

Finding the optimal parameters ???

This is a model of reaction-diffusion system as can be found in the following figure (1).

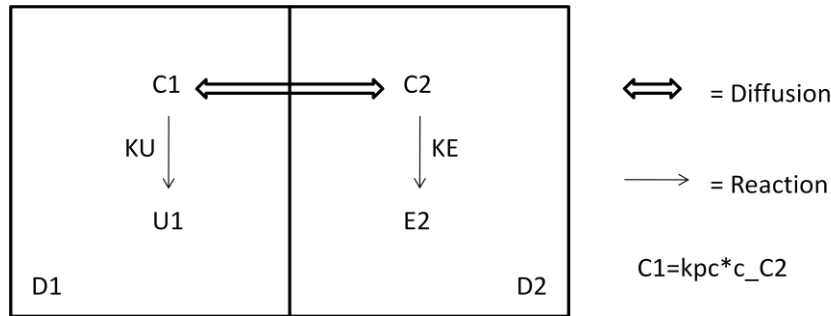


Figure (1)

In the above model, KU and KE are rate constants. $D1$ and $D2$ are diffusion coefficients in subdomain 1 and 2 respectively. kpc is a partition coefficient between $C1$ and $C2$. I have modeled this system in Comsol 3.5a and run the system for a time span of 600 sec in the interval of 200 sec i.e. (0:200:600). (You can find it in the attached file test.mph) Then I computed the solution which are given in the following figures (2,3).

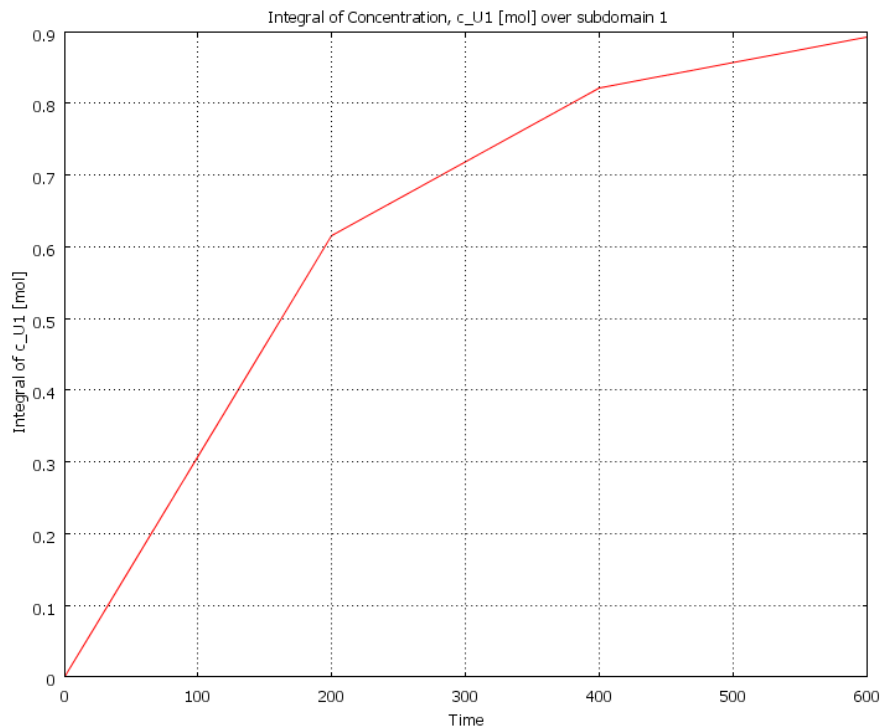


Figure (2)

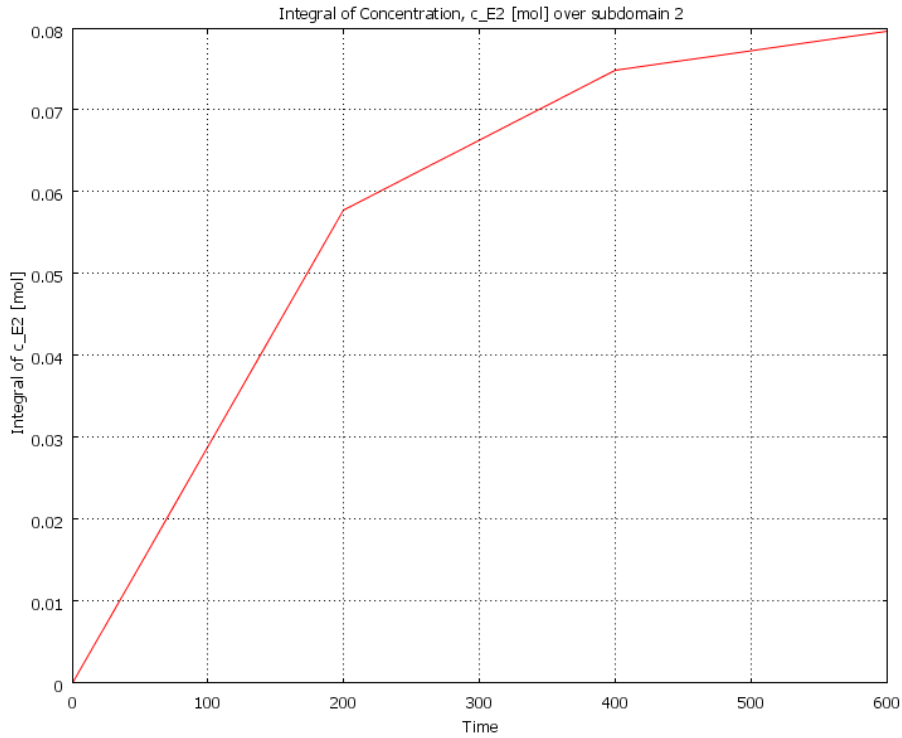


Figure (3)

Now my objective is to find the best-fitted parameters (KU , KE , kpc , $D2$) such that the solution is closest the data given in the following table.

Species with domains	At time $t=200$	At time $t=400$	At time $t=600$
U1 (Integral of Concentration, c_{U1} [mol] over domain 1)	.35	.5	.6
E1 (Integral of Concentration, c_{E2} [mol] over domain 2)	0.04	.06	.07