Monolithic reactor (PDE modes)

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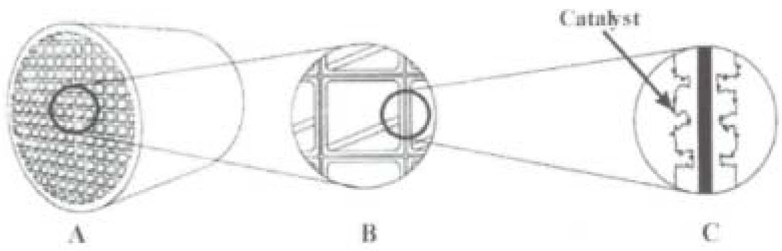
Monolithic reactors
(Model assumptions)



The figure shows the monolithic reactor, A, channel wall, B, and porous ceramic (washcoat), C, with catalyst. The illustration is from [1]

- The following model simulates the catalytic abatement of a volatile organic compound (VOC), in this case a contaminant in a waste gas.
- Assumptions
  - Since the concentrations of contaminants from the waste gases are usually very low, the heat release from the oxidation is negligible.
  - The flow is laminar and the axial diffusion of the reactants is small compared to the convective flow. So axial diffusion is neglected.
  - A diameter of the monolith channel : 0.625mm
  - Sides of length (square) : 0.645mm

Boundary and inlet conditions

- The conditions at the channel inlet z=0 are uniform concentration and a fully developed velocity profile.
- The velocity can be analytically derived using the Hagen-Poiseuille law.

$$V_z = 2U_m(1 - x^2 - y^2)$$

Parameter	Meaning
V_z	Velocity
U_m	Average velocity
x, y	coordinates

Gas phase equation

- The equation describing the process for the gas in the monolith channel is as follows.

$$U(x,y)\frac{\partial c}{\partial z'} = \frac{\partial}{\partial x'}(D\frac{\partial c}{\partial x'}) + \frac{\partial}{\partial y'}(D\frac{\partial c}{\partial y'})$$

Parameter	Meaning
$U(x,y)$	Velocity profile
D	Diffusion coefficient
c	Concentration
x, y, z	Space coordinates

Solid phase equation

- The equation for the washcoat describes the simultaneous reaction and diffusion in the porous network of the washcoat.
- The temperature dependence of the reaction is accounted through the Arrhenius law

$$\frac{\partial}{\partial x'}\left(D^{eff}\frac{\partial c}{\partial x'}\right)+\frac{\partial}{\partial y'}\left(D^{eff}\frac{\partial c}{\partial y'}\right)+Q=0$$

$$Q=-ke^{\left(-\frac{E}{RT}\right)}c$$

Parameter	Meaning
D^{eff}	Effective diffusion coefficient
Q	Reaction rate
k	Constant
E	Activation energy
T	Temperature
R	Gas constant

Scaling

- Scaled variables

$$V(x,y) = U(x,y)/U_m, \;\; x = x^{'}/Ra, \;\; y = y^{'}/Ra$$

$$z = z^{'}/L, \;\; C = c/C_0$$

- Scaled equation

$$U(x,y)K_1 \frac{\partial c}{\partial z} = \frac{\partial}{\partial x}(D\frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(D\frac{\partial C}{\partial y})$$

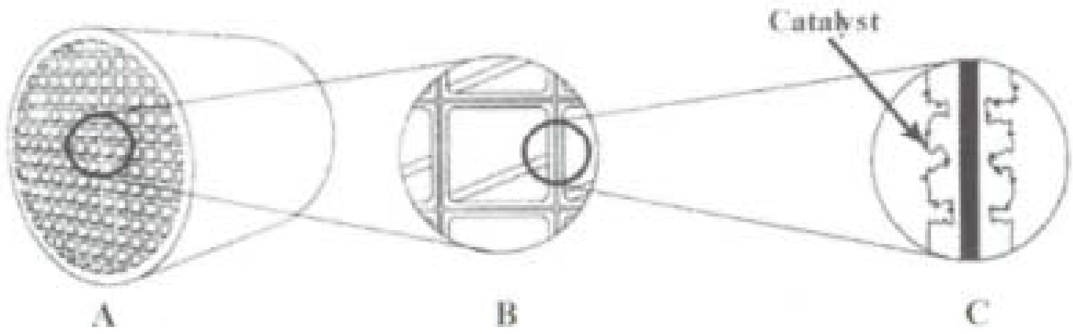
$$\frac{\partial}{\partial x}(D^{eff}\frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(D^{eff}\frac{\partial C}{\partial y}) - K_2 C = 0$$

$$K_1 = \frac{U_m Ra^2}{L}$$

$$K_2 = -ke^{(-\frac{E}{RT})}Ra^2$$

Monolithic reactors

The figure shows the monolithic reactor, A, channel wall, B, and porous ceramic (washcoat), C, with catalyst. The illustration is from [1]



