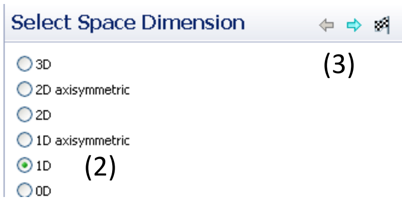
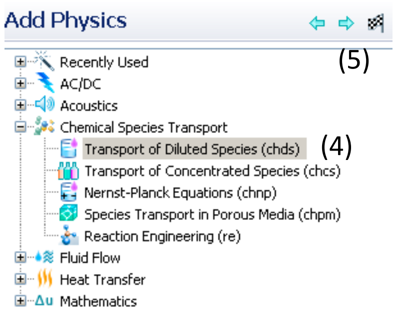
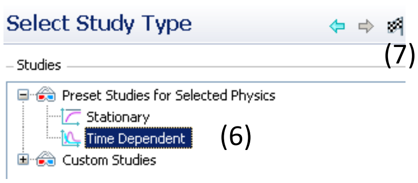
Problem Type Specification







(1) Open COMSOL 4.1 and save file. Remember to save file often.

(2) Under **Select Space Dimension**, select 1D.

(3) Click on the blue next arrow to add physics.

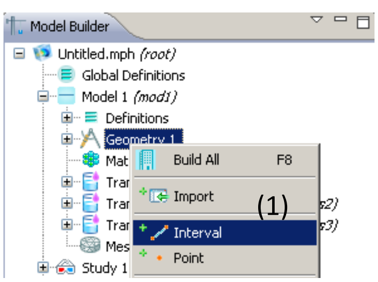
(4) Double click "Transport of Diluted Species (chds)". Repeat two more times for a total of three species (c, c2, c3).

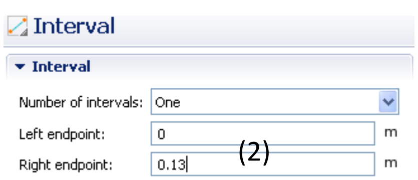
(5) Click on blue next arrow.

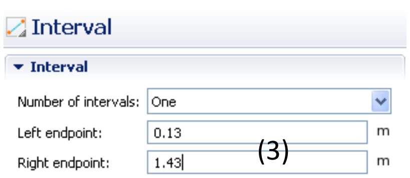
(6) Select "Time Dependent".

(7) Click checkered flag to finish.

Geometry Creation







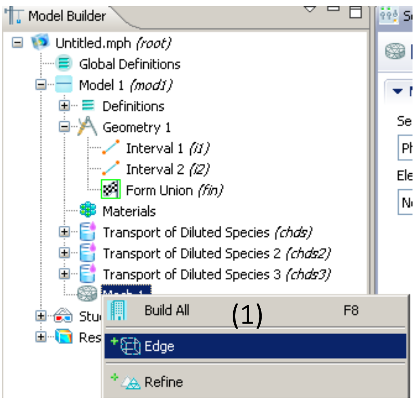
(1) Right click on "Geometry 1" and select to add new "Interval". Repeat to create two intervals.

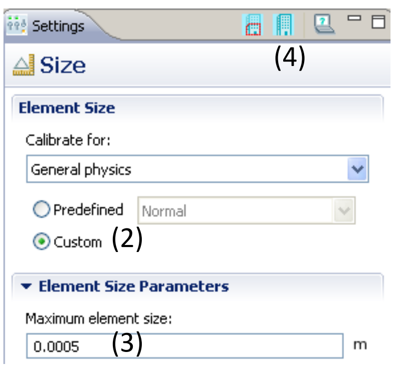
(2) Click on "Interval 1". Input 0 m for left endpoint and 0.13m for right endpoint. This represents the tumor.

(3) Click on "Interval 2" and input 0.13m for left endpoint and 1.43 for right endpoint. This line represents the tissue. Click on the "Build All" icon.

(4) Under **Graphics**, click on the green expand icon to fit geometry to screen.

