9. ZADATAK

Izračunati fugacitet amonijaka pri temperaturi od 200 °C i tlakovima od a) 100 atm; b) 400 atm, na temelju izraza:

$$\ln f = \ln p - \frac{1}{RT}\int_0^p \alpha\, dp$$

Integral riješiti grafički na temelju mjernih podataka navedenih u tablici. Površinu odrediti primjenom trapezne jednadžbe. Ordinatu $p \to 0$ odrediti linearnom ekstrapolacijom.

Podaci:

***p*/atm**	20	60	100	150	200	250	300	400
***v*/cm^{3}mol^{-1}**	1866	570,8	310,9	176,7	107,4	74,2	59,6	47,7

Približna metoda:

(iz 6. zadatka)

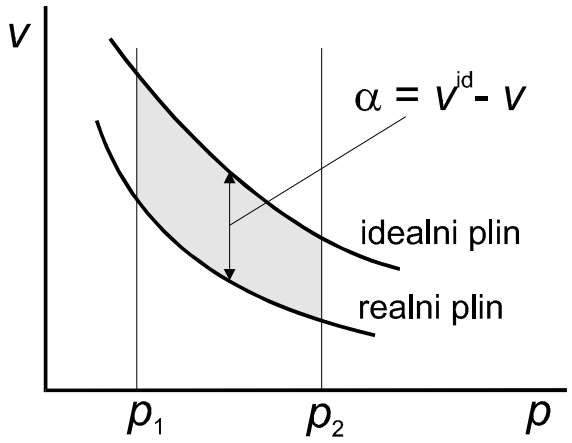
$$RTd\ln f = vdp$$

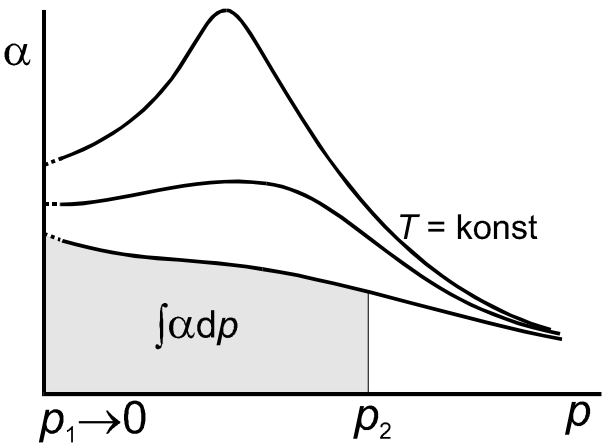
$$RT\ln\varphi = -\int_0^p \alpha dp$$

$$\ln f = \ln p - \frac{1}{RT}\int_0^p \alpha dp$$

Definicija odstupanja

$$\alpha = v^{\mathrm{id}} - v = \frac{RT}{p} - v = \frac{RT}{p}\left(1 - z\right)$$





Zadatak:

$T = 200\ °\mathrm{C}$

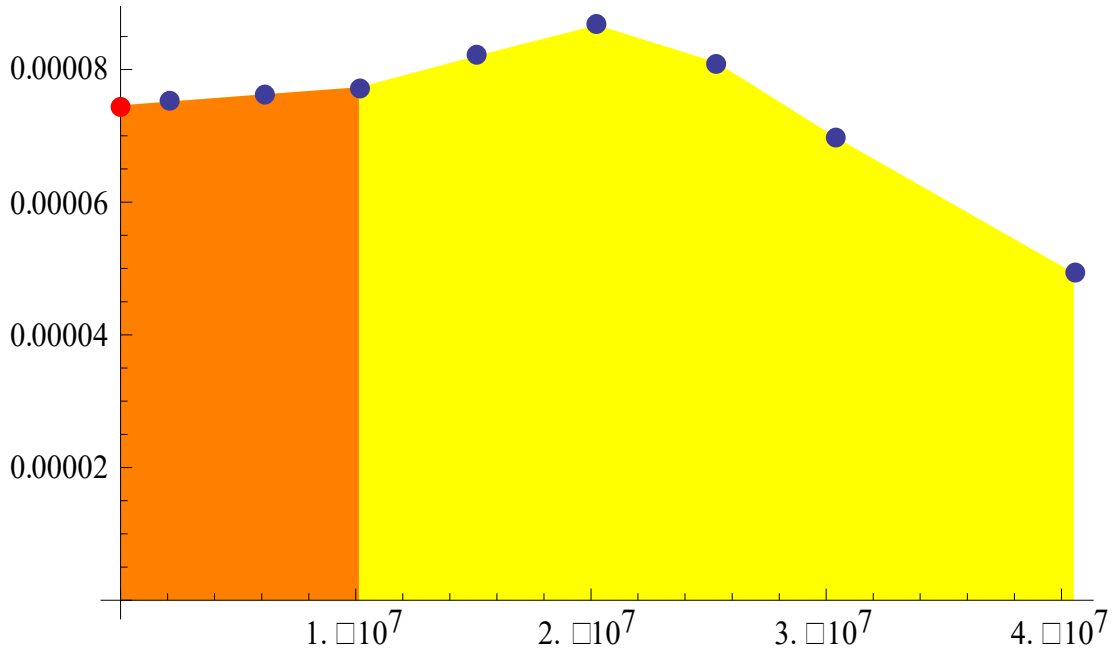
$p = 100\ \mathrm{atm}\ (400\ \mathrm{atm})$

