

Open Book Exam, Puu 3020, December 11<sup>th</sup>, 2012  
Thermochemical Conversion Technology

15:00-17.00

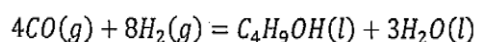
1. Gasification of some biomass resulted in a producer gas of the following composition: 12 mol % CO, 11 mol % H<sub>2</sub>, 16 mol % CO<sub>2</sub>, 55 mol % N<sub>2</sub> and 6 mol % CH<sub>4</sub>. The producer gas can be directly burned (=combusted) to produce energy.

Calculate higher heating (HHV) and lower heating (LHV) values of the producer gas (per mol producer gas) using the **standard combustion enthalpies**,  $\Delta_c H^\circ(298)$ , of the gas components given in the table:

Component	$\Delta_c H^\circ(298)$ , kJ mol <sup>-1</sup>	Component	$\Delta_c H^\circ(298)$ , kJ mol <sup>-1</sup>
CO (g)	-283	N <sub>2</sub> (g)	0
H <sub>2</sub> (g)	-286	CH <sub>4</sub> (g)	-889
CO <sub>2</sub> (g)	0		

Standard enthalpy of water vaporisation at 298 K,  $\Delta_{vap} H^\circ(H_2O)$ , is 44.0 kJ mol<sup>-1</sup>.

2. Synthesis of 1-butanol from syngas proceeds according to the equation:



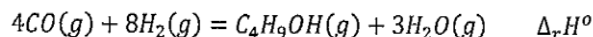
Calculate the efficiencies for the conversion using the formulas below. Higher heating values (HHV) and molar masses for the components are given in the data section at the end.

- a. **Energy efficiency** =  $\frac{HHV(\text{products})}{HHV(\text{reactants})} * 100\%$
- b. **Mass efficiency** =  $\frac{\text{mass of the fuel products}}{\text{mass of the fuel reactants}} * 100\%$  \*
- c. **Carbon efficiency** =  $\frac{\text{moles carbon in the fuel products}}{\text{moles carbon in the fuel reactants}} * 100\%$  \*

\* Note: fuel components exclude H<sub>2</sub>O.

d. How much water is formed per 1 kg of butanol?

3. For the reaction (synthesis of 1-butanol from syngas):



calculate:

- Standard reaction enthalpy at 298 K,  $\Delta_r H^\circ(298)$ , using standard formation enthalpies,  $\Delta_f H^\circ(298)$ , of the components (see data section).
- Standard reaction entropy at 298 K,  $\Delta_r S^\circ(298)$ , using standard entropy values,  $S_m^\circ(298)$ , of the components (see data section).
- Change of the heat capacity at 298 K,  $\Delta_r C_{p,m}^\circ(298)$ , using standard heat capacities,  $C_{p,m}^\circ(298)$ , of the components (see data section).
- Standard reaction enthalpy at 600 K,  $\Delta_r H^\circ(600)$ , using the data obtained in points 3a-3c. Assume that  $\Delta_r C_{p,m}^\circ = \text{const}$  in the temperature range 298-600 K.
- Thermodynamic equilibrium constant at 600 K,  $K$ , using the data obtained in points 3a-3c. Again assume that  $\Delta_r C_{p,m}^\circ = \text{const}$  in the temperature range 298-600 K.

Data section (for tasks 2 and 3).

Component	Molar mass, g mol <sup>-1</sup>	HHV, kJ mol <sup>-1</sup>	$\Delta_f H^\circ(298)$ , kJ mol <sup>-1</sup>	$S_m^\circ(298)$ , J K <sup>-1</sup> mol <sup>-1</sup>	$C_{p,m}^\circ(298)$ , J K <sup>-1</sup> mol <sup>-1</sup>
CO(g)	28.0	283	-110.5	198	29.2
H <sub>2</sub> (g)	2.0	286	0	131	28.8
C <sub>4</sub> H <sub>9</sub> OH(l)	74.1	2670	not needed		
C <sub>4</sub> H <sub>9</sub> OH(g)		not needed	-277	362	108
H <sub>2</sub> O(l)	18.0	0	not needed		
H <sub>2</sub> O(g)		not needed	-242	189	33.6

\* Note: some values are given in kJ, while others are in J.