Super Brief FRAP Note

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Abstract

This is an extension of my previous FRAP code in which I better encode the reaction process, and I further allow the product particles to diffuse (if someone doesn't like that, they can just put the k_{off} value for that particle to be 0). This is going to fucking suck, so I am (for the moment) only writing this note to help me to verify the validity of my equations.

MODEL

I will allow all the particles to possible diffuse in order to induce symmetry in my program. I want the only exceptional particles to be due to the binding process. The reaction I am modeling is

$$A + B \leftrightarrow C \tag{1}$$

In order to take into account the FRAP process, I need to define what happens when you bind bleached particles with unbleached particles. Therefore, I define the more detailed reaction scheme as follows:

$$Au + Bu \leftrightarrow Cuu$$

$$Au + Bb \leftrightarrow Cub$$

$$Ab + Bu \leftrightarrow Cbu$$

$$Ab + Bb \leftrightarrow Cbb$$

The ultimate goal is to model the following reaction scheme under a FRAP experiment:

$$A + B \leftrightarrow C$$

$$C \leftrightarrow D$$

$$D \leftrightarrow A + E$$

In order to model the first reaction, I need the following equations:

- Au
  - Initial Volume: $Au(x,0) = \widetilde{Au}(x)$
  - Initial Surface: $\sigma_{Au}(0) = \widetilde{\sigma_{Au}}$
  - Diffusion: $\frac{\partial Au}{\partial t} = D_{Au}\frac{\partial^2 Au}{\partial x^2}$
  - Left Flux: $\frac{\partial Au}{\partial x}\Big|_{x=0} = 0$
  - Right Flux: $-D_{Au}\frac{\partial Au}{\partial x}\Big|_{x=L} = k_{on}^{Au}Au(L,t) - k_{off}^{Au}\sigma_{Au}(t)$
  - Reaction:

$$\frac{\mathrm{d}\sigma_{Au}}{\mathrm{d}t} = k_{on}^{Au}Au(L,t) - (k_{off}^{Au} + k_{bind}^{uu}\sigma_{Bu} + k_{bind}^{ub}\sigma_{Bb})\sigma_{Au} + k_{dis}^{uu}\sigma_{cuu} + k_{dis}^{ub}\sigma_{Cub}$$

- Bu
  - Initial Volume: $Bu(x,0) = \widetilde{Bu}(x)$
  - Initial Surface: $\sigma_{Bu}(0) = \widetilde{\sigma_{Bu}}$
  - Diffusion: $\frac{\partial Bu}{\partial t} = D_{Bu} \frac{\partial^2 Bu}{\partial x^2}$
  - Left Flux: $\frac{\partial Bu}{\partial x}\Big|_{x=0} = 0$
  - Right Flux: $-D_{Bu} \frac{\partial Bu}{\partial x}\Big|_{x=L} = k_{on}^{Bu} Bu(L,t) - k_{off}^{Bu} \sigma_{Bu}(t)$
  - Reaction:

$$\frac{\mathrm{d}\sigma_{Bu}}{\mathrm{d}t} = k_{on}^{Bu} Bu(L,t) - (k_{off}^{Bu} + k_{bind}^{uu} \sigma_{Au} + k_{bind}^{bu} \sigma_{Ab}) \sigma_{Bu} + k_{dis}^{uu} \sigma_{Cuu} + k_{dis}^{bu} \sigma_{Cbu}$$

- Ab
  - Initial Volume: $Ab(x,0) = \widetilde{Ab}(x)$
  - Initial Surface: $\sigma_{Ab}(0) = \widetilde{\sigma_{Ab}}$
  - Diffusion: $\frac{\partial Ab}{\partial t} = D_{Ab} \frac{\partial^2 Ab}{\partial x^2}$
  - Left Flux: $\frac{\partial Ab}{\partial x}\Big|_{x=0} = 0$
  - Right Flux: $-D_{Ab} \frac{\partial Ab}{\partial x}\Big|_{x=L} = k_{on}^{Ab} Ab(L,t) - k_{off}^{Ab} \sigma_{Ab}(t)$
  - Reaction:

$$\frac{\mathrm{d}\sigma_{Ab}}{\mathrm{d}t} = k_{on}^{Ab} Ab(L,t) - (k_{off}^{Ab} + k_{bind}^{bu} \sigma_{Bu} + k_{bind}^{bb} \sigma_{Bb}) \sigma_{Ab} + k_{dis}^{bu} \sigma_{Cbu} + k_{dis}^{bb} \sigma_{Cbb}$$

