An investigation on the use of the diffusion theory computational models to characterize the antibacterial action of ZnO

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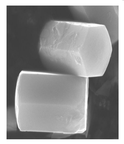
Abstract

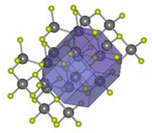
Antimicrobial action of micro- and nanoscale ZnO particles has been documented, but the fundamental physical mechanisms driving these actions are still not identified. We hypothesize that one of the key mechanisms behind the antibacterial action of ZnO is rooted in interactions between ZnO surfaces and extracellular material. An investigation was done of the biological components of that interaction using diffusion theory and more specifically Brownian motion computational models to look at the interaction of Zn+2 and O-2 ions with staphylococcus aureus bacteria. The analysis allowed us to find a correlation between the thickness of the staphylococcus aureus bacteria and the amount of the zinc and oxygen ions present in the solution.

Introduction

- Fundamental mechanisms driving antibacterial action for ZnO is still unknown.
- Antimicrobial behavior of ZnO is initiated by interactions of surfaces

Zinc Oxide Crystal Structure





- ZnO has Hexagonal structure composed of alternating layers of Zn^{2+} and O^{2-} ions
- Structure yields net charge at hexagonal (polar) faces and neutral charge on rectangular (non-polar) sides
- Nature of these crystallographic faces (neutral, negative, positive) could be very different.

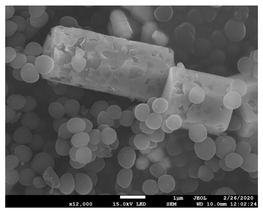
Diffusion and Forward-Euler Method

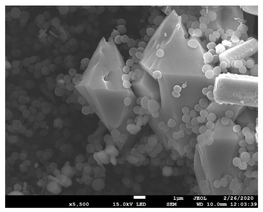
Diffusion is a process of random motion of particles of which there is a net flow of matter from higher concentration to lower concentration.

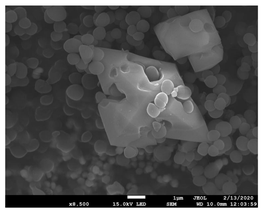
- Staphylococcus is a type of bacteria that constitutes it as one of the most common infections.
- We want to investigate the diffusion of Zn and O ions from the extracellular to the intracellular environment through the staph. extracellular wall and investigate the concentration after diffusion,
- We need to create a computational model to investigate the diffusion of the ions through the wall with the use of some differential equations.

Bacterial Growth Inhibition

- **Interaction of Staphylococcus Aureous**







Differential Equation Set up

- Differential Equation that will help us solve the actual equation.

```
def ode_FE(f, U_0, dt, T):
    N_t = int(round(float(T)/dt))
    # Ensure that any list/tuple returned from f_ is wrapped as array
    f_ = lambda u, t: asarray(f(u, t))
    u = zeros((N_t+1, len(U_0)))
    t = linspace(0, N_t*dt, len(u))
    u[0] = U_0
    for n in range(N_t):
        u[n+1] = u[n] + dt*f_(u[n], t[n])
    return u, t
```

- Equations used to define and solve the differential equations.

$$\frac{du_0}{dt} = s'(t),$$

$$\frac{du_i}{dt} = \frac{\beta}{\Delta x^2}(u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)) + g_i(t), \quad i = 1, \ldots, N-1,$$

$$\frac{du_N}{dt} = \frac{2\beta}{\Delta x^2}(u_{N-1}(t) - u_N(t)) + g_N(t)\,.$$

- Where u signifies the concentration and N the number of times that we run the simulation.

Solution of the Differential Equation and Model

- **Defining the equations into code and using an actual solution of u to run the simulation and using N= 2 and L which is the length of the outer wall L = 1.5 cm.**

```
def rhs(u, t):
    N = len(u) - 1
    rhs = zeros(N+1)
    rhs[0] = dsdt(t)
    for i in range(1, N):
        rhs[i] = (beta/dx**2)*(u[i+1] - 2*u[i] + u[i-1]) + \
                 g(x[i], t)
    rhs[N] = (beta/dx**2)*(2*u[N-1] + 2*dx*dudx(t) -
                           2*u[N]) + g(x[N], t)
    return rhs

def u_exact(x, t):
    return (3*t + 2)*(x - L)

def dudx(t):
    return (3*t + 2)

def s(t):
    return u_exact(0, t)

def dsdt(t):
    return 3*(-L)

def g(x, t):
    return 3*(x-L)

def test_rod_diffusion_hand():
    global beta, dx, L, x       # needed in rhs
    L = 1.5
    beta = 0.5
    N = 2
    x = linspace(0, L, N+1)
    dx = x[1] - x[0]
    u = zeros(N+1)

    U_0 = zeros(N+1)
    U_0[0] = s(0)
    U_0[1:] = u_exact(x[1:], 0)

    u_hand = zeros((3, len(U_0)))
    u_hand[0,:] = -3.0, -1.5, 0.0    # spatial indices: 0, 1 and 2
    u_hand[1,:] = -3.45, -1.725, 0.0
    u_hand[2,:] = -3.90, -1.95, 0.0

    dt = 0.1

    u, t = ode_FE(rhs, U_0, dt, T=1.2)

    tol = 1E-12
    for i in [0, 1, 2]:
        print u_hand[i,:]
        print u[i,:]
        diff = abs(u_hand[i,:] - u[i,:]).max()
        assert diff < tol, 'diff=%.16g' % diff
        print 'diff=%g at t=%g' % (diff, t[i])

if __name__ == '__main__':
    test_rod_diffusion_hand()
```

Conclusions

- Our model signifies that as you increase the length of which the ions move through for the extracellular wall the final concentration will decrease.
- We would need to figure out a way to generalize the code more instead of using it to evaluate the solutions that we did by hand.
- Thus, the employment of the Forward Euler Method is needed.

```
[-3.  -1.5  0. ]
[-3.  -1.5  0. ]
diff=0 at t=0
[-3.45  -1.725  0.   ]
[-3.45  -1.725  0.   ]
diff=0 at t=0.1
[-3.9  -1.95  0.  ]
[-3.90000000e+00 -1.95000000e+00 -3.94745964e-17]
diff=4.44089e-16 at t=0.2
```