Diffusion through stagnant gas film and reaction at solid surface

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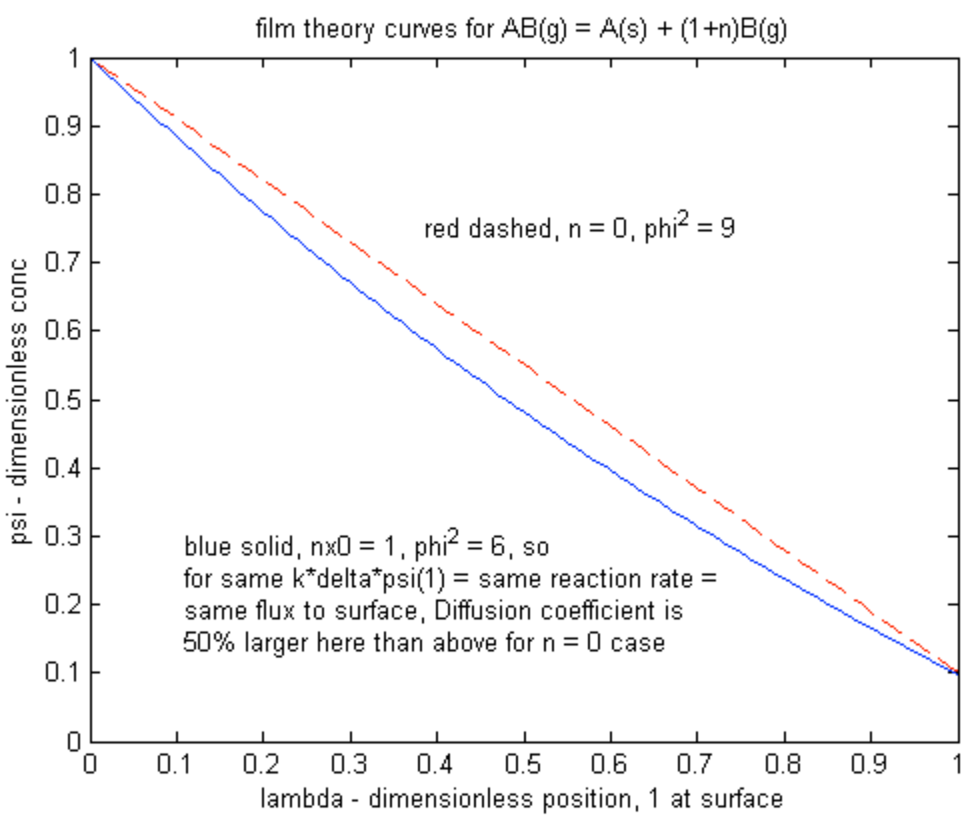
Notation follows that of Middleman and Hochberg, Process Engineering Analysis in Semiconductor Fabrication, McGraw-Hill (1993), pp. 501-503. The reaction at the surface is AB(g) = A(s) + (1+n)B(g).

