

### Initial Value Problem Solved in Comsol 4.1.

Copyright Bruce A. Finlayson, 2010

See also *Introduction to Chemical Engineering Computing*, Wiley (2006).

Consider next the problem posed by Eq. (8.24-26) for a reactor oxidizing SO<sub>2</sub> to form SO<sub>3</sub> (Young and Finlayson, 1973). After some manipulation, the equations are

$$\frac{dX}{dz} = -50R', \quad \frac{dT}{dz} = -4.1(T - T_{surr}) + 1.02 \cdot 10^4 R' \quad (8.24)$$

where the reaction rate is

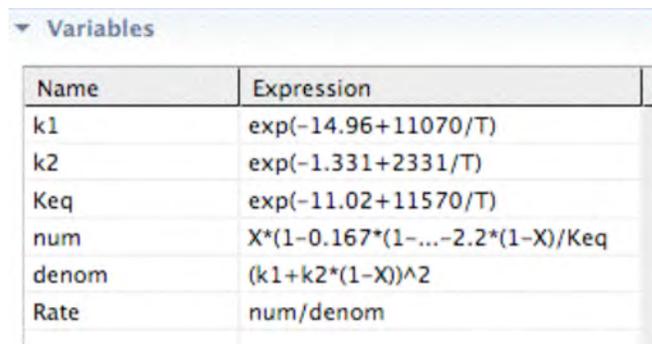
$$R' = \frac{X[1 - 0.167(1 - X)]^{1/2} - 2.2(1 - X)/K_{eq}}{[k_1 + k_2(1 - X)]^2} \quad (8.25)$$

$$\ln k_1 = -14.96 + 11070/T, \quad \ln k_2 = -1.331 + 2331/T, \quad K_{eq} = -11.02 + 11570/T \quad (8.26)$$

with the parameters:  $T_{surr} = 673.2$ ,  $T(0) = 673.2$ ,  $X(0) = 1$ . The variable  $X$  is the concentration of SO<sub>2</sub> divided by the inlet concentration,  $1 - X$  is the fractional conversion, and  $T$  is the temperature in °K. The first equation is the mole balance on SO<sub>2</sub>, and the second is the energy balance. The first term on the right-hand side of Eq. (8.24) represents cooling at the wall; the second term there is the heat of reaction. Because there are two variables, you need two equations.

**Step One: Choose the Problem.** Open Comsol Multiphysics and choose 0D in the Model Wizard (the time dimension serves as the length dimension). Expand 'Global ODEs and DAE interface folder' and select 'Global ODEs and DAEs(ge)'; select 'Time Dependent' and click Finish.

**Step Two: Define Equation.** Under the Model node, choose Definitions and create the Variables as shown in Figure 8.7b. Under ODEs and DAEs, right click to Global Equations. Set the two equations as shown in Figure 8.7c, which agree with Eq. 8.24. The initial conditions on  $X$  and  $T$  are set here, too.



Name	Expression
k1	exp(-14.96+11070/T)
k2	exp(-1.331+2331/T)
Keq	exp(-11.02+11570/T)
num	X*(1-0.167*(1-...-2.2*(1-X)/Keq
denom	(k1+k2*(1-X))^2
Rate	num/denom

Figure 8.7b. Variables

▼ Global Equations

$$f(u, u_t, u_{tt}, t) = 0, \quad u(t_0) = u_0 \quad u_t(t_0) = u_{t0}$$

Name	f(u,ut,utt,t)	Initial value (u_0)	Initial...(u_t0)
X	Xt+50*Rate	1	0
T	Tt+4.1*(T-Tsurr)-Rate*1.02e4	673.2	0

Figure 8.7c. Equations

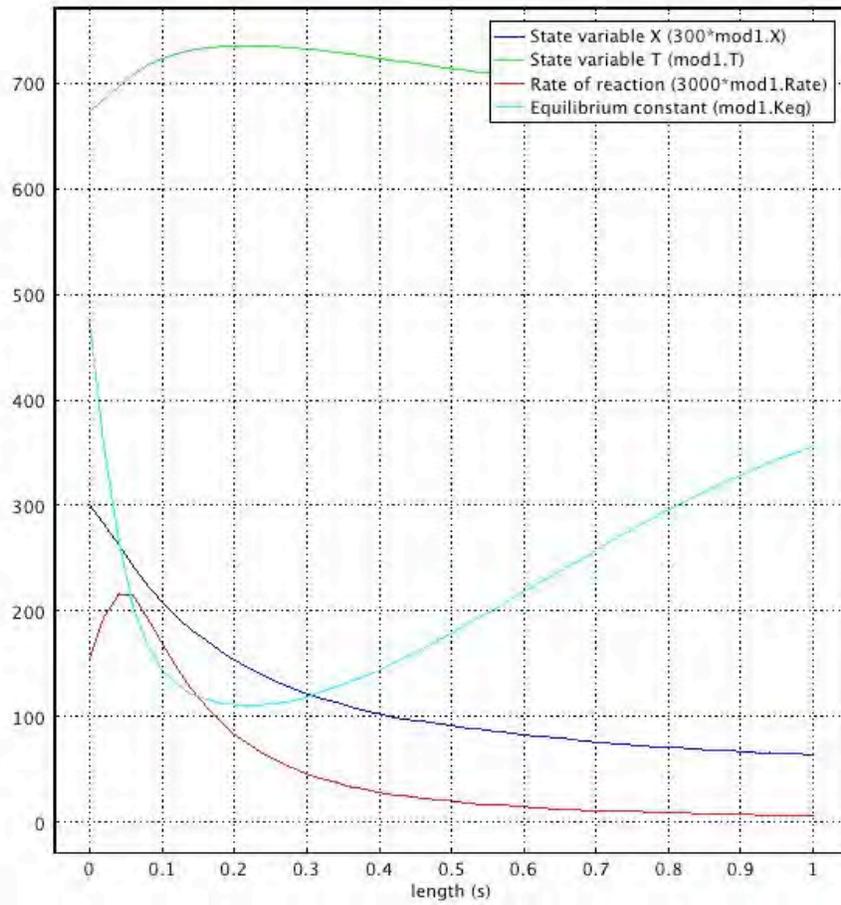
**Step Three: Solve.** Under Study, choose Time Dependent and note that the range of solution is from 0 to 1, as desired. Right click on Study, =.

**Step Four: Plot.** The plot should appear automatically. If not, choose Results under Model Builder; right click to 1D Plot Group. If that already exists, choose it. Right click on 1D Plot Group and choose Global. Then create the expressions to plot as shown in Figure 8.7d. The results (X, T, Rate, and Keq) are all scaled so that they appear on the graph. The X-Axis Data is changed to Expression, and set to t, so that the description can be changed to length. Unfortunately, in version 4.1 the units of (s) will be displayed. In this problem there are no units in the length, which is dimensionless. It is useful to see what part of the reactor is doing the most work and to see how the equilibrium constant changes with temperature, which changes with axial position.

▼ Expressions

Expression	Unit	Description
300*mod1.X		State variable X
mod1.T		State variable T
3000*mod1.Rate	1	Rate of reaction
mod1.Keq	1	Equilibrium constant

Figure 8.7d. Expressions to Plot to obtain Figure 8.7.



**Figure 8-7. Results for SO2 reactor, Eq. (8-24-26)**