p}v^2 - \left(b^2 + \frac{RTb}{p} - \frac{a\alpha}{p}\right)v - \frac{a\alpha b}{p} = 0$$

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

Jednadžbe stanja III. stupnja



Jednadžbe stanja III. stupnja



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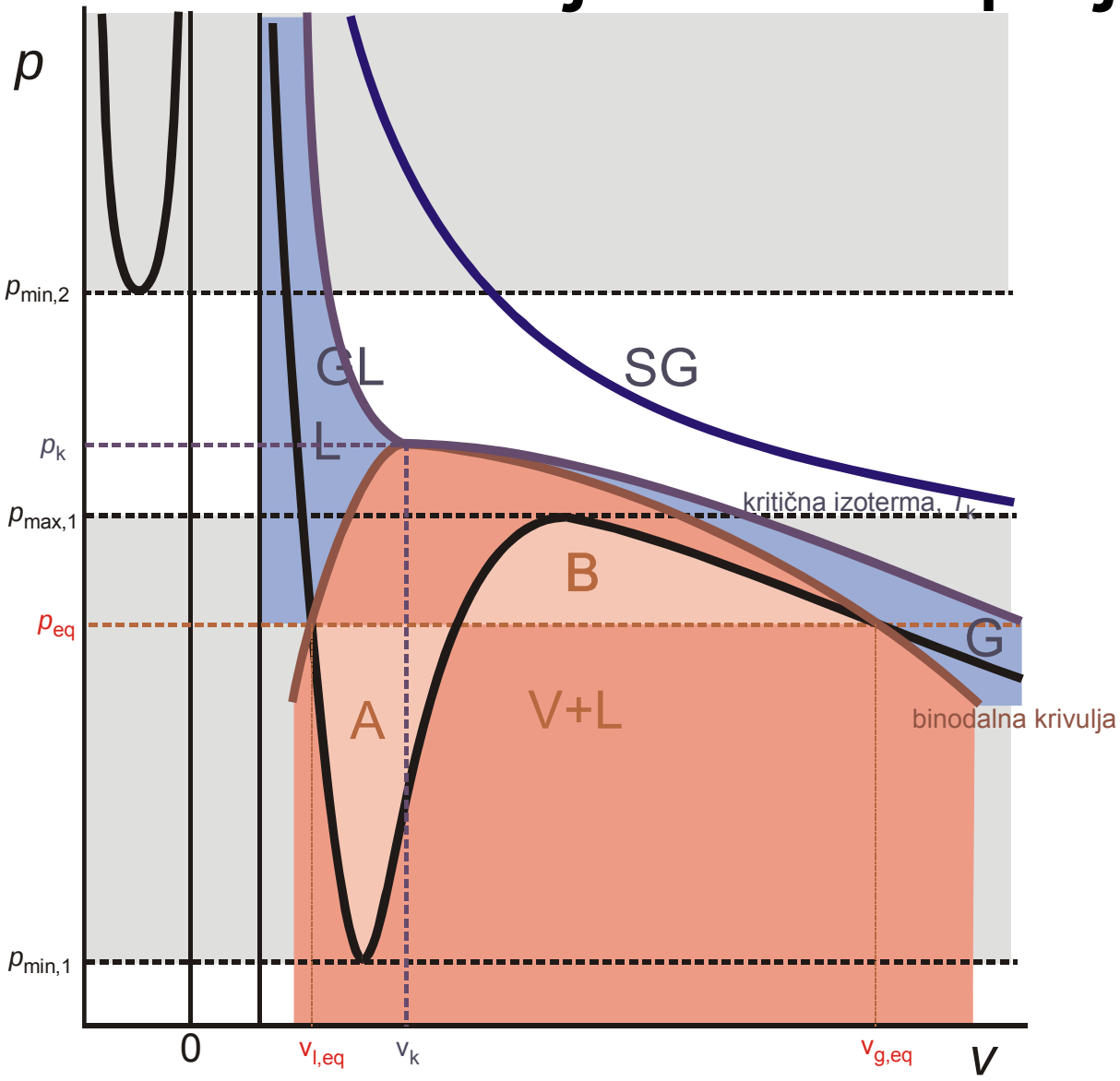

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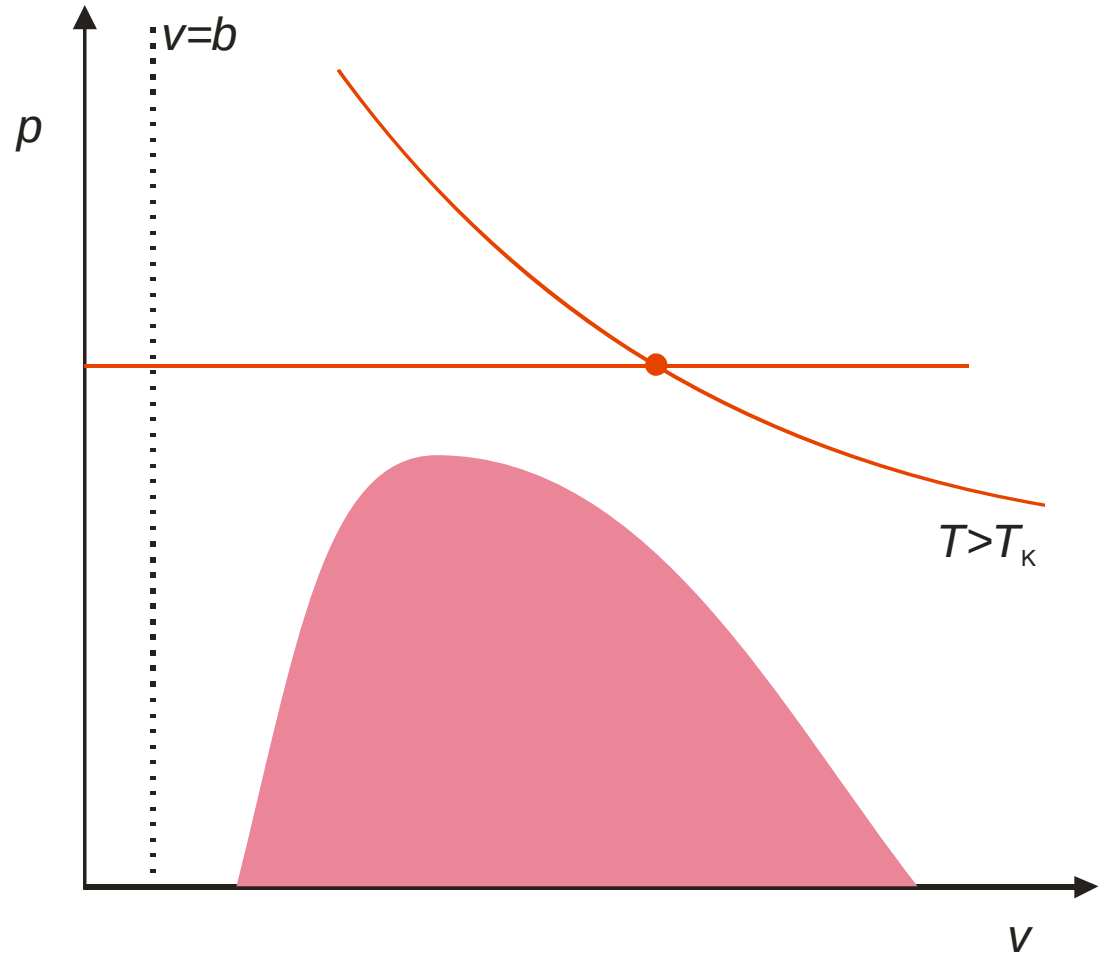