- In this model, we will use the following parameter values :
- At scaling equation

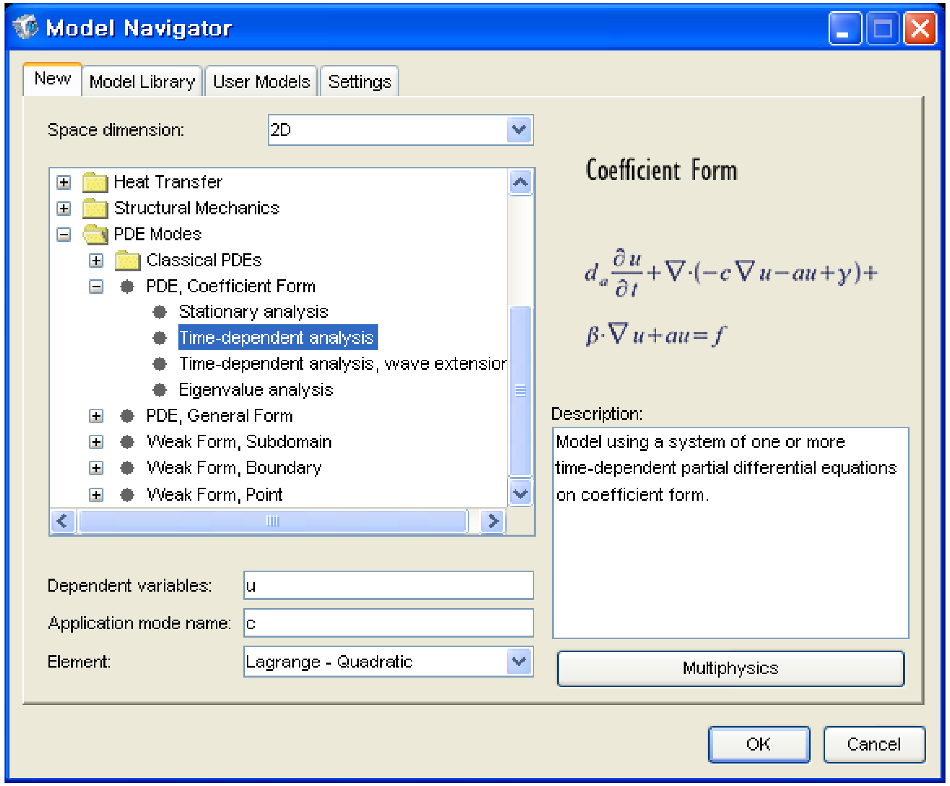
- K_1=0.39

- K_2=11.2

- D=0.88 (in this case cm^2s^{-1})

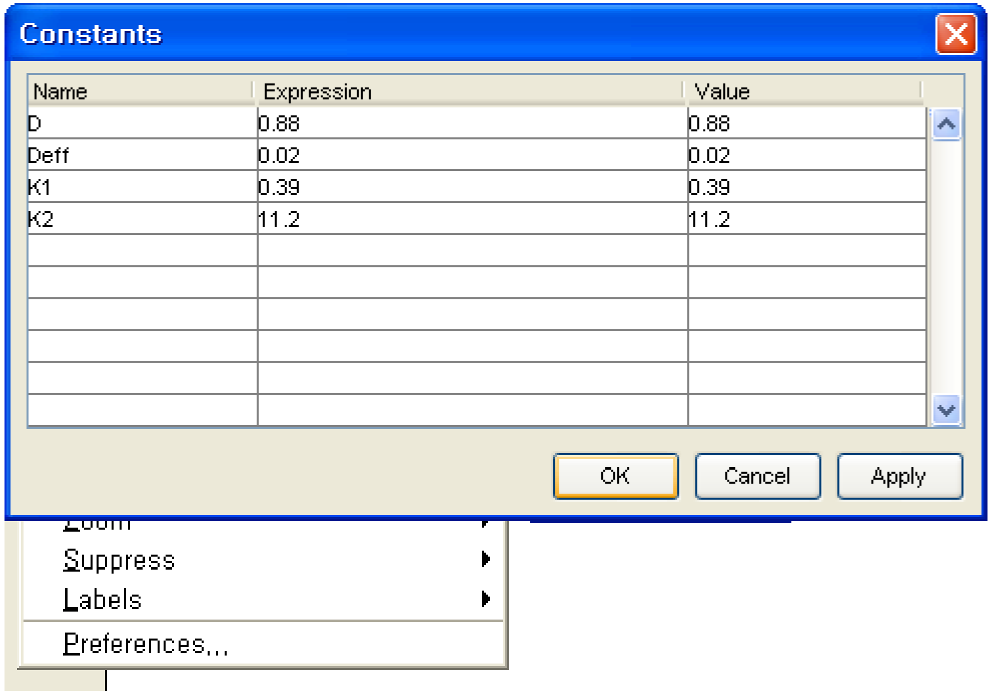
- D^{eff}=0.02 (cm^2s^{-1})

