

Biophysical Journal, Volume 112

Supplemental Information

A Model for the Transient Subdiffusive Behavior of Particles in Mucus

Matthias Ernst, Thomas John, Marco Guenther, Christian Wagner, Ulrich F. Schaefer, and Claus-Michael Lehr

```

%% Input

L = 500e-9; % distance between permeable membranes in m

R = 100e-9; % particle radius in m

N = 10000; % number of time steps / iterations

M = 10000; % number of particles

T = 10; % total time in s

ts = T/N; % time step in s

time = ts*(0:N-1); % time in s

pM = 0.5; % permeation parameter in 1/sqrt(s)

r = 1 - pM*sqrt(ts); % reflection probability

V = 0.004; % dynamic viscosity in Pa*s

kb = 1.38e-23; % Boltzmann constant in J/K

Temp = 310.15; % absolute temperature in K

D0 = (kb*Temp)/(6*pi*V*R); % diffusion coefficient (Stokes-Einstein) in m2/s

%% simulation

x_0 = repmat(L*rand(M,1),1,N);

dx = sqrt(2*D0*ts);

xpos = x_0;

for m = 1:M

    for n = 1:N-1

        step = dx*randn;

        xpos(m,n+1) = xpos(m,n) + step;

        if mod(xpos(m,n),L) + step > L && rand < r

            xpos(m,n+1) = xpos(m,n) - step + 2*L - 2*mod(xpos(m,n),L);

        elseif mod(xpos(m,n),L) + step < 0 && rand < r

            xpos(m,n+1) = xpos(m,n) - step - 2*mod(xpos(m,n),L);

        end

    end

```

```

end

end

msd = mean((xpos-x_0).^2,1); % mean squared displacement in m
Deff = msd(end)/(2*T); % effective diffusion coefficient in m2/s

%% Output

% Create figure

figure1 = figure;

% Create axes

axes1 = axes('Parent',figure1,'YScale','log','YMinorTick','on',...
    'XScale','log',...
    'XMinorTick','on');

box(axes1,'on');

hold(axes1,'all');

% Create multiple lines using matrix input to loglog

loglog1 = loglog(time,[msd;2*D0*time;2*Deff*time],'Parent',axes1);

set(loglog1(1),...
    'DisplayName','normal diffusion with D0 and effective diffusion coefficient (r > 0)');

set(loglog1(2),'DisplayName','normal diffusion with D0 and r = 0');

set(loglog1(3),'DisplayName','normal diffusion with Deff');

% Create xlabel

xlabel('time [s]');

% Create ylabel

ylabel('MSD [m2]');

```

```
% Create legend
```

```
legend(axes1,'show','Location','NW');
```