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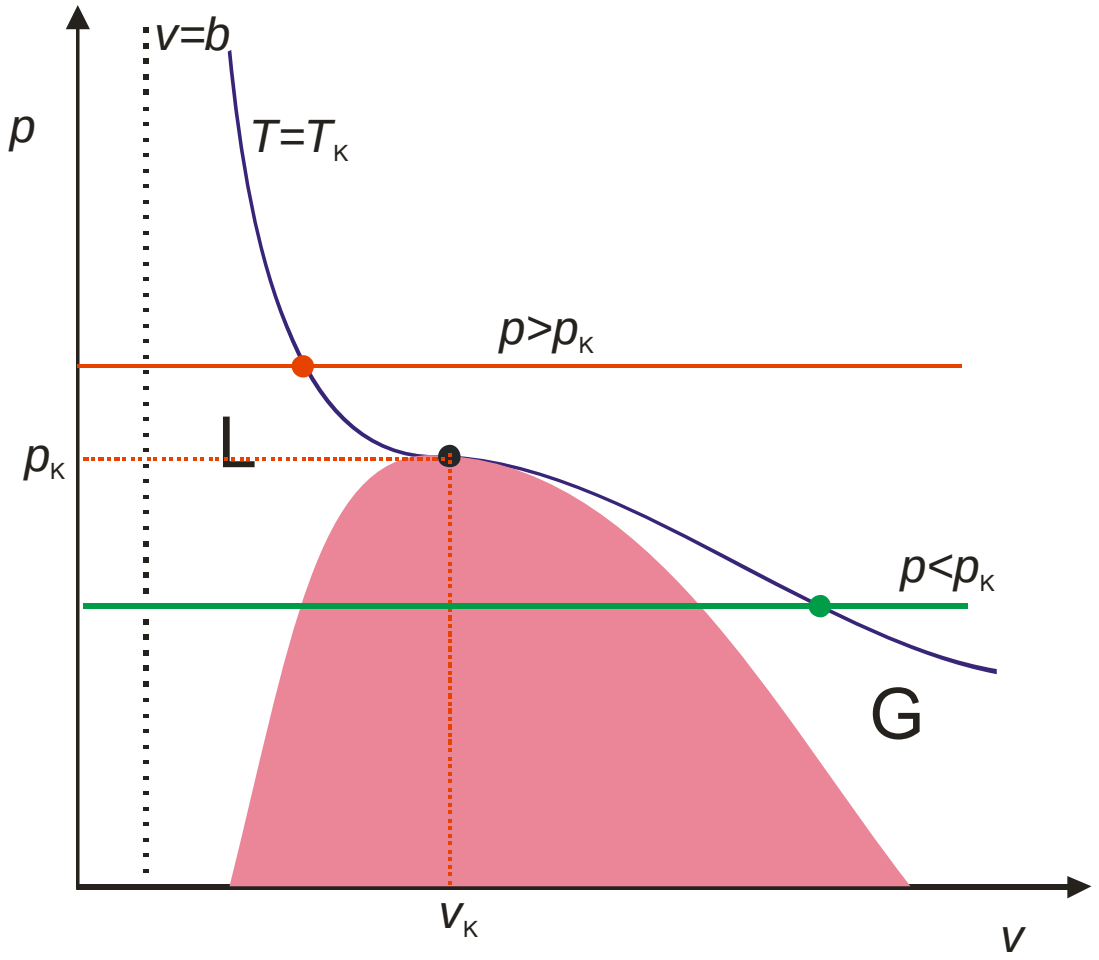
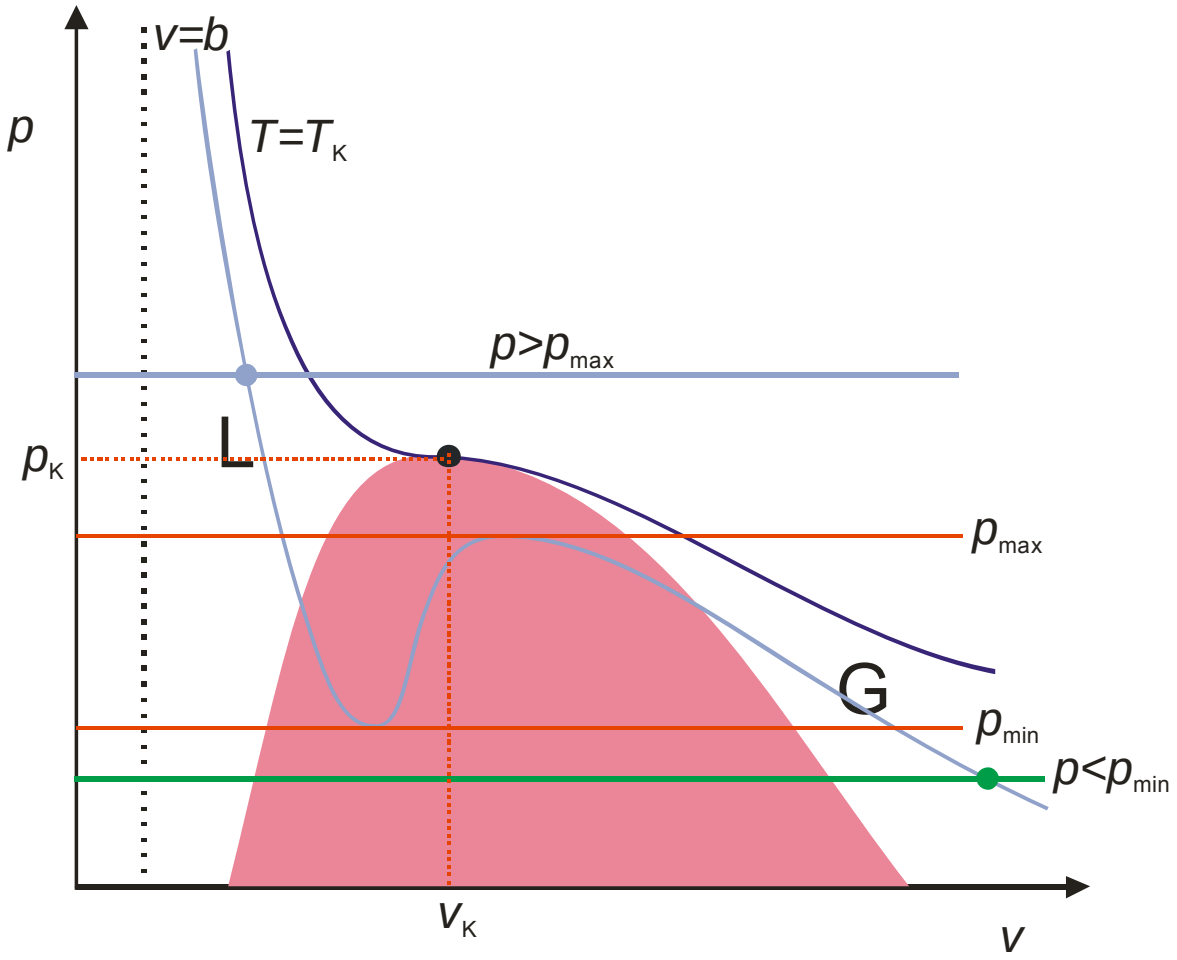
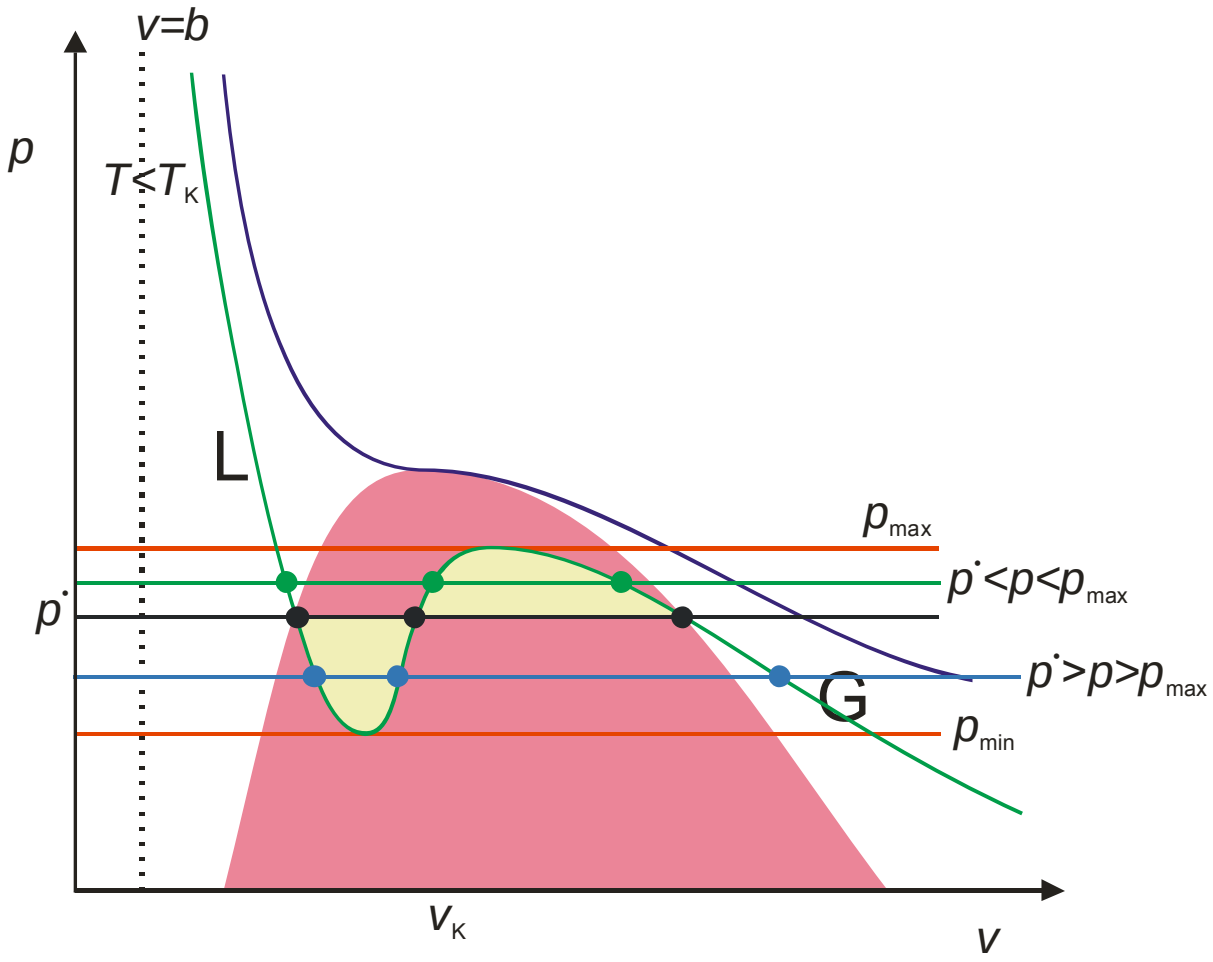


