

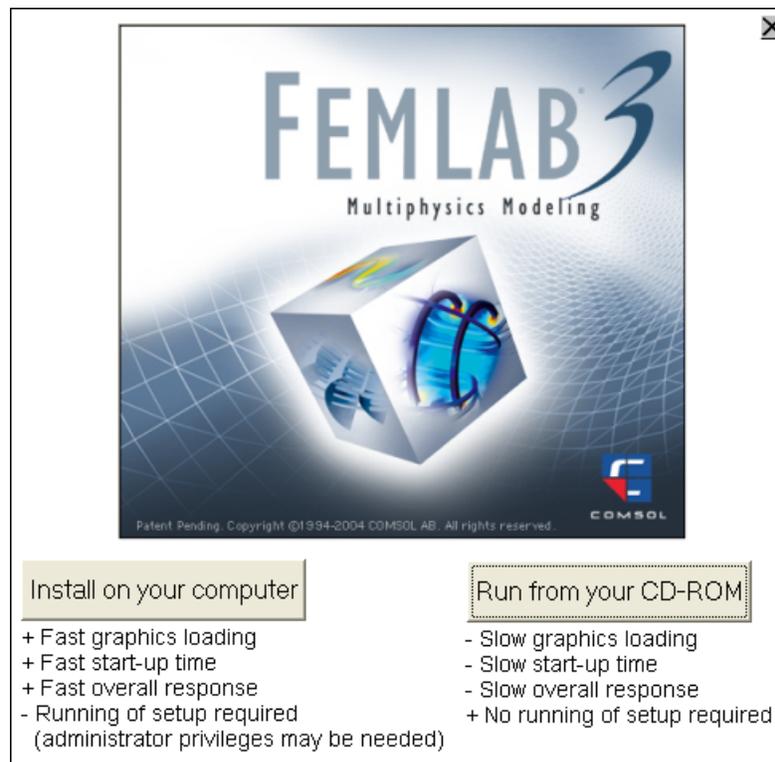
RADIAL EFFECTS IN TUBULAR REACTORS

We are going to study an elementary, exothermic, second order reversible reaction: $A + B \rightleftharpoons 2C$ in a tubular reactor (liquid phase, laminar flow regime) using FEMLAB. The reactor is cooled by a cooling jacket with variable coolant temperature. We will discuss the details of the reactor model after the basics of FEMLAB are covered.

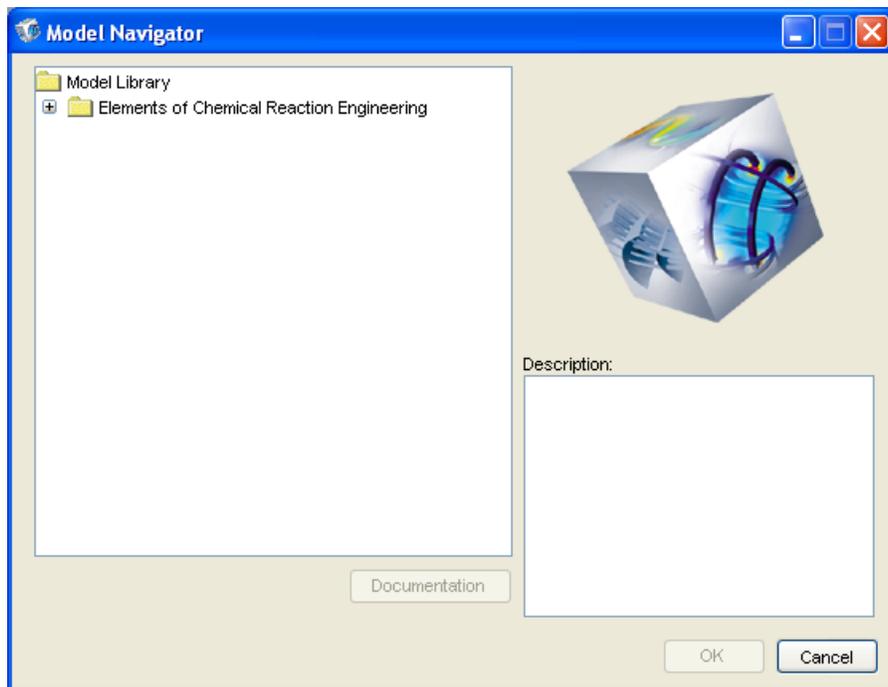
Starting the FEMLAB30F-ECRE CD-ROM

The distributed CD-ROM contains the ECRE (*Elements of Chemical Reaction Engineering*) version of FEMLAB and it has been tested on Windows 2000/XP computers. You can use it on your own machine or on CAEN Lab computers to run FEMLAB. You can run directly from the CD-ROM or install the program to your hard drive and run it from there.

