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Zbirka rešenih nalog iz Fizikalne kemije I

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A) Enačbe stanja in plinski zakoni

1) Živosrebrni termometer meri temperaturo od 0 do 50 °C. Jakec ne želi v šolo ter posledično naredi še eno neumnost – s pomočjo lučke ga pregreje na 51 °C. Za koliko pri tem naraste tlak v notranjosti živosrebrnega termometra?

Iz grafa priloženega na koncu zbirke pri nizkih tlakih najprej odčitamo koeficienta α in κ za živo srebro:

$\alpha=1{,}8*10^{-4}\ K^{-1}$

$\kappa=3{,}9*10^{-6}\ bar^{-1}$

$$\left(\frac{\partial P}{\partial T}\right)_V=\frac{\alpha}{\kappa}=46\ \frac{bar}{K}$$

$$\left(\frac{\partial P}{\partial T}\right)_V\approx\left(\frac{\Delta P}{\Delta T}\right)_V$$

$$\Delta T=1K\ \Longrightarrow\ \Delta P=\left(\frac{\partial P}{\partial T}\right)_V\Delta T=46\,bar$$

2) S pomočjo van der Waalsove enačbe izračunajte volumen 0,454 kg acetilena pri tlaku 34 bar ter temperaturi 18 °C.

$b=51{,}2\ mL\ mol^{-1}$

$a=4{,}46*10^{6}\ bar\ mL^{2}\ mol^{-2}$

Acetilen ima molekulsko formulo C_2H_2 ter M=26 g/mol.

$$n=\frac{m}{M}=17{,}45\ mol$$

Volumna iz van der Waalsove enačbe ne moremo eksplicitno izraziti:

$$\left(P+a\frac{n^2}{V^2}\right)(V-bn)=nRT$$

Posledično bomo morali volumen acetilena iskati numerično kot ničlo spodnje funkcije:

$$f(V)=\left(P+a\frac{n^2}{V^2}\right)(V-bn)-nRT=0$$

Za prvi poskus bomo uporabili volumen idealnega plina pri identičnih pogojih:

$$V=\frac{nRT}{P}=12{,}4*10^3\ ml$$

Nato izdelamo sledečo tabelo:

V [mL]	f(V) [bar mL]
$12{,}4*10^3$	$0{,}707*10^5$
$11*10^3$	$0{,}35*10^5$
$10*10^3$	$0{,}11*10^5$
$9*10^3$	$-0{,}11*10^5$

f(V) spremeni predznak in posledično zavzame ničlo med 9 in 10 L. Posledično lahko volumen acetilena ocenimo na 9,5 L.

3) Izrazite koeficiente α, β in κ za 1 mol van der Waalsovega plina z vsemi količinami razen s tlakom. Pokažite, da je βP= α/κ.

Van der Waalsov plin sledi van der Waalsovi enačbi:

$$\left(P + a\frac{n^2}{V^2}\right)(V - bn) = nRT$$

$$n = 1 \implies \left(P + \frac{a}{V^2}\right)(V - b) = RT$$

$$P = \frac{RT}{V - b} - \frac{a}{V^2} \; ter \; T = \frac{1}{R}\left(P + \frac{a}{V^2}\right)(V - b)$$

Ker naloga prepoveduje izražanje s tlakom, moramo na mesto njega vedno vstaviti gornji levi izraz:

$$\beta = \frac{1}{P}\left(\frac{\partial P}{\partial T}\right)_V = \frac{1}{P} * \frac{R}{V - b} = \frac{RV^2}{RTV^2 - a(V - b)}$$

Ker volumna iz van der Waalsove enačbe ne moremo eksplicitno izraziti, se poslužimo dvojnega ulomka:

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = \frac{1}{V}\frac{1}{\left(\frac{\partial T}{\partial V}\right)_P} = \frac{1}{V} * \frac{R}{-\frac{2a}{V^3}(V - b) + \left(P + \frac{a}{V^2}\right)} = \frac{R(V - b)V^2}{RTV^3 - 2a(V - b)^2}$$

$$\kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T = -\frac{1}{V}\frac{1}{\left(\frac{\partial P}{\partial V}\right)_T} = -\frac{1}{V} * \frac{1}{-\frac{RT}{(V-b)^2} + \frac{2a}{V^3}} = \frac{V^2(V - b)^2}{-2a(V - b)^2 + RTV^3}$$

$$\beta P = \frac{\alpha}{\kappa}$$

$$\frac{RV^2}{RTV^2 - a(V - b)} * \frac{RTV^2 - a(V - b)}{(V - b)V^2} = \frac{R(V - b)V^2}{RTV^3 - 2a(V - b)^2} * \frac{-2a(V - b)^2 + RTV^3}{V^2(V - b)^2}$$

$$\frac{R}{(V - b)} = \frac{R}{(V - b)}$$

$$1 = 1$$

4) Z uporabo Hagen-Watson-Ragatzovega diagrama iz priloge izračunajte volumen 1 kg O_2 pri -88 °C ter 45,3 bar.

T_K=154,4 K

P_K=50,4 bar

Najprej moramo izračunati reducirano temperaturo in tlak:

$$T_R = \frac{T}{T_K} = \frac{185{,}15K}{154{,}4\ K} = 1{,}2$$

$$P_R = \frac{P}{P_K} = \frac{45{,}3bar}{50{,}4\ bar} = 0{,}9$$

Z uporabo Hagen-Watson-Ragatzovega diagrama iz priloge pri gornjih vrednostih reducirane temperature in tlaka odčitamo vrednost faktorja kompresibilnosti z:

$$z = 0{,}8$$

$$z = \frac{PV}{nRT} \Longrightarrow V = \frac{znRT}{P} = \frac{zmRT}{MP} = 8{,}5\ L$$

5) Za 1 mol plina, ki sledi enačbi P(V-nb)=nRT, izrazite faktor kompresibilnosti z, drugi virialni koeficient b_2 ter Boylovo temperaturo T_B.

