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Mathematical Modeling of Cell Packings

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Abstract

The concept of packing density of cells is discussed in this paper. In particular it is well known that in two extreme cell packing cases, the value of packing density are $\frac{1}{3}, \frac{1}{2}$. But most often perfect packing of cells may not be possible. To find the packing density in such non-idealized packing of cells, I had introduced a prototype random sequential adsorption model whose solution is derived mathematically. Finally, the limiting packing density of the cells in non-idealized conditions is determined and it is found be in good agreement with the average of the possible packing density values in idealized situations.

Keywords: Packing Density, Random Sequential Adsorption, Recurrence Relation, Exponential Series, Limiting Packing Density.

1. Introduction

To begin with we suppose that the joint area for lymphocyte-RBC adhesion is *a*. If the surface area of the cell is *S*, then tentatively we may assume that there are $M = \frac{S}{a}$ possible binding areas. But one practical problem that we may encounter in this assumption is that the number *M* that can fit a cell will not be exactly $\frac{S}{a}$ because that value would require a perfect fit, and the bound RBCs do not have the mobility to readjust. In fact, we can compare this situation to that of the classical "parking problem" in which cars arrive randomly and park along a curb, the number that can fit depending upon just how they arrive. In this paper, I will describe mathematical way of cell packing.

2. Describing the Model

Considering the simplest discrete version, consider a grid of extended adhesive sites in one dimension, and suppose that any cell that adheres to a site precludes the two adjacent sites from being used. Let *n* denote the packing density of the cells. There are clearly two extreme cell packing. In one extreme, they pile up as close to each other as possible, occupying every other site, for a density $n = \frac{1}{2}$. In the other extreme, gaps of two sites are left that cannot be filled, so that $n = \frac{1}{3}$. All final packings (which can accept no more cells) must then satisfy $\frac{1}{3} \le n_\infty \le \frac{1}{2}$. If the cells are adsorbed sequentially but randomly, what is the mean final packing density? Or equivalently the mean density of accepted sites under the

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restriction of next neighbor exclusion? The purpose of this model is to answer these questions and determine its distribution.

To solve this prototypical Random Sequential Adsorption (RSA) problem, I use Flory's technique (applied originally to pair-bond formation on a polymer chain). Suppose a segment of $k > 2$ unoccupied sites, say 1, 2, . . . , k with 0 and $k + 1$ occupied, has when filled to "jamming" (no cell can be added) an average of A_k vacant sites remaining. Clearly, $A_1 = 1, A_2 = 2, A_3 = 2$. But a cell dropped randomly on the unoccupied segment will adhere with equal probability $\frac{1}{k-2}$ to one of the available sites 2, . . . , $k - 1$. If it adheres at site j, there remains one empty sub-lattice of $j - 1$ sites, and one of $k - j$ sites. Hence for $k > 2$, we have the recurrence relation

$$A_k = \frac{1}{k-2}\sum_{j=2}^{k-1}\left(A_{j-1} + A_{k-j}\right) = \frac{2}{k-2}\sum_{j=1}^{k-2}A_j \quad (2.1)$$

3. Solving the Model

To solve (2.1), we note that $(k-1)A_{k+1} - (k-2)A_k = 2\left(\sum_{j=1}^{k-1}A_j - \sum_{j=1}^{k-2}A_j\right) = 2A_{k-1}$ (3.1)

If we now define $B_k = A_{k+1} - A_k$ (3.2) then $B_1 = A_2 - A_1 = 2 - 1 = 1, B_2 = A_3 - A_2 = 2 - 2 = 0$.

Using (3.1), we get

$$2A_k - 2A_{k-1} = \left[kA_{k+2} - (k-1)A_{k+1}\right] - \left[(k-1)A_{k+1} - (k-2)A_k\right] = kA_{k+2} - 2(k-1)A_{k+1} + (k-2)A_k \quad (3.3)$$

Now equation (3.3) can be re-written as $k\left(A_{k+2} - A_{k+1}\right) - (k-2)\left(A_{k+1} - A_k\right) - 2\left(A_k - A_{k-1}\right) = 0$

In view of (3.2), we get $kB_{k+1} - (k-2)B_k - 2B_{k-1} = 0$ (3.4) where $B_1 = 1, B_2 = 0$.

