Miscele by Tom

Due gas (vedi tabella) sono miscelati a volume costante. Determinare: $n, \chi, MW_m, w_i, \bar{c}_{vm}, \bar{c}_{pm}, c_v, c_p, R, T_m, p_i, V, V_i \; e \; \gamma_m$.

Specie	Massa kg	MW	N freedom	T
N2	8	28	5	300
CO2	2	44	7	800
Tot	10			
Ro	8314.5	J/kmolK		
p	101300	Pa		
	n Kmole	χ,p/pm,V/V	χ*MW	wi=mi/m
N2	0.28571	0.862745	24.15686	0.8
CO2	0.04545	0.137255	6.039216	0.2
Tot	0.33117	1	30.19608	

$$n_{N_2} = \frac{m_{N_2}}{MW_{N_2}} = \frac{8}{28} = 0.286 \qquad n_{CO_2} = \frac{m_{CO_2}}{MW_{CO_2}} = \frac{2}{44} = 0.0455$$

$$n_m = n_{N_2} + n_{CO_2} = 0.286 + 0.0455 = 0.331$$

$$\chi_{N_2} = \frac{n_{N_2}}{n_m} = \frac{0.286}{0.331} = 0.865 \qquad \ldots$$

$$MW_m = \chi_{N_2} MW_{N_2} + \chi_{CO_2} MW_{CO_2} = \frac{m_m}{n_m} = \frac{10}{0.331} = 30.27$$

$$w_{N_2} = \frac{m_{N_2}}{m_m} = \frac{8}{10} = 0.8 \qquad \ldots$$

$$\bar{c}_{vN_2} = \bar{R}\frac{5}{2} = 8315 \cdot \frac{5}{2} = 20.8 \cdot \frac{kJ}{kmole \cdot K} \qquad \bar{c}_{vCO_2} = \bar{R}\frac{7}{2} = 8315 \cdot \frac{7}{2} = 29.1 \cdot \frac{kJ}{kmole \cdot K}$$

$$\bar{c}_{vm} = \bar{c}_{vN_2}\chi_{N_2} + \bar{c}_{vCO_2}\chi_{CO_2} = 20.8 \cdot 0.865 + 29.1 \cdot (1 - 0.865) = 21.9 \cdot \frac{kJ}{kmole \cdot K}$$

$$\bar{c}_{pm} = \bar{c}_{vm} + \bar{R} = 21.93 + 8.315 = 30.2 \cdot \frac{kJ}{kmole \cdot K}$$

$$c_{v_{N_2}} = \frac{\bar{c}_{vN_2}}{MW_{N_2}} = \frac{20.8}{28} = 743 \cdot \frac{J}{kg \cdot K} \qquad \ldots.$$

$$c_{v_m} = \frac{\bar{c}_{vm}}{MW_m} = \frac{21.9}{30.27} = 724 \cdot \frac{J}{kg \cdot K}$$

$$R = \frac{\bar{R}}{MW_m} = \frac{8315}{30.27} = 275 \cdot \frac{J}{kg \cdot K}$$

$$T_M = \frac{c_{v_{N_2}} w_{N_2} T_{N2} + c_{v_{CO_2}} w_{CO_2} T_{CO2}}{c_{vm}} = \frac{743 \cdot 0.8 \cdot 300 + 661 \cdot 0.2 \cdot 800}{724} = 392.5K$$

$$p_{N2} = p_m \chi_{N_2} = 101.3 \cdot 0.865 = 87.6 \cdot kPa \qquad \ldots$$

$$V_m = \frac{n_{N_2} \bar{R} T_m}{p_{N_2}} = \frac{n_m \bar{R} T_m}{p_m} = \frac{0.331 \cdot 8315 \cdot 393}{101{,}300} = 10.7 \cdot m^3$$

$$V_{N_2} = V_m \chi_{N_2} = \frac{n_{N_2} \bar{R} T_m}{p_m} = 10.7 \cdot 0.865 = 9.22 \cdot m^3 \qquad \ldots$$