$$n = 1 \implies P(V-b) = RT$$

$$V = \frac{RT}{P} + b$$

$$n = 1 \implies PV_i = RT$$

$$V_i = \frac{RT}{P}$$

$$z = \frac{V}{V_i} = \frac{\frac{RT}{P} + b}{\frac{RT}{P}} = 1 + \frac{Pb}{RT}$$

$$b_2 = \lim_{P\to 0}\left(\frac{\partial z}{\partial P}\right)_T = \lim_{P\to 0}\frac{b}{RT} = \frac{b}{RT}$$

$$\lim_{P\to 0}\left(\frac{\partial z}{\partial P}\right)_{T_B} = 0 \implies T_B = \infty$$

6) N_2O_4 disociira s stopnjo disociacije α=0,185. Kolikšna je povprečna molska masa nastale plinske mešanice? Na koliko pri tem naraste tlak, če je njegova začetna vrednost 1,2 bar. Kolikšna sta parcialna tlaka plinov plinske mešanice? Temperatura in volumen sta konstantna.

$$N_2O_4(g) \rightleftharpoons 2NO_2(g)$$

t=0 n_0 0 $\Sigma = n_0$

t=∞ $n_0(1-\alpha)$ $2\alpha\, n_0$ $\Sigma = n_0(1+\alpha)$

$$\bar{M} = \sum_i^k X_i\, M_i = X_1M_1 + X_2M_2$$

$$\bar{M} = \frac{n_0(1-\alpha)}{n_0(1+\alpha)}M_1 + \frac{2n_0}{n_0(1+\alpha)}M_2 = 77{,}6\; g/mol$$

$$P_\infty = \frac{n_\infty RT}{V}$$

$$P_0 = \frac{n_0 RT}{V}$$

$$\frac{P_\infty}{P_0} = \frac{n_\infty}{n_0} = \frac{n_0(1+\alpha)}{n_0} = (1+\alpha)$$

$$P_\infty = P_0(1+\alpha) = 1{,}42\; bar$$

$$P_1 = X_1P_\infty = \frac{n_0(1-\alpha)}{n_0(1+\alpha)}P_\infty = 0{,}977\; bar$$

$$P_2 = P_\infty - P_1 = 0{,}443\; bar$$

B) Prvi zakon termodinamike

1) Posodo idealnega plina z volumnom 10 L in tlakom 25 bar odpremo. Kolikšno delo opravi plin na okolico s tlakom 1 bar, če sta temperatura plina in okolice enaka?

Začnemo z definicijo volumskega dela:

$$W = -\int_{V_1}^{V_2} P_0\, dV == -\int_{V_1}^{V_2} P_2\, dV = -P_2(V_2 - V_1)$$

Ker sta temperaturi plina in okolice enaka:

$$P_1V_1 = P_2V_2 \implies V_2 = \frac{P_1V_1}{P_2}$$

$$W = -P_2\left(\frac{P_1V_1}{P_2} - V_1\right) = -P_1V_1 + P_2V_1 = (P_2 - P_1)V_1 = -24\ kJ$$

2) Izračunajte delo pri segretju 200 cm^3 vode pri tlaku 1 bar od 25 do 50 °C. Kolikšni sta prenesena toplota ter sprememba entalpije.

$\alpha=2,1*10^{-4}\ K^{-1}$

$\rho=1\ g/cm^3$

$\overline{c_P} = 75,3\ \frac{J}{mol\ K}$

Začnemo z definicijo volumskega dela:

$$W = -\int_{V_1}^{V_2} P_0\, dV$$

Ker ne poznamo začetnega in končnega volumna, integracijo s pomočjo definicije α prenesemo na začetno in končno temperaturo:

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P \implies dV = \alpha V dT$$

$$W = -\int_{T_1}^{T_2} P_0\, \alpha V dT = -P_0\alpha V(T_2 - T_1) = -0,105\ J$$

Toplota prenesena pri konstantnem tlaku je enaka spremembi entalpije:

$$Q_P = \Delta H = \int_{T_1}^{T_2} n\,\overline{c_P} dT = \frac{\rho V}{M}\overline{c_P}(T_2 - T_1) = 20,92\ kJ$$

3) Joule-Thomsonov koeficient van der Waalsovega plina je izražen kot

$$\mu_{JT} = \frac{1}{c_P}\left(\frac{2a}{RT} - b - \frac{3abP}{R^2T^2}\right)$$

Izpeljite izraz za inverzno temperaturo kot funkcijo tlaka.

$$\mu_{JT}(T_i) = 0$$

$$\frac{1}{c_P}\left(\frac{2a}{RT_i} - b - \frac{3abP}{R^2T_i^2}\right) = 0$$

$$\left(\frac{2a}{RT_i} - b - \frac{3abP}{R^2T_i^2}\right) = 0$$

$$bR^2T_i^2 - 2aRT_i + 3abP = 0$$

Dobimo kvadratno enačbo – spomnimo se njene rešitve:

$$ax^2 + bx + c = 0 \implies x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$T_i = \frac{2aR \pm \sqrt{4a^2R^2 - 12ab^2R^2P}}{2bR^2}$$

$$T_i = \frac{a}{bR}\left(1 \pm \sqrt{1 - \frac{3b^2}{a}P}\right)$$

4) Izračunajte delo pri reverzibilni a) izotermni oziroma b) adiabatni ekspanziji 2 mol idelanega plina z 10 L ter 25 °C na 20 L.

$$\overline{c_V} = \frac{5}{2}R$$

a) izotermna ekspanzija

$$W = -nRTln\frac{V_2}{V_1} = -3{,}44\ kJ$$

b) adiabatna ekspanzija

$$\overline{c_P} = \overline{c_V} + R = \frac{7}{2}R$$

$$\gamma = \frac{\overline{c_P}}{\overline{c_V}} = 1{,}4$$

$$W = n\overline{c_V}T_1\left[\left(\frac{V_2}{V_1}\right)^{\gamma-1} - 1\right] = -3\ kJ$$

5) Izpeljite enačbo, ki povezuje začetno in končno temperaturo z začetnim in končnim volumnom, pri reverzibilni adiabatni spremembi 1 mol plina, ki sledi van der Waalsovi enačbi.