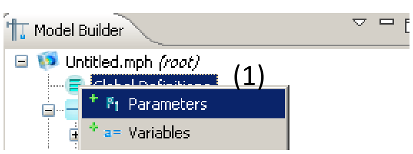
Meshing

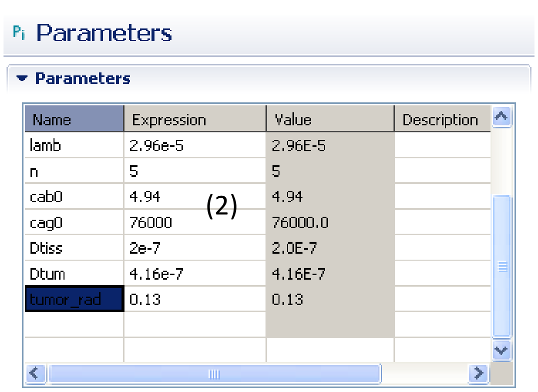




(1) Right Click on "Mesh 1" and select to add new "Edge" meshing type.
(2) Click on "Size" from "Mesh 1". Under Element Size, click bubble for "Custom". This will allow you to modify the meshing parameters.
(3) Under Element Size Parameters, input 0.0005 m for Maximum element size.
(4) Click the blue build all icon. The mesh should now have 2860 edge (mesh) elements.

Governing equations, source terms, I.C., B.C.

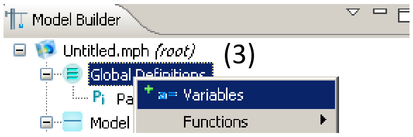


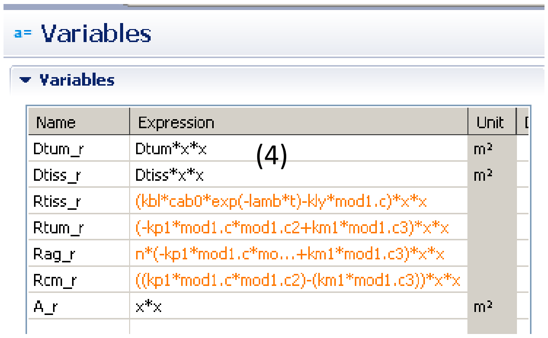


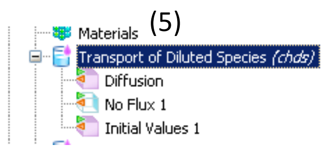
Constants:

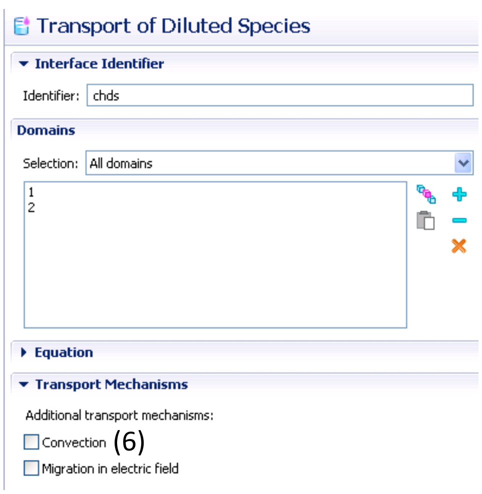
(1) In **Model Builder**, right click on "Global Definitions" and select to add new list of "Parameters".
(2) Define the following parameters

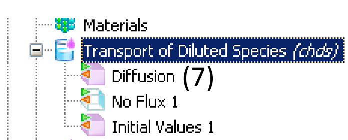
Name	Expression
kbl	4.60e-5
kly	1.78e-5
kp1	5.00e-5
km1	1.00e-5
lamb	2.96e-5
n	5
cab0	4.94
cag0	76000
Dtiss	2.00e-7
Dtum	4.16e-7
tumor_rad	0.13

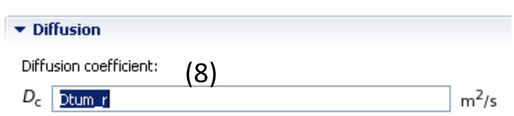


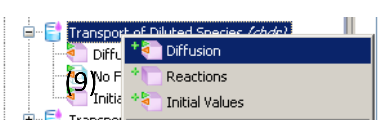












Expressions:

(3) Right click on "Global Definitions" and select to add new list of "Variables"

(4) Define the following expressions

Name	Expression
A_r	x*x
Dtum_r	Dtum* x*x
Dtiss_r	Dtiss* x*x
Rtiss_r	(kbl*cab0*exp(-lamb*t)-kly*mod1.c) * x*x
Rtum_r	(-kp1* mod1.c* mod1.c2+km1* mod1.c3) * x*x
Rag_r	n*(-kp1* mod1.c* mod1.c2+km1* mod1.c3) * x*x
Rcm_r	(kp1* mod1.c* mod1.c2-km1* mod1.c3) * x*x

