**Instructions for COMSOL Modeling Project Part 3**

***Make sure you read all the instructions before you start (or else you will have to do a lot of backtracking and ultimately more work).***

1. Download the COMSOL instructions for this part and complete the step-by-step guide to modeling the drug release from a biomatrix.
2. Write a short report that includes the following (be sure to provide a brief caption and comment for each figure):
3. 1D, semi-log plot of the concentrations of all chemical species within the biomatrix material OD model.
4. 3D surface maps of concentration profile of *free* drug at 1 hour (3600s) and 16 hours (57,600s). (Be sure to use the same color scales for these plots and the ones in part C below.)
5. 3D surface maps of concentration profile of *free* + *peptide-bound* drug at 1 and 16 hours. (Use same color scales in all 4 plots from part B and C.)
6. 1D plot of total drug (free + peptide bound) concentration across modeling domain, but only plot for the time series starting at 0, 2.5 hr, 5 hr, …, 15 hr. (Hint: changing the “time selection” from “from list” to “manual” can speed this part up.

*If you are having trouble downloading the parameter list, here is the list you can type in manually.*

|  |  |  |  |
| --- | --- | --- | --- |
| T\_in | 300[K] | 300 K | Inlet temperature |
| kf\_mm | 7.336e-3[s^-1] | 0.007336 1/s | Reaction rate constant, matrix-degradation following Michaelis-Menten kinetics |
| Km | 0.01[mol/m^3] | 0.01 mol/m³ | Michaelis-Menten constant |
| kf\_d | 1.5e4[m^3/(s\*mol)] | 15000 m³/(s·mol) | Forward reaction rate constant, drug dissociation |
| kr\_d | 13.5[1/s] | 13.5 1/s | Reverse reaction rate constant, drug dissociation |
| ce\_init | 2e-3[mol/m^3] | 0.002 mol/m³ | Initial concentration enzyme, biomaterial matrix |
| cnE\_init | 2e-3[mol/m^3] | 0.002 mol/m³ | Initial concentration enzyme, nerve cell tissue |
| cmp\_init | 1e-2[mol/m^3] | 0.01 mol/m³ | Initial concentration matrix-bound peptide, biomaterial matrix |
| cmpd\_init | 1e-2[mol/m^3] | 0.01 mol/m³ | Initial concentration matrix-bound drug-peptide species, biomaterial matrix |
| c\_solv | rhoh2o/Mnh2o | 55556 mol/m³ | Concentration, solvent (water) |
| Dd | 8.93e-11[m^2/s] | 8.93E-11 m²/s | Diffusion coefficient matrix-bound drug, biomaterial matrix |
| Dmp | 0[m^2/s] | 0 m²/s | Diffusion coefficient matrix-bound peptide, biomaterial matrix |
| Dmpd | 0[m^2/s] | 0 m²/s | Diffusion coefficient matrix-bound drug-peptide species, biomaterial matrix |
| Dp | 1.58e-10[m^2/s] | 1.58E-10 m²/s | Diffusion coefficient drug, biomaterial matrix |
| Dpd | 8.3e-11[m^2/s] | 8.3E-11 m²/s | Diffusion coefficient peptide, biomaterial matrix |
| De | 5e-11[m^2/s] | 5E-11 m²/s | Diffusion coefficient enzyme, biomaterial matrix |
| DsD | 8.3e-11[m^2/s] | 8.3E-11 m²/s | Diffusion coefficient drug, surroundings |
| DsP | 1.68e-10[m^2/s] | 1.68E-10 m²/s | Diffusion coefficient peptide, surroundings |
| DsPD | 9.31e-11[m^2/s] | 9.31E-11 m²/s | Diffusion coefficient drug-peptide species, surroundings |
| DsE | 5.5e-11[m^2/s] | 5.5E-11 m²/s | Diffusion coefficient enzyme, surroundings |
| DnD | 8.93e-11[m^2/s] | 8.93E-11 m²/s | Diffusion coefficient drug, nerve cell tissue |
| DnP | 1.58e-10[m^2/s] | 1.58E-10 m²/s | Diffusion coefficient peptide, nerve cell tissue |
| DnPD | 8.3e-11[m^2/s] | 8.3E-11 m²/s | Diffusion coefficient drug-peptide species, nerve cell tissue |
| DnE | 5e-11[m^2/s] | 5E-11 m²/s | Diffusion coefficient enzyme, nerve cell tissue |
| Mnd | 10[kg/mol] | 10 kg/mol | Molar mass, drug |
| Mnp | 1[kg/mol] | 1 kg/mol | Molar mass, peptide |
| Mnpd | 11[kg/mol] | 11 kg/mol | Molar mass, drug-peptide species |
| Mne | 50[kg/mol] | 50 kg/mol | Molar mass, enzyme |
| Mnh2o | 0.018[kg/mol] | 0.018 kg/mol | Molar mass, solvent (water) |
| rhoh2o | 1000[kg/m^3] | 1000 kg/m³ | Density solvent (water) |