Solving Mass Balances with Recycle using Comsol Multiphysics

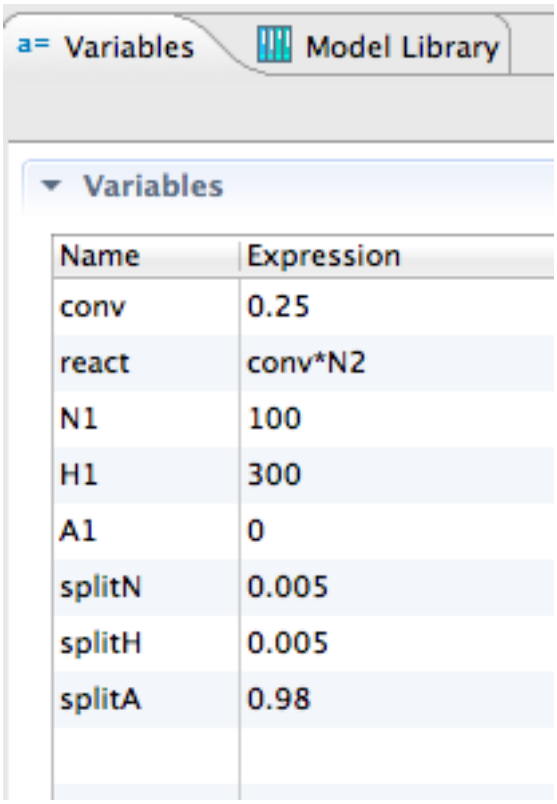
1. Mass Balance with Specified Reaction and Recycle
2. Mass Balance with Equilibrium Reaction and Recycle

Problem in Figure 5.8 – Mass Balance with Specified Reaction and Recycle

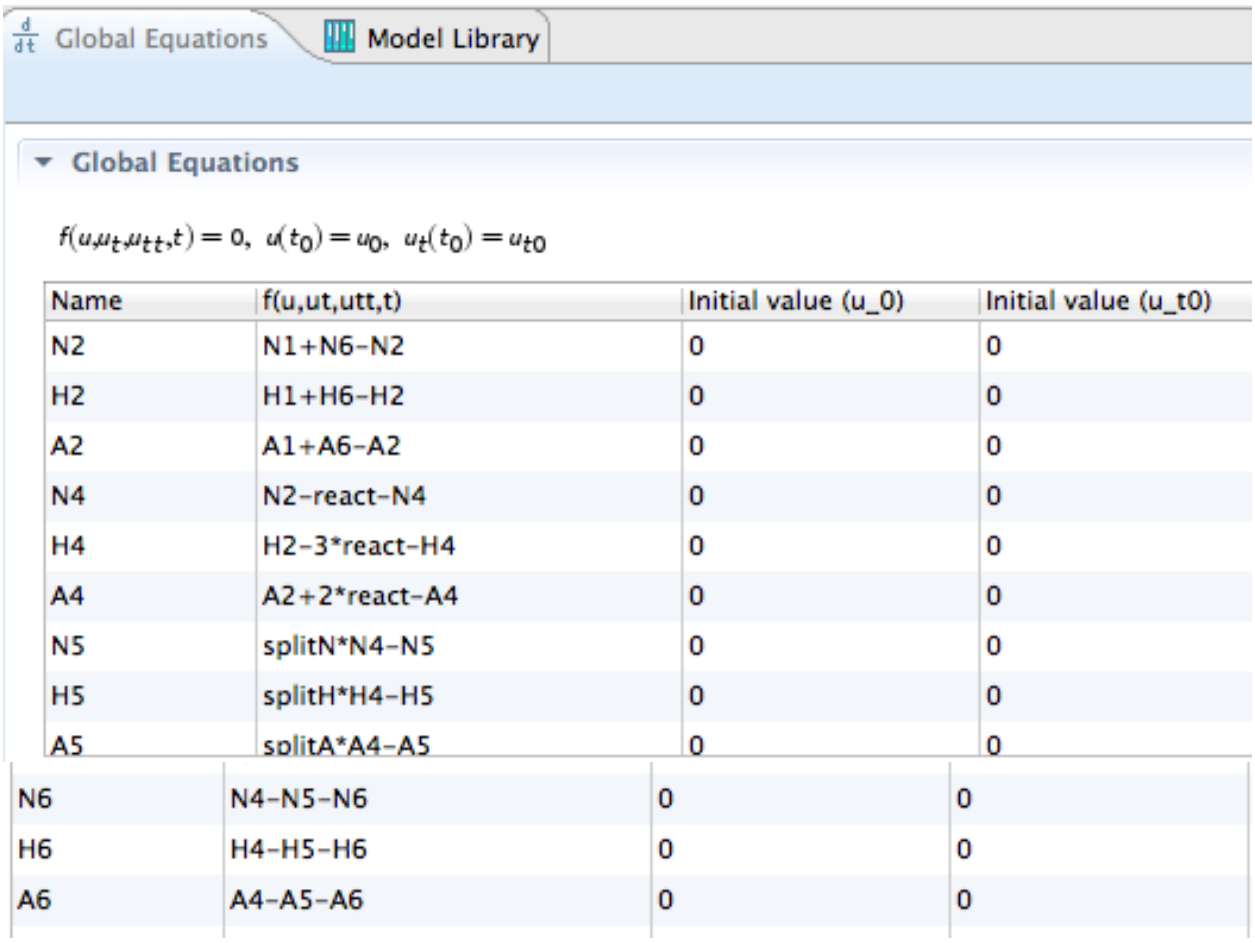
Consider the problem posed on page 72: an ammonia process with nitrogen and hydrogen feed with 25% conversion per pass (in Reactor) and a specified separation at the Separator.