$$\gamma_m = \frac{\bar{c}_{pm}}{\bar{c}_{vm}} = \frac{30.2}{21.9} = 1.377$$

j/kmolK	cv	cv*χ	Cp	cp*χ
N2	20786.3	17933.24	29100.75	25106.529
CO2	29100.8	3994.221	37415.25	5135.4265
	medio	21927.46		30241.956
	J/kgK			
	cv	cv wi	cp	cp wi
N2	742.366	593.8929	1039.313	831.45
CO2	661.381	132.2761	850.3466	170.06932
	Medio	726.169		1001.5193
γ	1.37918			
	wi cv T	wi cp T	R	R wi
N2	178168	249435	296.9464	237.55714
CO2	105821	136055.5	188.9659	37.793182
Somma	283989	385490.5		275.35032
Tm	391.078	384.9057		
		V costante	p costante	
	Vm	10.63016	10.46238	
	pi	Vi	Vi	
N2	87396.1	9.171114	9.026366	
CO2	13903.9	1.459041	1.436013	
		10.63016	10.46238	

Farokhi problem 7.4

Write the chemical reaction for the complete combustion of JP-4 and air. JP-4 has the formula $CH_{1.93}$. Also, calculate the stoichiometric fuel-to-air ratio for this blended jet fuel.

$$CH_{1.93} + x(O_2 + 3.76N_2) \rightarrow CO_2 + yH_2O + z3.76N_2$$

$$x = z \qquad 2y = 1.93 \qquad 2x = 2 + y$$

$$2x = 2 + \frac{1.93}{2} \quad \rightarrow \quad 2x = \frac{4 + 1.93}{2} \quad \rightarrow \quad x = \frac{5.93}{4}$$

$$CH_{1.93} + \frac{5.93}{4}(O_2 + 3.76N_2) \rightarrow CO_2 + \frac{1.93}{2}H_2O + \frac{5.93}{4}3.76N_2$$

$$f = \frac{\dot{m}_f}{\dot{m}_0} = \frac{1 \cdot 12 + 1 \cdot 1.93}{\frac{5.93}{4}(2 \cdot 16 + 3.76 \cdot 2 \cdot 14)} = 0.0684$$

Farokhi problem 7.5

Calculate the lower and higher heating values of octane, C_8H_{18},in the stoichiometric chemical reaction with oxygen at a reference temperature of 298.16 K and the pressure of 1 bar ($h_{VapH_2O} = 2243kJ/kg$).

CO_2	Carbon dioxide	Gas	−393.522	−8.944
CO	Carbon monoxide	Gas	−110.53	−3.947
H_2	Hydrogen	Gas	0	0
H	Hydrogen atom	Gas	217.999	217.999
OH	Hydroxyl radical	Gas	39.463	2.321
H_2O	Water	Gas	−241.827	−13.435
H_2O_2	Hydrogen peroxide	Gas	−136.106	−4.003
C_2H_5OH	Ethyl alcohol	Liquid	−277.20	−6.026
C_3H_8	Propane	Gas	−103.90	−2.3614
C_4H_{10}	Butane	Gas	−126.148	−2.175
C_8H_{18}	Octane	Gas	−208.447	−1.8285
C_8H_{18}	Octane	Liquid	−249.93	−2.1924

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

$$Q_{ext} = \sum_j \left[n_j \bar{c}_{pj}\left(T_2 - T_f\right)\right]_{prod} - \sum_i \left[n_i \bar{c}_{pi}\left(T_1 - T_f\right)\right]_{rea} + \Delta H_{RPf}$$

$$Q_{ext} = \Delta H_{RPf} = \sum_j \left[n_j \Delta \bar{\mathrm{h}}^0_{fj}\right]_{prod} - \sum_i \left[n_i \Delta \bar{\mathrm{h}}^0_{fi}\right]_{rea} = -8 \cdot 393 - 9 \cdot 242 - (-208)$$

$$= -5114 \cdot 10^3 \cdot kJ$$

$$LHV = \frac{-Q_{ext}}{m_f} = \frac{5114 \cdot 10^3}{12 \cdot 8 + 1 \cdot 18} = 44.9 \cdot 10^3 \cdot \frac{kJ}{kg}$$

$$HHV = LHV + \frac{m_{H_2O}}{m_{C_8H_{18}}} \mathrm{h}_{VapH_2O} = 44.9 \cdot 10^3 + \frac{18 \cdot 9}{12 \cdot 8 + 1 \cdot 18} 2243 = 48.1 \cdot 10^3 \cdot \frac{kJ}{kg}$$

