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Reaction: $$SiCl_{4(g)} + 2H_{2(g)} \rightarrow Si_{(s)} + 4HCl_{(g)}$$

Part A: Determine the minimum possible temperature in the reactor to achieve 75% utilization of $SiCl_4$. State any assumptions made.

Assumptions:

1) P=100 Pa. This is a very low operating pressure thus the vapor phase can be assumed to be ideal.
2) Poynting correction is insignificant.
3) Lewis-Randall reference state is assumed for the Si solid phase.
4) The reference fugacity for the gaseous species is 1 bar.

Applying the definition of equilibrium constant

$$K = \frac{\left(\frac{f_{HCl}}{f_{HCl}^\circ}\right)^4 \left(\frac{f_{Si}}{f_{Si}}\right)}{\left(\frac{f_{SiCl_4}}{f_{SiCl_4}^\circ}\right)\left(\frac{f_{H_2}}{f_{H_2}^\circ}\right)^2}$$

Substituting in the reference fugacities (1 bar) and eliminating the solid term,

$$K = \frac{\left(y_{HCl}P\right)^4}{\left(y_{SiCl_4}P\right)\left(y_{H_2}P\right)^2} = \frac{{y_{HCl}}^4}{y_{SiCl_4}{y_{H_2}}^2}P \qquad (1)$$

Now, we will calculate the composition of the vapor phase at equilibrium,

Extent of reaction: $\xi = 0.75$

For mole fractions: $y_i = \frac{n_i^\circ + \upsilon_i \xi}{n^\circ + \upsilon \xi}$

Where n_i° = initial number of moles of species i

n° = initial number of moles of all species

υ_i =stoichiometric coefficient of species i

$\upsilon = \sum \upsilon_i$

Substituting the above relations into Equation (1)

$$K = \frac{\left(\frac{4(0.75)}{3+(1)(0.75)}\right)^4}{\left(\frac{1-0.75}{3+(1)(0.75)}\right)\left(\frac{2-(2)(0.75)}{3+(1)(0.75)}\right)^2}(0.001bar)$$

K=0.3456

(Note: The units of the pressure must be consistent with the units of the reference state)

Now, we will determine K(298K),

$$K(298K) = \exp\left(\frac{-\Delta g^\circ_{rxn}}{RT}\right)$$

The data of all the species is presented in the table below:

	$SiCl_4$	H_2	Si	HCl
Δg_f^o (kJ/mol)	-622.76	0	0	-95.29
Δh_f^o (kJ/mol)	-662.75	0	0	-92.312
A	12.700	3.249	2.879	3.156
B (10^{-3})	0.255	0.422	0.297	0.623
D (10^5)	-1.744	0.083	-0.498	0.151

Solving for the gibbs energy of reaction

$$\Delta g^\circ_{rxn} = \sum_{prod} g^\circ_f - \sum_{reac\tan ts} g^\circ_f$$

$$\Delta g^\circ_{rxn} = 4(-95.29) - (-622.76) = 241.6\frac{kJ}{mol}$$

Solving for K(298K),

$$K(298K) = \exp\left(\frac{-241.6\times 10^3 \frac{J}{mol}}{(8.314\frac{J}{mol-K})(298K)}\right) = 4.47\times 10^{-43}$$

To determine the minimum temperature of reactor, we will use the following relation:

$$\ln\left(\frac{K}{K(298K)}\right) = \left\{\left[-\frac{\Delta h^\circ_{rxn}}{R} + \Delta A(298) + \frac{\Delta B}{2}(298)^2 - \frac{\Delta D}{298}\right]\left(\frac{1}{T} - \frac{1}{298}\right) + \Delta A \ln\left(\frac{T}{298}\right) + \frac{\Delta B}{2}(T-298) + \frac{\Delta D}{2}\left(\frac{1}{T^2} - \frac{1}{298^2}\right)\right\}$$

Solving for heat of reaction at 298K,

$$\Delta h^{\circ}_{rxn} = \sum_{prod} h^{\circ}_f - \sum_{reac\tan t} h^{\circ}_f$$

$$\Delta h^{\circ}_{rxn} = 4(-92.312) - (-662.75) = 293.5 \frac{kJ}{mol}$$

Solving for the delta terms,

$$\Delta X = \sum_{prod} X_i - \sum_{reac\tan t} X_i$$

$$\Delta A = -3.695, \Delta B = 1.69 \times 10^{-3}, \Delta D = 1.684 \times 10^{5}$$

Substituting all the values into Equation (2) and solve for T,

$$\boxed{T = 1747K}$$

Part B: Indicate the effect of each of the following process changes on the minimum possible operating temperature to obtain a utilization of 75%. Explain your reasoning.

(a) Decrease the reactor pressure

$$K = \frac{y_{HCl}{}^{4}}{y_{SiCl_4} y_{H_2}{}^{2}} P$$

As the extent of reaction remains constant, K is directly proportional to P. Thus as P decreases, K will decrease. K is function of T. By Le Chatelier's Principle, for an endothermic reaction, K decreases when T decreases.

Thus the decrease in reactor pressure will result in a decrease in the minimum possible operating temperature.

(b) Dilute the feed stream to a ratio of 1 mol $SiCl_4$: 100 mol H_2

$$K = \frac{\left(\frac{n_{HCl}}{n_T}\right)^4}{\left(\frac{n_{SiCl_4}}{n_T}\right)\left(\frac{n_{H_2}}{n_T}\right)^2} P = \frac{\left(n_{HCl}\right)^4}{\left(n_{SiCl_4}\right)\left(n_{H_2}\right)^2} \frac{P}{n_T}$$

A change in the feed stream caused a change in the number of moles of H_2 and the total number of moles present. The number of moles of $SiCl_4$ and HCl remain constant. Thus the feed stream of 1 mol $SiCl_4$: 100 mol H_2 caused n_{H2} and n_T to increase. K will decrease. Similar to the above argument, T will decrease when K decreases.

Thus the dilution of feed stream will result in a decrease in the minimum possible operating temperature.

Both strategies are able to lower the minimum operating temperature.