Jednadžbe stanja III. stupnja



Jednadžbe stanja III. stupnja



Jednadžbe stanja III. stupnja

$$v = \frac{zRT}{p}$$

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

SRK $$z^3 - z^2 - \left(\frac{b^2 p^2}{R^2 T^2} + \frac{bp}{RT} - \frac{a\alpha p}{R^2 T^2} \right) z - \frac{a\alpha bp^2}{R^3 T^3} = 0$$

PR $$z^3 - \left(1 - \frac{bp}{RT} \right) z^2 - \left(\frac{3b^2 p^2}{R^2 T^2} + \frac{2bp}{RT} - \frac{a\alpha p}{R^2 T^2} \right) z - \left(\frac{a\alpha bp^2}{R^3 T^3} - \frac{b^2 p^2}{R^2 T^2} - \frac{b^3 p^3}{R^3 T^3} \right) = 0$$

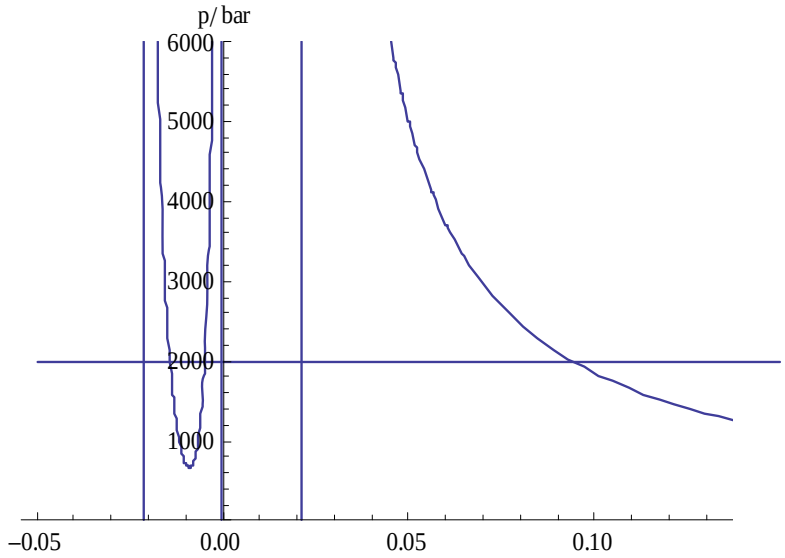
Jednadžbe stanja III. stupnja

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

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

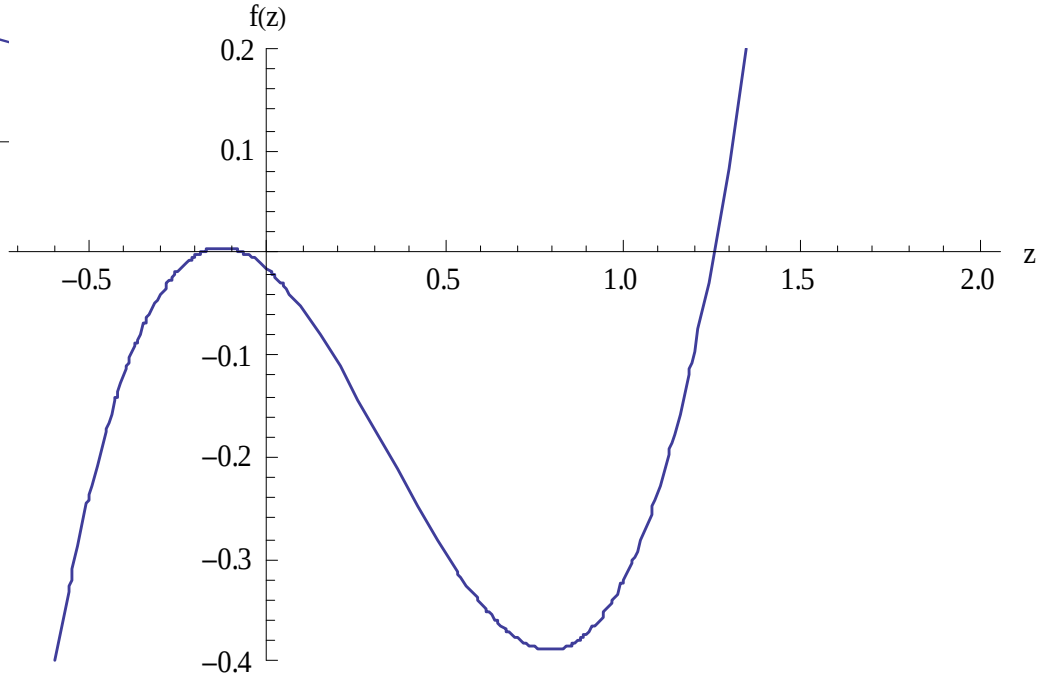
PR $$z^3 - \left(1 - B\right)z^2 + \left(A - 3B^2 - 2B\right)z - \left(AB - B^2 - B^3\right) = 0$$

Jednadžbe stanja III. stupnja



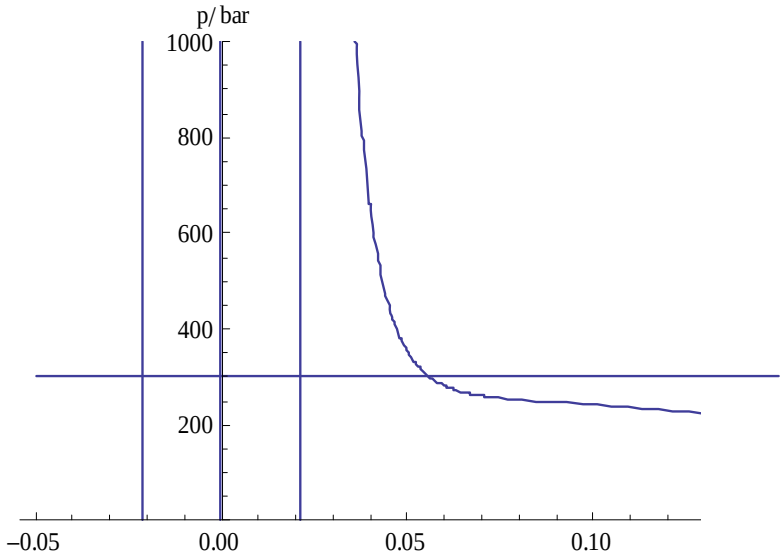
Temperature iznad kritične
Vrlo visoki tlakovi

Jednadžbe stanja III stupnja nisu pogodne za područje visokih temperatura i tlakova