Farokhi problem 7.9

One mole of octane is burned with 120% theoretical air. Assuming that the octane and air enter the combustion chamber at 25*C* and the excess oxygen and nitrogen in the reaction will not dissociate, calculate

(a) the fuel–air ratio

(b) the equivalence ratio ϕ

(c) the adiabatic flame temperature T_{af}

Assume: $\bar{c}_{p\mathrm{CO_2}} = 61.9 kJ/kmol \cdot K, \bar{c}_{p\mathrm{O_2}} = 37.8 kJ/kmol \cdot K,\ \bar{c}_{p\mathrm{N_2}} = 33.6 kJ/kmol \cdot K\ \bar{c}_{p\mathrm{H_2O}} = 52.3 kJ/kmol \cdot K$

%Oss	1.2		FA7.9					
Reagenti	n	MW	h0f	Prodotti	n	MW	h0f	cp
C8H18	1	114	-208.447	CO2	8	44	-393.522	61.9
O2	15	32		H2O	9	18	-241.827	52.3
N2	56.4	28		N2	56.4	28		33.6
Tot	72.4			O2	2.5	32		37.8
Tot	298.15			Tot	75.9			
mf	114		ΔH	-5.116E+06				
mair	2059.2			Stima	Valore medio esatto			
f	0.05536		Cpm	38.938603	36.4777			
fst	0.06643		T	2029.2633	2146.04			
ϕ	0.83333		Dif	-324,038				
Tf guess	2029		Err%	-6.334E+00				

$$C_8H_{18} + x(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + x3.76N_2$$

$$2x = 16 + 9 \quad \rightarrow \quad x = 25/2 = 12.5$$

$$C_8H_{18} + 12.5(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 12.5 \cdot 3.76N_2$$

$$\alpha = 1.2$$

$$C_8H_{18} + \alpha x(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + yO_2 + \alpha x3.76N_2$$

$$y = x(\alpha - 1) = 12.5 \cdot 0.2 = 2.5$$

$$C_8H_{18} + 15(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 2.5O_2 + 15 \cdot 3.76N_2$$

(a) the fuel–air ratio

$$f = \frac{\dot{m}_f}{\dot{m}_0} = \frac{8 \cdot 12 + 18 \cdot 1}{15(2 \cdot 16 + 3.76 \cdot 2 \cdot 14)} = \frac{114}{2059} = 0.0554$$

(b) the equivalence ratio ϕ

$$\phi = \frac{f}{f_{st}} = \frac{0.0554}{\frac{8 \cdot 12 + 18 \cdot 1}{12.5(2 \cdot 16 + 3.76 \cdot 2 \cdot 14)}} = \frac{1}{\alpha} = 0.833$$

(c) the adiabatic flame temperature T_{af}

$$Q_{ext} = \sum_j \left[n_j \bar{c}_{pj}(T_2 - T_f)\right]_{prod} - \sum_i \left[n_i \bar{c}_{pi}(T_1 - T_f)\right]_{rea} + \Delta H_{RPf}$$

$$Q_{ext} = 0 = \sum_j \left[n_j \bar{c}_{pj}(T_2 - T_f)\right]_{prod} + \Delta H_{RPf}$$

$$\Delta H_{RPf} = \sum_j \left[n_j \Delta \bar{\mathrm{h}}^0_{fj}\right]_{prod} - \sum_i \left[n_i \Delta \bar{\mathrm{h}}^0_{fi}\right]_{rea} = 10^3\big(-8 \cdot 394 - 9 \cdot 242 - (-1 \cdot 208)\big)$$