$\overline{c_V} = A + BT$

Van der Waalsov plin sledi van der Waalsovi enačbi:

$$\left(P + a\frac{n^2}{V^2}\right)(V - bn) = nRT$$

$$n = 1 \implies \left(P + \frac{a}{V^2}\right)(V - b) = RT \implies P = \frac{RT}{V - b} - \frac{a}{V^2}$$

Notranja energija je funkcija volumna in temperature:

$$U = f(V,T) \Rightarrow dU = \left(\frac{\partial U}{\partial V}\right)_T dV + \left(\frac{\partial U}{\partial T}\right)_V dT$$

$$\left(\frac{\partial U}{\partial T}\right)_V = \overline{c_V} = A + BT$$

Notranji tlak enega mola van der Waalsovega plina pa je enak:

$$\left(\frac{\partial U}{\partial V}\right)_T = \frac{a}{V^2}$$

$$dU = \frac{a}{V^2}dV + (A + BT)dT$$

Po drugi strani pa velja tudi prvi zakon termodinamike:

$$dU = đQ + đW$$

Pri adiabatni spremembi torej:

$$đQ = 0 \Longrightarrow\ dU = đW = -PdV = -\frac{RT}{V - b}dV + \frac{a}{V^2}dV$$

Izenačimo spremembi notranje energije po prvem in drugem načinu:

$$dU = dU \ \Longrightarrow \frac{a}{V^2}dV + (A + BT)dT = -\frac{RT}{V - b}dV + \frac{a}{V^2}dV$$

$$(A + BT)dT = -\frac{RT}{V - b}dV$$

Ločimo spremenljivki in integriramo:

$$\int_{T_1}^{T_2}\left(\frac{A}{T} + B\right)dT = \int_{V_1}^{V_2} -\frac{R}{V - b}dV$$

$$Aln\frac{T_2}{T_1} + B(T_2 - T_1) = -Rln\frac{V_2 - b}{V_1 - b}$$

6) Izrazite razliko med specifično toploto pri stalnem tlaku ter specifično toploto pri stalnem volumnu za 1 mol van der Waalsovega plina z vsemi količinami razen s tlakom.

Van der Waalsov plin sledi van der Waalsovi enačbi:

$$\left(P + a\frac{n^2}{V^2}\right)(V - bn) = nRT$$

$$n = 1 \implies \left(P + \frac{a}{V^2}\right)(V - b) = RT$$

$$P = \frac{RT}{V - b} - \frac{a}{V^2} \; ter \; T = \frac{1}{R}\left(P + \frac{a}{V^2}\right)(V - b)$$

$$c_P - c_V = \left[P + \left(\frac{\partial U}{\partial V}\right)_T\right]\left(\frac{\partial V}{\partial T}\right)_P$$

Ker volumna iz van der Waalsove enačbe ne moremo eksplicitno izraziti, se poslužimo dvojnega ulomka:

$$c_P - c_V = \left[P + \left(\frac{\partial U}{\partial V}\right)_T\right]\frac{1}{\left(\frac{\partial T}{\partial V}\right)_P}$$

Notranji tlak enega mola van der Waalsovega plina pa je enak:

$$\left(\frac{\partial U}{\partial V}\right)_T = \frac{a}{V^2}$$

$$c_P - c_V = \left[P + \frac{a}{V^2}\right]\frac{R}{-\frac{2a}{V^3}(V - b) + \left(P + \frac{a}{V^2}\right)} = \frac{R}{1 - \frac{2a(V-b)}{V^3\left(P+\frac{a}{V^2}\right)}}$$

Ker naloga prepoveduje izražanje s tlakom, moramo na mesto njega vedno vstaviti gornji levi izraz:

$$c_P - c_V = \frac{R}{1 - \frac{2a(V-b)^2}{RTV^3}}$$

C) Drugi zakon termodinamike

1) Izračunajte spremembo entropije, če 1 mol N_2 izobarno segrejemo iz 300 na 1000 °C.

$\overline{c_P} = A + BT + CT^2 \; ter \; A = 26{,}983 \; B = 5{,}91 * 10^{-3} \; C = -3{,}376 * 10^{-7}$

$$\Delta S = \int_{T_1}^{T_2} \frac{\overline{c_P}}{T} dT = \int_{T_1}^{T_2} \frac{A}{T} dT + \int_{T_1}^{T_2} B dT + \int_{T_1}^{T_2} CT dT$$

$$\Delta S = A ln \frac{T_2}{T_1} + B(T_2 - T_1) + \frac{C}{2}(T_2^2 - T_1^2) = 36{,}48 \; \frac{J}{K}$$

2) Izračunajte spremembo entropije, entalpije in notranje energije za sledeči proces segrevanja 1 mol vode:

$$H_2O(l, 20\ \text{°C}) \rightarrow H_2O(g, 250\ \text{°C})$$

P=1 atm

$\overline{c_P}(l) = 75{,}3 \; \frac{J}{mol\ K}$

$\overline{c_P}(g) = 36{,}0 \; \frac{J}{mol\ K}$

$\Delta \overline{H}(izp) = 40668 \; \frac{J}{mol}$

$$\Delta S = \int_{T_1}^{T_V} \frac{\overline{c_P}(l)}{T} dT + \frac{\Delta \overline{H}(izp)}{T_V} + \int_{T_V}^{T_2} \frac{\overline{c_P}(g)}{T} dT$$

$$\Delta S = \overline{c_P}(l) ln \frac{T_V}{T_1} + \frac{\Delta \overline{H}(izp)}{T_V} + \overline{c_P}(g) ln \frac{T_2}{T_V} = 139{,}3 \; \frac{J}{K}$$

$$\Delta H = \int_{T_1}^{T_V} \overline{c_P}(l)\, dT + \Delta \overline{H}(izp) + \int_{T_V}^{T_2} \overline{c_P}(g)\, dT$$

$$\Delta H = \overline{c_P}(l)(T_V - T_1) + \Delta \overline{H}(izp) + \overline{c_P}(g)(T_2 - T_V) = 52090\, J$$

$$H = U + PV \;\Longrightarrow U = H - PV \;\Longrightarrow dU = dH - PdV - VdP$$

$$P = const. \Longrightarrow dP = 0 \;\Longrightarrow\; dU = dH - PdV$$

Predpostavimo idealno obnašanje vodne pare:

$$\Delta U = \Delta H - P\Delta V = \Delta H - P\big(V(g) - V(l)\big) \approx \Delta H - PV(g) = \Delta H - RT_2 = 47739\, J$$

3) Izračunajte preneseno delo in toploto ter spremembo notranje energije, entalpije in entropije za vsak korak sledečega krožnega procesa enega mola idealnega plina ter za celoten krožni proces.