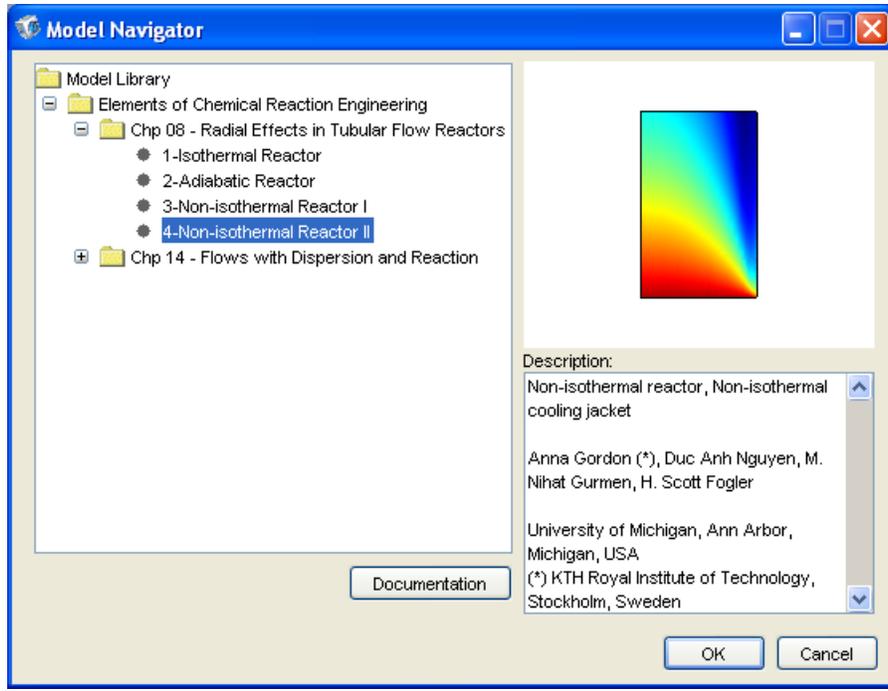
1. Insert the CD-ROM and wait until the launcher starts (may take up to 3 minutes)
 - If the launcher does not start automatically
 - i. Go to your CD-ROM drive directory
 - ii. Double-click on FEMLAB-launcher.exe
2. You should see the launcher interface as shown below



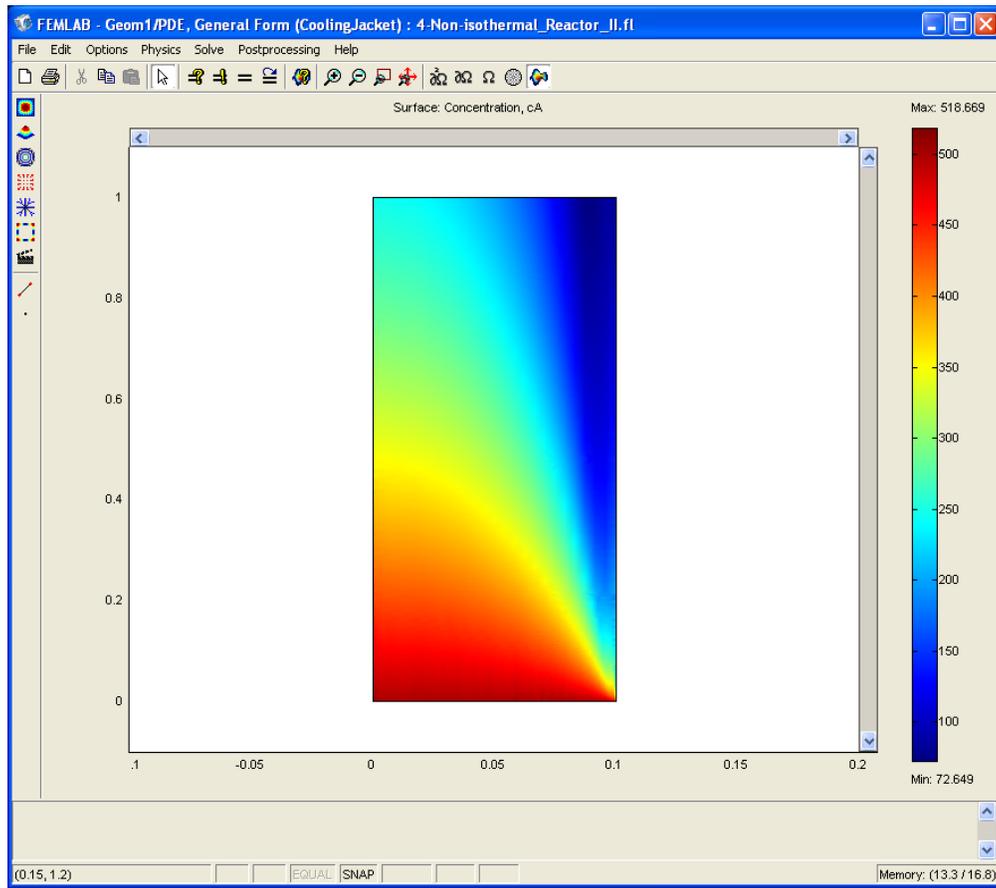
3. Click on the button with the appropriate method (Try to run the program from the CD-ROM if you cannot install it on the computer you are working with for some reason)
 - If you choose the installation option, shortcuts will be placed on your **Desktop** and **Start→Programs** menu so you can start FEMLAB. There will be also an uninstallation program in the **Start→Programs** location.
 - If you don't have administrative rights on the computer you are working, the default installation directory would not work. However, you can change it to your **Desktop** and install there.
4. Now, start FEMLAB either from the CD-ROM or from the installed shortcuts to see the **Model Navigator** as shown below (start-up may take up to 3-5 minutes from CD-ROM)



