

How to calculate the diffusion coefficient D given a sedimentation coefficient s , a frictional ratio k and partial specific volume \bar{v} , but not the molecular weight M . We have:

Diffusion coefficient and sedimentation coefficient:

$$\begin{array}{|l|} \hline D = \frac{RT}{Nf} \\ \hline \text{Equ. 1} \\ \hline \end{array} \quad \begin{array}{|l|} \hline s = \frac{M(1 - \bar{v}\rho)}{Nf} \\ \hline \text{Equ. 2} \\ \hline \end{array} \quad \begin{array}{|l|} \hline \frac{s}{D} = \frac{M(1 - \bar{v}\rho)}{RT} \\ \hline \text{Equ. 3} \\ \hline \end{array} \quad (\text{Svedberg's law})$$

Frictional coefficient of a sphere ($f/f_0 = 1$):

$$\begin{array}{|l|} \hline f_0 = 6\pi\eta r \\ \hline \text{Equ. 4} \\ \hline \end{array} \quad (\text{Stokes – Einstein Equation, where } \eta \text{ is the viscosity of the solvent.})$$

For the volume of a sphere we have:

$$\begin{array}{|l|} \hline Vol_{sphere} = \frac{4}{3}\pi r^3 \\ \hline \text{Equ. 5} \\ \hline \end{array} \quad \text{or} \quad \begin{array}{|l|} \hline \frac{M\bar{v}}{N} = Vol_{sphere} \\ \hline \text{Equ. 6} \\ \hline \end{array}$$

and for the frictional ratio we have:

$$\begin{array}{|l|} \hline \frac{f}{f_0} = k \\ \hline \text{Equ. 7} \\ \hline \end{array}$$

For a spherical particle, $f/f_0 = 1$, and the radius of the sphere in Eqn. 5 matches the radius of the sphere with the volume calculated in Eqn. 6, and they can be equated and a molar mass can be calculated:

$$\begin{array}{|l|} \hline M = \frac{4N\pi r^3}{3\bar{v}} \\ \hline \text{Equ. 8} \\ \hline \end{array} \quad \text{and from Eqn 4 we have:} \quad \begin{array}{|l|} \hline r = \frac{f_0}{6\pi\eta} \\ \hline \text{Equ. 9} \\ \hline \end{array}$$

Substitute Eqn. 9 into Eqn. 8 to get:

$$\begin{array}{|l|} \hline M_0 = \frac{4N\pi}{3\bar{v}} \left(\frac{f_0}{6\pi\eta} \right)^3 \\ \hline \text{Equ. 10} \\ \hline \end{array}$$

solve Eq. 2 for M and equate with Eq. 10:

$$\begin{array}{|l|} \hline M_0 = \frac{sNf_0}{(1 - \bar{v}\rho)} = \frac{4N\pi}{3\bar{v}} \left(\frac{f_0}{6\pi\eta} \right)^3 \\ \hline \text{Equ. 11} \\ \hline \end{array}$$

This is only true if s is appropriate for f_0

If we parameterize the diffusion coefficient from the frictional ratio, \bar{v} and s , we can use Equ. 1 to calculate D . In order to do so, we need to first figure out what f_0 is. We can do that using Equ. 4, which relates f_0 , and therefore ultimately D , to the radius of a sphere. But which sphere? It has to be the sphere that has the same volume as the particle sedimenting with molar mass M and partial specific volume, \bar{v} . But we do not have M explicitly. M appears in Equ. 2, and also in Equ. 8. Substituting the Stokes Einstein relationship into Equ. 8 we get an equation that can be solved for f_0 as a function of s and \bar{v} alone:

$$\frac{s N f_0}{(1 - \bar{v} \rho)} = \frac{4 N \pi}{3 \bar{v}} \left(\frac{f_0}{6 \pi \eta} \right)^3$$

Equ. 12

solving for f_0 we get:

$$\frac{s N}{(1 - \bar{v} \rho)} = \frac{4 N \pi}{3 \bar{v}} \frac{f_0^2}{(6 \pi \eta)^3}$$

Equ. 13

Simplifying further:

$$9 \eta \pi \sqrt{\frac{2 \bar{v} s \eta}{(1 - \bar{v} \rho)}} = f_0$$

Equ. 14

The corresponding D for a given f_0 can be easily determined from Equ. 1.

Once f_0 is available, any other f can be determined from the frictional ratio (Equ. 7), just use Equ. 1 to derive D . Once both s and D are available, together with the partial specific volume, M can also be derived by solving Equ. 3 for M .