$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du \tag{11.89}$$

The purity is defined as

$$P_{\Delta t,i} = \frac{\int_{t_1}^{t_2} y_i F \, dt}{\sum_k \int_{t_1}^{t_2} y_k F \, dt} \tag{11.90}$$

or the amount of solute i eluted in Δt divided by the total sum of all solutes eluted in Δt.

The key in the above analysis is σ. The value of σ will depend on dispersion and adsorption kinetics. With a more detailed analysis it can be shown that

$$\sigma^2 = \frac{v}{kal} \tag{11.91}$$

where v is the superficial fluid velocity (i.e., volumeteric flow rate divided by column diameter A), ka is the surface "reaction" rate consisting of a reaction rate (k) and available surface area (a), and l is column length. The reader may note that σ^2 in eq. 11.91 equals a flow rate divided by the reaction rate and is effectively a Peclet Number. The value of σ^2 depends on rate controlling step; for example[†]

$$\sigma^2 \propto \frac{vd^2}{l} \qquad \text{(internal diffusion control)} \tag{11.92}$$

$$\sigma^2 \propto \frac{v^{1/2}/d^{3/2}}{l} \qquad \text{(external film control)} \tag{11.93}$$

$$\sigma^2 \propto \frac{vd^2}{Dl} \qquad \text{(Taylor dispersion)} \tag{11.94}$$

In the above equations d is the diameter of the particle used to pack the column and D is the effective diffusion coefficient of the solute.

Consider the problem of scale-up of a chromatography process to handle increasing amount of product. One approach might be to increase solute concentration while using the same column. The danger here is that the packing would become saturated, which would reduce purity and yield. Another approach might be to increase both d and A so as to maintain a constant particle-size-to-bed-diameter ratio. Such an approach maintains flow patterns, but note from eqs. 11.92 to 11.94 that σ would increase if d increased. Higher values of σ indicate broadening of peaks and reduced resolution, yield, and purity. Another approach is to fix d and increase both v and l, but maintain the ratio of v to l constant. While this approach will mathematically keep σ constant, there are practical limitations. Lengthening the column increases pressure drop. Since many packings are soft, they compress further, thereby increasing pressure drop, reducing flow, and altering flow patterns. Some chromatography columns have been made in segments, each less than

[†]See P. A. Belter, E. L. Cussler, and W. S. Hu, *Bioseparations,* John Wiley & Sons, New York, 1988.