LPCVD reactor - simplest model possible

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$$A_{(g)} + S_{(s)} \rightarrow PS_{(s)} + B_{(g)}$$

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 $S_{(S)}$ represents the silicon wafer surface, and $PS_{(S)}$ is the film product deposited by the reaction. The surface reaction between wafers can be represented by an effectiveness factor times the rate that would be obtained if wafer surfaces were exposed to the reactant gas concentration in the annulus. For plug flow of gas in the annular space between wafer stack and tube wall, the balance on the gas-phase reactant $A_{(g)}$ is:

$$\frac{dC_{\rm A}}{dz} = -\left(\frac{\eta k ({\rm m/s}) A_L ({\rm m^2/m})}{Q ({\rm m^3/s})}\right) C_{\rm A} ({\rm mol/m^3}) \quad ; \quad A_L = A_V \left(\frac{d_g}{d_g + d_w}\right) (\pi R_w^2) \quad ; \quad A_V ({\rm m^2/m^3}) = \left(\frac{2}{d_g}\right) (\pi R_w^2) \quad ; \quad A_V ({\rm m^2/m^3}) = \left(\frac{2}{d_g}\right) (\pi R_w^2) (\pi R_w^2) (\pi R_w^2) (\pi R_w^2) = \left(\frac{2}{d_g}\right) (\pi R_w^2) (\pi R_w^2) (\pi R_w^2) = \left(\frac{2}{d_g}\right) (\pi R_w^2) (\pi R_w^2)$$

where η is the effectiveness factor, A_L is the wafer area per unit length of the stack, A_V is the wafer area per unit volume of gas between wafers, d_g is the distance between wafers, d_w is the thickness of a wafer, and R_w is the wafer radius.

Assume that the concentration gradient between wafers in the axial z direction is small. The balance on $A_{(g)}$ over a ring-shaped control volume between two wafers gives, in dimensionless form:

$$\left(\frac{d^2\psi}{d\lambda^2} + \frac{1}{\lambda}\frac{d\psi}{d\lambda}\right) - \phi^2\psi = 0 \quad \text{B.C. at} \quad \lambda = 0 \quad \frac{d\psi}{d\lambda} = 0 \quad \text{at} \quad \lambda = 1 \quad \psi = 1$$

where $\psi = C_A(\lambda)/C_A(1)$, $\lambda = r/R_w$, $\phi_w = R_w(m) \left(\frac{k'(1/s)}{D(m^2/s)}\right)^{1/2}$

The last term is the Thiele modulus. The effectiveness factor for these cylindrical coordinates is:

$$\eta = \left(\frac{2}{\Phi_w}\right) \left(\frac{I_1(\phi_w)}{I_0(\phi_w)}\right)$$

where the I are modified (hyperbolic) Bessel functions of the first kind, and of order 1 and 0.

The primary objective in the design of the reactor is to get uniform film deposition rate across the radius of the wafers. To do that we want to get an effectiveness factor close to one, for which the reactant concentration across the wafer radius will be almost constant. To do this we want a small value of Thiele modulus. The radius R_w is fixed by the need to make a lot of circuits per wafer. Operating at low pressure can increase the diffusivity D and, thus, decrease the Thiele modulus.

Now back to the rate constants:
$$k'(1/s) = k(m/s) A_V(m^2/m^3) = \left(\frac{2k}{d_g}\right)$$

As d_g decreases, k' increases, Φ_w increases, η decreases, and uniformity decreases - but you can process more wafers in one batch. A tradeoff in reactor design.