$\overline{c_V} = \frac{5}{2}R$

$T_1 = 300\ K\ ter\ P_1 = 1\ atm$

izohorno $T_2 = 900\ K$

izotermno $P_3 = P_1 = 1\ atm$

$\overline{c_P} = \overline{c_V} + R = \frac{7}{2}R$

1→2 izohora

$$\frac{\mathrm{P_1}}{\mathrm{T_1}} = \frac{\mathrm{P_2}}{\mathrm{T_2}} \Longrightarrow \mathrm{P_2} = \frac{\mathrm{P_1T_2}}{\mathrm{T_1}} = 3\ atm$$

$$V = const \Longrightarrow dV = 0 \Longrightarrow đW = -PdV = 0 \Longrightarrow W = 0$$

$$dU = đQ \Longrightarrow \Delta U = Q = \int_{T_1}^{T_2} \overline{c_V} dT = \overline{c_V}(T_2 - T_1) = 900\ R$$

$$\Delta H = \int_{T_1}^{T_2} \overline{c_P} dT = \overline{c_P}(T_2 - T_1) = 1500\ R$$

$$\Delta S = \int_{T_1}^{T_2} \frac{\overline{c_V} dT}{T} = \overline{c_V} ln\frac{T_2}{T_1} = \frac{3}{2}Rln3$$

2→3 izoterma $\Longrightarrow\ T_3 = 900\ \Longrightarrow\ T = const\ \Longrightarrow dT = 0$

$$dU = \overline{c_V}dT = 0 \Longrightarrow \Delta U = 0$$

$$dH = \overline{c_P}dT = 0 \Longrightarrow \Delta H = 0$$

$$W = -Q = -RTln\frac{V_3}{V_2}$$

$$P_3V_3 = P_2V_2 \Longrightarrow \frac{V_3}{V_2} = \frac{P_2}{P_3} \Longrightarrow W = -Q = -RT_2ln\frac{P_2}{P_3} = -900Rln3$$

$$\Delta S = -\int_{P_2}^{P_3} \frac{RdP}{P} = -Rln\frac{P_3}{P_2} = Rln3$$

3→1 $\Longrightarrow\ P = const\ \Longrightarrow\Longrightarrow dP = 0\ \Longrightarrow$ **izobara**

$$\Delta H = Q = \int_{T_3}^{T_1} \overline{c_P} dT = \overline{c_P}(T_1 - T_3) = -1500\ R$$

$$\Delta U = \int_{T_3}^{T_1} \overline{c_V} dT = \overline{c_V}(T_1 - T_3) = -900\ R$$

$$W = -\int_{V_3}^{V_1} P_3 dV = -P_3V_1 + P_3V_3 = -P_1V_1 + P_3V_3$$

$$PV = RT \implies W = -RT_1 + RT_3 = 600\ R$$

$$\Delta S = \int_{T_3}^{T_1} \frac{\overline{c_P} dT}{T} = \overline{c_P} ln \frac{T_1}{T_3} = -\frac{5}{2} R ln 3$$

celokupen krožen proces

$$Q_{\circlearrowleft} = Q_1 + Q_2 + Q_3 = 388{,}8\ R$$

$$W_{\circlearrowleft} = W_1 + W_2 + W_3 = -388{,}8\ R$$

$$\Delta U_{\circlearrowleft} = Q_{\circlearrowleft} + W_{\circlearrowleft} = 0$$

$$\Delta H_{\circlearrowleft} = \Delta H_1 + \Delta H_2 + \Delta H_3 = 0$$

$$\Delta S_{\circlearrowleft} = \Delta S_1 + \Delta S_2 + \Delta S_3 = 0$$

4) Izračunajte spremembo entropije ireverzibilnega procesa zmrzovanja enega mol podhlajene vode pri tlaku 1 atm

$$H_2O(l, -10\ °\mathrm{C}) \rightarrow H_2O(s, -10\ °\mathrm{C})$$

Kolikšni sta spremembi entropije okolice in celotnega vesolja?

$$\overline{c_P}(l) = 75{,}3\ \frac{J}{mol\ K}$$

$$\overline{c_P}(s) = 37{,}2\ \frac{J}{mol\ K}$$

$$\Delta \overline{H}(tal, 0\ °\mathrm{C}) = 6008\ \frac{J}{mol}$$

$$\Delta \overline{H}(tal, -10\ °\mathrm{C}) = 5627\ \frac{J}{mol}$$

$$\Delta S(proces) = \int_{T_1}^{T_Z} \frac{\overline{c_P}(l) dT}{T} + \frac{\Delta \overline{H}(tal, 0\ °\mathrm{C})}{T_Z} + \int_{T_Z}^{T_1} \frac{\overline{c_P}(s) dT}{T}$$

$$\Delta S(proces) = \overline{c_P}(l) ln \frac{T_Z}{T_1} + \frac{\Delta \overline{H}(tal, 0\ °\mathrm{C})}{T_Z} + \overline{c_P}(s) ln \frac{T_1}{T_Z} = -20{,}59\ \frac{J}{K}$$

$$\Delta S(okolica) = \frac{\Delta \overline{H}(tal, -10\ °\mathrm{C})}{T_1} = 21{,}38\ \frac{J}{K}$$

$$\Delta S(vesolja) = \Delta S(okolica) + \Delta S(proces) = 0{,}79\ \frac{J}{K}$$

5) 200 g kositra z začetno temperaturo 100 °C vržemo v adiabatno posodo, v kateri je 100 g vode s temperaturo 25 °C. Izračunajte zmesno temperaturo, spremembo entropije kositra, vode ter adiabatne posode.

