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! 1. Hess -- směs =====
DspHH2 =-242          ! [kJ mol-1]
                                -242
DspHCH4=2*-242+-394--75    ! [kJ mol-1]
                                -803
DspHCO = -394--110       ! [kJ mol-1]
                                -284
DH=0.50*DspHH2+0.20*DspHCH4+0.10*DspHCO
                                -310
n=101325/R/273.15        ! [mol m-3]
                                44.615
Qvyh=-DH*n              ! [kJ m-3]
                                13831
Qvyh/1000               ! [MJ mol-1]
                                13.831

! 2. Entalpická bilance =====
! H2 + 1/2 O2 -> H2O
DH298=-241.8e3          ! [J mol-1]
                                -2.418 · 10+05
def CpH20=30+10.7e-3*T+0.335e5/T↑2 ! [JK-1 mol-1]
def intCpH20=30*T+10.7e-3*T↑2/2-0.335e5/T
T=298
                                298
intCp298=intCpH20      ! (= hodnota pro T=298)
                                9302.7
solve T=4000 DH298+intCpH20-intCp298 ! [K]
                                4598.8

! 3. Kirchhoffova věta =====
! C6H5NO2 + 3 H2 -> C6H5NH2 + 2 H2O
n=1000/M(C6H5NO2)      ! [mol]
                                8.1229
Q=-2.8e6                ! [J]
                                -2.8 · 10+06
DHskut=Q/n              ! [J mol-1]
                                -3.4471 · 10+05
DH298=101e3+2*-242e3 - 55e3 ! [J mol-1]
                                -4.38 · 10+05
DCp=102+2*33-110-3*28  ! [JK-1 mol-1]
                                -26
DHteor=DH298+DCp*(250-25) ! [J mol-1]
                                -4.4385 · 10+05
proc=100*DHskut/DHteor  ! [√%]
                                77.663

! 4. Adiabatická teplota vč. fázového přechodu ==
! 3 Fe3O4(s) + 8 Al(s) -> 4 Al2O3(s) + 9 Fe(s)
DH298=4*-1676e3 - 3*-1121e3 ! [J mol-1]
                                -3.341 · 10+06
def HFe=(1808-298)*55+13e3+(T-1808)*46 ! [J mol-1]
def HAl2O3=(2373-298)*133+50e3+(T-2373)*193 ! [J mol-1]
solve T DH298+4*HAl2O3+9*HFe      ! [K]
                                3164.5

! 5. Kirchhoffova věta =====
! C(s) + CO2 -> 2 CO
DH1_298=172.45e3       ! [J mol-1]
                                1.7245 · 10+05
! 2 C(s) + O2 -> 2 CO
DH2_298=-110.53e3*2 ! [J mol-1]
                                -2.2106 · 10+05
def CpCO=27+0.0042*T
def CpCO2=33.4+0.019*T
def CpO2=27+0.0042*T
def CpC=4.0+0.017*T
x=integ T=298,1200 2*CpCO-CpC-CpCO2
                                -3673.3
DH1=DH1_298+x
                                1.6878 · 10+05
x=integ T=298,1200 2*CpCO-2*CpC-CpO2
                                -2994.8
DH2=DH2_298+x
                                -2.2405 · 10+05
pomer=(-DH1)/DH2 ! O2:CO2
                                0.75328

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