5. You can browse through the available example problems that correspond to the chapters of the *Elements of Chemical Reaction Engineering* book.
6. The **Documentation** button provides you background information on the system and how the model file can be created on a full version of FEMLAB.
7. Select the fourth example from chapter 8 as shown below and Click **OK**

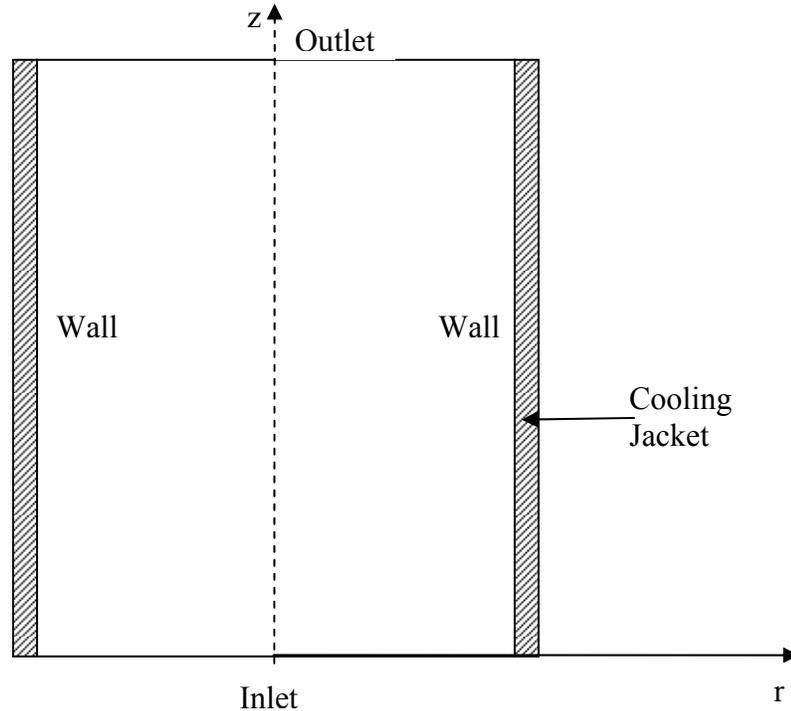


8. Now, you should see the FEMLAB result as the surface plot of concentration A in the reactor with the base-case parameters



In the rest of the document we will first discuss the theoretical basis of the mathematical model constructed in FEMLAB. Then, we will go through some step-by-step virtual experiments to answer the questions at the end of this problem set.

Description of the model



The system is described by three partial differential equations on a two dimensional surface. This surface represents a cross-section of the tubular reactor in the z - r -plane. The borders of the two- dimensional surface represent the inlet, outlet, the wall of the reactor and the center line. This means that the three differential equations only will be solved for half the reactor. This can be done because the reactor is axisymmetrical. The partial differential equations represent one mass balance for the fluid inside the reactor, and two energy balances, one for the fluid inside the reactor and one for the coolant in the cooling jacket.

The PDEs and ODE are:

Mass Balance, species A

$$D_p \frac{1}{r} \frac{\partial C_A}{\partial r} + D_p \frac{\partial^2 C_A}{\partial r^2} + D_p \frac{\partial^2 C_A}{\partial z^2} - 2U \left(1 - \left(\frac{r}{R} \right)^2 \right) \frac{\partial C_A}{\partial z} + r_A = 0$$

The boundary conditions for the mass balance are

Inlet (z=0) $C_A(r,0) = C_{A0}$

At the wall (r=R=radius) $\frac{\partial C_A}{\partial r}(R,z) = 0$

Center (symmetry) line $\frac{\partial C_A}{\partial r}(0,z) = 0$

In reality, there is no need to specify a boundary condition for the outlet boundary. FEMLAB, however, requires that a boundary condition is selected for all boundaries. The boundary condition selected for the outlet is not a true boundary condition, meaning that it doesn't put any restrictions to the calculations but keeps the outlet boundary open.