$$= -5122 \cdot \frac{MJ}{kmol_{C_8H_{18}}}$$

$$c_{pm_{prod}} = \sum \chi_j \bar{c}_{pj} = \frac{8 \cdot 61.9 + 9 \cdot 52.3 + 2.5 \cdot 37.8 + 15 \cdot 3.76 \cdot 33.6}{8 + 9 + 2.5 + 15 \cdot 3.76} = 38.9 \cdot \frac{kJ}{kmol \cdot K}$$

$$n_m c_{pm_{prod}} \big(T_2 - T_f\big) = -\Delta H_{RPf}$$

$$T_2 = T_f - \frac{\Delta H_{RPf}}{n_m c_{pm_{prod}}} = 298.15 + \frac{5122 \cdot 10^3}{(8 + 9 + 2.5 + 15 \cdot 3.76)38.9} = 2030 \cdot K$$

■ TABLE 7.2

Molar Specific Heats of Various Gases

Gases at low pressures $\bar{c}_{p0}$= kJ/kmol · K θ = T(K)/100

Gas		Range K	Max. error (%)
N_2	$\bar{c}_{p0} = 39.060 - 512.79\theta^{-1.5} + 1072.7\theta^{-2} - 820.40\theta^{-3}$	300–3500	0.43
O_2	$\bar{c}_{p0} = 37.432 + 0.0201020\theta^{1.5} - 178.57\theta^{-1.5} + 236.88\theta^{-2}$	300–3500	0.30
H_2	$\bar{c}_{p0} = 56.505 - 702.74\theta^{-0.75} + 1165.0\theta^{-1} - 560.70\theta^{-1.5}$	300–3500	0.60
CO	$\bar{c}_{p0} = 69.145 - 0.704630\theta^{0.75} - 200.77\theta^{-0.5} + 176.76\theta^{-0.75}$	300–3500	0.42
OH	$\bar{c}_{p0} = 81.564 - 59.350\theta^{0.25} + 17.329\theta^{0.75} - 4.2660\theta$	300–3500	0.43
HO	$\bar{c}_{p0} = 59.283 - 1.7096\theta^{0.5} - 70.613\theta^{-0.5} + 74.889\theta^{-1.5}$	300–3500	0.34
H_2O	$\bar{c}_{p0} = 143.05 - 183.54\theta^{0.25} + 82.751\theta^{0.5} - 3.6989\theta$	300–3500	0.43
CO_2	$\bar{c}_{p0} = -3.7357 + 30.529\theta^{0.5} - 4.1034\theta + 0.024198\theta^2$	300–3500	0.19
NO_2	$\bar{c}_{p0} = 46.045 + 216.10\theta^{-0.5} - 363.66\theta^{-0.75} + 232.550\theta^{-2}$	300–3500	0.26
CH_4	$\bar{c}_{p0} = 672.87 + 439.74\theta^{0.25} - 24.875\theta^{0.75} + 323.88\theta^{-0.5}$	300–2000	0.15
C_2H_4	$\bar{c}_{p0} = 95.395 + 123.15\theta^{0.5} - 35.641\theta^{0.75} + 182.77\theta^{-3}$	300–2000	0.07
C_2H_6	$\bar{c}_{p0} = 6.895 + 17.26\theta - 0.6402\theta^2 + 0.00728\theta^3$	300–1500	0.83
C_3H_8	$\bar{c}_{p0} = -4.042 + 30.46\theta - 1.571\theta^2 + 0.03171\theta^3$	300–1500	0.40
C_4H_{10}	$\bar{c}_{p0} = 3.954 + 37.12\theta - 1.833\theta^2 + 0.03498\theta^3$	300–1500	0.54

Source: Adapted from Van Wylen and Sonntag 1985.