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 Stationary 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.



Then in Global ODEs/Global Equations, insert the variables and equations as follows. See Figure 5.8 for the structure. Notice that the equations one must solve are under f(u,ut,utt,t), and the term there is what must be zero. Thus, if the equation is N2=N1+N6, the f is given as N1+N6-N2.



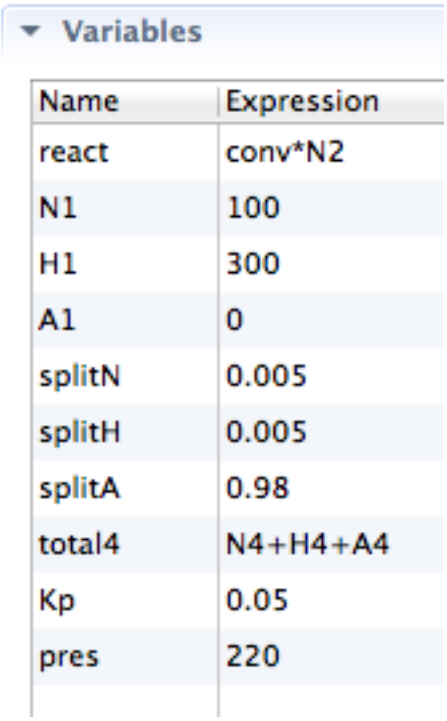
Name	f(u,ut,utt,t)	Initial value (u_0)	Initial value (u_t0)
N2	N1+N6-N2	0	0
H2	H1+H6-H2	0	0
A2	A1+A6-A2	0	0
N4	N2-react-N4	0	0
H4	H2-3*react-H4	0	0
A4	A2+2*react-A4	0	0
N5	splitN*N4-N5	0	0
H5	splitH*H4-H5	0	0
A5	splitA*A4-A5	0	0
N6	N4-N5-N6	0	0
H6	H4-H5-H6	0	0
A6	A4-A5-A6	0	0

Step 3, Solve the Problem: Right click on Study 1 and choose Compute. The problem converges and gives the same answers as in Figure 5.8.

It would be nice if variables could be defined as vectors, but that is harder. Of course, it could be done using LiveLink with MATLAB, but if you have MATLAB it is easier just do solve the problem in MATLAB, as shown in Chapter 3. The exercise shown here is just to show you how to solve mass balances with recycle in Comsol Multiphysics.

Problem in Figure 5.10 – Mass Balance with Equilibrium Reaction and Recycle

The problem above is modified so that the conversion is determined by chemical equilibrium, using Eq. (5.6). The variables now include the equilibrium constant, *Kp*, and the pressure, *pres*. The former specification of *conv* is not used, since it is determined from the equations.