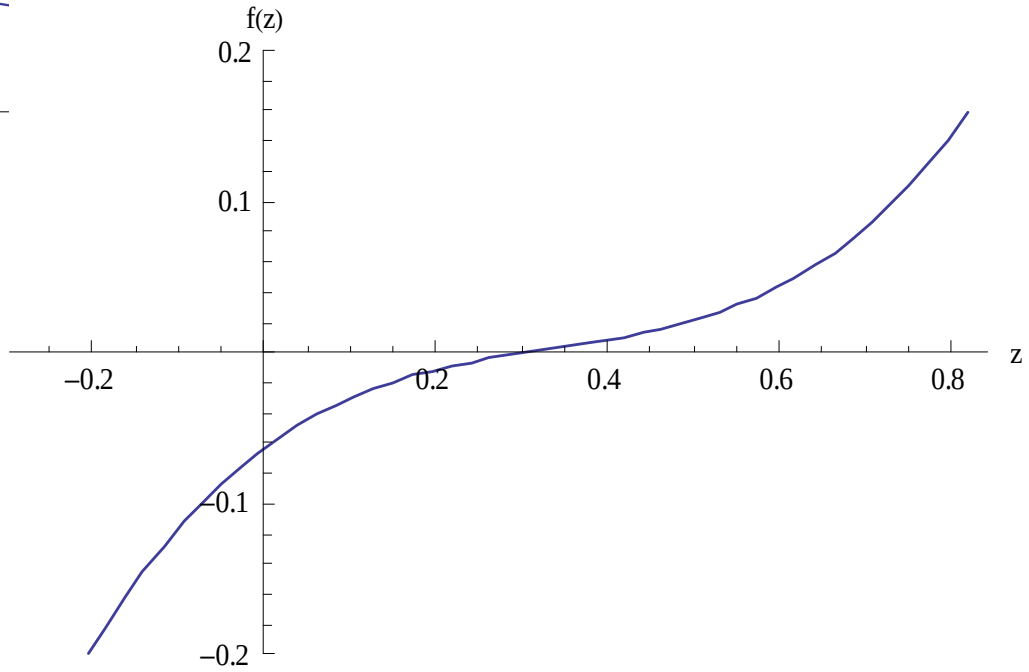


Voda, SRK

Jednadžbe stanja III. stupnja

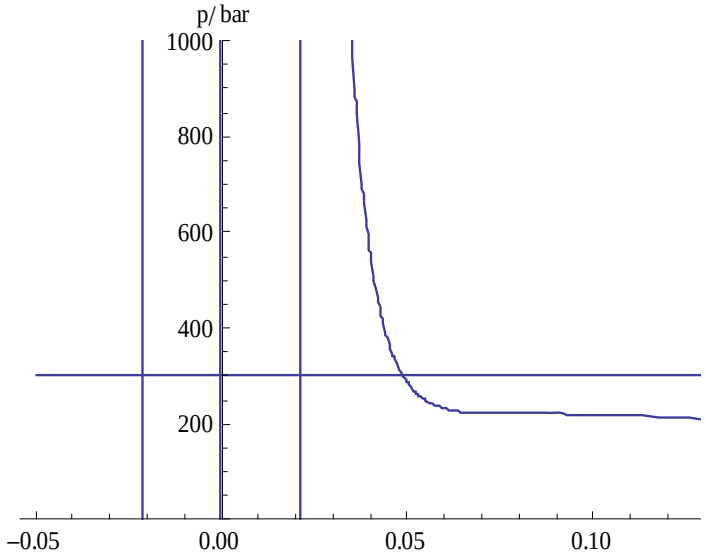


Temperature iznad kritične
Niži tlakovi

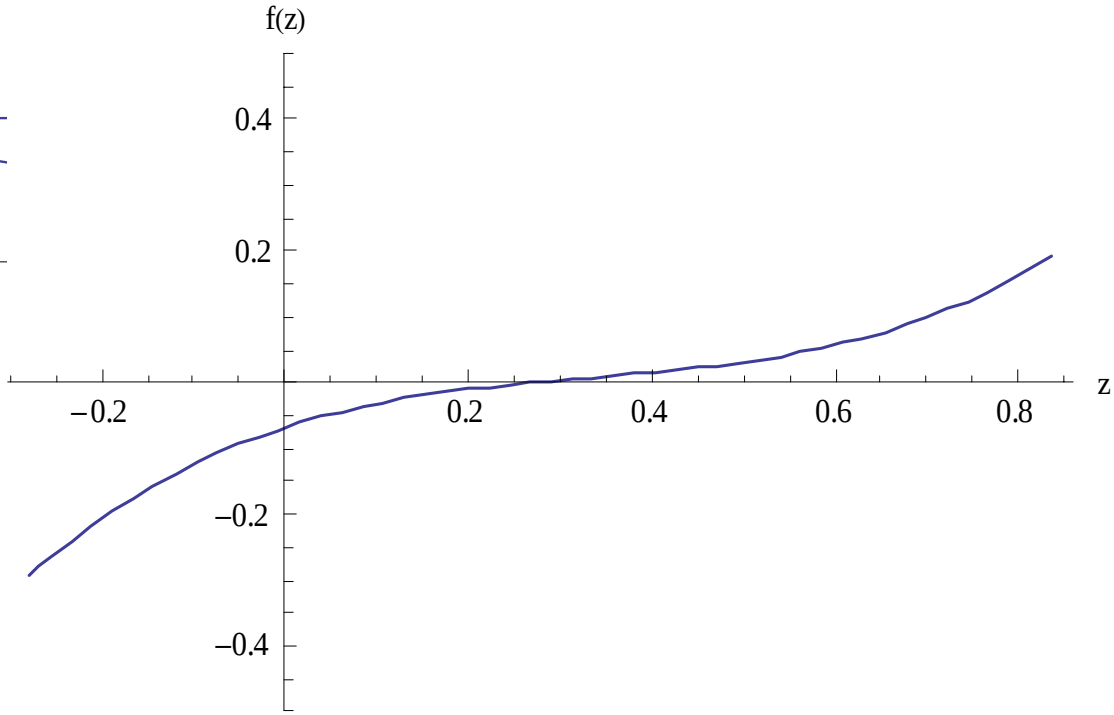


Voda, SRK

Jednadžbe stanja III. stupnja

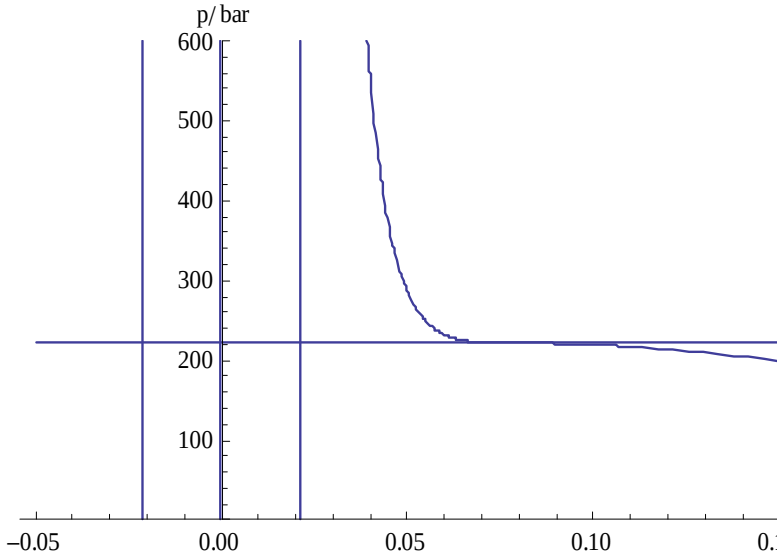


Kritična temperatura
Visoki (ali ne previsoki) tlakovi

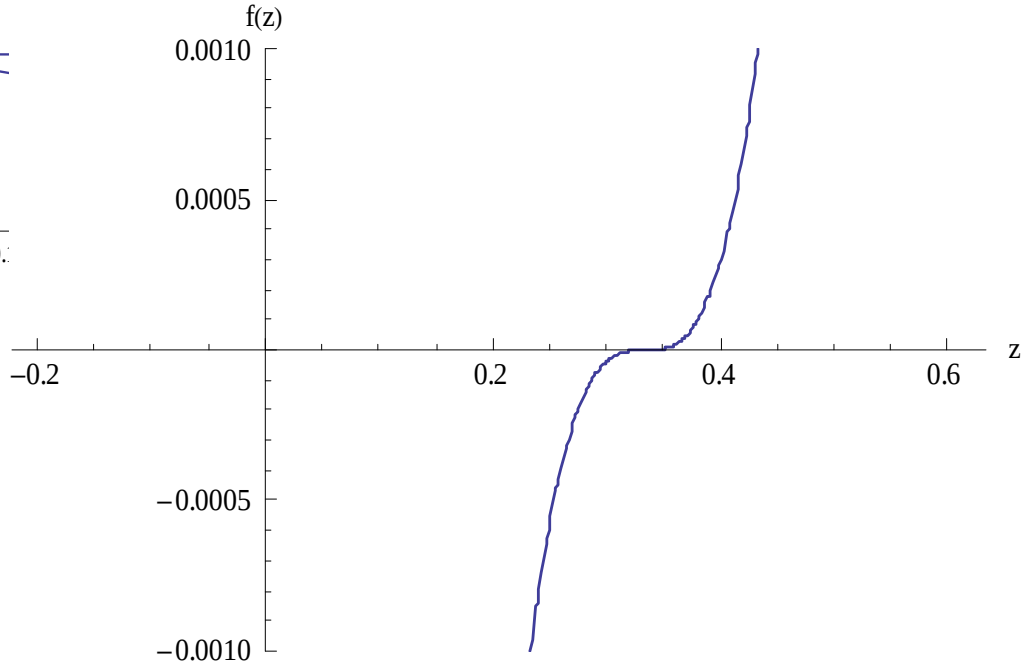


Voda, SRK

Jednadžbe stanja III. stupnja

