Thermodynamics **Test June 19th 2024**

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☐1	☐1	☐1	☐1	☐1	☐1	☐1	☐1
☐2	☐2	☐2	☐2	☐2	☐2	☐2	☐2
☐3	☐3	☐3	☐3	☐3	☐3	☐3	☐3
☐4	☐4	☐4	☐4	☐4	☐4	☐4	☐4
☐5	☐5	☐5	☐5	☐5	☐5	☐5	☐5
☐6	☐6	☐6	☐6	☐6	☐6	☐6	☐6
☐7	☐7	☐7	☐7	☐7	☐7	☐7	☐7
☐8	☐8	☐8	☐8	☐8	☐8	☐8	☐8
☐9	☐9	☐9	☐9	☐9	☐9	☐9	☐9

⟵ Please enter you student number, and write your name above.

NAME, First Name :

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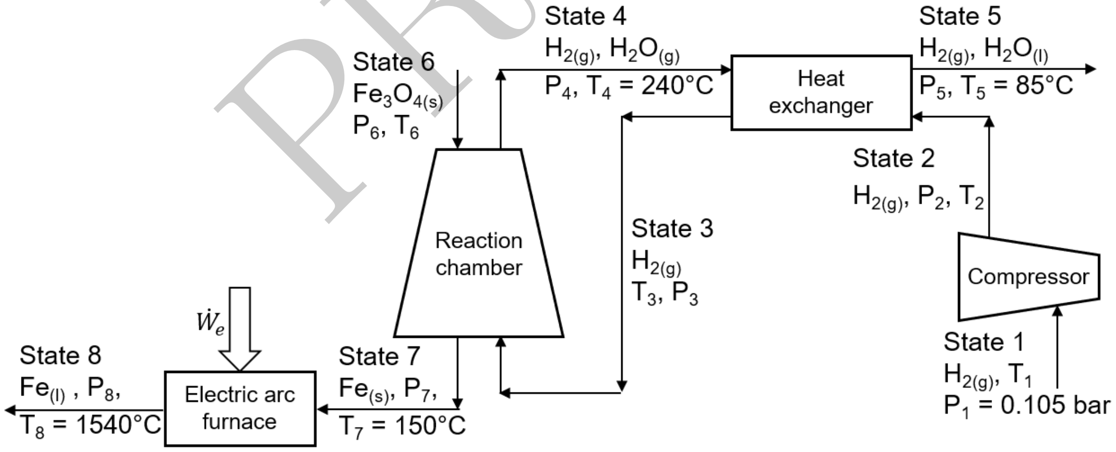
Duration : 3 h - All documents and all calculators authorised - No computer or tablet, no wifi no 4/5G

Thermodynamic data

Molar masses : $M_{Fe_3O_4} = 231.5\,$g/mol, $M_{H_2} = 2.016\,$g/mol, $M_{H_2O} = 18.02\,$g/mol, $M_{Fe} = 55.85\,$g/mol
Iron latent heat of melting at 1540 °C : $L_m = 247\,$kJ/kg
Hydrogen specific heat capacity at constant pressure : $\overline{C}_{P_{H_2}} = 28.8\,$J/(mol K)
Water specific heat capacities : $\overline{C}_{P_{H_2O}} = 1.867\,$kJ/(kg K), $\overline{C}_{H_2O} = 4.184\,$kJ/(kg K)

1 Direct reduction of iron by pure hydrogen (15 points)



Iron production is among the most carbon-intensive manufacturing processes, producing about 7% of world-wide CO_2 emissions. In order to reduce them, alternative processes are currently tested. A new promising ironmaking process is the pure hydrogen direct reduction (H-DR) of iron ore (assumed here as Fe_3O_4) schematised in the figure above. The main process unit is the adiabatic reaction chamber ($\dot{W}_s = 0$) in which this total reaction takes place : $Fe_3O_{4(s)} + 4H_{2(g)} \rightarrow 3Fe_{(s)} + 4H_2O_{(g)}$

The other process units are an isothermal compressor and an adiabatic heat exchanger to respectively compress and heat the hydrogen stream and an electric arc furnace (EAF) converting electric power ($\dot{W}_e$) into heat (efficiency $\eta_{EAF} = 0.925$) to obtain liquid iron. Except P_1 given in figure, all other pressures are 1.00 bar.

Reduction reaction (1.5pts)

Question 1 From the data provided and by clearly explicating your reasoning, give the literal expression of $\Delta_r H^\circ_{298}$ of the reduction reaction.

☐ Empty ☐ 0 ☐ 1 ☐ 2

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Question 2 What is the numerical value of $\Delta_r H^\circ_{298}$ in kJ/mol ?

	☐ 0	☐ 1	☐ 2	☐ 3	☐ 4	☐ 5	☐ 6	☐ 7	☐ 8	☐ 9
☐ +	☐ 0	☐ 1	☐ 2	☐ 3	☐ 4	☐ 5	☐ 6	☐ 7	☐ 8	☐ 9
☐ −	☐ 0	☐ 1	☐ 2	☐ 3	☐ 4	☐ 5	☐ 6	☐ 7	☐ 8	☐ 9

Question 3 From the data provided and by clearly explicating your reasoning, give the literal expression of $\Delta_r G^\circ_{298}$ of the reduction reaction.