- Bb
  - Initial Volume: $Bb(x,0) = \widetilde{Bb}(x)$
  - Initial Surface: $\sigma_{Bb}(0) = \widetilde{\sigma_{Bb}}$
  - Diffusion: $\frac{\partial Bb}{\partial t} = D_{Bb} \frac{\partial^2 Bb}{\partial x^2}$
  - Left Flux: $\frac{\partial Bb}{\partial x}\Big|_{x=0} = 0$
  - Right Flux: $-D_{Bb} \frac{\partial Bb}{\partial x}\Big|_{x=L} = k_{on}^{Bb} Bb(L,t) - k_{off}^{Bb} \sigma_{Bb}(t)$
  - Reaction:

$$\frac{\mathrm{d}\sigma_{Bb}}{\mathrm{d}t} = k_{on}^{Bb} Bb(L,t) - (k_{off}^{Bb} + k_{bind}^{ub} \sigma_{Au} + k_{bind}^{bb} \sigma_{Ab}) \sigma_{Bb} + k_{dis}^{ub} \sigma_{Cub} + k_{dis}^{bb} \sigma_{Cbb}$$

- Cuu
  - Initial Volume: $Cuu(x,0) = \widetilde{Cuu}(x)$
  - Initial Surface: $\sigma_{Cuu}(0) = \widetilde{\sigma_{Cuu}}$
  - Diffusion: $\frac{\partial Cuu}{\partial t} = D_{Cuu} \frac{\partial^2 Cuu}{\partial x^2}$
  - Left Flux: $\frac{\partial Cuu}{\partial x}\Big|_{x=0} = 0$
  - Right Flux: $-D_{Cuu} \frac{\partial Cuu}{\partial x}\Big|_{x=L} = k_{on}^{Cuu} Cuu(L,t) - k_{off}^{Cuu} \sigma_{Cuu}(t)$
  - Reaction:

$$\frac{\mathrm{d}\sigma_{Cuu}}{\mathrm{d}t} = k_{on}^{Cuu} Cuu(L,t) - (k_{off}^{Cuu} + k_{dis}^{uu})\sigma_{Cuu} + k_{bind}^{uu} \sigma_{Au} \sigma_{Bu}$$

- Cub
  - Initial Volume: $Cub(x,0) = \widetilde{Cub}(x)$
  - Initial Surface: $\sigma_{Cub}(0) = \widetilde{\sigma_{Cub}}$
  - Diffusion: $\frac{\partial Cub}{\partial t} = D_{Cub} \frac{\partial^2 Cub}{\partial x^2}$
  - Left Flux: $\frac{\partial Cub}{\partial x}\Big|_{x=0} = 0$
  - Right Flux: $-D_{Cub} \frac{\partial Cub}{\partial x}\Big|_{x=L} = k_{on}^{Cub} Cub(L,t) - k_{off}^{Cub} \sigma_{Cub}(t)$
  - Reaction:

$$\frac{\mathrm{d}\sigma_{Cub}}{\mathrm{d}t} = k_{on}^{Cub} Cub(L,t) - (k_{off}^{Cub} + k_{dis}^{ub})\sigma_{Cub} + k_{bind}^{ub} \sigma_{Au} \sigma_{Bb}$$

- Cbu
  - Initial Volume: $Cbu(x,0) = \widetilde{Cbu}(x)$
  - Initial Surface: $\sigma_{Cbu}(0) = \widetilde{\sigma_{Cbu}}$
  - Diffusion: $\frac{\partial Cbu}{\partial t} = D_{Cbu} \frac{\partial^2 Cbu}{\partial x^2}$
  - Left Flux: $\frac{\partial Cbu}{\partial x}\Big|_{x=0} = 0$
  - Right Flux: $-D_{Cbu} \frac{\partial Cbu}{\partial x}\Big|_{x=L} = k_{on}^{Cbu} Cbu(L,t) - k_{off}^{Cbu} \sigma_{Cbu}(t)$
  - Reaction:

$$\frac{\mathrm{d}\sigma_{Cbu}}{\mathrm{d}t} = k_{on}^{Cbu} Cbu(L,t) - (k_{off}^{Cbu} + k_{dis}^{bu})\sigma_{Cbu} + k_{bind}^{bu} \sigma_{Ab} \sigma_{Bu}$$

- Cbb
  - Initial Volume: $Cbb(x,0) = \widetilde{Cbb}(x)$
  - Initial Surface: $\sigma_{Cbb}(0) = \widetilde{\sigma_{Cbb}}$
  - Diffusion: $\frac{\partial Cbb}{\partial t} = D_{Cbb}\frac{\partial^2 Cbb}{\partial x^2}$
  - Left Flux: $\frac{\partial Cbb}{\partial x}\Big|_{x=0} = 0$
  - Right Flux: $-D_{Cbb}\frac{\partial Cbb}{\partial x}\Big|_{x=L} = k_{on}^{Cbb}Cbb(L,t) - k_{off}^{Cbb}\sigma_{Cbb}(t)$
  - Reaction:

$$\frac{\mathrm{d}\sigma_{Cbb}}{\mathrm{d}t} = k_{on}^{Cbb}Cbb(L,t) - (k_{off}^{Cbb} + k_{dis}^{bb})\sigma_{Cbb} + k_{bind}^{bb}\sigma_{Ab}\sigma_{Bb}$$

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