$\overline{c_P}(H_2O) = 75{,}3\ \frac{J}{mol\ K}$

$\overline{c_P}(Sn) = 25{,}5\ \frac{J}{mol\ K}$

M(Sn)=118,7 g/mol

$$\frac{m(Sn)}{M(Sn)}\overline{c_P}(Sn)(T(Sn) - T_z) = \frac{m(H_2O)}{M(H_2O)}\overline{c_P}(H_2O)(T_z - T(H_2O))$$

$$T_Z = 305{,}1\ K$$

$$\Delta S(Sn) = \int_{T(Sn)}^{T_z} \frac{m(Sn)\overline{c_P}(Sn)}{M(Sn)T} dT = \frac{m(Sn)\overline{c_P}(Sn)}{M(Sn)} ln\frac{T_z}{T(Sn)} = -8{,}66\ \frac{J}{K}$$

$$\Delta S(H_2O) = \int_{T(H_2O)}^{T_z} \frac{m(H_2O)\overline{c_P}(H_2O)}{M(H_2O)T} dT = \frac{m(H_2O)\overline{c_P}(H_2O)}{M(H_2O)} ln\frac{T_z}{T(H_2O)} = 9{,}71\ \frac{J}{K}$$

$$\Delta S(posoda) = \Delta S(Sn) + \Delta S(H_2O) = 1{,}05\ \frac{J}{K}$$

6) Izračunajte entropijo in molsko entropijo mešanja 1 mol O_2 s 3 mol N_2 pri 25 °C ter stalnem tlaku.

$$\Delta S_m = -R\sum_{i=1}^{k} n_i\, lnX_i = -R(n_1 lnX_1 + n_2 lnX_2) = 18{,}7\ \frac{J}{K}$$

$$\Delta\overline{S_m} = \frac{\Delta S_m}{n_1 + n_2} = 4{,}67\ \frac{J}{mol\ K}$$

D) Gibbsova in Helmholtzova prosta energija

1) Pri temperaturi 298 K ter tlaku 1 bar poteče zgorevanje oktana po sledeči kemijski enačbi:

$$C_8H_{18}(g) + \frac{25}{2}O_2(g) \rightarrow 8CO_2(g) + 9H_2O(g)$$

Izračunajte spremljajoči spremembi Gibbsove in Helmholtzove proste energije.

ΔU=-5109 kJ

ΔS=422 J/K

$$A = U - TS \implies dA = dU - TdS - SdT$$
$$T = const \implies dT = 0 \implies dA = dU - TdS \implies \Delta A = \Delta U - T\Delta S = -5235\ kJ$$
$$G = A + PV \implies dG = dA + PdV + VdP$$
$$P = const \implies dP = 0 \implies dG = dA + PdV \implies \Delta G = \Delta A + P\Delta V$$
$$\Delta G = \Delta A + P(V_P - V_R)$$
$$PV = nRT \implies \Delta G = \Delta A + RT(n_P - n_R) = -5226\ kJ$$

2) Z vsemi količinami razen s tlakom izrazite notranji tlak mola idealnega oziroma van der Waalsovega plina.

Idealni plin sledi splošni plinski enačbi:

$$PV = nRT;\ n = 1 \implies PV = RT \implies P = \frac{RT}{V}$$
$$\left(\frac{\partial U}{\partial V}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_V - P = T\frac{R}{V} - P = P - P = 0$$

Van der Waalsov plin sledi van der Waalsovi enačbi:

$$\left(P + a\frac{n^2}{V^2}\right)(V - bn) = nRT$$
$$n = 1 \implies \left(P + \frac{a}{V^2}\right)(V - b) = RT \implies P = \frac{RT}{V - b} - \frac{a}{V^2}$$
$$\left(\frac{\partial U}{\partial V}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_V - P = T\frac{R}{V - b} - \frac{RT}{V - b} + \frac{a}{V^2} = \frac{a}{V^2}$$

3) Volumen tekoče vode je pri tlaku 1 bar podan z enačbo:

$$V = V_0(1 + aT + bT^2 + cT^2)$$

kjer T predstavlja temperaturo v °C. Poiščite notranji tlak vode ter razliko c_P-c_V pri 1 °C.

a=-6,427*10^{-5}

b=8,5053*10^{-6}

c=-6,79*10^{-8}

κ=5,18*10^{-5} bar^{-1}

ρ_0=1 g/cm^3

$$\left(\frac{\partial U}{\partial V}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_V - P = T\frac{\alpha}{\kappa} - P$$

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = \frac{1}{V_0}V_0(a + 2bT + 3cT^2) = -4{,}746 * 10^{-5}\ K^{-1}$$

$$\left(\frac{\partial U}{\partial V}\right)_T = T\frac{\alpha}{\kappa} - P = -252\ bar$$

$$c_P - c_V = \left[\left(\frac{\partial U}{\partial V}\right)_T + P\right]\left(\frac{\partial V}{\partial T}\right)_P = \left[\left(\frac{\partial U}{\partial V}\right)_T + P\right]\alpha V_0 = \left[\left(\frac{\partial U}{\partial V}\right)_T + P\right]\alpha\frac{m}{\rho_0}$$

$$c_P - c_V = \left[\left(\frac{\partial U}{\partial V}\right)_T + P\right]\alpha\frac{nM}{\rho_0} = 0{,}0214\ \frac{J}{mol\ K}$$

4) Izrazite Joule-Thomsonov koeficient za 1 mol idealnega oziroma van der Waalsovega plina z vsemi količinami razen s tlakom.

Idealni plin sledi splošni plinski enačbi:

$$PV = nRT;\ n = 1\ \Rightarrow PV = RT\ \Rightarrow V = \frac{RT}{P}; P = \frac{RT}{V}; T = \frac{PV}{R}$$

$$\mu_{JT} = \frac{V(\alpha T - 1)}{c_P}$$

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = \frac{1}{V}\frac{R}{P} = \frac{1}{T}$$

$$\mu_{JT} = \frac{V(T^{-1}T - 1)}{c_P} = 0$$

Van der Waalsov plin sledi van der Waalsovi enačbi:

$$\left(P + a\frac{n^2}{V^2}\right)(V - bn) = nRT$$

$$n = 1\ \Rightarrow\ \left(P + \frac{a}{V^2}\right)(V - b) = RT\ \Rightarrow\ P = \frac{RT}{V - b} - \frac{a}{V^2};\ T = \frac{1}{R}\left(P + \frac{a}{V^2}\right)(V - b)$$

$$\mu_{JT} = \frac{V(\alpha T - 1)}{c_P} = \frac{T\left(\frac{\partial V}{\partial T}\right)_P - V}{c_P} = \frac{1}{c_P}\left[\frac{T}{\left(\frac{\partial T}{\partial V}\right)_P} - V\right] = \frac{1}{c_P}\left[\frac{RT}{-\frac{2a(V-b)}{V^3} + \left(P + \frac{a}{V^2}\right)} - V\right]$$

$$\mu_{JT} = \frac{1}{c_P}\left[\frac{RT}{-\frac{2a(V-b)}{V^3} + \frac{RT}{(V-b)}} - V\right] = \frac{1}{c_P}\frac{2aV(V-b)^2 - RTbV^3}{RTV^3 - 2a(V-b)^2}$$