Outlet (z=L=length) $\frac{\partial C_A}{\partial z}(r,L) = 0$ (fully-developed flow)

Energy balance inside the reactor

$$k \frac{1}{r} \frac{\partial T}{\partial r} + k \frac{\partial^2 T}{\partial r^2} + k \frac{\partial^2 T}{\partial z^2} - 2U \left(1 - \left(\frac{r}{R} \right)^2 \right) \rho C_p \frac{\partial T}{\partial z} - r_A (-\Delta H_{Rx}) = 0$$

The boundary conditions for the energy balance are

Inlet (z=0) $T(r,0) = T_0$

At the wall (r=R=radius) $-\frac{\partial T}{\partial r}(R,z) = \frac{U_k}{k}(T - T_a)$

Center (symmetry) line $\frac{\partial T}{\partial r}(0,z) = 0$

As for the mass balance, the boundary condition at the outlet for the energy balance is chosen in such way to keep the outlet boundary open.

Outlet (z=L=length) $\frac{\partial T}{\partial z}(r,L) = 0$ (fully-developed flow)

Energy balance of the coolant in the cooling jacket

$$\frac{dT_a}{dz} = \frac{2\pi R U_k (T - T_a)}{m_c C_{pc}}$$

The boundary condition for the cooling jacket is

The cooling jacket is described by a one dimensional line. Therefore, we only need an inlet boundary condition for the cooling jacket.

$$\text{Inlet (z=0)} \quad T_a(0) = T_{a0}$$

Constant Model Parameters

Parameters for the model (Note: for each parameter, the left-hand-side part of the equal sign (e.g. Diff) is used for the **Name** of constant and the right-hand-side part of the equal sign (e.g. 1E-9) is used for the **Expression**):

- Diffusivity of all species, $Diff = 1E-9 \text{ m}^2/\text{s}$
- Activation energy, $E = 95238 \text{ J/mol}$
- Rate constant, $A = 1.1E8 \text{ m}^6/(\text{mol}\cdot\text{kg}\cdot\text{s})$
- Gas constant, $R = 8.314 \text{ J/mol}\cdot\text{K}$
- Inlet temperature, $T_0 = 320 \text{ K}$
- Total flowrate, $v_0 = 0.0005 \text{ m}^3/\text{s}$
- Reactant concentrations in the feed, $C_{A0} = C_{B0} = 500 \text{ mol/m}^3$
- Reactor radius, $Ra = 0.1 \text{ m}$
- Catalyst density, ρ_{Cat} , $\text{rhoCat} = 1500 \text{ kg/m}^3$
- Heat of reaction, ΔH_{Rx} , $dHrx = -83680 \text{ J/mol}$
- Equilibrium constant at 303 K, $Keq_0 = 1000 @ 303 \text{ K}$
- Thermal conductivity of the reaction mixture, $ke = 0.559 \text{ J/m}\cdot\text{s}\cdot\text{K}$
- Average density of the reaction mixture, ρ , $\text{rho} = 1000 \text{ kg/m}^3$
- Heat capacity of the reaction mixture, $Cp = 4180 \text{ J/kg}\cdot\text{K}$
- Overall heat transfer coefficient, $U_k = 1300 \text{ J/m}^2\cdot\text{s}\cdot\text{K}$
- Inlet temperature of the coolant, $Ta_0 = 298 \text{ K}$
- Heat capacity of the coolant, $Cp_J = 4180 \text{ J/kg}\cdot\text{K}$
- Coolant flowrate, $m_J = 0.01 \text{ kg/s}$

Variable Model Parameters

The definitions for the variables used in this model are (Note: for each expression in FEMLAB form, the left-hand-side part of the equal sign (e.g. u0) is used for the **Name** of the variable and the right-hand-side part of the equal sign (e.g. v0/(pi*Ra^2)) is used for the **Expression**):

- The superficial flow rate, $u_0 = \frac{v_0}{\pi \cdot (Ra)^2}$.