Species 1: antibody

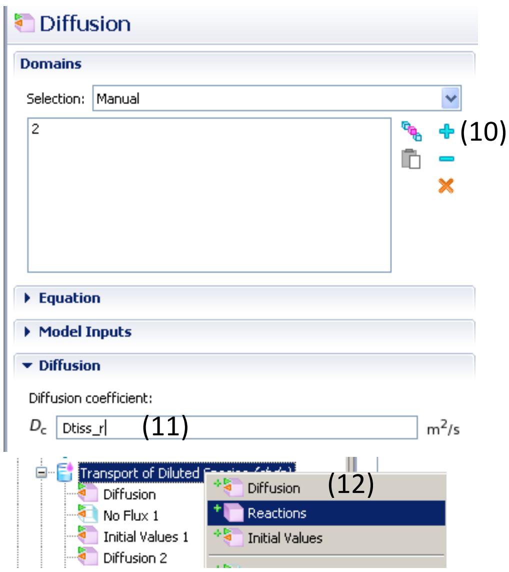
(5) Expand and click on "Transport of Diluted Species (chds)".

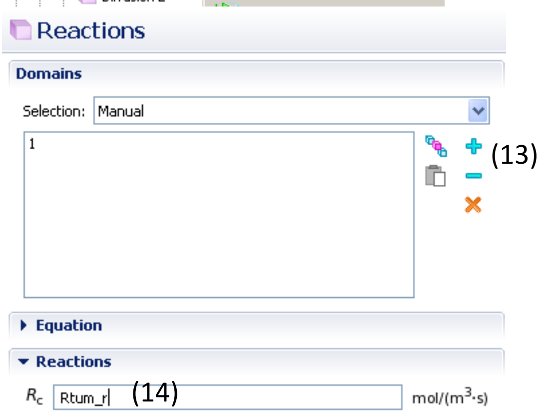
(6) Under Transport Mechanisms, uncheck box for "Convection".

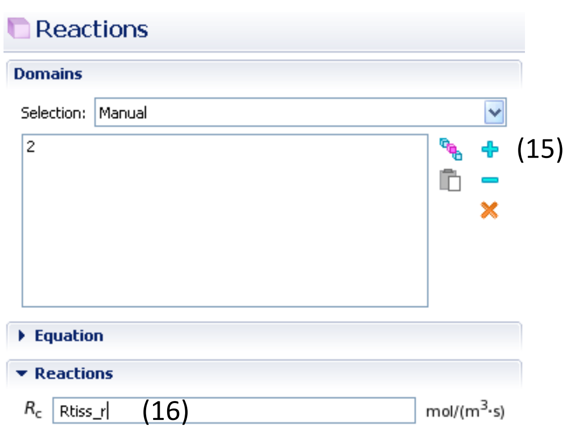
(7) Under "Transport of Diluted Species (chds)" click "Diffusion".

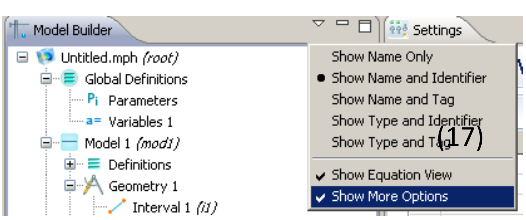
(8) Set Diffusion coefficient to Dtum_r.

(9) Right click on "Transport of Diluted Species (chds)" and add new "Diffusion" parameter.









(10) Under **Graphics**, select domain 2 and click the blue add icon.

(11) Set diffusion coefficient to Dtiss_r.

(12) Right click on “Transport of Diluted Species (chds)” and select to add new “Reactions”. Repeat to have two new “Reactions” parameter.

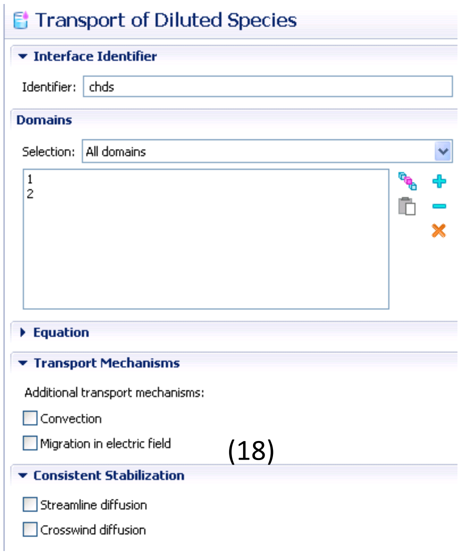
(13) Click on “Reactions 1” and click on subdomain 1 in the **Graphics** window and click blue add icon.

