

Problem 1. Reactive Random Walks

Take the reactive random walk code that you were provided for class. Before running any codes think about what might change relative to the results that we obtained in class if you run the code with

- (i) 10 times fewer particles
- (ii) 100 times fewer particles
- (iii) A diffusion coefficient that is 10 times smaller
- (iv) A diffusion coefficient that is 10 times bigger
- (v) A reaction rate that is ten times bigger
- (vi) A reaction rate that is ten times smaller

Try and deduce what you would expect to happen, particularly in relation to the effects of incomplete mixing. Do you expect it to kick in earlier, later, at the same time? Do you expect it to change the late time scaling of $t^{-1/4}$ etc.? Use physical reasoning or any theoretical argument you can think of to justify your answers.

Now actually run the code under these circumstances. To get statistically meaningful results run each of the cases above for a minimum of ten realizations averaging over each of them. Beware that this could be time consuming so have the code running while you are doing other work. Do these results align with your physical reasoning and expectations? If not, rethink your arguments to make them consistent with what you observe.

Problem 2. Reactive Random Walks 2

Change the reactive random walk code so that your domain is of size $[-100,100]$. Now set up an initial condition so that all particles associated with one species start at $x=-5$ and all of the other species particles are located at $x=5$. You can assume that a unit mass pulse of particles is the initial condition in all cases (i.e. $C_A(t=0) = \delta(x-5)$ and $C_B(t=0) = \delta(x+5)$). Run the code with $D=1$; and assume that the probability of reaction given collocation equals 1 (i.e. the reaction rate k is big enough to ensure that any collocating particles must react). Run the code with several situations with differing numbers of particles and compare your solutions with what you would expect from the results we developed for instantaneous reactions in previous chapters (i.e. the case where we said $C_A C_B = 0$). How do the results compare to the theory and depend on particle numbers? Do mismatches, if they occur, make sense to you? Again make sure to run several realizations to get statistically meaningful results. I will not tell you at what times to make comparisons or number of particles to use, but use your own reasoning and understanding to pick values that may be interesting. In particular pick times so that the size of the domain is not important.

Problem 3. Shear Flows

For this problem you may want to look at the notes "Extra Notes on Shear" available from the class website.

We may have discussed this in class briefly, but it is something I want to make sure you all understand well. Consider a case where you have a shear flow in 2d filled with A and B particles uniformly. From everything you have learned already you should know that in the

absence of any heterogeneous flow this system will initially behave as if it were well mixed and that at late time when incomplete mixing effects kick in the scaling of the consumption of reactants will slow from a scaling of t^{-1} to $t^{-1/2}$ (because it is two dimensional). Using the dominant balance arguments we discussed in class (or any other method you like), explain this late time scaling.

Now if the domain has a shear flow in it (i.e. a velocity $u = \alpha y$), we know that the scaling will transition from t^{-1} to $t^{-1/2}$ as in the absence of shear flow, but given sufficient time it will revert to a t^{-1} scaling again. Use the same dominant balance arguments to explain this transition.

Hint: Recall that the term $C'_A C'_B$, which is the term that needs to be closed for the dominant balance argument, can be modeled as $C'_A C'_B = \chi G_{peak}$ where χ is a constant, whose specific value we are not worried about just yet and G_{peak} is the value of the peak of Greens function for the equivalent conservative transport problem.

If you do not understand what I am asking for here please make sure to come by my office and ask.

Also, if you do not know what the Greens function for shear flow is it is on slide 5 of the extra notes.