In FEMLAB form: u0 = v0/(pi*Ra^2)

- The superficial, laminar, flow rate, $u_z = 2 \cdot u_0 \left(1 - \left(\frac{r}{Ra} \right)^2 \right)$

In FEMLAB form: uz = 2*u0*(1-(r/Ra).^2)

- The conversion, $x_A = \frac{c_{A0} - c_A}{c_{A0}}$

In FEMLAB form: xA = (cA0-cA)/cA0

- The concentration of B, $c_B = c_{B0} - c_{A0} \cdot x_A$

In FEMLAB form: cB = cB0-cA0*xA

- The concentration of C, $c_C = 2 \cdot c_{A0} \cdot x_A$

In FEMLAB form: cC = 2*cA0*xA

- The rate of reaction:

- Before adding the energy balance:

$$r_A = -A \cdot \exp\left(\frac{-E}{R \cdot T_0}\right) \cdot \rho_{Cat} \cdot \left(c_A \cdot c_B - \frac{c_C^2}{K_{eq}} \right)$$

In FEMLAB form: rA = -A*exp(-E/R/T0)*rhoCat*(cA.*cB-cC.^2/Keq)

- After adding the energy balance:

$$r_A = -A \cdot \exp\left(\frac{-E}{R \cdot T}\right) \cdot \rho_{Cat} \cdot \left(c_A \cdot c_B - \frac{c_C^2}{K_{eq}} \right)$$

In FEMLAB form: rA = -A*exp(-E/R/T)*rhoCat*(cA.*cB-cC.^2/Keq)

- The temperature dependent equilibrium constant,

- Before adding the energy balance:

$$K_{eq} = K_{eq0} \cdot \exp\left(\frac{\Delta H_{Rx}}{R} \left(\frac{1}{303} - \frac{1}{T_0}\right)\right)$$

In FEMLAB form: $Keq = Keq0 * \exp(dHrx/R * (1/303 - 1/T0))$

- After adding the energy balance:

$$K_{eq} = K_{eq0} \cdot \exp\left(\frac{\Delta H_{Rx}}{R} \left(\frac{1}{303} - \frac{1}{T}\right)\right)$$

In FEMLAB form: $Keq = Keq0 * \exp(dHrx/R * (1/303 - 1/T))$

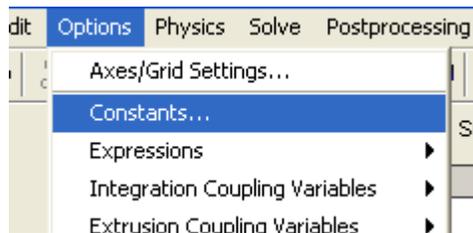
- The heat production term, $Q = (-r_A) \cdot (-\Delta H_{Rx})$

In FEMLAB form: $Q = (-rA) * (-dHrx)$

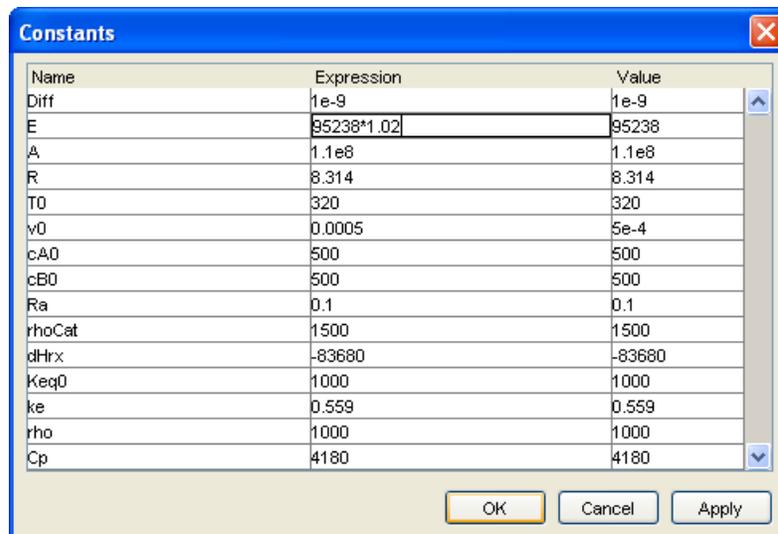
How to change the constant model parameters

Let's increase the activation energy, E, by 2%

1. Select the menu **Options** → **Constants**



2. Select E in the list and add *1.02 to the end of the **Expression**



- To solve the model with the new parameter click the equal sign from the toolbar as shown below