☐ Empty ☐ 0 ☐ 1 ☐ 2

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Question 4 What is the numerical value of $\Delta_r G^\circ_{298}$ in kJ/mol ?

	☐ 0	☐ 1	☐ 2	☐ 3	☐ 4	☐ 5	☐ 6	☐ 7	☐ 8	☐ 9
☐ +	☐ 0	☐ 1	☐ 2	☐ 3	☐ 4	☐ 5	☐ 6	☐ 7	☐ 8	☐ 9
☐ −	☐ 0	☐ 1	☐ 2	☐ 3	☐ 4	☐ 5	☐ 6	☐ 7	☐ 8	☐ 9

Reaction chamber (5.5pts)

Question 5 Give the RICE chart of the reaction knowing that $\dot{n}_6 = 45.2\,\text{mol/s}$ and $\dot{n}_3/\dot{n}_6 = 7.50$. Specify the value of $\dot{\xi}_{max}$ (or $\dot{x}_{max}$) and the quantity of all species at equilibrium.

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Question 6 Knowing that $T_3 = 1009\,^{\circ}\mathrm{C}$ give and demonstrate the literal expression of T_6 as function of the given data. ☐Empty ☐0 ☐1 ☐2 ☐3 ☐4

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Question 7 Give the numerical value of T_6 in °C.

☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9
☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9
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☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9

Question 8 Demonstrate the literal expression of $\dot{S}_{cre}$ as function of the given data. ☐Empty ☐0 ☐1 ☐2 ☐3 ☐4

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Question 9 Give the numerical value of $\dot{S}_{cre}$ in W/K.

	☐0	☐1	☐2	☐3	☐4	☐5	☐6	☐7	☐8	☐9
☐+	☐0	☐1	☐2	☐3	☐4	☐5	☐6	☐7	☐8	☐9
☐−	☐0	☐1	☐2	☐3	☐4	☐5	☐6	☐7	☐8	☐9

Heat exchanger (2pts)

Question 10 Assuming from now on that $\dot{n}_4 = 339\,\text{mol/s}$ with molar fraction $x_{H_2} = 0.44$ ($\dot{n}_6 = 45.2\,\text{mol/s}$ and $\dot{n}_3/\dot{n}_6 = 7.50$), give and demonstrate the literal expression of T_2 as function of the given data.

☐Empty ☐0 ☐1 ☐2 ☐3 ☐4

Question 11 Give the numerical value of T_2 in °C.

☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9
☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9

Reversible isothermal compressor (2pts)

Question 12 Assuming from now on that $T_2 = 357\,\text{K}$ ($\dot{n}_6 = 45.2\,\text{mol/s}$ and $\dot{n}_3/\dot{n}_6 = 7.50$), give and demonstrate the literal expression of the exchanged $\dot{W}_s$ as function of the given data.

☐Empty ☐0 ☐1 ☐2 ☐3 ☐4

Question 13 Give the numerical value of $\dot{W}_s$ in MW.

☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9
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☐+ ☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9
☐− ☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9

Electric arc furnace (2pts)

Question 14 Assuming from now on that $\dot{n}_7 = 136\,\text{mol/s}$, give and demonstrate the literal expression of the exchanged $\dot{W}_e$ as function of the given data. ☐Empty ☐0 ☐1 ☐2 ☐3 ☐4

Question 15 Give the numerical value of $\dot{W}_e$ in MW.

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☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9
☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9
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☐0 ☐1 ☐2 ☐3 ☐4 ☐5 ☐6 ☐7 ☐8 ☐9

Conclusion (1pts)

Question 16 How would you explain that $\Delta_r G^\circ_{298}$ of the reaction is positive and $\dot{S}_{cre}$ including all inlets and outlets is also positive ? ☐Empty ☐0 ☐1 ☐2 ☐3 ☐4

2 Classical blast furnace vs direct reduction (6pts)

Iron production is classically performed in a blast furnace where coke (produced from coal) is involved in two reactions : (i) it is burnt with pure oxygen to release CO_2 and heat ; (ii) it reduces iron ore (Fe_3O_4) into iron and CO_2. These reactions will be assumed to take place at constant pressure (1 atm) and constant temperature (2000 K). The bast furnace is considered adiabatic. Coke will be assumed to be pure C in the form of graphite (same enthalpy, entropy and heat capacity).

Additional data : The CO_2 emission of coke production process is 0.2 kg(CO_2)/kg(coke). The annual production of iron is 1.39 GTon. The annual worldwide CO_2 emissions are 35 GTon.

Question 17 What is the fraction f of CO_2 emissions due to iron production in the blast furnace relative to total world-wide CO_2 emissions ?

☐ Empty ☐ 0 ☐ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7 ☐ 8 ☐ 9 ☐ 10 ☐ 11 ☐ 12