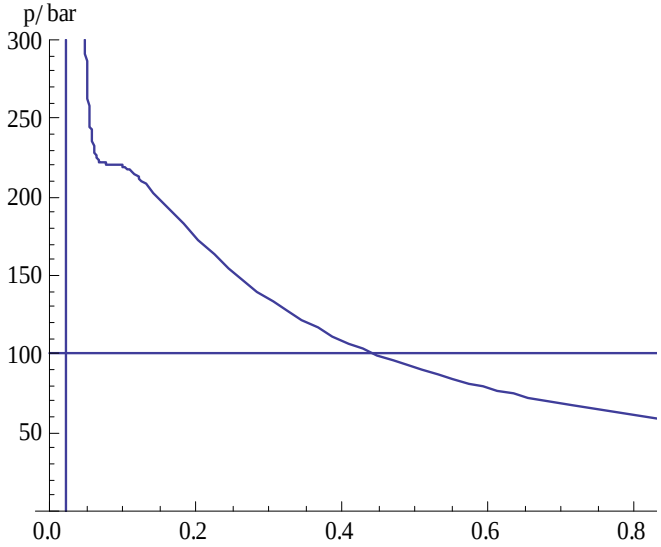


Kritična temperatura
Kritični tlak

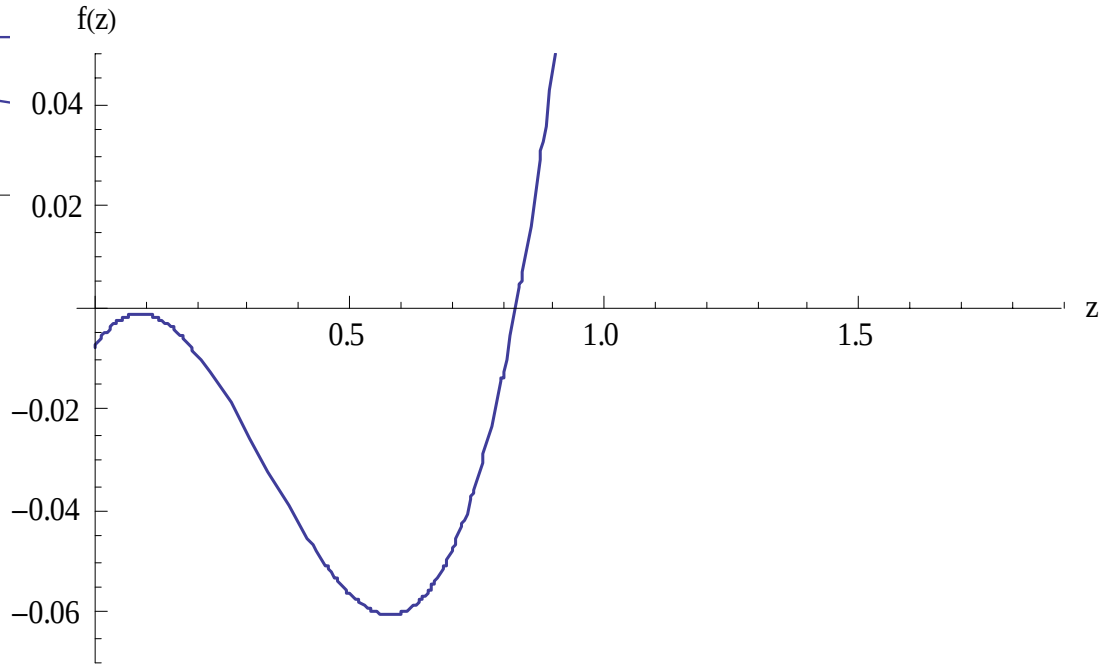


Voda, SRK

Jednadžbe stanja III. stupnja

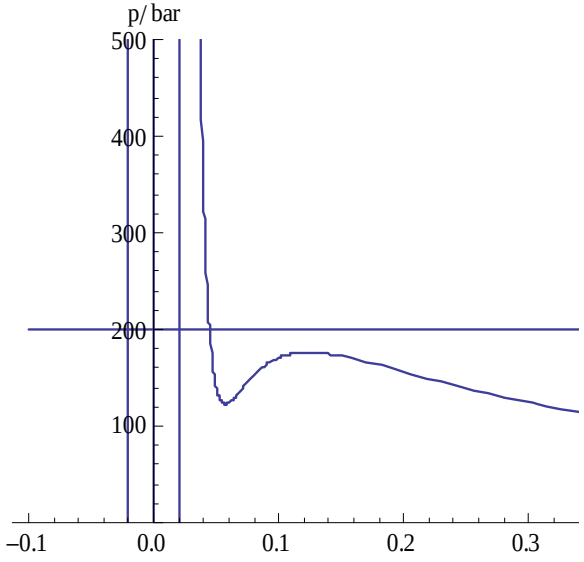


Kritična temperatura
Tlak ispod kritičnog

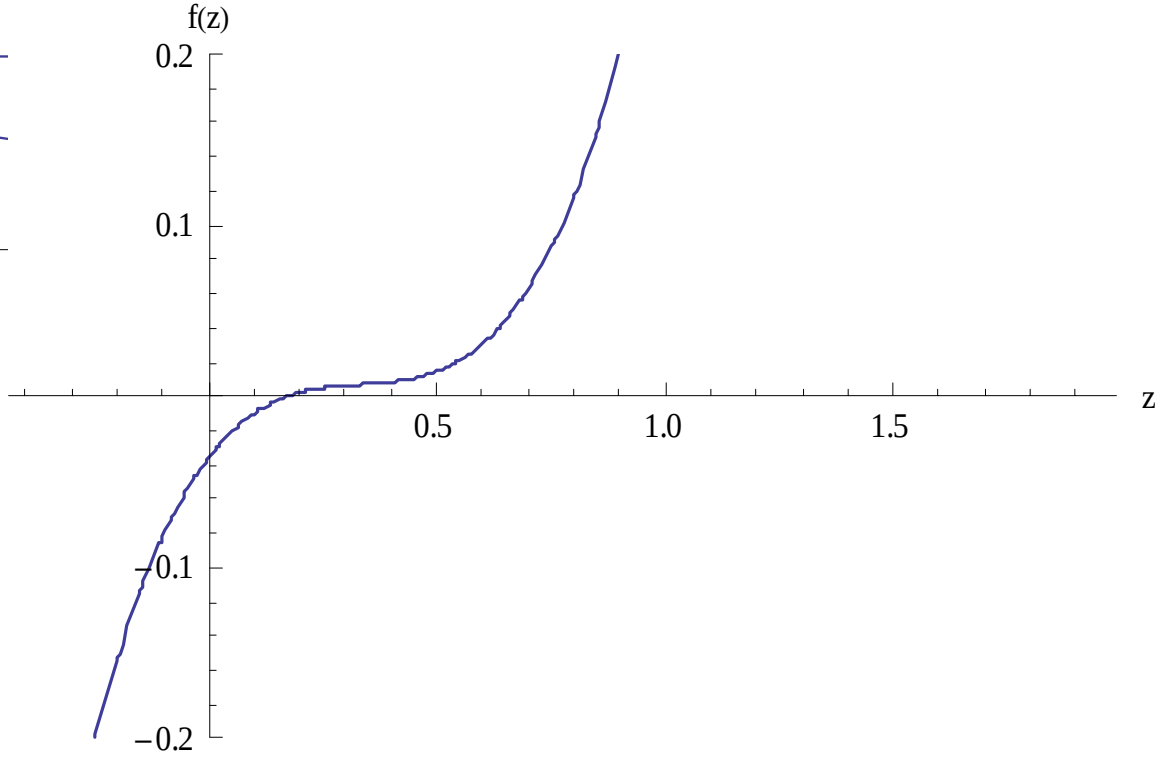


Voda, SRK

Jednadžbe stanja III. stupnja

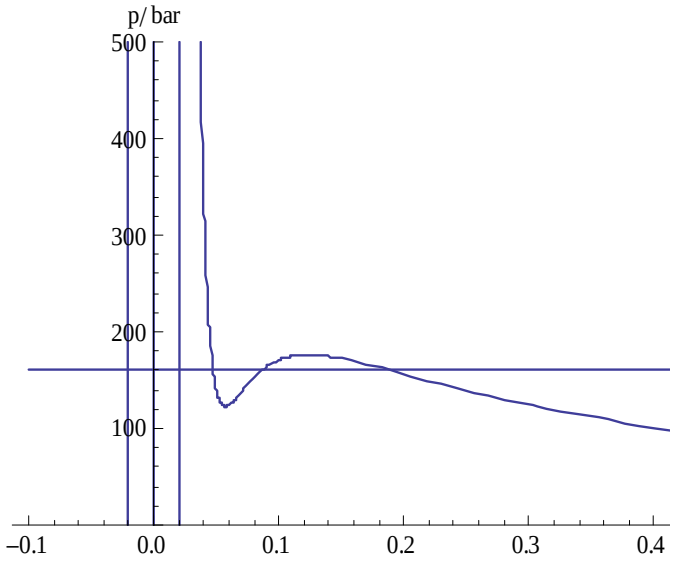


Subkritična temperatura
Tlak veći od p_{max},
Visok (ali ne previsok)