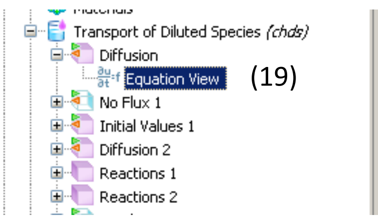
(14) Input Rtum_r under Reactions.

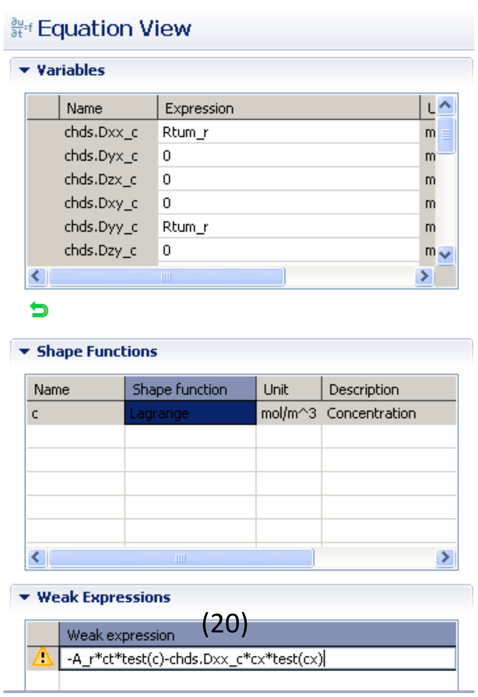
(15) Click on “Reactions 2” and click on subdomain 2 in the **Graphics** window and click blue add icon.

(16) Input Rtiss_r under Reactions.

(17) On the **Model Builder** title bar, click on the upside-down triangle to open the drop down menu. Click on “Show Equation View” and “Show More Options” to activate both actions.





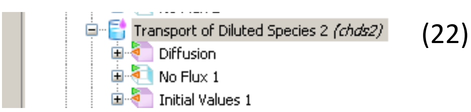


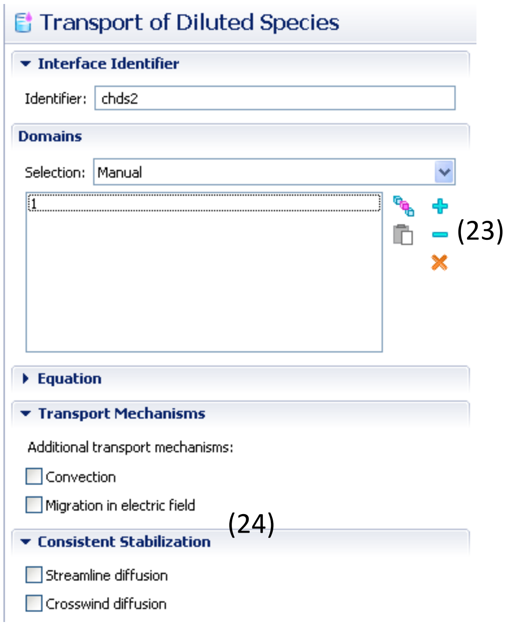
(18)Click on “Transport of Diluted Species (chds)”. Under Transport Mechanisms, uncheck box for “Convection”. Under Consistent Stabilization, uncheck boxes for “Streamline diffusion” and “Crosswind diffusion”.

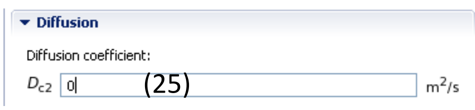
(19)Under “Transport of Diluted Species (chds)”, expand “Diffusion” and click on “Equation View”.

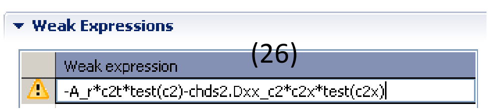
(20)In **Equation View**, under Weak Expression, multiply the existing equation with A_r to result with - A_r*ct*test(c)- chds.Dxx_c*cx*test(cx).

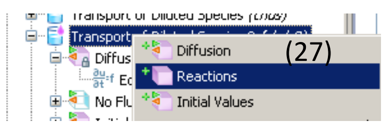
(21)Repeat steps (19) and (20) for “Diffusion 2”.