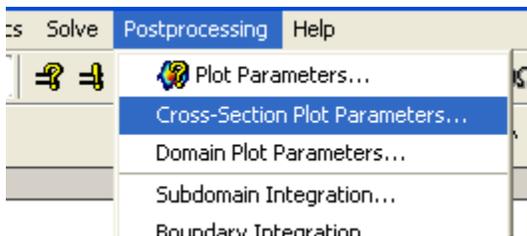
How to construct cross-section plots

Let's draw a conversion profile at the mid point of the reactor

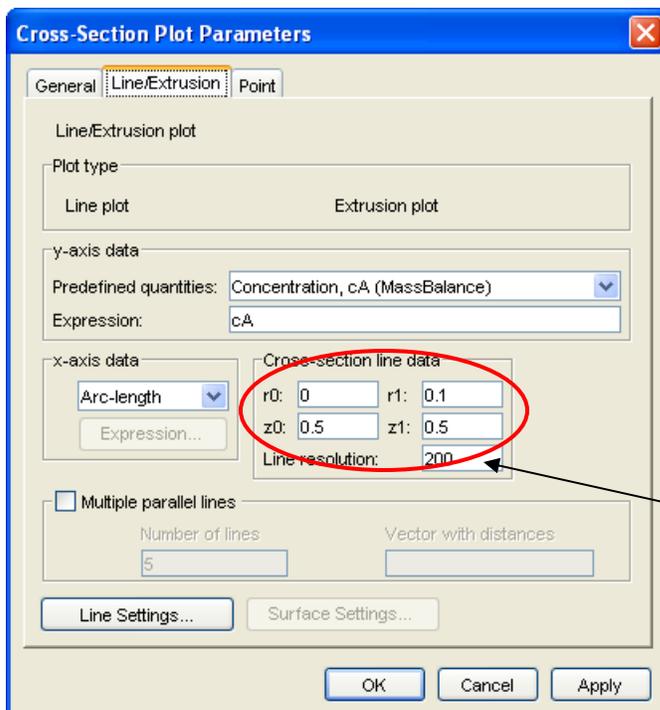
- First, make sure FEMLAB is in **Postprocessing Mode** by selecting the button circled below



- Select **Postprocessing** → **Cross-Section Plot Parameters**

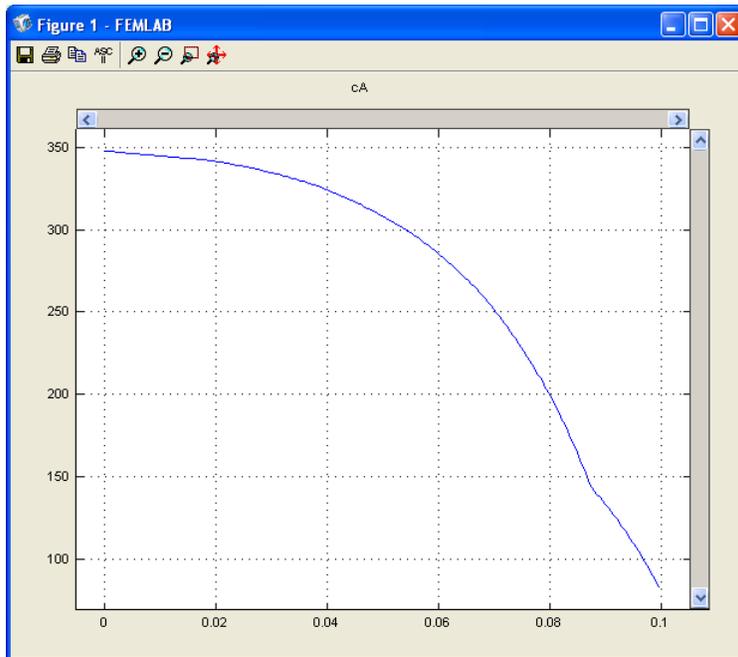


- Select the **Line/Extrusion** tab and fill in the values as shown below to create a cross-section plot at the reactor

