Diffusion of Vitamin B12 Across a Mesoporous Metal Organic Framework

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Abstract

The rate of uptake and the rate of release of a Vitamin B12 solution (dissolved in water) at 2 different temperatures (room temperature and 37 C) by the mesoporous metal organic framework TbMOF-100 were measured at 1-hour intervals using a spectrophotometer. Through the usage of the Beer-Lambert law, the concentration of the stock solution was calculated based on the absorbance values obtained with the spectrophotometer. These values allowed for the quantification of the rate of uptake and rate release of Vitamin B12 by the TbMOF-100, while the value of the coefficient of diffusion for this 2-phase system was calculated using Fick's laws of diffusion.

Problem Statement

To study the kinetics of diffusion of biomolecules into new types of porous materials at different temperatures. Consider the initial rate of uptake, the diffusion rate, and the coefficient of diffusion for a 2-phase system consisting of TbMOF-100 and Vitamin B12 solution.

Porous metal–organic frameworks (MOFs) are highly crystalline inorganic–organic hybrids, and they are constructed by assembling metal ions or metal-containing clusters known as secondary building units (SBUs) with multidentate organic ligands via coordination bonds into a three-dimensional structure (Ma.) The research experiment conducted dealt with the applications of MOFs for biocatalysis. A study of the diffusion of vitamins into metal-organic frameworks is relevant, because it provides information that is necessary to determine the efficiency of encapsulating the vitamin within the mesoporous structure.

Mathematical Approach

Calculating the Coefficient of Diffusion

An approximation of the true value of the diffusion coefficient for this 2-phase system can be calculated through the usage of the following formula:

$$\theta_f = \frac{\beta}{\beta+1} + \sum_{i=1}^{\infty} \frac{6\beta e^{-\lambda_i^2 \tau}}{9(1+\beta)+\beta^2\lambda_i^2}$$

In this model, the equation has been cast in dimensionless form through the use of Laplace transforms as follows:

$$\theta_f = \frac{C_f}{C_0},\quad \beta = \frac{V_f}{\Phi V_b},\ \text{and}\ \tau = \frac{tD_{eff}}{R^2}$$

Where Cf is the concentration in the solution in water at time t, C_o is the initial concentration of the Vitamin B12 solution, V_f is the volume of the solution, V_b is the volume of the TbMOF-100 crystals, D_{eff} is the diffusion coefficient of the solution, and R is the radius of the crystal structure. Furthermore, in this model, λi are the solutions to the equation,

$$\tan\lambda_i = \frac{3\lambda_i}{3+\beta\lambda_i^2},$$

Incubation Time (in hours)	Vitamin B12 Solution Absorbance	Vitamin B12 Solution Concentration (in mM)
0	0.591903	2.23
1	0.505663	1.91
2	0.506142	1.91
3	0.471538	1.78
4	0.468357	1.77
5	0.440578	1.66
6	0.435000	1.64
19.3	0.345054	1.30

Table 1: *Vitamin B12 Solution Absorbances and Concentrations*

Incubation Time (in hours)	Concentration Absorbed by TbMOF-100 (in mM)
0	0
1	0.32
2	0.32
3	0.45
4	0.46
5	0.57
6	0.59
19.3	0.93

