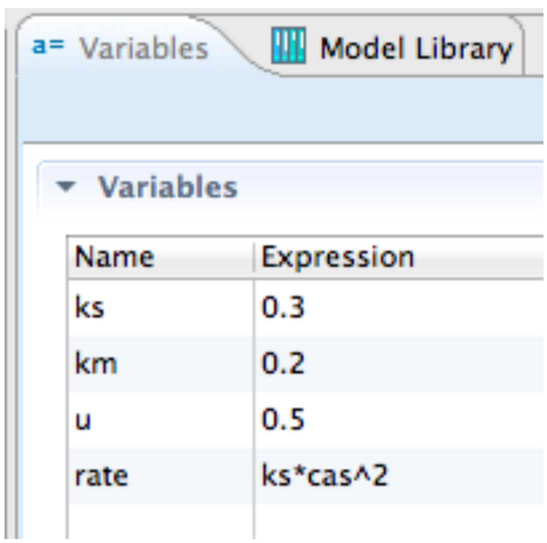
Solving Chemical Reactors with Mass Transfer Limitations using Comsol Multiphysics

Consider the problem posed on page 155[1]: a chemical reactor with mass transfer limitations. The reaction rate is determined by the concentration on the catalyst, which is different from the concentration in the bulk, flowing stream. The equations are:

$$u\frac{dC_A}{dz} = -2k_s C_{A,s}^2, \quad u\frac{dC_B}{dz} = 2k_s C_{A,s}^2 \quad u\frac{dC_C}{dz} = 0$$
$$k_m a(C_A - C_{A,s}) = k_s C_{A,s}^2$$
$$C_A(0) = 2, \quad C_B(0) = 0, \quad C_C(0) = 2$$

Step 1, Begin: Open Comsol Multiphysics and choose the 0D option, right arrow; then Global ODEs and DAEs (ge) (under Mathematics/ODE and DAE Interfaces); then right arrow and finally Time Dependent and the Finish flag.

Step 2, Prepare the Model: Model 1 opens, with Global ODEs and DAEs (ge). In Model/Definitions right click and choose variables. Insert the following variables.



Name	Expression
ks	0.3
km	0.2
u	0.5
rate	ks*cas^2

The surface area per volume, *a*, is included in the variable *km*.

Then in Global ODEs/Global Equations, insert the equations as follows. Notice that the equations one must solve are under f(u,ut,utt,t), and the term there is what must be zero.