Variables

Name	Expression
react	conv*N2
N1	100
H1	300
A1	0
splitN	0.005
splitH	0.005
splitA	0.98
total4	N4+H4+A4
Kp	0.05
pres	220

The Global Equations are modified by adding the following equation for *conv*.

conv	Kp-total4*(A4/(N4*H4*H4*H4)^0.5)/pres

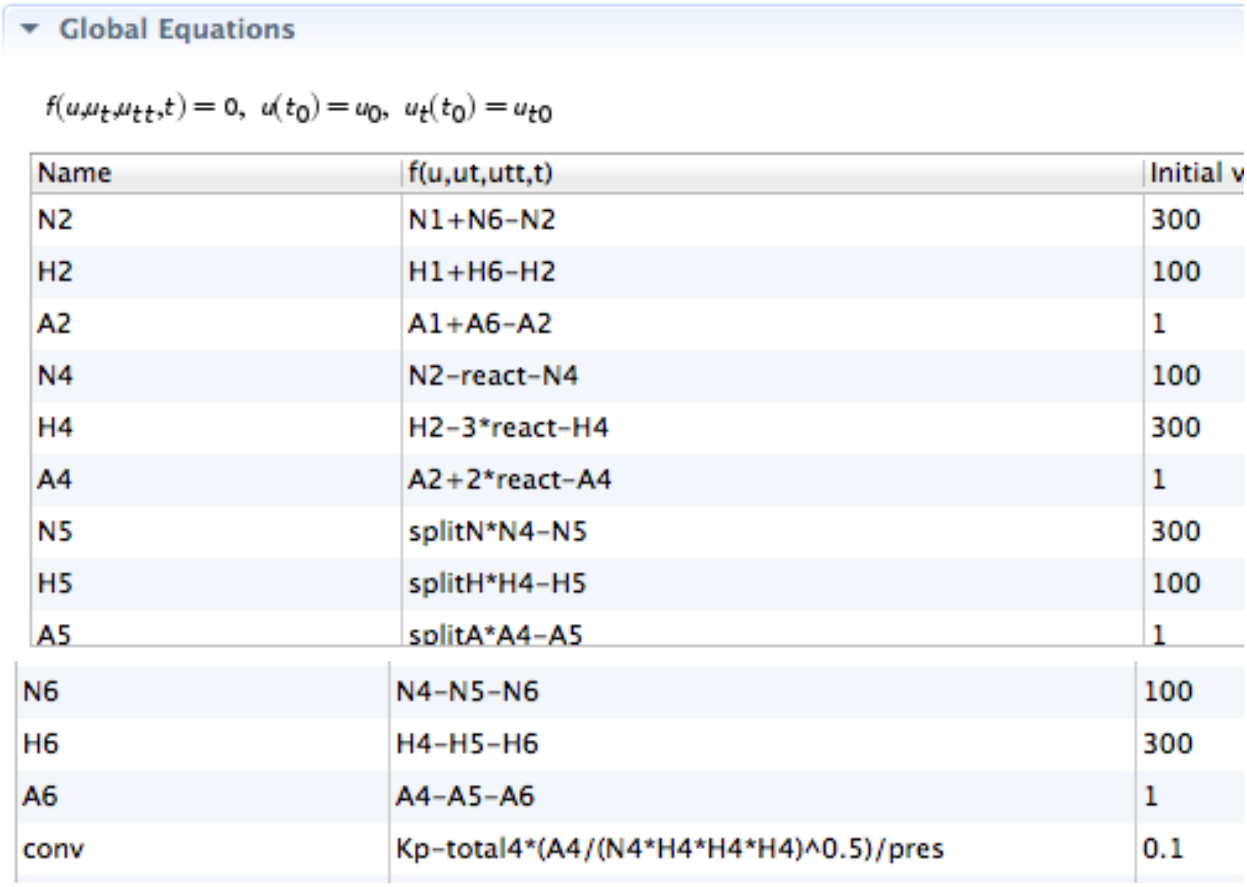
Since the equilibrium expression uses mole fractions, it is necessary to modify Eq. (5.6) so that it is in terms of molar flow rates.

$$K_p = \frac{y_{NH_3}}{(y_{N_2} y_{H_2}^3)^{0.5}} \frac{1}{p} \quad \text{becomes} \quad K_p = \frac{n_{total} n_{NH_3}}{(n_{N_2} n_{H_2}^3)^{0.5}} \frac{1}{p}$$

