SOLUTION FYS9310 problem 200-11
(Defects, Si vacancy charge state, intermediate-easy)

Restate problem:
Derive equation 2.13 in the textbook.

$$C_s(x) = kC_0 \cdot (1-x)^{(k-1)} \quad \text{[eq2.13]}$$

(x is the fraction solidified, k is the equilibrium segregation coefficient, k=C_s/C_L. C_s is the concentration in the solid, C_L is the concentration in the liquid. The well mixed approximation implies that the concentration in the liquid is always homogenous.

Solution:
We can solve by setting up a differential equation or an integral equation for the problem and then either solve these in a general way or just show that that the given equation is a solution (ignoring the possibility that there can be other solutions).

We consider the situation when the fraction x is solidified. We demand that the total amount of impurities is conserved. Before it is solidified the total number of impurities is V_0 $C_0$where V_0 is the volume of the liquid and C_0 the initial concentration. So we have

$$V_0 C_0 = \int_0^x V_0 C_s \cdot (t) \mathrm{d}t + C_s(x) V_0 (1-x) \frac{1}{k} \qquad \text{[eq 1]}$$

The first term on the right is the total number of impurity atoms in the solid. (If t is the fraction solidified, then the increment in that reaction is dt and V_0dt is the incremental volume solidified. The second term on the right is the number of impurity atoms in the melt; $V_0(1$-$x)$ is the volume of the melt. It has a constant concentration which is $C_s(x_s)/k$.

We can then test that the solution [eq2.13] satisfies the integral equation [eq1].

$$V_0 C_0 = \int_0^x V_0 C_0 k \cdot (1-t)^{(k-1)} \mathrm{d}t + kC_0 \cdot (1-x)^{(k-1)} V_0 (1-x) \frac{1}{k}$$

$$1 = \int_0^x k(1-t)^{(k-1)} \mathrm{d}t + (1-x)^{(k-1)}(1-x)$$

$$1 = 1-(1-x)^k + (1-x)^k = 1$$

So the expression in [eq2.13] is a solution of the integral equation.

We could also let Maple solve the integral equation. I transformed it to a differential equation with initial condition using the following Maple commands

$$eq1 := C[0] = \int_0^x Cs(t)\,\mathrm{d}t + \frac{Cs(x)\,(1-x)}{k} \qquad init1 := C_s(0) = k \cdot C_0$$

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> sol:=dsolve({diff(eq1,x),init1},Cs(x));
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$$sol := Cs(x) = (1-x)^{k-1}\, k\, C_0$$