Table 2: *Concentration Absorbed by TbMOF-100*

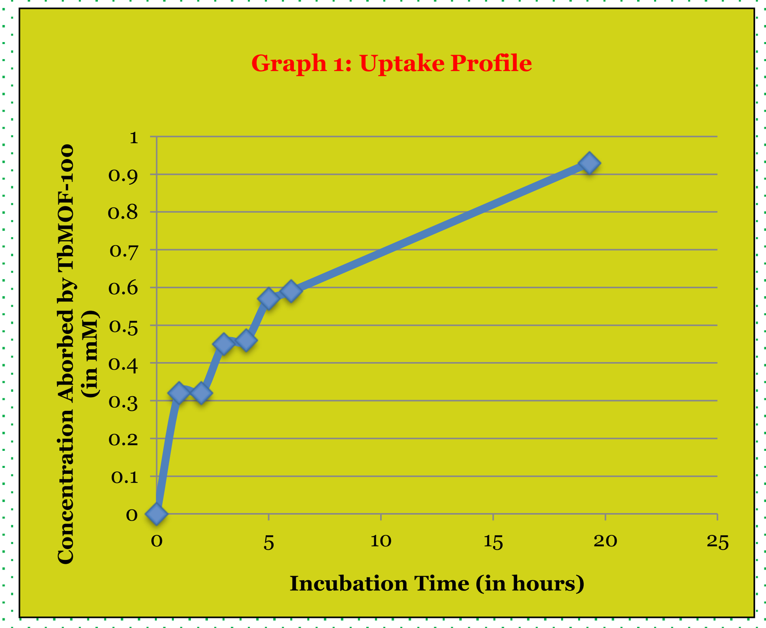
Discussion

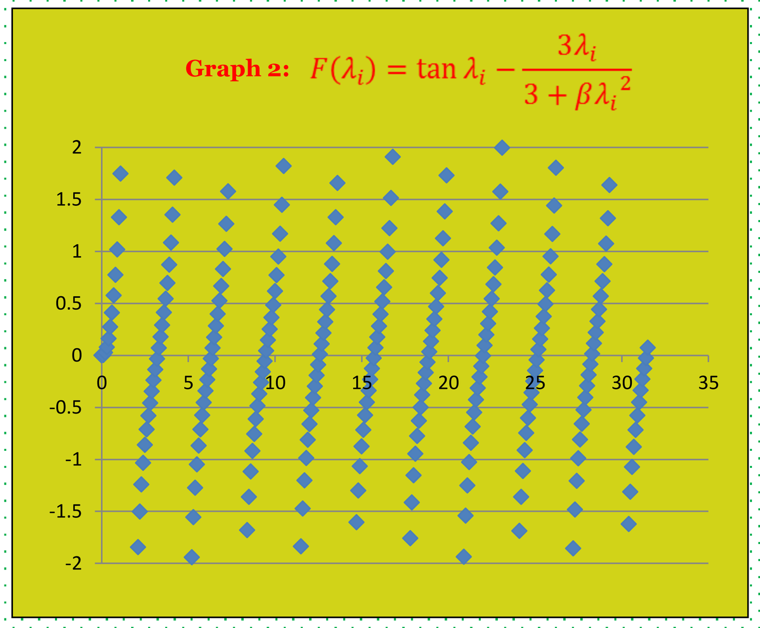
The objective of this project was to calculate the initial rate of uptake, the rate of uptake at a random incubation time, and the coefficient of diffusion for this 2-phase system. The objectives of this project were met. The initial rate of uptake was calculated to be 0.0880783051 mM/hour using the first derivative of the best-fit line for the data.

This characteristic is also supported by the graphical representation of the data, since the graph of the data is concave down. In addition, the coefficient of diffusion for this 2-phase system was found to be 44 nm^2/ hour, which was also expected, since this positive value confirms that diffusion of the Vitamin B12 into the mesoporous material did indeed occur

Conclusions

As expected, the initial rate of uptake was higher that the rate of uptake at later incubation times. In addition, the coefficient of diffusion was calculated to be 44 nm^2/ hour. This confirms that the TbMOF-100 is a porous material as its value for the coefficient of diffusion can be explained by its porous structure, which allows for the capture of the Vitamin B12 inside its cages. Several recommendations could be given to provide a more accurate result for the value of the coefficient of diffusion for this system. It would be useful to conduct the experiment to measure the uptake profile on a sonicator (which is pictured in the appendices,) to keep the Vitamin B12 solution constantly mixed. Another recommendation, would be to construct a new model to compute the coefficient of diffusion, that took into account the non-spherical structure of the TbMOF-100.





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