5) Izrazite odvod $\left(\frac{\partial P}{\partial V}\right)_S$ z merljivimi količinami. Uporabite dobljeno enačbo za 1 mol idealnega plina.

$$S = f(P, V)$$

$$dS = \left(\frac{\partial S}{\partial P}\right)_V dP + \left(\frac{\partial S}{\partial V}\right)_P dV$$

$$S = const \implies dS = 0 \implies 0 = \left(\frac{\partial S}{\partial P}\right)_V (\partial P)_S + \left(\frac{\partial S}{\partial V}\right)_P (\partial V)_S$$

$$0 = \left(\frac{\partial S}{\partial P}\right)_V \left(\frac{\partial P}{\partial V}\right)_S + \left(\frac{\partial S}{\partial V}\right)_P$$

$$-1 = \left(\frac{\partial S}{\partial P}\right)_V \left(\frac{\partial P}{\partial V}\right)_S \left(\frac{\partial V}{\partial S}\right)_P$$

$$\left(\frac{\partial P}{\partial V}\right)_S = -\frac{1}{\left(\frac{\partial S}{\partial P}\right)_V \left(\frac{\partial V}{\partial S}\right)_P} = -\frac{\left(\frac{\partial S}{\partial V}\right)_P}{\left(\frac{\partial S}{\partial P}\right)_V} = -\frac{\left(\frac{\partial S}{\partial T}\right)_P \left(\frac{\partial T}{\partial V}\right)_P}{\left(\frac{\partial S}{\partial T}\right)_V \left(\frac{\partial T}{\partial P}\right)_V} = -\frac{\frac{c_P dT}{T\partial T}\frac{1}{\alpha V}}{\frac{c_V dT}{T\partial T}\frac{\kappa}{\alpha}} = -\frac{\gamma}{V\kappa}$$

Idealni plin sledi splošni plinski enačbi:

$$PV = nRT;\ n = 1 \implies PV = RT \implies V = \frac{RT}{P}; P = \frac{RT}{V}$$

$$\kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T = \frac{1}{V}\frac{RT}{P^2} = \frac{P}{P^2} = \frac{1}{P}$$

$$\left(\frac{\partial P}{\partial V}\right)_S = -\frac{\gamma}{V\kappa} = -\gamma\frac{P}{V}$$

$$\int \frac{dP}{P} = -\gamma \int \frac{dV}{V}$$

$$lnP = -\gamma lnV + const$$

$$lnP + \gamma lnV = const$$

$$lnPV^{\gamma} = const$$

$$PV^{\gamma} = konst$$

6) Izrazite odvod $\left(\frac{\partial H}{\partial U}\right)_T$ z merljivimi količinami. Uporabite dobljeno enačbo za 1 mol idealnega plina.

$$\left(\frac{\partial H}{\partial U}\right)_T = \frac{\left(\frac{\partial H}{\partial V}\right)_T}{\left(\frac{\partial U}{\partial V}\right)_T} = \frac{\left(\frac{\partial H}{\partial P}\right)_T \left(\frac{\partial P}{\partial V}\right)_T}{\left(\frac{\partial U}{\partial V}\right)_T} = \frac{\left[-T\left(\frac{\partial V}{\partial T}\right)_P + V\right]\left(-\frac{1}{\kappa V}\right)}{T\left(\frac{\partial P}{\partial T}\right)_V - P} = \frac{V[\alpha T - 1]}{\kappa V\left(T\frac{\alpha}{\kappa} - P\right)} = \frac{\alpha T - 1}{\alpha T - \kappa P}$$

Idealni plin sledi splošni plinski enačbi:

$$PV = nRT;\ n = 1 \ \Longrightarrow PV = RT \ \Longrightarrow V = \frac{RT}{P}; P = \frac{RT}{V}; T = \frac{PV}{R}$$

$$\kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T = \frac{1}{V}\frac{RT}{P^2} = \frac{P}{P^2} = \frac{1}{P}$$

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = \frac{1}{V}\frac{R}{P} = \frac{1}{T}$$

$$\left(\frac{\partial H}{\partial U}\right)_T = \frac{\alpha T - 1}{\alpha T - \kappa P} = \frac{T^{-1}T - 1}{T^{-1}T - P^{-1}P} = \frac{0}{0}$$

E) Odprti sistemi

1) Etilenglikol pri atmosferskem tlaku vre pri 197 °C. Pri kateri temperaturi vre etilenglikol, če je zunanji tlak 0,040 bar?

M=62 g/mol

ΔH_{izp}=799 J/g

$$ln\frac{P_2}{P_1} = -\frac{\Delta\overline{H_{izp}}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$ln\frac{P_2}{P_1} = -\frac{\Delta H_{izp}M}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$T_1 = 101{,}5\ °\mathrm{C}$$

2) Sublimacijska in izparilna krivulja uranovega heksafluorida UF_6 sledita sledečim enačbam:

$$(s): log\frac{P}{torr} = 10{,}648 - \frac{2559{,}5}{T}$$

$$(l): log\frac{P}{torr} = 7{,}5396 - \frac{1511{,}3}{T}$$

Določite tlak in temperaturo trojne točke. Pri kateri temperaturi bi UF_6 sublimiral, če je zunanji tlak 1 bar?

$$P_3(s) = P_3(l)$$

$$10{,}648 - \frac{2559{,}5}{T_3} = 7{,}5396 - \frac{1511{,}3}{T_3}$$

$$T_3 = 337{,}2\ K$$

$$log\frac{P_3}{torr} = 7{,}5396 - \frac{1511{,}3}{T_3}$$

$$P_3 = 1142\ torr$$

$$log\frac{P_s}{torr} = 10{,}648 - \frac{2559{,}5}{T_S}$$

$$T_S = 329{,}3\ K$$

3) Izračunajte temperaturo tališča živega srebra pod površjem Zemlje pri tlaku 100 bar. Pri tlaku 1 bar se živo srebro tali pri -38,87 °C.

