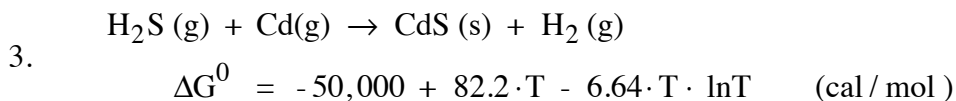
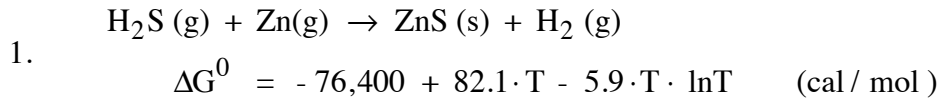


Assignment #3: Thermodynamics & Deposition

(due to Wednesday, February 27, 2017)

- 1) You are involved in deposition ZnS and CdS films for infrared optical coatings. Thermodynamic data reveal:



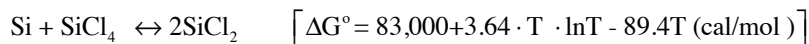
- Are these reactions endothermic or exothermic?
- In practice, reactions 1 and 2 are carried out at 680°C and 600°C, respectively. From the vapor pressures of Zn and Cd at these temperatures, estimate the $P_{\text{H}_2\text{S}} / P_{\text{H}_2}$ ratio for each reaction, assuming equilibrium conditions.

partial pressure of Zinc is given via $\log(p) = -\frac{7070}{T} + 9.41$ (T in K; p in mmHg)

partial pressure of Cadmium is given via $\log(p) = -\frac{5940}{T} + 9.02$ (T in K; p in mmHg)

A. C. Egerton, Vapor Pressure of Zinc, Cadmium and Mercury; Phil. Mag., Vol. 33, p. 33, 1917

- 2) Epitaxial deposition of Si can be achieved by disproportionation reaction



The reaction is carried out in a closed long tubular atmospheric pressure reactor whose diameter is 15 cm. Deposition of Si occurs on a substrate maintained at 750°C and located 25 cm away from the source, which is heated to 900°C.

- Assuming that the thermodynamic equilibrium prevails at the source and substrate, calculate the flux of SiCl_2 transported to the substrate if the gas viscosity is 0.8 mPoise. [Hint: You may assume a linear pressure drop between the source and substrate].
- Consider the same reactor in which one-dimensional steady-state diffusion and convection processes occur together with a homogeneous first-order chemical reaction (not pure viscous flow as previous question). Assume the concentration $C(x)$ of a given species satisfies the ordinary differential equation

$$D \cdot \frac{d^2C}{dx^2} - v \cdot \frac{dC}{dx} - K \cdot C = 0,$$

where K is the chemical rate constant and x is the distance along the reactor. If the boundary conditions are $C(x=0) = 1$ and $C(x=1 \text{ m}) = 0$ derive an expression for $C(x)$. Plot this expression for the concentration profiles if $D = 1000 \text{ cm}^2/\text{s}$, $v = 100 \text{ cm/s}$, and $K=1 \text{ s}^{-1}$. What is the flux at 25 cm away from the source ($C(x=0)$)?