(d) Evaluate also the flame temperature by considering non constant specific heat.

$$\bar{h}_j = \left(\int_{T_f}^{T_2} \bar{c}_{pj} dT + \Delta \bar{\mathrm{h}}^0_{fj}\right) \qquad \overline{\bar{c}_{pj}} = \frac{1}{T_2 - T_f}\int_{T_f}^{T_2} \bar{c}_{pj} dT \qquad \theta = \frac{T}{100}$$

$$\bar{c}_{p_{CO_2}} = \frac{1}{T_2 - T_f}\int_{T_f}^{T_2} 100 \sum (a_i \theta^{e_i}) d\left(\frac{T}{100}\right) = \frac{1}{T_2 - T_f}\left[100 \frac{\sum a_i \theta^{e_i + 1}}{e_i + 1}\right]_{T_f}^{T_2} = \frac{1}{T_2 - T_f}\left[T \frac{\sum a_i \theta^{e_i}}{e_i + 1}\right]_{T_f}^{T_2}$$

$$\bar{c}_{p_{CO_2}} = \frac{1}{T_2 - T_f}\left[-3.736 \cdot T + \frac{30.53}{1.5} \cdot T\left(\frac{T}{100}\right)^{0.5} - \frac{4.103}{2} \cdot T\left(\frac{T}{100}\right)^{1} + \frac{0.02420}{3} \cdot T\left(\frac{T}{100}\right)^{2}\right]_{T_f}^{T_2}$$

$$\bar{c}_{p_{CO_2}} = \frac{1}{T_2 - T_f}[(-7{,}580 + 168{,}013 - 84{,}465 + 6{,}738)$$

$$- (-1{,}113 + 10{,}478 - 1{,}824 + 21.38)] = \frac{1}{2029 - 298.15}[100{,}706 - 7{,}562]$$

$$= 53.81 \cdot kJ/kmol \cdot K$$

$$T_2 = T_f - \frac{\Delta H_{RPf}}{n_m c_{pm_{prod}}} = 298.15 + \frac{5122 \cdot 10^3}{(8 + 9 + 2.5 + 15 \cdot 3.76)36.45} = 2146 \cdot K$$

Si deve iterare e si ha:

$$T_2 = T_f - \frac{\Delta H_{RPf}}{n_m c_{pm_{prod}}} = 298.15 + \frac{5122 \cdot 10^3}{(8 + 9 + 2.5 + 15 \cdot 3.76)36.74} = 2133 \cdot K$$

$$T_2 = T_f - \frac{\Delta H_{RPf}}{n_m c_{pm_{prod}}} = 298.15 + \frac{5122 \cdot 10^3}{(8 + 9 + 2.5 + 15 \cdot 3.76)36.71} = 2134 \cdot K$$

Da https://www.grc.nasa.gov/www/CEAWeb/ceaThermoBuild.htm per CO2:

$$h_{2029} - h_{298.15} = 93.19 \frac{kJ}{mole}$$

$$\bar{c}_{p_{CO_2}} = \frac{h_{2029} - h_{298.15}}{2029 - 298.15} = \frac{93.19 \cdot 1000}{2029 - 298.15} = 53.84 \cdot kJ/kmol \cdot K$$

Prodotti	Δh	Δh n	cpm		
CO2	93,144	745,156	53.81429		
H2O	74,735	672,613	43.1781		
N2	57,157	3,223,638	33.02233		
O2	60,291	150,727	34.83301		
	Tot	4,792,134			
https://www.grc.nasa.gov/www/CEAWeb/ceaThermoBuild.htm					
	CO2	T1	298.15	T2	2029
Cost	Esp	Cp	Int	Cp	Int
-3.7357	0	-3.7357	-1113.8	-3.7357	-7,580
30.529	0.5	52.71449	10477.88	137.51612	186,013
-4.1034	1	-12.2343	-1823.83	-83.25799	-84,465
0.024198	2	0.215104	21.37778	9.9619319	6,738
		36.9596	7561.635	60.484363	100,706
				Diff	93,144
H2O		T1	298.15	T2	2029
Cost	Esp	Cp	Int	Cp	Int
143.05	0	143.05	42650.36	143.05	290,248
-183.54	0.25	-241.179	-57526	-389.5393	-632,300
82.751	0.5	142.8863	28401.04	372.7471	504,203
-3.6689	1	-10.9388	-1630.71	-74.44198	-75,521
		33.81853	11894.68	51.815856	86,630
					74,735
N2		T1	298.15	T2	2029
Cost	Esp	Cp	Int	Cp	Int
39.06	0	39.06	11645.74	39.06	79,253
-512.79	-1.5	-99.6064	59395.31	-5.610693	22,768
1072.7	-2	120.6726	-35978.5	2.6056386	-5,287
-820.4	-3	-30.9543	4614.515	-0.098215	100
		29.17186	39677.03	35.956731	96,834
					57,157
O2		T1	298.15	T2	2029
Cost	Esp	Cp	Int	Cp	Int
37.432	0	37.432	11160.35	37.432	75,950
0.020102	1.5	0.103488	12.34202	1.837225	1,491
-178.57	-1.5	-34.6862	20683.36	-1.953824	7,929
236.88	-2	26.64764	-7944.99	0.5753926	-1,167
		29.49696	23911.06	37.890794	84,202
					60,291