***p*/atm**	20	60	100	150	200	250	300	400
***v*/cm^{3}mol^{-1}**	1866	570,8	310,9	176,7	107,4	74,2	59,6	47,7

$$v^{\mathrm{id}} = \frac{RT}{p} = \frac{8{,}314 \cdot (200 + 273{,}15)}{20 \cdot 101325} = 1{,}94116 \cdot 10^{-3}\,\mathrm{m^3 mol^{-1}}$$

$$\alpha = v^{\mathrm{id}} - v = 1{,}94116 \cdot 10^{-3} - 1{,}866 \cdot 10^{-3} = 7{,}51641 \cdot 10^{-5}\,\mathrm{m^3 mol^{-1}}$$

***v*$^{\mathrm{id}}$/cm^{3}mol^{-1}**	1941,16	647,055	388,233	258,822	194,116	155,293	129,411	97,0582
α/cm^{3}mol^{-1}	75,1641	76,2547	77,3328	82,1219	86,7164	81,0931	69,8109	49,3582



Linearna ekstrapolacija

$$\alpha(p=0) = 75{,}1641\cdot 10^{-6} + \frac{(76{,}2547 - 75{,}1641)\cdot 10^{-6}}{(60-20)101325}(0-20)101325$$

$$\alpha(p=0) = 7{,}46188\cdot 10^{-5}\,\mathrm{m^3 mol^{-1}}$$

Trapezna formula:

$$A = (p_{i+1} - p_i)\frac{\alpha_i + \alpha_{i+1}}{2}$$

$$A_1 = (20-0)\cdot 101325\,\frac{7{,}46188\cdot 10^{-5} + 75{,}1641\cdot 10^{-6}}{2}$$

A_1=151,768
A_2=306,85
A_3=311,245
A_4=403,919
A_5=427,689
A_6=425,083
A_7=382,259
A_8=603,741

a)

$$p = 100 \text{ atm}$$

$$\int_0^{100\text{ atm}} \alpha dp = 151,768 + 306,85 + 311,245 = 769,863$$

$$\ln f = \ln p - \frac{1}{RT}\int_0^p \alpha dp$$

$$f = \exp\left(\ln p - \frac{1}{RT}\int_0^p \alpha dp \right) =$$

$$= \exp\left(\ln\left(100 \cdot 101325\right) - \frac{769,863}{8,314 \cdot \left(200 + 273,15\right)} \right)$$

$$f = 8,33149 \text{ MPa}$$

$$\varphi = \frac{f}{p} = 0,822254$$

b)

$$p = 400 \text{ atm}$$

$$\int_0^{400\text{ atm}} \alpha dp = 3012,55$$

$$\ln f = \ln p - \frac{1}{RT}\int_0^p \alpha dp$$

$$f = \exp\left(\ln p - \frac{1}{RT}\int_0^p \alpha dp \right) =$$

$$= \exp\left(\ln\left(400 \cdot 101325\right) - \frac{3012,55}{8,314 \cdot \left(200 + 273,15\right)} \right)$$

$$f = 18,8446 \text{ MPa}$$

$$\varphi = \frac{f}{p} = 0,464953$$