1. This question is about the preparation of pure silicon for solar cells

Thousands of tonnes of silicon are produced each year to be used in solar cells. First, metallurgical grade silicon, MGS, is made by reducing quartz (SiO_2, the major component of sand) with carbon in the form of coke and charcoal.

The MGS produced is typically between 98.5 and 99.5 % pure – nowhere near pure enough for the electronics industry. Typical impurities include metals such as iron and aluminium.

sand purified silicon

(a) Write an equation for the reaction between quartz and carbon to form silicon.

High purity silicon can be made from silane (SiH_4) and its derivatives. In one such scheme, silicon is first reacted with HCl at 300 °C to form trichlorosilane and hydrogen. The trichlorosilane is then reduced in a hydrogen environment to form pure silicon.

(b) i) What is the bond angle in silane?

ii) Write the equation for the reduction of trichlorosilane with hydrogen.

This method is rather energy intensive – a more environmentally friendly method has recently been developed which requires a tenth of the energy. In this method ethanol reacts with silicon to form triethoxysilane and hydrogen. Upon heating, the triethoxysilane forms silane gas and tetraethoxysilane in a disproportionation reaction. The silane gas can be decomposed at high temperatures to give pure silicon.

(c) i) Write the equation for the disproportionation of triethoxysilane.

ii) Air must be excluded from the process to avoid the spontaneous ignition of the silane gas. Suggest an equation for this reaction.

An earlier method used to purify the silicon was *zone refining*. In this technique, a bar of impure silicon is melted at one end and then the melt zone is gradually moved along the bar, allowing the silicon to re-solidify behind this zone. Since the impurities are more soluble in the liquid silicon rather than the solid, as the silicon re-solidifies, the impurities become more concentrated in the moving melt zone and hence end up in the last region that re-solidifies.

During zone refining, the concentration, C_x, of a given impurity at position x in the re-solidified bar is given by:

$$C_x = kC_0(1-x)^{k-1}$$

where C_0 is the initial concentration of impurity (usually expressed in number of atoms of impurity per million atoms); x is distance along the bar from the start, expressed as a fraction between 0 and 1; k is a constant known as the *distribution coefficient* whose value depends on the particular impurity. For aluminium, $k = 2.00 \times 10^{-3}$; for iron, $k = 8.00 \times 10^{-6}$.

(d) i) If the initial concentration of aluminium impurity is 3300 ppm atoms, calculate the maximum local concentration of aluminium remaining (in ppm) after one melting, assuming the last 5% of the silicon bar is discarded.

ii) Assuming the only impurity present is iron at 1300 ppm atoms, calculate the minimum percentage of the silicon that would need to be discarded in order to reach the level desirable for photocells, <10 ppm.