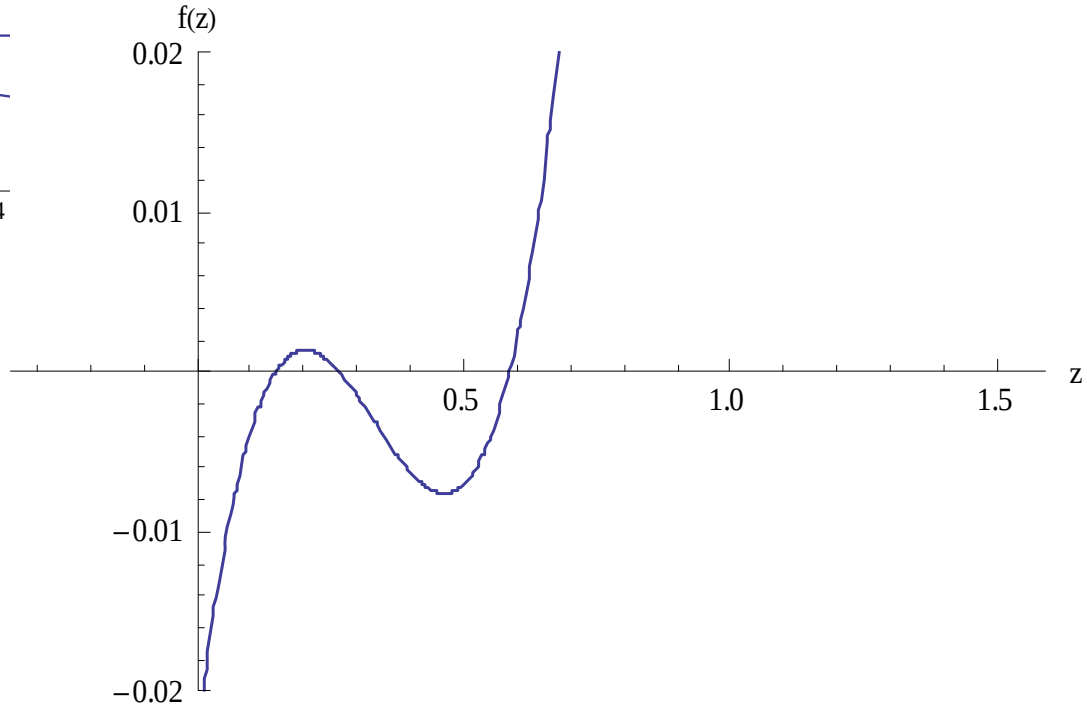


Voda, SRK

Jednadžbe stanja III. stupnja

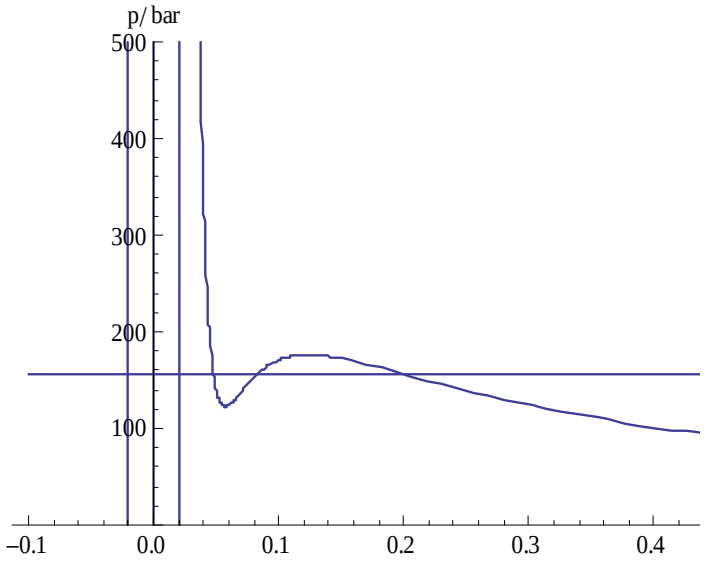


Subritična temperatura
Tlak veći od ravnotežnog
Tlak manji od p_{max}

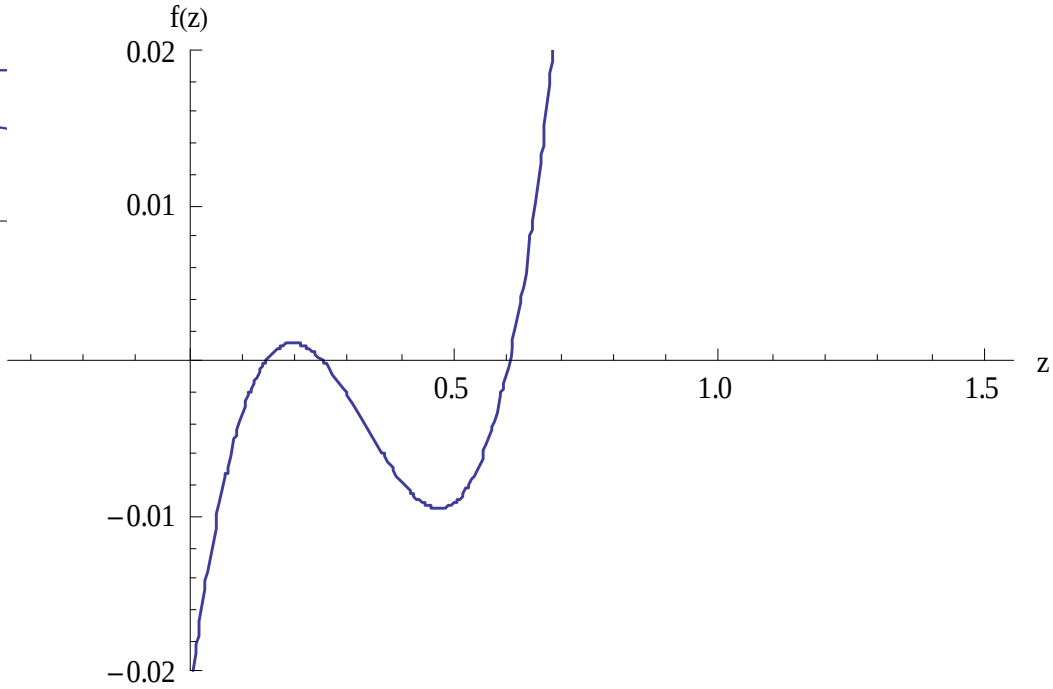


Voda, SRK

Jednadžbe stanja III. stupnja

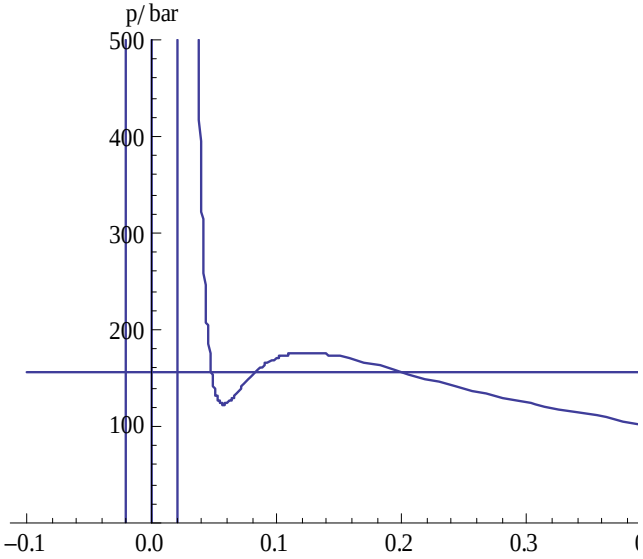


