KMC Bacteria Hopping And Trapping Notes

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I. Problem Description

In a 3D domain, some flagellated bacteria will swim with a two state motion called a "run" and "tumble". The flagella "runs" in a straight direction for a few body lengths by bundling and rotating its flagella. After a few body lengths, the flagella unravels its bundle, which causes it to slow and tumble. It then goes off in a new random direction having been re-oriented by its tumble. In doing this, it is believed that bacteria sample the domain to construct a gradient of a food source or a specific chemical. In this motion, it is often presumed that the run time is much longer than its tumble time and so the diffusion can be estimated by considering its average run length and run time.

In a porous medium, it has been observed that flagellated bacteria employ a different two state motion called "hopping" and "trapping" [1]. The bacteria will swim or "hop" in a straight direction until it gets stuck or "trapped" due to the confinement of neighboring pores. While trapped, the bacteria re-orients and goes off in an almost random direction; it has a slightly higher chance of going back the way it came from, but we will assume its re-orientation angle to be uniformly distributed. The bacteria spends a larger time trapped than in its hop state. Hence an estimation of their diffusivity through the porous medium can be obtained from the average hop length $\langle \ell \rangle$ and trapped time $\langle \tau \rangle$–instead of the average hop time as in the homogenous space "run" and "tumble" motion.

The motion of flagellated bacteria through porous media was observed and measured in porous distributions with pores of characteristic sizes (a) 3.6 μm, (b) 2.5 μm, and (c) 1.9 μm [1]. It was observed that smaller pore sizes increased the effects of pore confinement. So, in smaller pore size distribution, the bacteria experience more trapping and less hopping.

The experimenters ran tests to measure the effect of bacteria crowding and concluded that their populations were dilute enough to rule out significant effects of bacteria collisions on their results; this suggests we can use the Fickian (free) diffusion model. They measured the velocity distributions of the bacteria in their experiments and set the threshold between the two states, hopping and trapping, to be half their measured value of the run velocity in a homogeneous domain; the threshold is 14 μm/s. They ran tests using several threshold velocities, between 8 and 20 μm/s, and found the choice of the threshold had little to no effect on their results. The experimenters measured re-orientation angle distributions of the bacteria during both their hopping and trapping states and found that in the hopping state, the bacteria swim straight ahead without much deviation and in the trapped state, the motion is almost random, with a slight tendency of the bacteria to turn around and head back the way it came from. We will assume the re-orientation angle to be random during that trapped state, and to be straight ahead in the hopping state.

The group also measured distributions of the hopping lengths and reported their means, $\langle \ell \rangle$, as (a) 3.24 μm, (b) 2.79 μm, and (c) 2.14 μm and distributions of the trapped times, but do not report the means, $\langle \tau \rangle$, of the trapped times. The group also reported their measurements of the diffusivities of the bacteria through the different pore distributions to be (a) (2 ± 0.25) μm^2/s, (b) (1 ± 0.25) μm^2/s, and (c) (0.5 ± 0.25) μm^2/s. They compared their measurements to a simple model in which the bacteria are assumed to perform a random walk of step length $\langle \ell \rangle$ and step time $\langle \tau \rangle$ and an estimated diffusivity D_{RW} given by

$$D_{RW} = \frac{\langle \ell \rangle^2}{3\langle \tau \rangle}. \tag{1}$$

To compare their predicted diffusivities to their measured diffusivities, they plotted them against each other and fit a line. Their line fit gave that the measured diffusivities, on average, were about 0.3 times that of the predicted diffusivites, or in other words, the measured diffusivities were about $\langle \ell \rangle^2/10\langle \tau \rangle$. From their predicted diffusivities, (a) 7 μm^2/s, (b) 3 μm^2/s, and (c) 2 μm^2/s, we can approximate their measurements of the mean trapped times, $\langle \tau \rangle$, by eqn. (1). We estimate the mean trapped times as (a) 0.5s, (b) 0.8649s, and (c) 0.7633s.

II. Subvolume KMC method with distributed hop hength and trapped time

Here we will present a KMC method that is essentially an alteration of the subvolume KMC method to allow for a distributed hop length ℓ to be sampled. Similar to the subvolume KMC method, we sample the amount of time spent in the lattice cell before hopping to another state, where the time spent in the lattice cell is called the trapped time τ. Then we sample a re-orientation direction and a hop length.

We apply this method to study the diffusion of bacteria in a porous media [1]. In order to simulate for the diffusivity, we will only require one bacteria in our simulations, which can be placed in any lattice of our 3D domain. At each iteration, the bacteria will be in another trapped state in the process of re-orienting itself to hop to another trapped state. We ignore the hop times and only consider the trapped times. Thus at each iteration, we sample a Poisson distribution (which is an estimation of the actual distribution) with an average set to half the trapped time $\langle \tau \rangle$;

we found that by using the half trapped time, rather than the whole trapped time, in the Poisson distribution, our diffusivity predictions are significantly better. We then sample a direction from a uniform distribution. Finally we sample another Poisson distribution (another approximation) fitted to the mean hop length $\langle \ell \rangle$.