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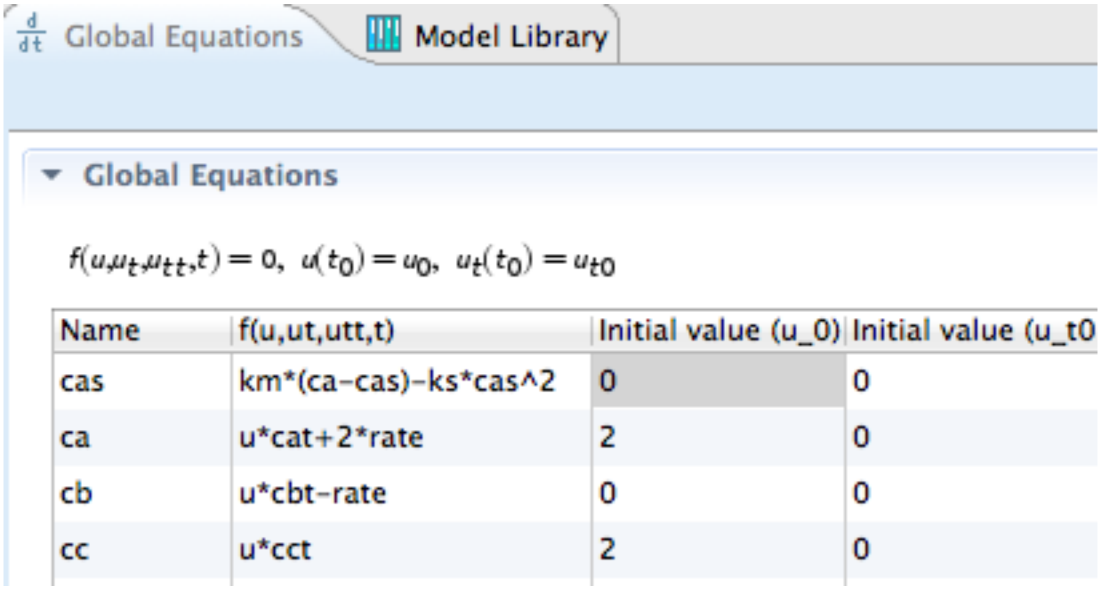
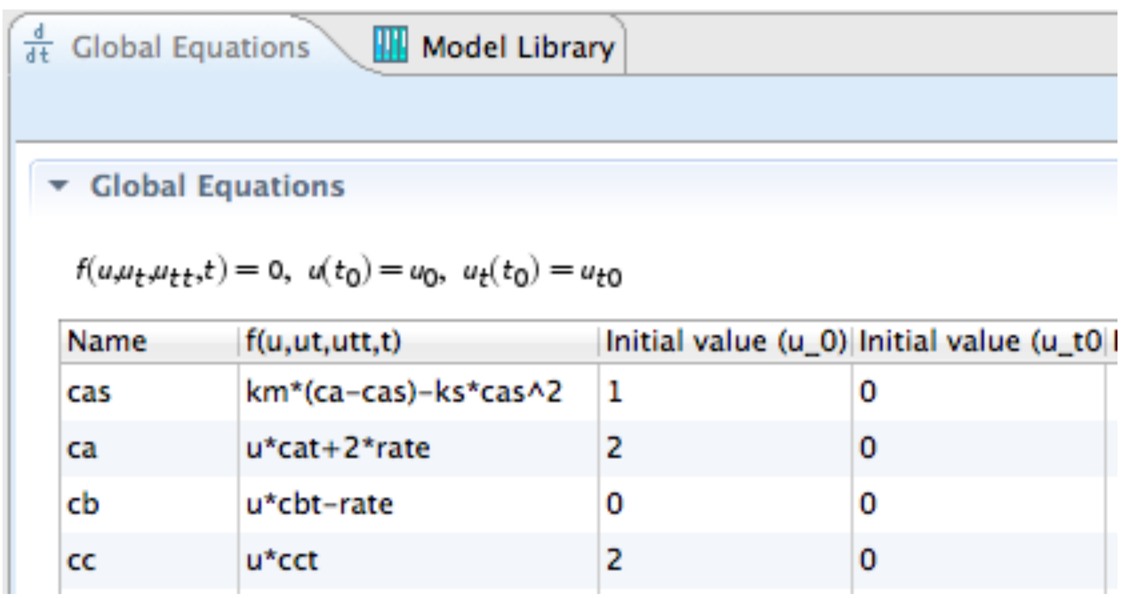
[1] Bruce A. Finlayson, Introduction to Chemical Engineering Computing, 2nd ed., Wiley (2012); ChemEComp.com for info, Buy Now .



Name	f(u,ut,utt,t)	Initial value (u_0)	Initial value (u_t0
cas	km*(ca-cas)-ks*cas^2	0	0
ca	u*cat+2*rate	2	0
cb	u*cbt-rate	0	0
cc	u*cct	2	0

Step 3, Solve the Problem: Open Study and click on Step 1: Time Dependent. The default value is to integrate from 0 to 1 and save the solution every 0.1. The variable is time, which is a stand-in for distance, *z*. Change this to go from 0 to 2.4. Right click on Study 1 and choose Compute. The problem fails to finish. If you open Results/ 1D Plot Group 1 you see that the cas starts out negative. It should never be lower than zero.

Step 4, Use a better guess for cas: Change the initial value of cas to 1. It must be between 0 and ca, which is 2 at the inlet, so the 1 is just a guess.



Name	f(u,ut,utt,t)	Initial value (u_0)	Initial value (u_t0
cas	km*(ca-cas)-ks*cas^2	1	0
ca	u*cat+2*rate	2	0
cb	u*cbt-rate	0	0
cc	u*cct	2	0

Step 5, Solve the Problem: Right click on Study 1 and choose Compute. This time the solution is correct. The figure is similar to 8.10 in the text, with the addition of the plot for *cas*. The difference between *ca* and *cas* shows the impact of the mass transfer resistance.