Now to solve (3.4) we can rewrite it as $k\left(B_{k+1} - B_k\right) = -2\left(B_k - B_{k-1}\right)$ (3.5) where $B_2 - B_1 = -1$.

Now for $k \geq 1$, from (3.5), we get

$$B_{k+1} - B_k = -\frac{2}{k}\left(B_k - B_{k-1}\right) = -\frac{2}{k}\times -\frac{2}{k-1}\left(B_{k-1} - B_{k-2}\right) = -\frac{2}{k}\times -\frac{2}{k-1}\times\cdots\times -\frac{2}{2}\left(B_2 - B_1\right)$$

Thus, $B_{k+1} - B_k = -\frac{2}{k}\times -\frac{2}{k-1}\times\cdots\times -\frac{2}{2}(-1) = \left(-1\right)^k\frac{2^{k-1}}{k!}$ (3.6)

Now in (3.6) substitute $k = 1, 2, 3, ..., r$ successively and add to get

$$\left(B_2 - B_1\right) + \left(B_3 - B_2\right) + \cdots + \left(B_r - B_{r-1}\right) + \left(B_{r+1} - B_r\right) = \sum_{k=1}^{r}\left(-1\right)^k\frac{2^{k-1}}{k!}$$

$$B_{r+1} - B_1 = \sum_{k=1}^{r}\left(-1\right)^k\frac{2^{k-1}}{k!} \quad (3.7)$$

Now the objective is to determine B_∞ which is obtained by considering the limit as $r \to \infty$ in (3.7). Doing this, we get

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$$B_\infty = \lim_{r\to\infty} B_{r+1} = B_1 + \sum_{k=1}^{\infty}(-1)^k \frac{2^{k-1}}{k!} \quad (3.8)$$

From exponential series, for any real number *x*, we know that $e^x = \sum_{k=0}^{\infty}\frac{x^k}{k!}$ and noting that $B_1 = 1$, from (3.8) we have

$$B_\infty = 1 + \sum_{k=1}^{\infty}(-1)^k \frac{2^{k-1}}{k!} = 1 + \frac{1}{2}\sum_{k=1}^{\infty}(-1)^k \frac{2^k}{k!} = 1 + \frac{1}{2}\left(\sum_{k=0}^{\infty}\frac{(-2)^k}{k!} - 1\right) = 1 + \frac{1}{2}\left(e^{-2} - 1\right)$$

Thus, $B_\infty = \dfrac{1+e^{-2}}{2}$ (3.9)

But we find that the limiting packing density n_∞ is given by the expression $n_\infty = 1 - B_\infty = 1 - \left(\dfrac{1+e^{-2}}{2}\right) = \dfrac{1-e^{-2}}{2}$ (3.10)

Thus from (3.10) we see that $n_\infty = 0.43233$ which is fairly close to the average of the minimum and maximum values of *n* namely $\frac{1}{2}(n_{\min} + n_{\max}) = \frac{1}{2}\left(\frac{1}{3} + \frac{1}{2}\right) = 0.4166$

4. Conclusion

Realizing the fact that the cells cannot be packed in the ideal form given by $M = \frac{S}{a}$, I have introduced a prototype Random Sequential Adsorption (RSA) model, through which obtained a recurrence relation in (2.1).

In section 3, detailed mathematical explanation is given to derive $B_{k+1} - B_k$ in (3.7). This expression enabled us to compute B_∞ as in (3.9). Using the fact that the limiting packing density n_∞ is the complement of B_∞ with respect to 1, I had finally arrived for nice expression for limiting packing density proving that $n_\infty = 0.4166$ approximately. We can notice that this value fits well in the specified range for all final cell packing values namely $\frac{1}{3} \le n_\infty \le \frac{1}{2}$. Moreover, we also observe that the derived value $n_\infty = 0.4166$ is fairly close enough to the average of minimum and maximum possible packing density of the cells which is 0.43233. Thus in this paper I had proved that the limiting packing density of the cells in non-idealized conditions is a fairly good estimate to the average of the possible packing density values in idealized situations.

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