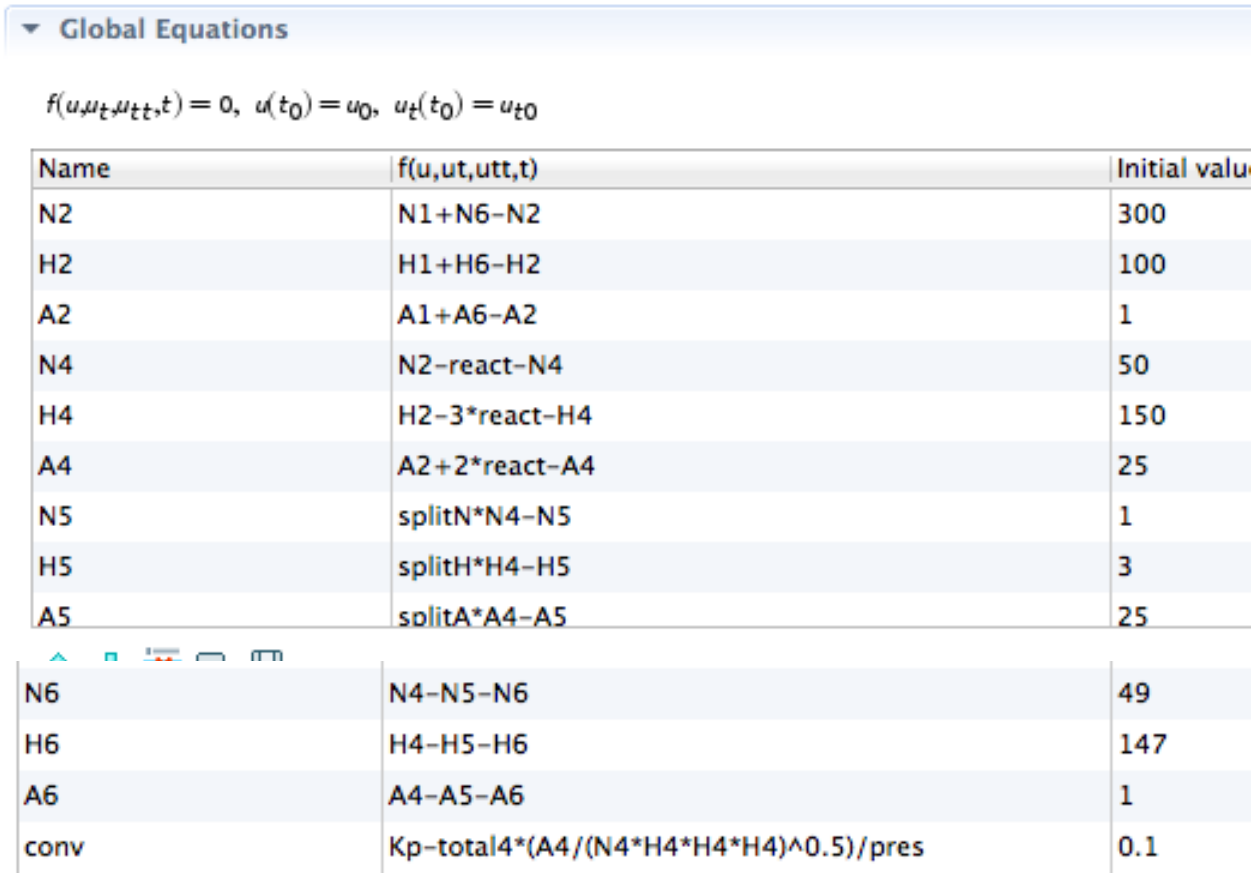
Notice that the equation determines the variable *conv*, but *conv* does not occur explicitly in the equation as expressed above. But, the flow rate of each species out of the reactor is determined by *conv*, using the equations above, so we add one equation with one new variable.

If one tries to start from an initial guess of all variables equal to zero, the problem cannot even get started, giving a singular matrix error. Various schemes were tried. If a

good approximation of the exact solution is provided as initial guess, the problem converges. When debugging a problem, this is a useful step because it suggests that the equations are correct, and it is the initial guess that needs to be improved. After several trials it was found that if the initial guess of all streams was the same as the inlet to the process plus some ammonia: nitrogen - 100, hydrogen - 300, ammonia -1, and the *conc* was set to 0.1, the problem converged.



In other cases, one may have to be ingenious to get a beginning solution. One option would be to work through the process without actually recycling anything, and then use that solution to begin, including the recycle stream. The following initial conditions worked, but if the ammonia in the recycle (A6) was changed to zero it did not work.



Name	f(u,ut,utt,t)	Initial valu
N2	N1+N6-N2	300
H2	H1+H6-H2	100
A2	A1+A6-A2	1
N4	N2-react-N4	50
H4	H2-3*react-H4	150
A4	A2+2*react-A4	25
N5	splitN*N4-N5	1
H5	splitH*H4-H5	3
A5	splitA*A4-A5	25
N6	N4-N5-N6	49
H6	H4-H5-H6	147
A6	A4-A5-A6	1
conv	Kp-total4*(A4/(N4*H4*H4*H4)^0.5)/pres	0.1