Effective hard-sphere model (EHM) and its analytical results

Theory

Intermolecular interactions have been introduced by Minton et. al. [1–4] in the effective hard-sphere model (EHM), where the size of effective particles depends on the magnitude of intermolecular interactions (Fig.S3).

![Figure S3. Association of two crystallins in macromolecular crowding for EHM. Sketch of two crystallins as reactants polymerising into a dimer as product for effective hard-sphere model (EHM), where dashed lines and blue spheres respectively represent the actual and effective sizes of crystallins.](image)

Since the SPT only gives $\gamma$ for hard-spheres, we implement EHM to introduce attractive interaction between crystallins. According to the approximation of EHM [1–3], if the interaction between particles is pairwise additive and isotropic [5], we have

$$\phi' = \frac{cB_2}{8M},$$

(1)

where $\phi'$ is effective packing fraction, $c$ is protein concentration and $M = 21kDa$ is the molar mass of crystallins. The second virial coefficient, $B_2$, reflects the pair interaction between crystallins:

$$B_2 = 4\pi N_a \int_0^\infty \left[ 1 - e^{-U(r)/kT} \right] r^2 dr,$$

(2)

where $U(r)$ is the interactive potential, $r$ is the distance between two molecules, $N_a$ is Avogadro number and $k$ is Boltzmann constant.

Therefore, $\phi'$ changes as a function of interaction between particles. The larger the attraction between proteins, the smaller the value of $\phi'$ (see Fig.S3). By substituting $\phi'$ for $\phi$ in Eq.5 in our main text, we obtain the activity coefficient of crystallins for EHM.

References