Model navigator



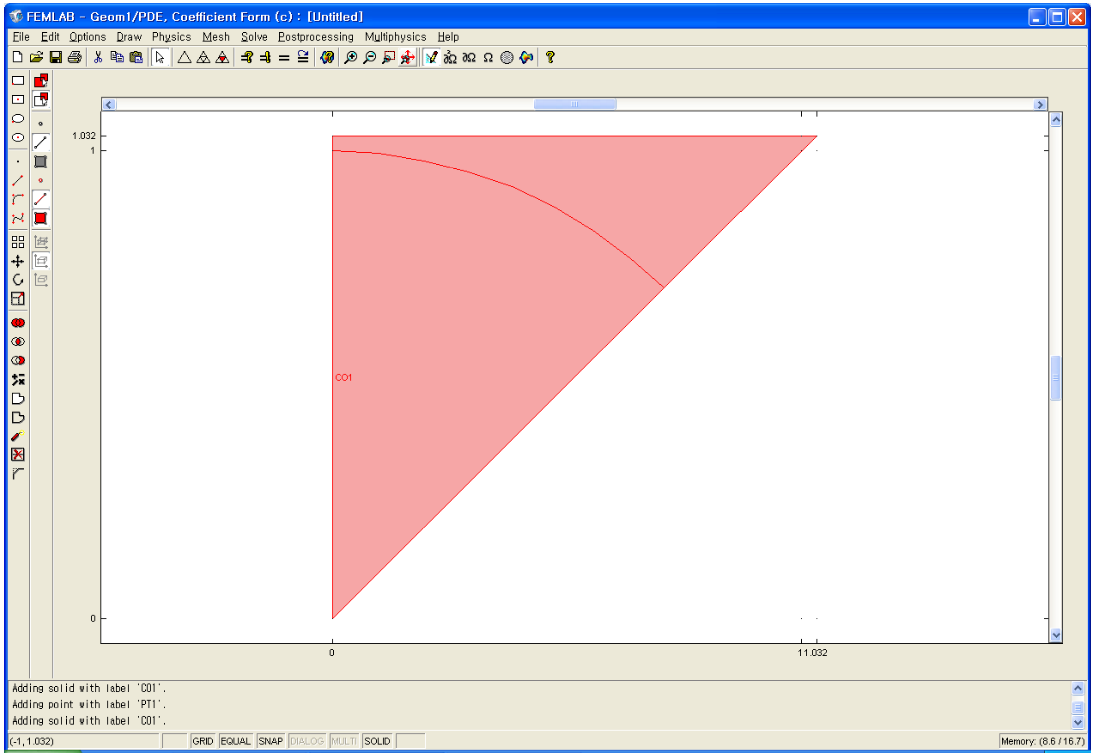
1. Select the **2D, Coefficient, Time-dependent** PDE mode in the **Model Navigator**. Use **Lagrange –Quadratic** elements.