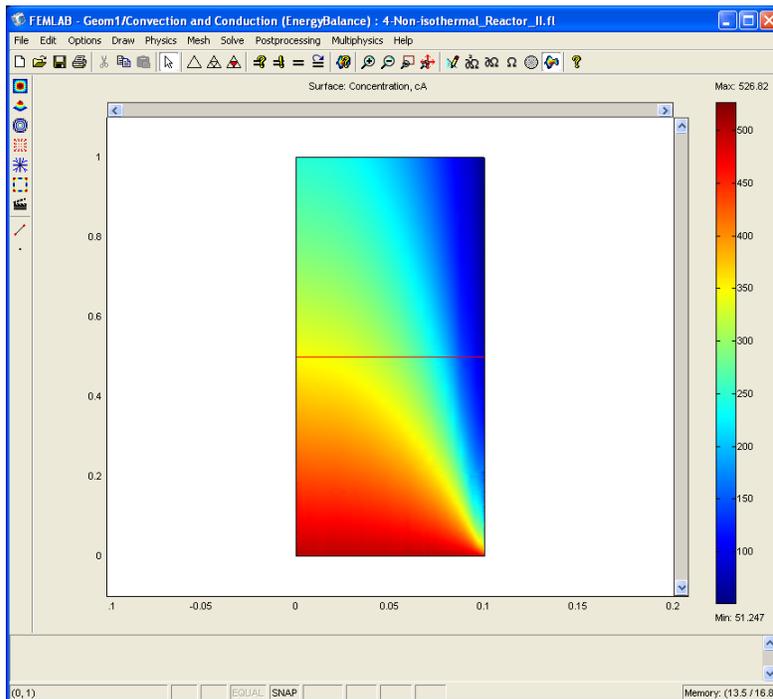


cross-section on the r-z plane from (0.0,0.5) to (0.1,0.5)

4. Press **Apply** to see the graph below



5. The main window will show a red line where the cross-section is taken



6. We can add more cross-section plots to the same graph shown in step 5 repeating step 3 and selecting Figure 1 from the **General** tab before defining a new cross section on the **Line/Extrusion** tab

How to find average conditions through integration

Let's calculate the average outlet conversion

1. After solving the model we have the concentration of A as a function of r and z, namely, $cA(r,z)$
2. At the outlet of the reactor ($z = 1$) the average flow rate of species A is defined mathematically as

$$\overline{FA} = \frac{\int_{r_{\min}=0}^{r_{\max}=0.1} (2\pi r)(uz \cdot cA(r,1))dr}{\pi R^2/2}$$

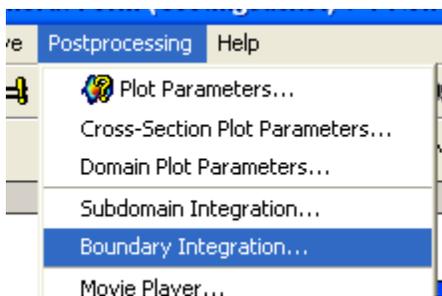
3. Similarly, at the entrance, the average flow rate of species A is

$$\overline{FA0} = \frac{\int_{r_{\min}=0}^{r_{\max}=0.1} (2\pi r)(uz \cdot cA(r,0))dr}{\pi R^2/2}$$

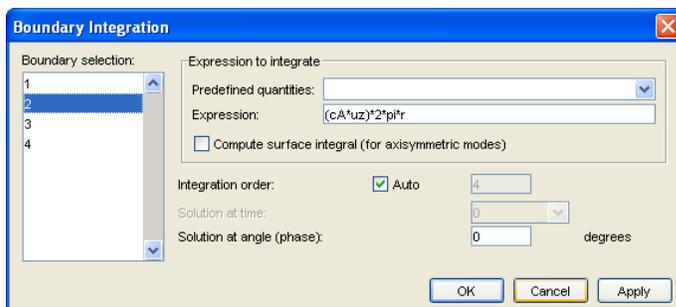
4. With these definitions, the average conversion at the outlet is defined as

$$\overline{X} = \frac{\overline{FA0} - \overline{FA}}{\overline{FA0}} \cdot 100$$

5. FEMLAB provides **Subdomain** and **Boundary Integration** for integrating arbitrary expressions that involve the solved variables
6. Select **Postprocessing** → **Boundary Integration**



7. First select **2** in the **Boundary Selection** for the inlet



8. Then enter $(cA*uz)*2*pi*r$ for the expression to be integrated

9. Click Apply

10. Value of the integral is reported at the bottom of the main FEMLAB window as

Value of line integral: 0.25, Expression: $(cA*uz)*2*pi*r$, Boundary: 2.

11. Repeat the same procedure for the third boundary

Value of line integral: 0.093119, Expression: $(cA*uz)*2*pi*r$, Boundary: 3.

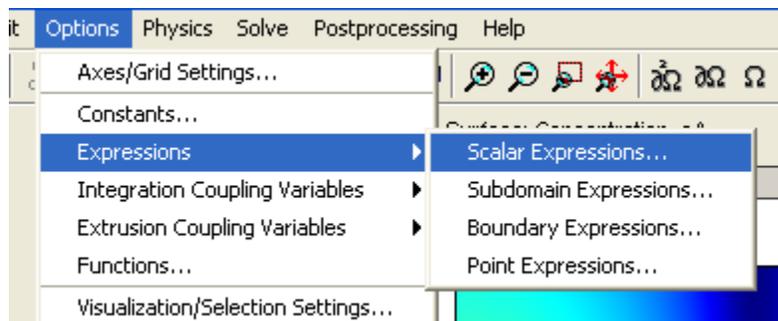
12. Now, perform the final operation manually