III. Results

We simulated the diffusion of a single bacteria in porous media with pore distributions of pore sizes (a) 3.6 μm, (b) 2.5 μm, and (c) 1.9 μm for 10 minutes per KMC iteration. Our results, averaged over the iterations, for the different pore size distributions are shown in figure 1. Our results in figure 1 reflect the effects of pore confinement on the bacterias diffusion rate through porous media, where smaller pore size distribution result in more pore confinement.

Our averaged diffusivity, over 10^5 iterations, for the pore size distributions are (a) 2.3 μm^2/s, (b) 1.0 μm^2/s, and (c) 0.67 μm^2/s. We plotted the measured diffusivities from the experiments [1] against our simulated diffusivities in figure 2. The line fit (black line) $y = 0.88 * x$, in figure 2, demonstrates that on average the percent error is less than 14% which is quite good considering the hop times and re-orientation direction distributions are ignored; we assumed the hop times and re-orientation directions to be negligible and uniformly distributed, respectively. The measured diffusivities in [4] are reported to the nearest 0.5 μm^2/s and so our simulated values for pores of sizes 1.9 μm and 2.5 μm agree quite well for this level of precision in the measured values. Our simulated diffusivity for pores of size 3.6 μm is closer to 2.5 μm^2/s than the reported measured value of about 2 μm^2/s , which we attribute to the bacteria spending less time trapped and more time hopping. Since our model assumes the hopping time to be negligible, we

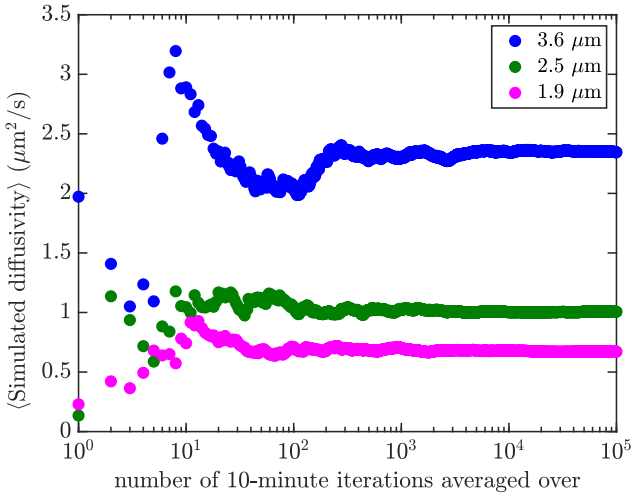

Figure 1. We ran 10-minute KMC simulations to measure the diffusivity of a bacteria swimming in porous media with the pore size distributions indicated and report, here, the average simulated diffusivity as a function of KMC iterations. Due to increased pore confinement effects, bacteria diffuse more slowly in media with smaller pore size distributions.

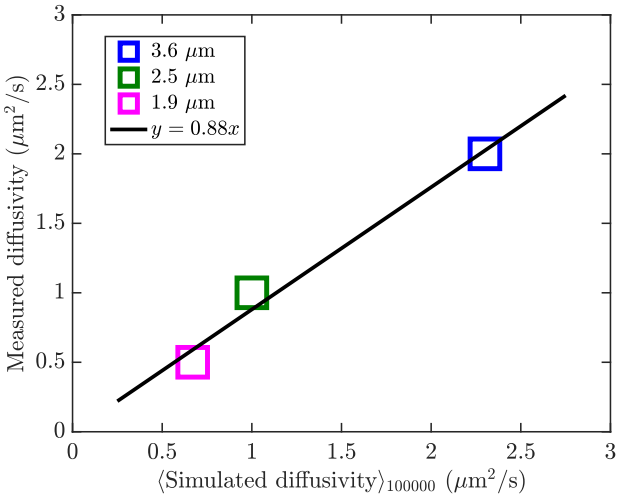

Figure 2. We compare our simulated diffusivities, averaged over 100000 10-minute simulations of a bacteria hopping and trapping in porous media with the pore size distributions indicated, to the measured diffusivities in experiments [1]. The black line is a line fit and demonstrates that on average our simulated calculations yield diffusivities about 14% larger than the experimentally measured diffusivities.

always underestimate the transition times and so our simulated values always overestimate the measured diffusivities.

Bibliography

[1] Tapomoy Bhattacharjee and Sujit S. Datta. Bacterial hopping and trapping in porous media. *Nature Communications*, 10(1), May 2019.