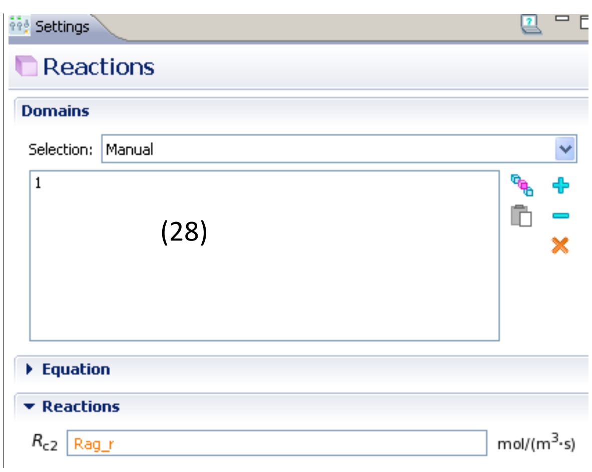












Species 2: antigen

(22)Click on “Transport of Diluted Species 2 (chds2)”.

(23)In **Transport of Diluted Species** window, select domain 2 and click the minus icon to inactivate.

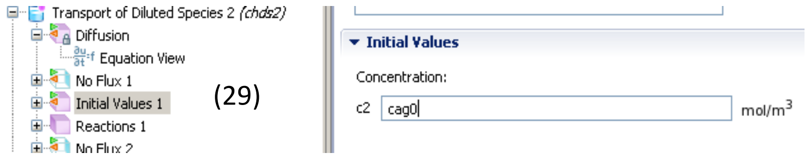
(24) Under Transport Mechanisms, uncheck box for “Convection”. Under Consistent Stabilization, uncheck boxes for “Streamline diffusion” and “Crosswind diffusion”.

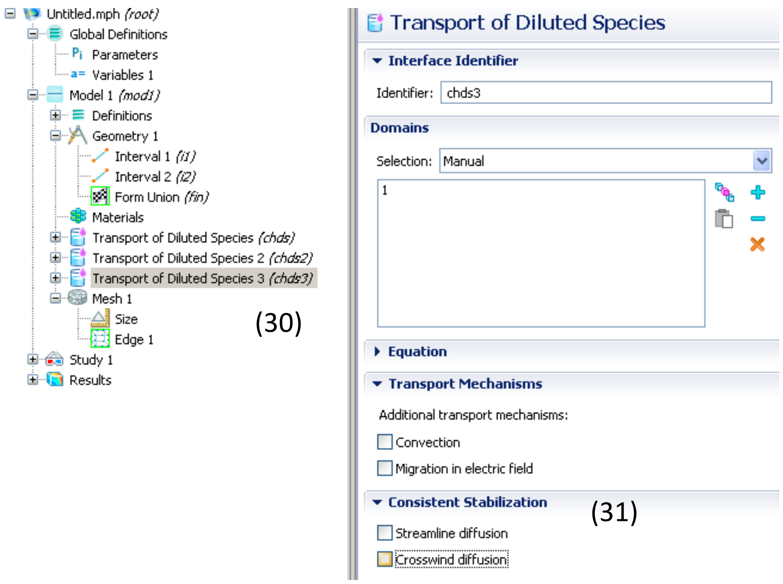
(25)Select “Diffusion” from the **Model Builder** window and input 0 for the diffusion coefficient.

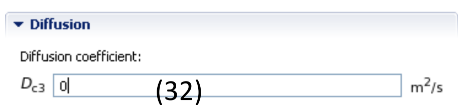
(26)Under “Diffusion” click on “Equation View”. In **Equation View**, multiply weak equation by with A_r .

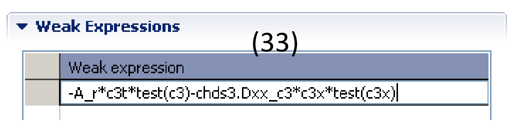
(27)Right click on “Transport of Diluted Species 2 (chds2)” and add new “Reactions” parameter.

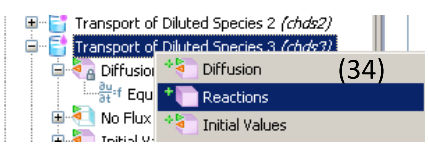
(28)Click domain 1 from **Graphics** window and click the blue add icon. This sets the reaction equation for just domain 1. Set Reactions to Rag_r.

