Enzyme-Substrate Dynamics & Michaelis-Menten Model

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Lab 6, C&SB 150, Spring 2019

May 10th, 2019

- Two .m files for today's lab: `enzymekin.m` and `QSSA_func.m` (download from CCLE lab assignment 6 portal).
- Can also download lecture8 note for more information on MM model.

Outline for today

- Review Michaelis-Menten Model.
- Model and simulate MM model through Matlab.
- Incorporate Quasi-Steady State Approximation (QSSA) into the model.

Michaelis-Menten Model

$$\mathrm{S} + \mathrm{E} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{SE} \xrightarrow{k_2} \mathrm{P} + \mathrm{E}$$

- Translate the chemical reaction into equations for each compartment.
- What quantity is not changing?

Quasi-Steady State Approximation (QSSA)

- What's the assumption?
- What's the amount of complex under the assumption of QSSA?
- What about $\frac{dP}{dt}$ and $\frac{dS}{dt}$?
- When is QSSA a good approximation and when is QSSA a bad approximation?

MM Model - System description in Matlab

```
function [dxdt] = QSSA_func(t,x,K1,K1MINUS,K2,e0)
% Single Substrate-Enzyme Reaction
% R1: S + E -- k1 --> ES
% R2: ES    -- k1minus --> E + S
% R3: ES    -- k2 --> E + P
% ----Original----
s=x(1); e=x(2); c=x(3); p=x(4);
dsdt = %% REPLACE %%;
dedt = %% REPLACE %%;
dcdt = %% REPLACE %%;
dpdt = %% REPLACE %%;
% ----sQSSA----
% Constraints
%     e(t) + c(t) = e0
% Assumption
%     dcdt ~ 0
%s_qssa = x(5); p_qssa = x(6);
% Pack output
dxdt=[dsdt;dedt;dcdt;dpdt];
return
```

MM Model - Simulation in Matlab

- Use `enzymkin.m` to simulate and plot the MM model.
- First, you need to enter corresponding parameters and initial conditions:

```
K1       = %% REPLACE %%;
K1MINUS = %% REPLACE %%;
K2       = %% REPLACE %%;

% Initial conditions x0.
s0 = %% REPLACE %%;
e0 = %% REPLACE %%;
c0 = %% REPLACE %%;
p0 = %% REPLACE %%;
```

Note:

- For question3, when you modify the code in `QSSA_func.m`, remember that you are adding two differential equations into your model. Therefore, make sure to also update the number of input/output variables to match the change.
- Also change the code for plotting in the `enzymkin.m` to accommodate for the modification (basically adding two items for plotting two more curves.)