$\frac{\Delta H_{tal}}{m} = 11{,}63\ \frac{J}{g}$

$\rho_l = 13{,}65 * 10^6\ \frac{g}{m^3}$

$\rho_s = 14{,}26\ * 10^6\ \frac{g}{m^3}$

$$\frac{dP}{dT} = \frac{\Delta H_{tal}}{T\Delta V_{tal}}$$

$$\Delta V_{tal} = V_l - V_s = m\left(\frac{1}{\rho_l} - \frac{1}{\rho_s}\right) = \frac{m(\rho_s - \rho_l)}{\rho_l \rho_s}$$

$$\frac{dP}{dT} = \frac{\Delta H_{tal}\rho_l\rho_s}{Tm(\rho_s - \rho_l)}$$

$$\int_{P_0}^{P} dP = \frac{\Delta H_{tal}}{m}\frac{\rho_l\rho_s}{(\rho_s - \rho_l)}\int_{T_0}^{T}\frac{dT}{T}$$

$$P - P_0 = \frac{\Delta H_{tal}}{m}\frac{\rho_l\rho_s}{(\rho_s - \rho_l)}\, ln\frac{T}{T_0}$$

$$T = -38{,}25\ °\mathrm{C}$$

4) V zaprti posodi z volumnom 10 L imamo 10 g H_2O. Pri kateri temperaturi, bo 5 g vodne pare v ravnotežju s 5 g tekoče vode?

$\Delta\overline{H_{izp}} = 40{,}7\ \frac{kJ}{mol}$

Ker imamo opravka z vodo poznamo temperaturo njenega vrelišča pri normalnem tlaku:

T_0=100 °C

P_0=1 atm

$$ln\frac{P}{P_0} = -\frac{\Delta\overline{H_{izp}}}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)$$

Za vodno paro predpostavimo idealno obnašanje:

$$PV = \frac{m_g}{M}RT\ \Rightarrow P = \frac{m_g RT}{MV}$$

$$ln\frac{m_g RT}{MVP_0} = -\frac{\Delta\overline{H_{izp}}}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)$$

Temperaturo bomo morali iskati numerično kot ničlo spodnje funkcije:

$$f(T) = \ln\frac{m_g RT}{MVP_0} + \frac{\Delta\overline{H_{izp}}}{RT} - \frac{\Delta\overline{H_{izp}}}{RT_0} = 0$$

Za prvi poskus bomo uporabili temperaturo vrelišča vode pri normalnem tlaku - 100 °C. Nato izdelamo sledečo tabelo:

T [K]	f(T)
373	-0,157
363	0,177

f(T) spremeni predznak in posledično zavzame ničlo med 100 in 90 °C. Posledično lahko temperaturo ocenimo na 95 °C.

5) Vodna ratopina etanola z masnim deležem 3% pri normalnem tlaku 760 torr vre pri 97,11 °C. Kolikšni so parni tlak vode in etanola ter celokupni parni tlak nad vodno raztopino etanola z molskim deležem 2% pri isti temperaturi?

$P^0_{H_2O} = 685$ torr

$$X_{et} = \frac{\frac{w_{et}}{M_{et}}}{\frac{w_{et}}{M_{et}} + \frac{w_{H_2O}}{M_{H_2O}}} = 0{,}012 \implies X_{H_2O} = 1 - X_{et} = 0{,}988$$

$$X_{et}K_{et} + X_{H_2O}P^0_{H_2O} = P$$

$$K_{et} = 6935\ torr$$

$$X_{et} = 0{,}02 \implies X_{H_2O} = 1 - X_{et} = 0{,}98$$

$$P_{et} = X_{et}K_{et} = 138{,}7\ torr$$

$$P_{H_2O} = X_{H_2O}P^0_{H_2O} = 671{,}3\ torr$$

$$P = P_{et} + P_{H_2O} = 810\ torr$$

6) Idealna vodna raztopina ima pri 100,5 °C tlak vodnih par P_A=100,75 kPa. Izračunajte njeno molalnost.

$$\Delta\overline{H_{izp}} = 40{,}7\ \frac{kJ}{mol}$$

Ker imamo opravka z vodo poznamo temperaturo njenega vrelišča pri normalnem tlaku:

T_0=100 °C

P_0=101,325 kPa

$$ln\frac{P_A^0}{P_0} = -\frac{\Delta\overline{H_{\imath zp}}}{R}\left(\frac{1}{T} - \frac{1}{T_o}\right)$$

$$P_A^0 = 103{,}11\ kPa$$

$$X_A = \frac{P_A}{P_A^0} = 0{,}9771$$

$$X_B = 1 - X_A = 0{,}0229$$

$$m = \frac{n_B}{m_A} = \frac{n_B}{n_A M_A} = \frac{X_B}{X_A M_A} = 1{,}301\ \frac{mol}{kg}$$

F) Kemijsko ravnotežje

1) Pri 400 °C ima reakcija

$$N_2(g) + 3H_2(g) \Leftrightarrow 2NH_3(g)$$

K_P^1 1,6*10^{-4}. Kolikšen je $\Delta G_1^{\ominus}$? Kolikšna sta pri isti temperaturi K_P^2 ter $\Delta G_2^{\ominus}$, če reakcijo preuredimo?

