

Week 7: Deterministic Chemical Kinetics

(You are at the halfway point of CAAM 210!)

Skeletal Outline

mca2driver

[this is where the majority of the work is]

`dx=mcaode(t,x,k) (x=[R Pr RPr P D I])`

[write down ODEs]

`[t, xout] = mygill(tfin, rtab, x, c)`

[edit last week's mygill to return all reactants, not just dimer]

`h=update(x)`

[same as last week]

mca2driver

1. Set parameters: tfin, tinc, nr, x0, c (nr=4)
2. Hard code rtab (same as last week)
3. Call mygill nr times, interpolating and storing the time and concentration [t, xout], the outputs of mygill, for run=1:nr

...

First we look only at what happens to dimer, to create figure 1.

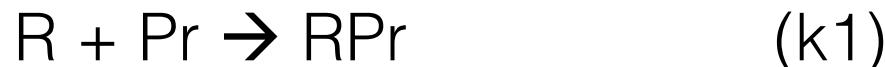
However, next we will look at all 6 chemicals, so we need to edit mygill so that it stores information for chemicals other than dimer. How do we do this?

mca2driver

1. Set parameters: tfin, tinc, nr, x0, c (nr=4)
2. Hard code rtab (same as last week)
3. Call mygill nr times, interpolating and storing the time and concentration [t, xout], the outputs of mygill, for run=1:nr
4. Plot mean and standard deviation, hold on [Stochastic]
5. Call ode23, which calls mcaode [Deterministic]
6. Superimpose deterministic dimer count on plot 1 to make first figure
7. Now run mygill only once (nr=1), and make the second figure with all the subplots by comparing stochastic to deterministic for each reactant

Task 1: write $dx = mcaode(t, x, k)$

Reactions are the same as last week. We're calling the propensities, k now (not c), with no necessary transformation.



The first one has already been done $dx(1,1) = -c_1x_1x_2 + c_2x_3 + c_3x_3$

Ode23

- $[t,x]=\text{ode23}(\text{function handle, timespan, initial values})$
 - Each element of the solution (and output) x is the solution at the time corresponding to that element in t .
 - Solves from start time to end time (specified in timespan)
 - Example: $[t,y]=\text{ode23}(@\text{vdp1},[0 \ 20],[2 \ 0]);$ (in MATLAB help)
- Our times are from 0 to t_{fin}
- Our initial values are in x_0 , which we set earlier in the driver (make sure it's a row vector)
- Function handles are tricky animals. Remember, our functions are hidden in `mcaode`. You have to call `mcaode` *within* `ode23` to pull out the functions you need. Then you need to tell `ode23` for which values to solve the ODE by using `@(t,x)`.

Task 2: ode23

- Let's write the one line of code that calls ode23 (and mcaode).
- You only need to call this once in your driver. You just access the different parts of its output (t , x) depending on which reactant you're considering.

mca2driver

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3. Call mygill nr times, interpolating and storing the time and concentration [t, xout], the outputs of mygill, for run=1:nr
4. Plot mean and standard deviation, hold on [Stochastic]
5. Call ode23, which calls mcaode [Deterministic]
6. Superimpose deterministic dimer count on plot 1 to make first figure [Stochastic]
7. Now run mygill only once (nr=1), and make the second figure with all the subplots by comparing stochastic to deterministic for each reactant