About diffusion

Fick's law states, that the rate of diffusion is proportional to the difference in concentration. We can write for the concentration of propane $[P]$ in inside the cell and outside the cell

$$\text{rate of flow} = D([P]_i - [P]_o),$$

where the constant D quantifies how readily propane diffuses across the membrane. It is usually represented as $D = \mu k_B T$, where k_B is Boltzmann's constant (about $1.3806488(13) \times 10^{-23}$ J/K), T is the temperature and μ is some kind of mobility value. We will grow our bacteria in 37°C so a good value for T is 310.16 K.

George Stokes has shown that the mobility for a spherical particle with radius r is

$$\mu = \frac{1}{6\pi\eta r},$$

where η is the dynamic viscosity of the fluid (Wikipedia). Radius of a water molecule is approximately 0.28 nm, although I didn't find very good sources for that [4]. In 40°C, the viscosity for water is $\eta = 0.653 \times 10^{-3} \frac{kg}{s\,m}$. This temperature was the closest available [3].

Based on information above, we can calculate D for 40°C or approximate it on 37°C by formula

$$D = \frac{k_B T}{6\pi\eta r}.$$

We may not need the equation for the constant D. In [2] there are many diffusion constants, including a constant for propane and water, which is $0.97 \times 10^{-5} \frac{\text{cm}^2}{\text{s}}$. It is to be noted that this value is for 25°C.

The differential equation for concentration of propane inside the cell is

$$\frac{d}{dt}[P]_i(t) = -\frac{D([P]_i(t) - [P]_o(t))}{V},$$

where V is the volume of the cell. It can be estimated to be 1 μm^3.

In our project, we want to harvest the propane for use as a fuel, so it might be reasonable assumption it is constantly taken away from the outside

of the cell. Furthermore, the outside of the cell is many times bigger than the inside, so it would be quite reasonable assumption that the concentration of propane on the outside is some small constant, maybe even zero if it is taken away efficiently. In any case, we have a simple way to estimate the diffusion of propane across the cell membrane.

Calculations

Calculation of D in Matlab when approximating 37°C:

```
>> kB = 1.3806488*10^(-23);
>> r = 2.4*10^(-10);
>> eta = 0.653*10^(-3);
>> T = 310.16;
>> D = (kB*T)/(6*pi*eta*r)

D =

   1.4496e-09
```

Calculation of D in Matlab when using right values for 40°C:

```
>> kB = 1.3806488*10^(-23);
>> r = 2.4*10^(-10);
>> eta = 0.653*10^(-3);
>> T = 313.16;
>> D = (kB*T)/(6*pi*eta*r)

D =

   1.4636e-09
```

We assumed that the mobility μ is for the medium, but what if it is for propane? The radius of propane is 4.397 Å which is 4.397×10^{-10} meters [5]. The viscosity is $\eta = 0.00011\frac{s}{m^2}$ for propane in 300 K [6]. With these, not perfect, values we obtain estimations for D, first approximation for 37°C, then more right value for 26.85°C.

```
>> kB = 1.3806488*10^(-23);
>> T = 310.16;
>> eta = 0.00011;
>> r = 4.397*10^(-10);
>> D = (kB*T)/(6*pi*eta*r)

D =

   4.6970e-09


>> kB = 1.3806488*10^(-23);
>> T = 300;
>> eta = 0.00011;
>> r = 4.397*10^(-10);
>> D = (kB*T)/(6*pi*eta*r)

D =

   4.5431e-09
```

These values differ a bit from both previous calculations with water and from the constant found from literature.

The problem in calculations right now is that the unit of these is $\frac{m^2}{s}$, 2D case, but we have 3D-case.

References

[1] E. L. Cussler *Mathematical Modelling in Systems Biology: An Introduction*,2012

[2] E. L. Cussler, *Diffusion: Mass Transfer in Fluid Systems*, (2nd ed.). New York: Cambridge University Press, 1997. Link to the book, Wikipedia article

[3] Table of viscosities

[4] Radius of the water

[5] Radius of propane

[6] Viscosity of propane