$$\frac{1}{2}N_2(g) + \frac{3}{2}H_2(g) \Leftrightarrow NH_3(g)$$

$$K_P^1 = \frac{P_{NH_3}^2}{P_{H_2}P_{N_2}^3}$$

$$\Delta G_1^{\ominus} = -RTlnK_P^1 = 48{,}91\ \frac{kJ}{mol}$$

$$K_P^2 = \frac{P_{NH_3}}{P_{H_2}^{\frac{3}{2}}P_{N_2}^{\frac{1}{2}}} = \sqrt{K_P^1} = 1{,}265 * 10^{-2}$$

$$\Delta G_2^{\ominus} = -RTlnK_P^2 = 24{,}46\ \frac{kJ}{mol}$$

2) Izračunajte K_P za sledečo reakcijo pri 25 °C

$$H_2(g) + \frac{1}{2}O_2(g) \Leftrightarrow H_2O(g)$$

$\Delta H_{tv}^{\ominus}(H_2O) = -241{,}818\ \frac{kJ}{mol}$

$S^{\ominus}(H_2O) = 188{,}825\ \frac{J}{molK}$

$S^{\ominus}(H_2) = 130{,}684\ \frac{J}{molK}$

$S^{\ominus}(O_2) = 205{,}138\ \frac{J}{molK}$

$$\Delta H_r^{\ominus} = \Delta H_{tv}^{\ominus}(H_2O) = -241{,}818\ \frac{kJ}{mol}$$

$$\Delta S_r^{\ominus} = S^{\ominus}(H_2O) - S^{\ominus}(H_2) - \frac{1}{2}S^{\ominus}(O_2) = -44{,}428\ \frac{J}{molK}$$

$$\Delta G_r^{\ominus} = \Delta H_r^{\ominus} - T\Delta S_r^{\ominus} = -228{,}572\ \frac{kJ}{mol}$$

$$\Delta G_r^{\ominus} = -RTlnK_P$$

$$K_P = 1{,}112 * 10^{40}$$

3) Pri temperaturi 318 K ter tlaku 1 bar je stopnja disociacije α spodnje reakcije 0,38

$$N_2O_4(g) \rightleftharpoons 2NO_2(g)$$

Določite stopnja disociacije α ter konstanto ravnotežja K_x pri tlaku 10 bar.

$$N_2O_4(g) \rightleftharpoons 2NO_2(g)$$

t=0 n_0 0 $\Sigma = n_0$

t=∞ $n_0(1-\alpha)$ $2\alpha n_0$ $\Sigma = n_0(1+\alpha)$

$$P_i = PX_i$$

$$K_P = \frac{P_{NO_2}^2}{P_{N_2O_4}} = \frac{X_{NO_2}^2 P^2}{X_{N_2O_4} P} = P\frac{\left(\frac{2n_0\alpha}{n_0(1+\alpha)}\right)^2}{\left(\frac{n_0(1-\alpha)}{n_0(1+\alpha)}\right)} = P\frac{4\alpha^2}{1-\alpha^2} = 0{,}68$$

$$K_P = K_X P \implies K_X = \frac{K_P}{P} = 0{,}068$$

$$K_X = \frac{4\alpha^2}{1-\alpha^2}$$

$$K_X = (4 + K_X)\alpha^2$$

$$\alpha = 0{,}129$$

4) Spodnja reakcija poteka pri konstantnem volumnu in temperaturi

$$H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$$

Če dodamo 1 mol H_2 ter 3 mol I_2, dobimo nekaj HI. V kolikor dodamo še 2 mol H_2, pa dobimo dvakrat toliko HI. Izračunajte K_P.

$$H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$$

t=0 1 3 0

t=∞ 1-x/2 3-x/2 x

$$H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$$

t=0 3 3 0

t=∞ 3-x 3-x 2x

$$P_i = PX_i$$

$$K_P = \frac{P_{HI}^2}{P_{I_2}P_{H_2}} = \frac{X_{HI}^2 P^2}{X_{I_2} P X_{H_2} P} = \frac{n_{HI}^2 n^2}{n^2 n_{I_2} n_{H_2}}$$

$$K_P^1 = K_P^2$$

$$\frac{x^2}{\left(1-\frac{x}{2}\right)\left(3-\frac{x}{2}\right)} = \frac{4x^2}{(3-x)^2}$$

$$12 - 8x = 9 - 6x$$

$$x = \frac{3}{2}$$

$$K_P = \frac{4x^2}{(3-x)^2} = 4$$

5) Spodnja reakcija poteka pri temperaturi 25 °C in tlaku 1 bar

$$2A(g) + 3B(g) \rightleftharpoons C(g) + 3D(g)$$

Če dodamo 2 mol A, 3 mol B ter 2 mol C, dobimo 2 mol D. Izračunajte ravnotežni konstanti K_x in K_p ter $\Delta G^{\ominus}$.

$$2A(g) + 3B(g) \rightleftharpoons C(g) + 3D(g)$$

t=0	1	3	2	0
t=∞	2/3	1	8/3	2

$$\sum n_i = \frac{19}{3}$$

$$P = 1\ bar \implies K_P = K_X$$

$$K_P = K_X = \frac{X_C X_D^3}{X_A^2 X_B^3} = \frac{n_C n_D^3 \sum n_i}{n_A^2 n_B^3} = 304$$

$$\Delta G^{\ominus} = -RTlnK_P = -14{,}171\ kJ$$

6) Pri temperaturi 1000 °C in tlaku 1 bar metan disociira po sledeči reakciji

$$CH_4(g) \rightleftharpoons 2H_2(g) + C(s)$$

Konstanta ravnotežja K_p znaša 128. Izračunajte stopnjo disociacije α ter ravnotežna molska deleža vodika in metana v plinski mešanici.

$$CH_4(g) \rightleftharpoons 2H_2(g) + C(s)$$

t=0	n_0	0	Σ= n_0
t=∞	$n_0(1-\alpha)$	$2\alpha\, n_0$	Σ= $n_0(1+\alpha)$

$$K_a = \frac{a_{H_2}^2 a_C}{a_{CH_4}} = \frac{a_{H_2}^2}{a_{CH_4}} = \frac{P_{H_2}^2}{P_{CH_4}} = K_P$$

$$P = 1\ bar \implies K_P = K_X$$

$$K_P = K_X = \frac{X_{H_2}^2}{X_{CH_4}} = \frac{\left(\frac{2\alpha n_0}{n_0(1+\alpha)}\right)^2}{\left(\frac{n_0(1-\alpha)}{n_0(1+\alpha)}\right)} = \frac{4\alpha^2}{1-\alpha^2}$$

$$K_P = (4 + K_P)\alpha^2$$

$$\alpha = 0{,}98$$

$$X_{CH_4} = \frac{1 - \alpha}{1 + \alpha} = 0{,}01$$

$$X_{H_2} = \frac{2\alpha}{1 + \alpha} = 0{,}99$$