DIAGNOSTIC 4

MODELING AND SIMULATION

Before attempting this diagnostic, you should read Chapter 9 of the cat book and do Exercise 9.2.

Corn Ethanol

The attached paper is from the Eleventh Industrial Mathematical and Statistical Modeling Workshop for Graduate Students; you can download it from `samsi.info/reports`. It describes a model of the enzyme processes that transform corn starch into glucose, which is the first step in corn ethanol production.

Your task is to re-implement the model presented in the paper and confirm[1] their results. You are welcome to work together to understand the paper and work out the details of the model, but we strongly encourage you to write your own implementation. These diagnostics are your best opportunity to sharpen your programming (and debugging!) skills.

Here are some suggestions to get you started:

1. For `ode45`, and some of your other functions, you will need to define a vector that contains the concentrations of each substrate. For the sake of consistency, I recommend putting them in the order of the initial conditions on page 27.

   ERROR ALERT: the left sides of these equations are wrong[2]; for example, the initial concentration of unavailable starch should be something like $S_{unavailable}(0)$, not $dS_{unavailable}/dt$ (that would be a rate of change, not a concentration).

2. Write a function called `reaction_rate` that takes a vector of concentrations and a reaction number (0 through 12) and returns the rate of the given reaction.

   Notice that each reaction rate depends on one enzyme concentration and one substrate concentration. You might find it useful to define two vectors that let you look up a reaction number and get the index of the relevant enzyme/substrate.

   ERROR ALERT: the values for k_{cat} in Figure 2.3 are actually in inverse seconds, not minutes as it says in the text.

   Test this function by calling it from the Command Window. Then make it a silent function before you go on.

3. Write a function called `rate_func` that defines a rate function for `ode45`. It should take time and a vector of concentrations

Figure 1: If you Google "corn ethanol," this image is *everywhere*. If it's under copyright, I pity the owner.

[1] Or refute...

[2] So very wrong.

as input variables and return a (column) vector of rates of change as an output variable.

If you compute all of the reaction rates and put them in a vector, you should be able to copy Equations 2.2 and 2.3 into your program almost verbatim.

FUDGE ALERT: Because rate constants are not available for two of the reactions, we have to fudge them. If you look closely[3] at the code on page 28, you will see that the authors set $r_4 = 0.05r_3$ and $r_7 = 0.05r_6$.

[3] I don't think they explain this fudge in the paper, which is bad form!

Test your function by calling it from the Command Window. Then make it a silent function before you go on.

4. Write a function called `corn` that uses `ode45` to simulate the enzyme process for 50 hours with the initial conditions on page 27.

   UNIT ALERT: Notice that the initial conditions are in *mMol*, but almost everything else in the paper is in *Mol*.

   See if your results look like the graph on page 27. If not, why not?