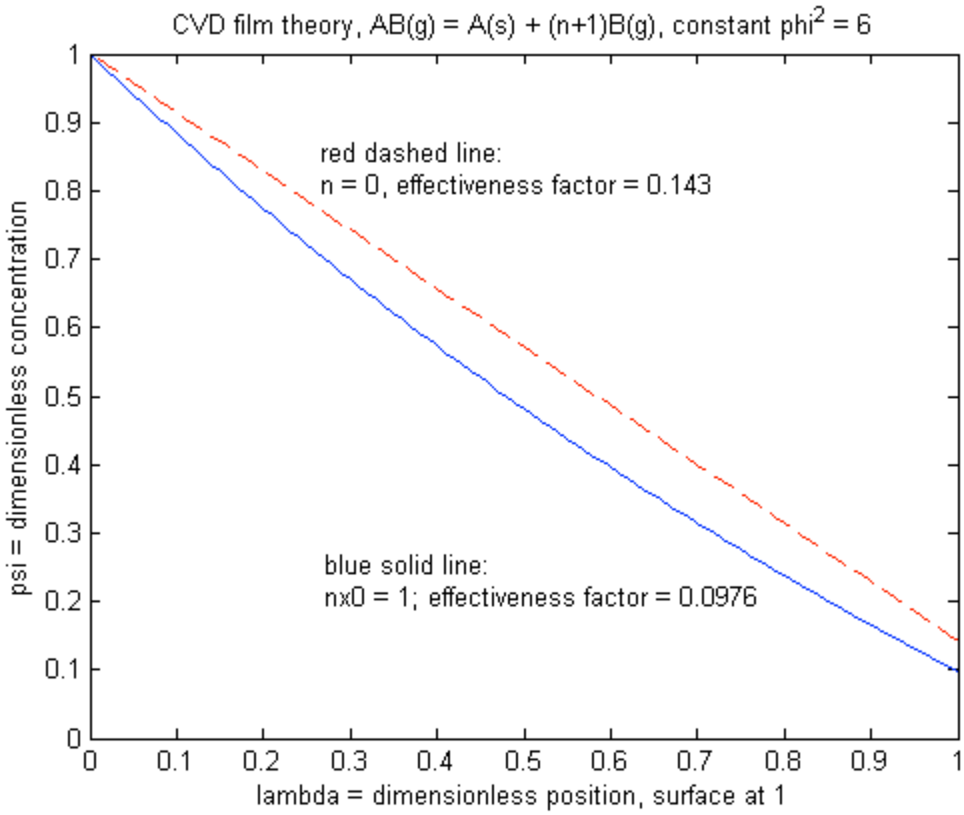
Define dimensionless variables:

$$\psi = \frac{x}{x_0} \quad \lambda = \frac{y}{\delta} \quad \phi^2 = \frac{k\delta}{D}$$

Below is a plot of dimensionless concentration ψ vs. dimensionless position λ for two example cases. In both, the dimensionless gas concentration at the surface is held constant at a value of 0.1. This also means the effectiveness factor equals 0.1 in both cases. In order to hold these the same, the value of the Thiele modulus differs between the two cases.



Below is plot for a case in which ϕ^2 is held constant.



The change in the slope with change in position for the *n* = 1 case can be explained mathematically in the following way. The reactant flux for binary diffusion is given by

$$N_{AB} = -CD\frac{dx_{AB}}{dy} + x_{AB}\left(N_{AB} + N_B\right)$$

$$N_{AB} = -CD\frac{dx_{AB}}{dy} + x_{AB}\left(N_{AB} - (1+n)N_{AB}\right)$$

$$\frac{dx}{dy} = -\left(\frac{N_{AB}}{CD}\right)\left(1+nx\right) \qquad \frac{d\psi}{d\lambda} = -\left(\frac{N_{AB}\delta}{CDx_0}\right)\left(1+nx_0\psi\right) = -\phi^2\psi_1\left(1+nx_0\psi\right)$$

For $n > 0$, as x and ψ decrease in the direction toward the reactive surface, *(dx/dy)* and $(d\psi / d\lambda)$ get less negative.

For *n* NOT = 0:

$$\frac{d\psi}{d\lambda} = -\phi^2\psi_1\left(1+nx_0\psi\right)$$

$$\psi = \left(\frac{1}{nx_0}\right)\left(\left(1+nx_0\right)e^{-nx_0\phi^2\psi_1\lambda} - 1\right)$$

Note that the value of ψ is dependent on the values of both nx_0 and ϕ^2.

$$\psi_1 = \left(\frac{1}{nx_0}\right)\left(\left(1+nx_0\right)e^{-nx_0\phi^2\psi_1} - 1\right)$$

Note that the above equation is not explicit in ψ_1.

For *n* = 0:

$$\frac{d\psi}{d\lambda} = -\phi^2\psi_1 = \text{constant}$$

$$\psi = 1 - \phi^2\psi_1\lambda$$

$$\psi\left(\lambda = 1\right) = \psi_1 = \frac{1}{1+\phi^2}$$

$\psi = 1 - \left(\frac{\phi^2}{1+\phi^2}\right)\lambda$ Note that the curve is uniquely determined by the value of ϕ^2

For all values of n:

$$\eta \equiv \frac{N_{AB}}{kCx_{AB,0}} = \frac{kCx_{AB,\delta}}{kCx_{AB,0}} = \frac{x_{AB,\delta}}{x_{AB,0}} = \psi_1$$