Farokhi problem 7.10

One mole of oxygen, O_2(g), is heated to 4000 K at the pressure of p_m. A fraction of the oxygen dissociates to oxygen atoms according to $xO_2 \rightarrow 2xO$. Assuming a state of equilibrium is reached in the mixture, calculate

(a) mole fraction of O_2 at equilibrium when p_m is 1 atm.

(b) mole fraction of O_2 at equilibrium when p_m is 10 atm.

Assume the equilibrium constant for the reaction $O_2 \leftrightarrow 2O$ is K_p= 2.19 atm at the temperature of 4000 K. Explain the effect of pressure on dissociation.

T(K)	$\frac{1}{2}\mathbf{O_2} \leftrightarrow \mathbf{O}$	$\frac{1}{2}\mathrm{H_2} \leftrightarrow \mathrm{H}$	$\frac{1}{2}\mathbf{H_2} + \frac{1}{2}\mathbf{O_2} \leftrightarrow \mathbf{OH}$	$\mathbf{H_2} + \frac{1}{2}\mathbf{O_2} \leftrightarrow \mathbf{H_2O}$
3500	-0.310	-0.231	0.160	0.712
4000	0.170	0.201	0.233	0.238

Logaritmo in base 10 delle cosanti d'equilibrio K

$$K = \frac{\chi_O}{\chi_{O_2}^{\frac{1}{2}}} p^{\frac{1}{2}} = 10^{0.170} = 1.479 \qquad K_p = \frac{\chi_O^2}{\chi_{O_2}} p = K^2 = 1.479^2 = 2.187$$

$$\mathrm{O_2} \rightarrow (1-x)\mathrm{O_2} + 2x\mathrm{O} \qquad n = 1 - \mathrm{x} + 2\mathrm{x} = 1 + \mathrm{x} \qquad \chi_{\mathrm{O}} = \frac{2\mathrm{x}}{1+\mathrm{x}} \qquad \chi_{\mathrm{O_2}} = \frac{1-\mathrm{x}}{1+\mathrm{x}}$$

$$\frac{\left(\frac{2\mathrm{x}}{1+\mathrm{x}}\right)^2}{\frac{1-\mathrm{x}}{1+\mathrm{x}}} p = K^2 = 1.479^2 = 2.187 \qquad \frac{4x^2}{1+x} p = K_p(1-x) \qquad 4x^2 p = 2.187(1-x^2)$$

$$x^2(4p + 2.187) = 2.187 \qquad x = \sqrt{\frac{2.187}{4p + 2.187}}$$

$$p_m = 1 \qquad x = \sqrt{\frac{2.187}{4 + 2.187}} = 0.595$$

$$\chi_{\mathrm{O}} = \frac{2 \cdot 0.595}{1 + 0.595} = 0.746 \qquad \chi_{\mathrm{O_2}} = \frac{1 - 0.595}{1 + 0.595} = 0.254$$

$$p_m = 10 \qquad x = \sqrt{\frac{2.187}{40 + 2.187}} = 0.228$$

$$\chi_{\mathrm{O}} = \frac{2 \cdot 0.228}{1 + 0.228} = 0.371 \qquad \chi_{\mathrm{O_2}} = \frac{1 - 0.228}{1 + 0.228} = 0.629$$