$$\bar{X} = \frac{0.25 - 0.093}{0.25} \cdot 100 = 62.8\% \approx 63\%$$

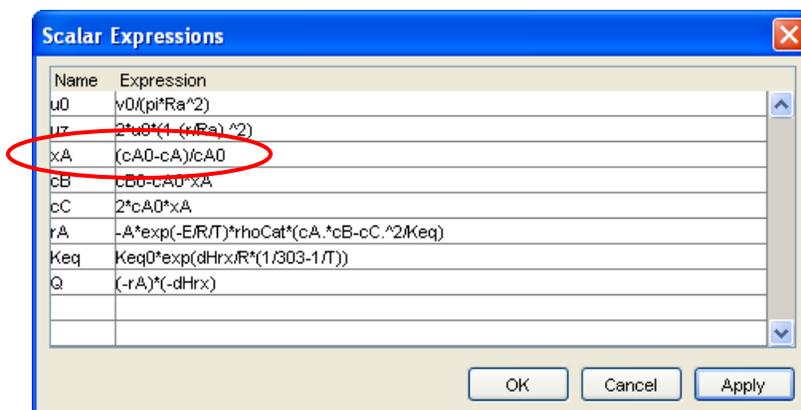
13. Note that we have omitted the term in the denominator shown in steps 3 and 4 because in step 12 they would have been cancelled out anyway.

How to define new expressions

1. The conversion, x_A , is not defined implicitly by the PDE's describing the physical system. Therefore it is defined explicitly in FEMLAB.
2. Select **Options** → **Expressions** → **Scalar Expressions**



3. In addition to other variables, the conversion, x_A , is defined as shown below



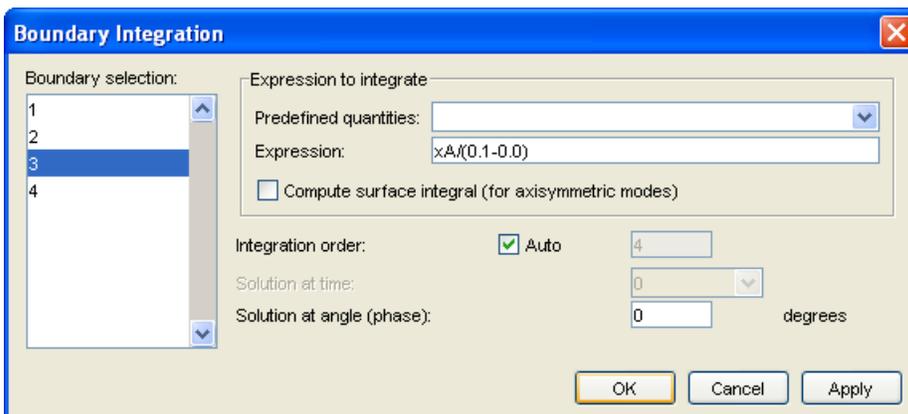
4. The expressions for uz, rA, Keq, etc. are used by FEMLAB to calculate the solution
5. The expressions for xA, cB and cC, however, are created for use in the postprocessing mode
6. You can use xA or any other scalar expression in the postprocessing mode (in graphs, etc.) instead of the predefined variables
7. To make a crossplot of the conversion xA, type the name of the scalar expression in the appropriate place as shown below



8. The average conversion at the outlet could have been also evaluated by realizing that for averaging xA we can perform the following integration

$$\overline{x_A} = \frac{\int_{r_{\min}=0}^{r_{\max}=0.1} x_A(r,1) dr}{r_{\max} - r_{\min}}$$

9. On **Boundary Integration** dialog entering the expression to be integrated as below results the same 62.9% \approx 63% we found earlier



10. The value is reported on the main FEMLAB window as

Value of line integral: 0.628575, Expression: xA/(0.1-0.0), Boundary: 3.

Questions

1. Analyze visually the FEMLAB solution for the base-case of the model and answer following questions:
 - a. Why is the concentration of A near the wall lower than the concentration near the center?
 - b. Where in the reactor do you find the maximum and minimum reaction rates? Why?
2. Now, we will change some of the parameters and rerun the model.
 - a. Increase the activation energy of the reaction by 5%. How do the conversion profiles change? How does the average outlet conversion change?
 - b. Decrease the original activation energy by 5%. How do the conversion profiles change? How does the average outlet conversion change?
 - c. Change the activation energy back to the original value.
 - d. Increase the thermal conductivity, k_e , by a factor of 10 and explain how this change affects the temperature profiles. At what radial position do you find the highest conversion?
 - e. Increase the coolant flow rate by a factor of 10 and explain how this change affects the conversion?
3. Describe your findings in 2-3 sentences when you varied the parameters (for all parts).
4. What would be your recommendation to maximize the average outlet conversion?