Subritična temperatura
Tlak jednak ravnotežnom



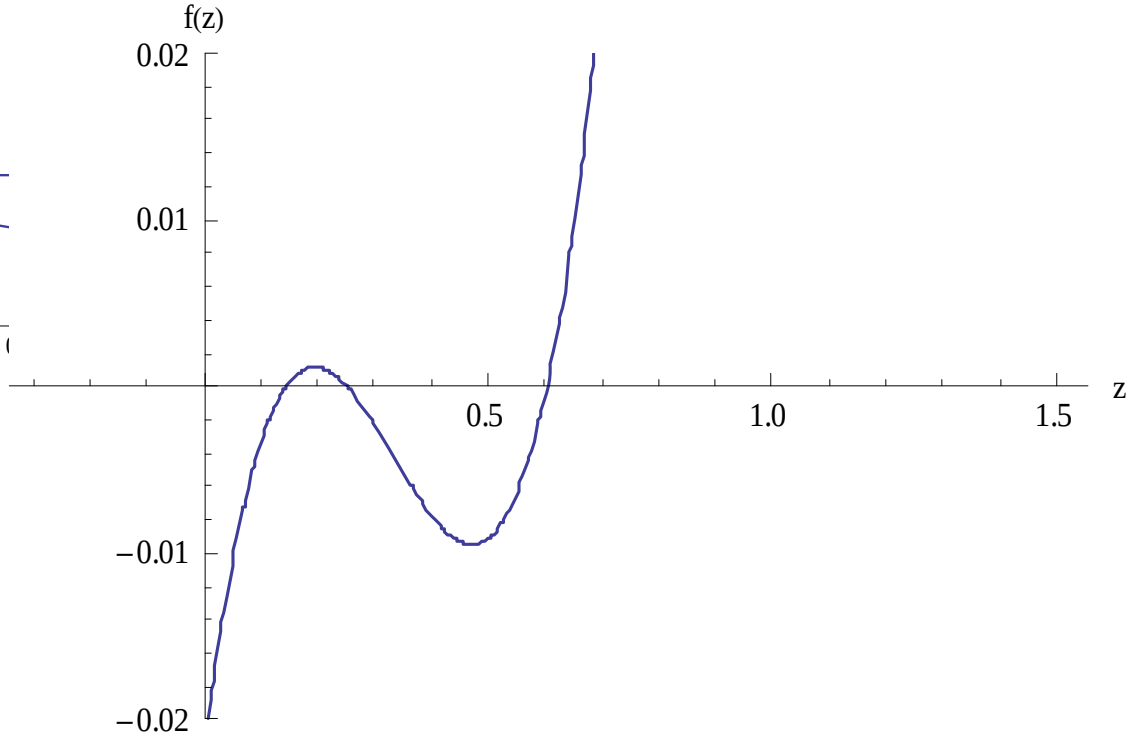
Voda, SRK

Jednadžbe stanja III. stupnja

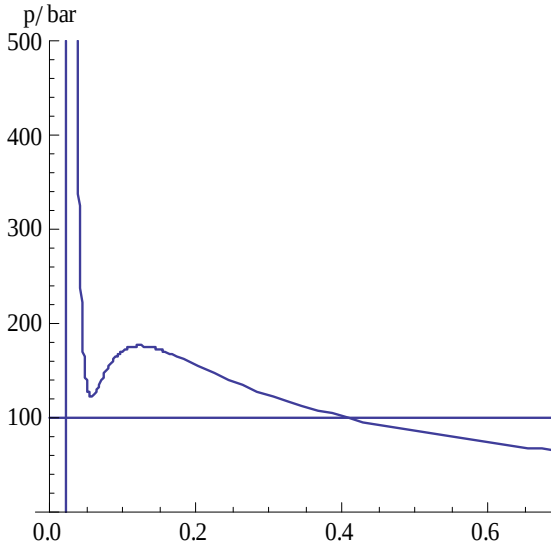


Voda, SRK

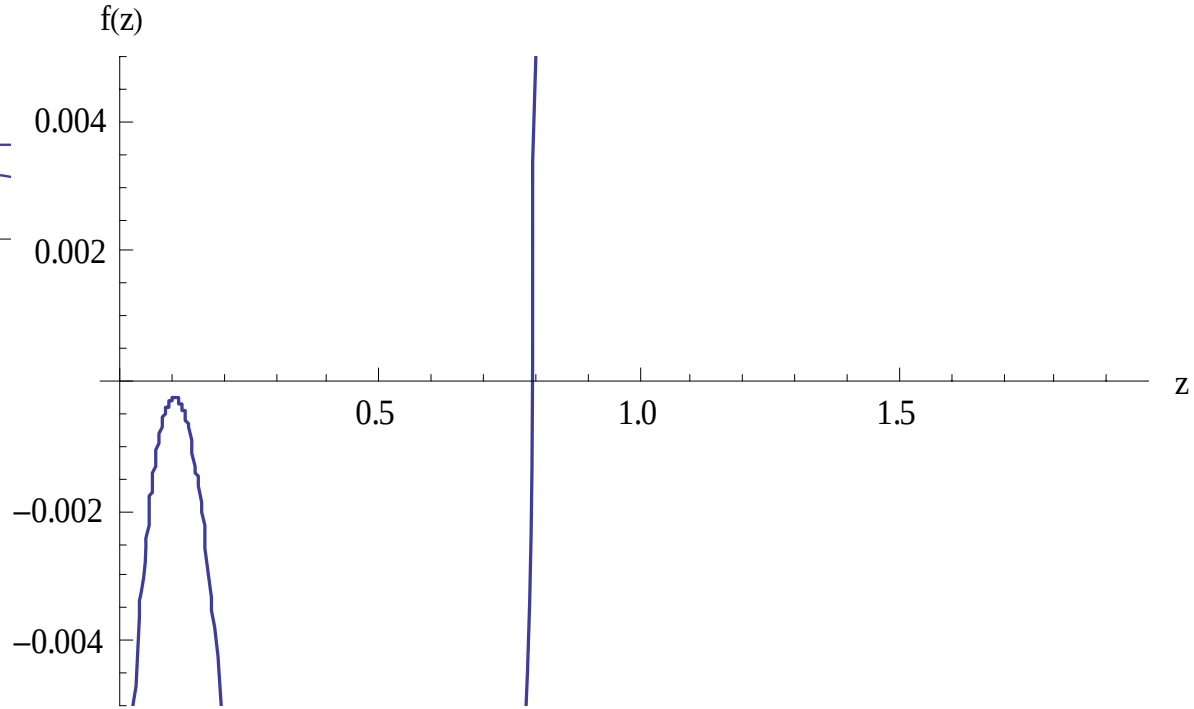
Subritična temperatura
Tlak manji od ravnotežnog
Tlak veći od p_{min}



