

Problem 1. Instantaneous Mixing-Driven Equilibrium Reactions

Consider a situation where two chemical solutes exist in water such that the product of their concentrations is given by a constant $c_1 c_2 = K$. When the water is not in equilibrium c_1 and c_2 will react to precipitate out a third species, which is immobile and whose concentration is c_3 . Define the difference in concentrations $u = c_1 - c_2$. Initially you have a one-dimensional domain entirely filled with a solution $u = 0$ (i.e. $c_1 = c_2 = \sqrt{K}$). You then at time $t = 0$, introduce a pulse of another mixture such that $u(x, t = 0) = \delta(x)$. Consider a system that only has solutes that diffuse with diffusion coefficient D .

(i) Write the full set of governing equations for how c_1 , c_2 and c_3 evolve as well as an equation for u .

(ii) Write an expression for the reaction rate r at which species 3 is created. Write it in a form that is made up of the product of a term that reflects only mixing (i.e. only depends on the form of u) and another term that reflects speciation (only depends on the specifics of the reaction).

(iii) For the particular setup considered write an explicit expression for the mixing term in the equation for r from (ii). Also write an explicit expression for the speciation term. In particular comment on their structure and anything interesting you might observe there.

(iv) Now consider the case $K = 4$ and $D = 10$ and plot the mixing term, the speciation term and the reaction rate r term at times $t = 0.1, 1, 10$ and 100 . Based on these plots, is there ever a time when it is reasonable to consider that the speciation term is constant (as has been done in many previous studies), or must we always consider it to vary? What are the consequences of not letting it vary and where would the error be greatest by neglecting the variation?

(v) What changes in (iv) if we decrease the diffusion coefficient to $D = 1$? Likewise what if we decrease K to 1? Discuss any changes you observe and hint at why these might happen.

(vi) For the times in (iv) and the case of $K = 4, D=10$, plot the concentrations of c_1 and c_2 at each of these times.

(vii) What changes if we now allow solutes 1 and 2 to advect with a uniform and constant velocity v ?

Problem 2. Dilution & Mixing

Consider a system with only diffusion with where you introduce a pulse of solute at time zero such that $C(x, t = 0) = \delta(x)$. Write down the solution for how this concentration will evolve in one, two and three dimensions (x,y and z respectively)

(i) For a one dimensional infinite system, calculate the scalar dissipation rate M . Calculate it in two ways

$$M = -\frac{1}{2} \frac{d \int_{-\infty}^{\infty} C^2 dx}{dt}$$

and

$$M = D \int_{-\infty}^{\infty} \frac{\partial C}{\partial x} \frac{\partial C}{\partial x} dx$$

to convince yourself that the formula we obtained in class that shows these are equal is correct.

In particular, discuss how the scalar dissipation rate scales with time

(ii) Without performing any new calculations do you expect mixing to be faster or slower when you increase the number of spatial dimensions to 2 or 3. Using intuition alone, explain why.

(iii) Now, using either of the expressions for M , calculate its evolution for the 2 and 3 dimensional scaling and deduce an expression for how M scales with time depending on the number of spatial dimensions d - i.e. $M \sim t^{f(d)}$, what is $f(d)$?

(iv) Finally, convince yourself of the scaling of the dilution index on slide 10 in the class notes that states $E = (4\pi Dt)^{d/2} e^{d/2}$.

(iv) Finally discuss what you see as the relationship between the dilution index and the scalar dissipation rate (or just $\int C^2 dV$ as you see fit). in particular compare and contrast the two, describing similarities and differences. Would you generally pick one over the other? If so, why?