Figure 11.31. Schematic of output from a chromatography column. The relative t_{max} values are used to calculate resolution, while the standard deviation of a peak ($\sigma t_{max,i}$) is used to estimate yields, purity, and capacity and is used in scale-up.

The yield is defined as the amount of a solute, such as i, collected between times t_1 and t_2 divided by the total amount of i injected into the column. Thus,

$$Y_{\Delta t,i} = \frac{\displaystyle\int_{t_1}^{t_2} y_i \, F \, dt}{\displaystyle\int_{0}^{\infty} y_i \, F \, dt} \qquad (11.86)$$

where y_i is the concentration of solute, i, and F is the solvent flow rate.

The value of y_i can be estimated from the peak height and shape if the peak is assumed to be Gaussian. This assumption leads to

$$y_i = y_{max,i} \, \exp\left[-\frac{(t - t_{max,i})^2}{2(\sigma t_{max,i})^2}\right] \qquad (11.87)$$

where $t_{max,i}$ is the time at which the maximum amount of i elutes, t is elution time, and $\sigma t_{max,i}$ is the standard deviation for peak i. Then the yield can be calculated as

$$Y_{\Delta t,i} = \tfrac{1}{2}\left\{\mathrm{erf}\left[\frac{(t_2 - t_{max,i})}{\sqrt{2}\,\sigma t_{max,i}}\right] - \mathrm{erf}\left[\frac{(t_1 - t_{max,i})}{\sqrt{2}\,\sigma t_{max,i}}\right]\right\} \qquad (11.88)$$

where erf is the error function as defined by