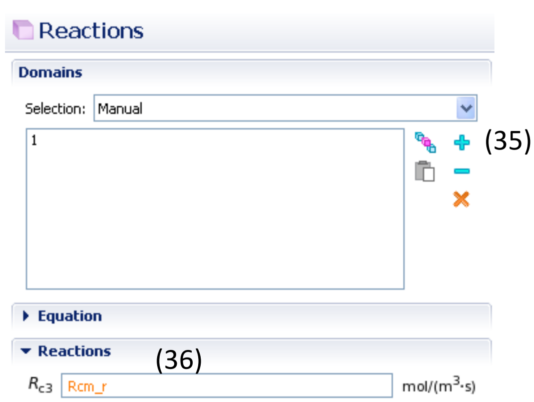












(29)Click on “Initial Values 1” and set to cag0.

Species 3: antibody-antigen complex

(30)Click on “Transport of Diluted Species 3 (chds3)”.

(31)In **Transport of Diluted Species** window, select domain 2 and click the minus icon. Under Transport Mechanisms, uncheck box for “Convection”. Under Consistent Stabilization, uncheck boxes for “Streamline diffusion” and “Crosswind diffusion”.

(32)Select “Diffusion” from the **Model Builder** window and input 0 for the diffusion coefficient.

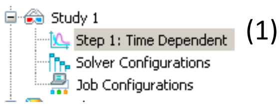
(33) In **Equation View**, multiple the weak expression by A_r .

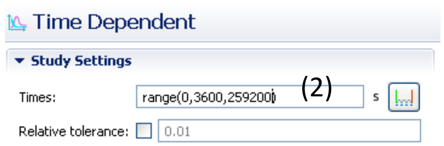
(34)Right click on “Transport of Diluted Species 3 (chds3)” and selec to add new “Reaction”.

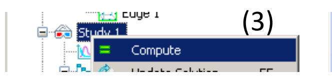
(35)Click domain 1 from **Graphics** window and click the blue add icon. This sets the reaction equation for just domain 1.

(36)Set Reactions to Rcm_r**.**

Solver Settings and Solution

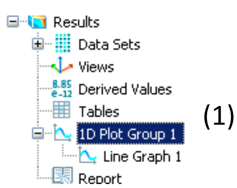


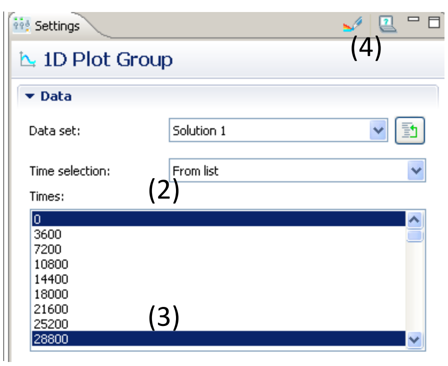


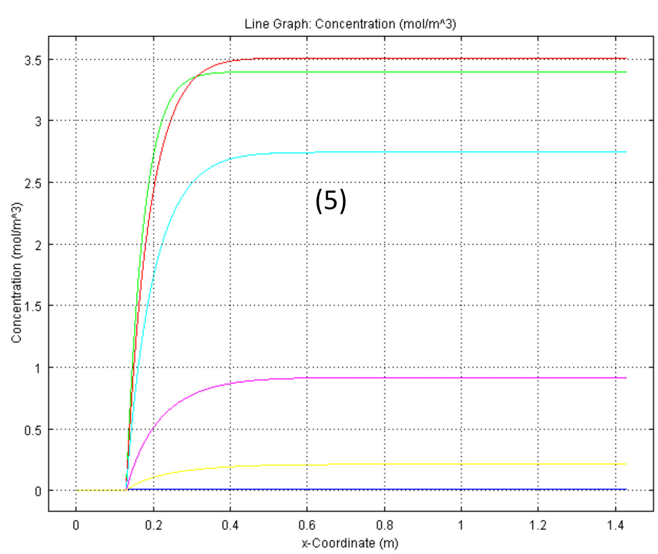


(1) Expand “Study 1” and select “Step 1: Time Dependent”.
(2) Set time range(0,3600,259200).
(3) Right click “Study 1” and select “Compute” to solve the problem.

Postprocessing







(1) Click on “1D Plot Group 1”.
(2) Under **1D Plot Group**, select “From List” from the drop down menu of Time selection.
(3) Hold the CTRL buttom and select the 6 desired times: 0, 28800, 57600, 172800, and 259200 in the Times area.
(4) Click the plot icon (rainbow pencil).
(5) The following concentration profile should result.