Jednadžbe stanja III. stupnja



Subritična temperatura
Tlak manji od od p_{min}



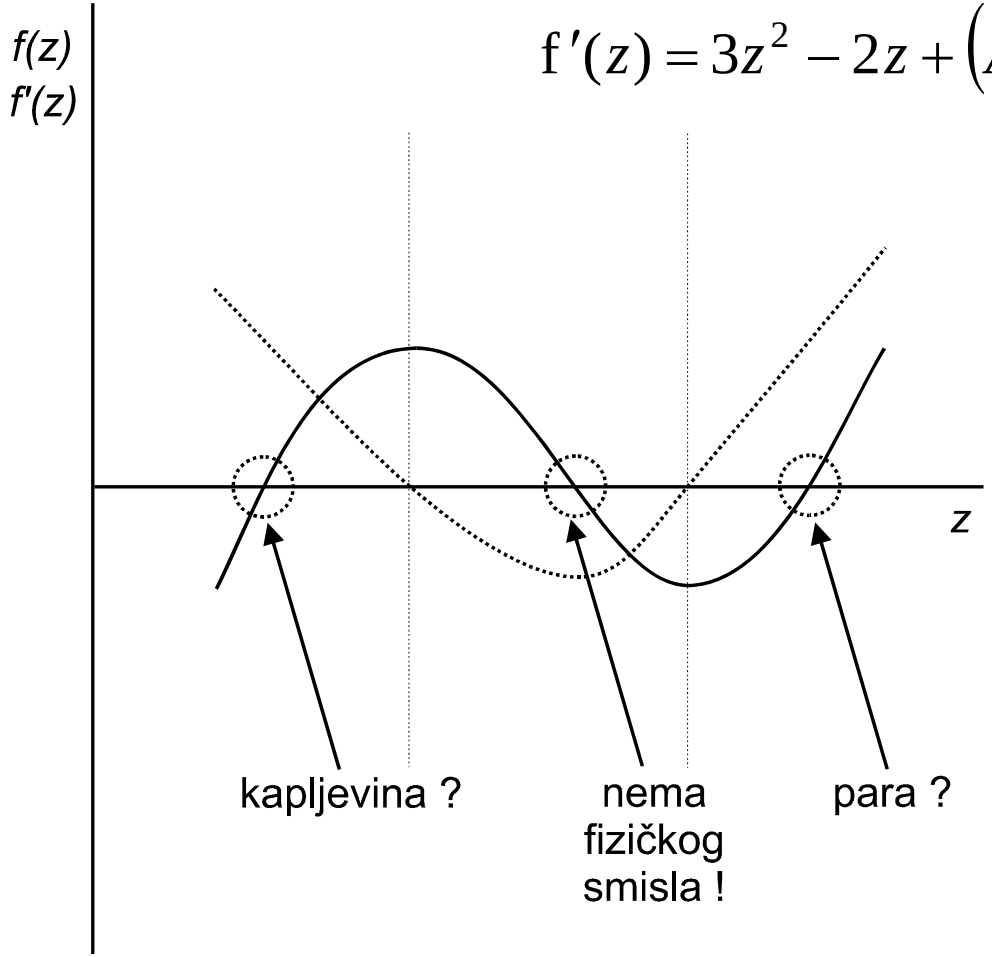
Voda, SRK

Način rješavanja

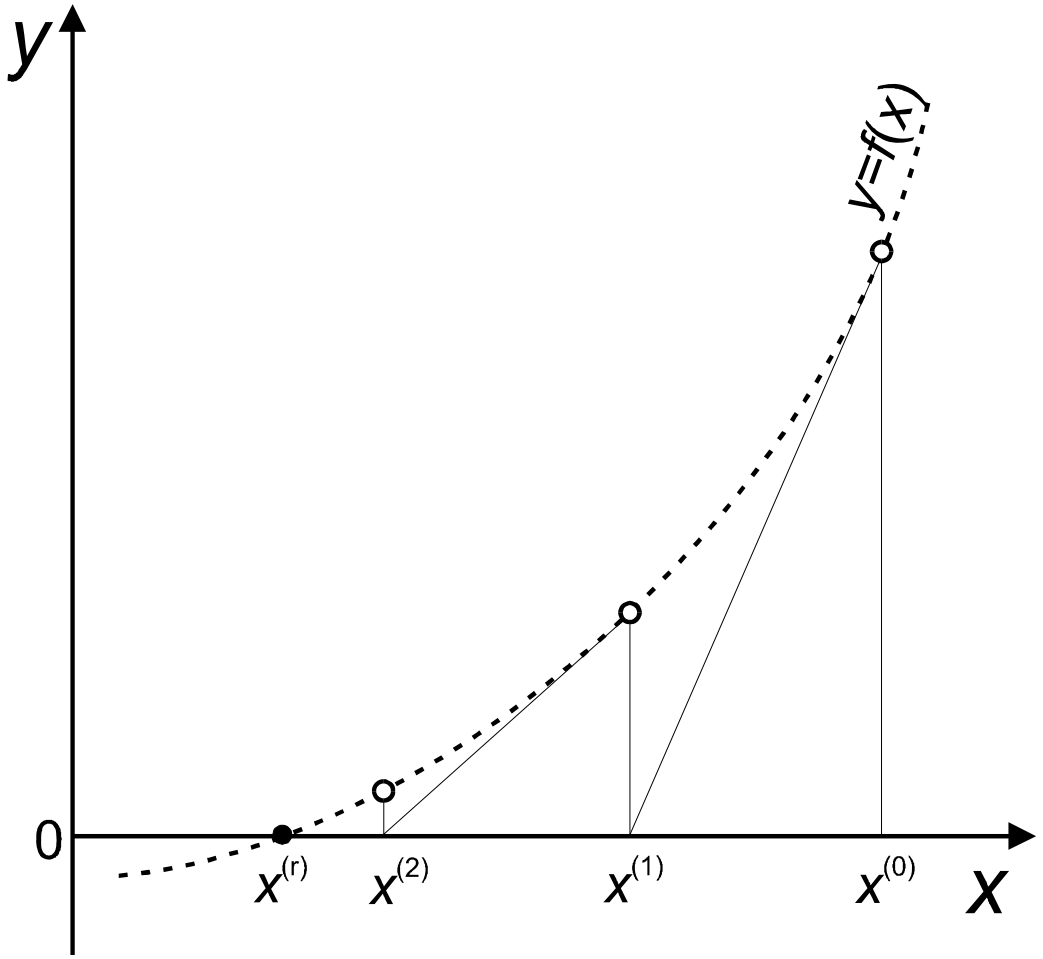
Soave Redlich Kwong

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

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



Način rješavanja



$$f(x) = 0$$

$$x^{(i+1)} = x^{(i)} - \frac{f\left(x^{(i)}\right)}{f'\left(x^{(i)}\right)}$$

Način rješavanja

Izbor početnih pretpostavki

kapljevina $z_0 = B$ $\qquad B = \frac{pb}{RT} = \frac{b}{v^{\mathrm{id}}}$

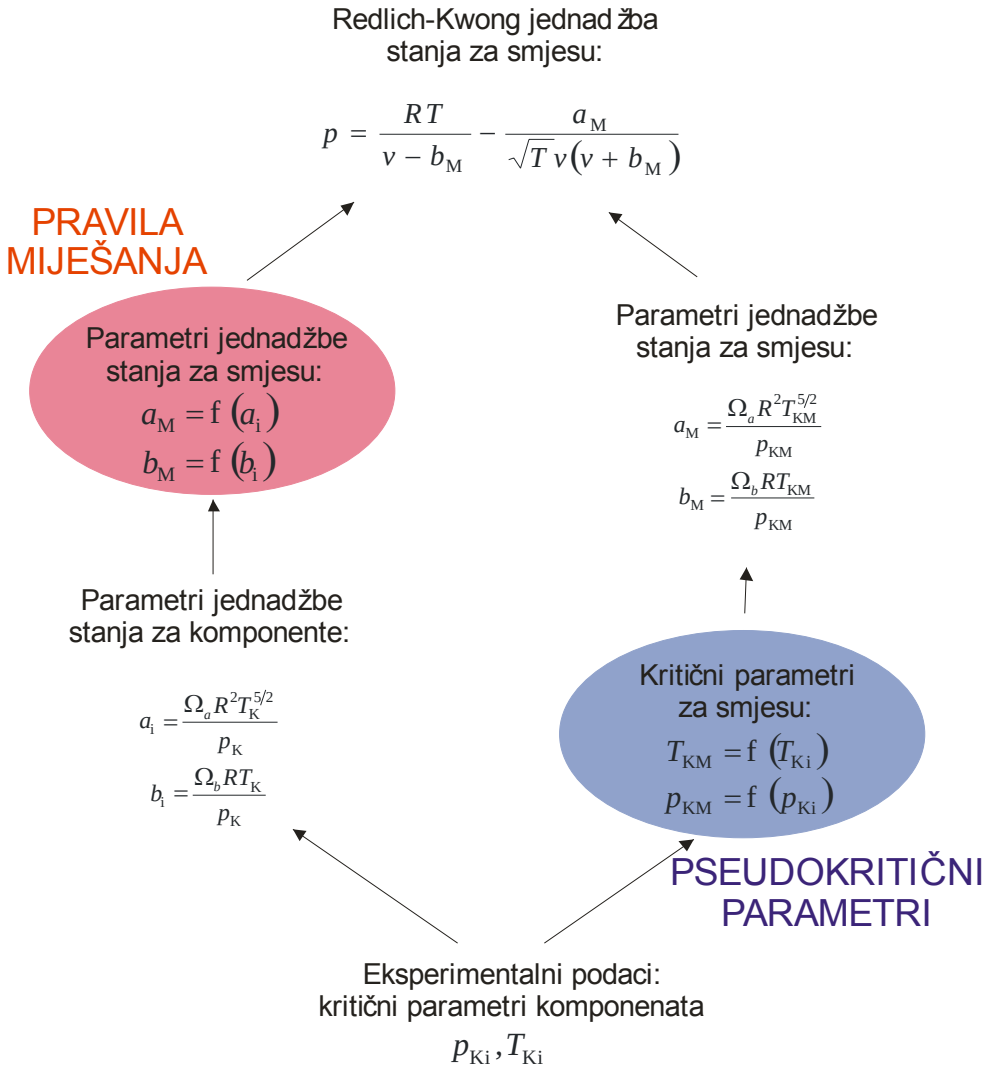
para $z_0 = 1$ $\qquad z = \frac{pv}{RT} = \frac{v}{v^{\mathrm{id}}}$

Primjer zadatka

Zadatak 1 – primjer.
Za smjesu *propan(1) – n–butan (2) – i–butan(3)* molarnih udjela $y1 = 0.4$, $y2 = 0.25$ izračunati koeficijent kompresibilnosti i molarni volumen pri sljedećim uvjetima:
a) p = _____, T = _____,
b) p = _____, T = _____,
c) p = _____, T = _____,
d) p = _____, T = _____.
Pretpostaviti da se smjesa vlada prema *Peng – Robinson* jednadžbi stanja. Kod proračuna primijeniti *pravila miješanja* .

Mijenja se:
- Komponente
- Sastav
- Jednadžba stanja (RK, SRK, PR)
- Način izračunavanja parametara smjese (pravila miješanja, pseudokritični parametri

Plinske smjese



Plinske smjese

Pseudokritični parametri

Prausnitz-Gunn (1958)

$$v_{\mathrm{KM}} = \sum y_{\mathrm{i}} v_{\mathrm{Ki}}$$

$$z_{\mathrm{KM}} = \sum y_{\mathrm{i}} z_{\mathrm{Ki}}$$

$$T_{\mathrm{KM}} = \sum y_{\mathrm{i}} T_{\mathrm{Ki}}$$

$$p_{\mathrm{KM}} = \frac{z_{\mathrm{KM}} R T_{\mathrm{KM}}}{v_{\mathrm{KM}}}$$

Plinske smjese

Pravila miješanja

RK

$$b_{\mathrm{M}} = \sum y_{\mathrm{i}} b_{\mathrm{i}}$$

$$B_{\mathrm{M}} = \sum y_{\mathrm{i}} B_{\mathrm{i}}$$

$$a_{\mathrm{M}} = \sum\sum y_{\mathrm{i}} y_{\mathrm{j}} a_{\mathrm{ij}}$$

$$a_{\mathrm{ij}} = \sqrt{a_{\mathrm{i}} a_{\mathrm{j}}}$$

$$A_{\mathrm{M}} = \sum\sum y_{\mathrm{i}} y_{\mathrm{j}} A_{\mathrm{ij}}$$

SRK, PR

$$b_{\mathrm{M}} = \sum y_{\mathrm{i}} b_{\mathrm{i}}$$

$$B_{\mathrm{M}} = \sum y_{\mathrm{i}} B_{\mathrm{i}}$$

$$(a\alpha)_{\mathrm{M}} = \sum\sum y_{\mathrm{i}} y_{\mathrm{j}} (a\alpha)_{\mathrm{ij}}$$

$$a_{\mathrm{ij}} = (1 - k_{\mathrm{ij}})\sqrt{a_{\mathrm{i}} a_{\mathrm{j}}}$$

$$A_{\mathrm{M}} = \sum\sum y_{\mathrm{i}} y_{\mathrm{j}} A_{\mathrm{ij}}$$

Umjesto zaključka

Mrežne stranice FKIT-a

- I numericki seminar - priprema.pdf
  (Uvodni seminar za prvu vježbu – Powerpoint prezentacija)
- I numericki seminar - popis zadataka.pdf
  (Tekstovi zadataka)
- I numericki seminar - jednadzbe stanja.pdf
  (Tekst s potrebnim formulama i tablicama termodinamičkih svojstava)
- TRS Upute za pisanje referata.pdf
  (Upute za pisanje referata)
- I seminarski zadatak - popis studenata 2010.pdf
  (Popisi)

Potvrditi e-mailom prijam zadatka!

Želim Vam ugodan rad!