Options and settings



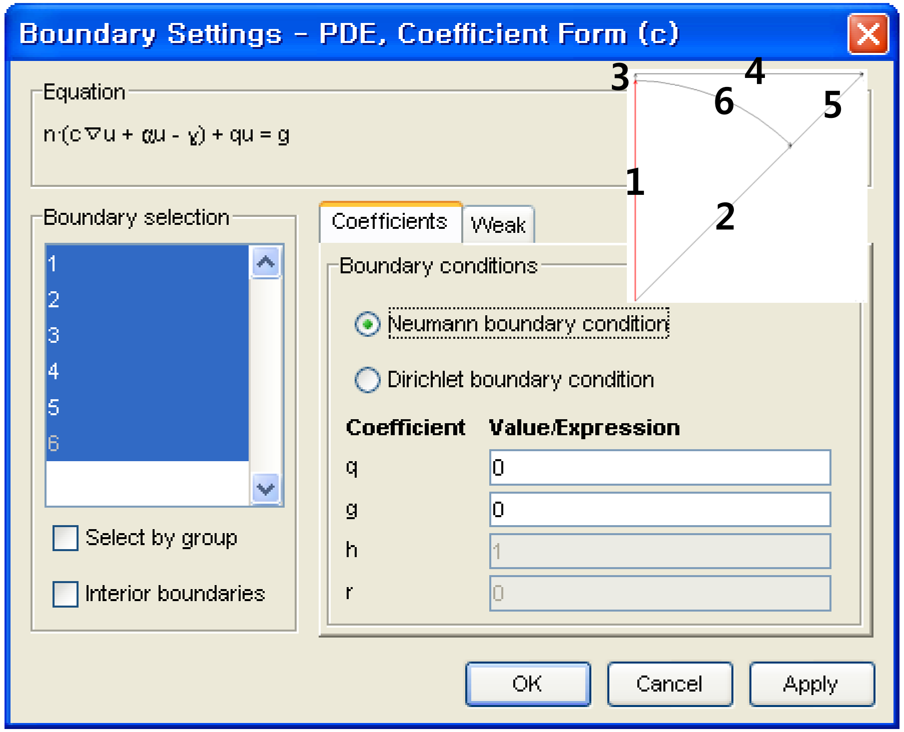
1. Set **Axis and Grid Settings** according to the following figure.
2. Enter the following constants.

Geometry modeling



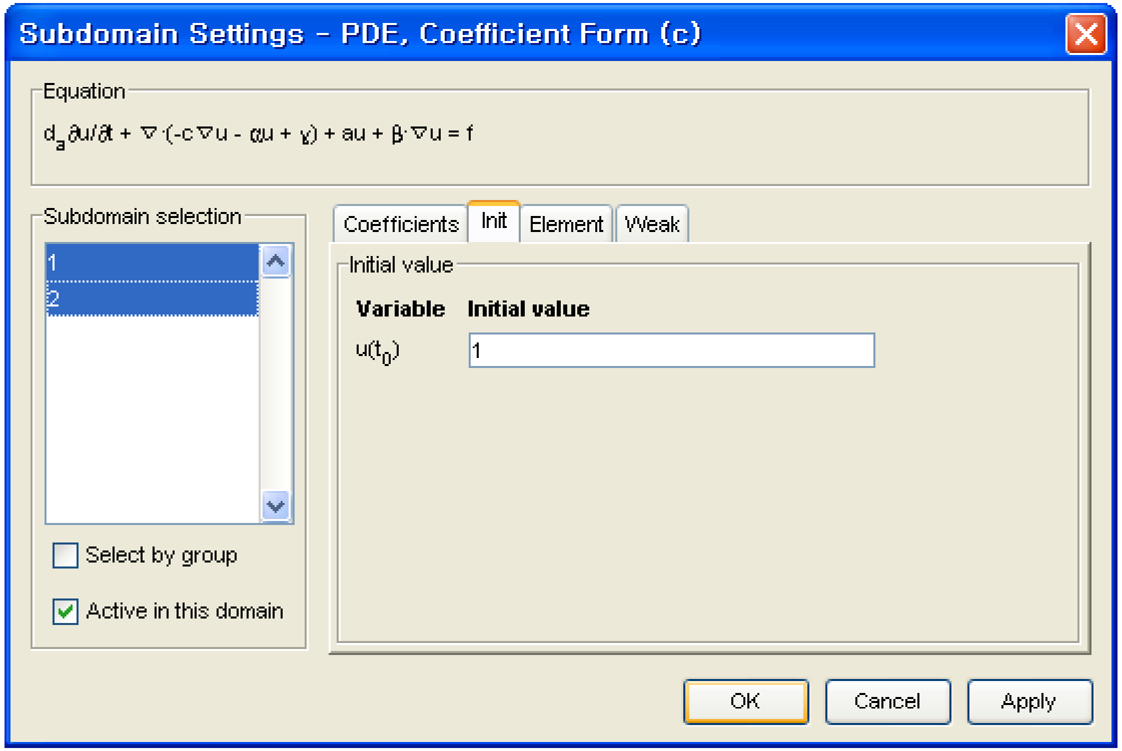
1. Draw a circle, C1, centered at (0, 0) with a radius of 1.
2. Draw a triangle, CO1, with the corner points (0, 0), (1.032, 1.032), (0, 1.032).
3. Form the composite object CO2 using the set formula CO1+CO1*C1.
4. Press the **Zoom Extents** button.

Physics settings (boundary)



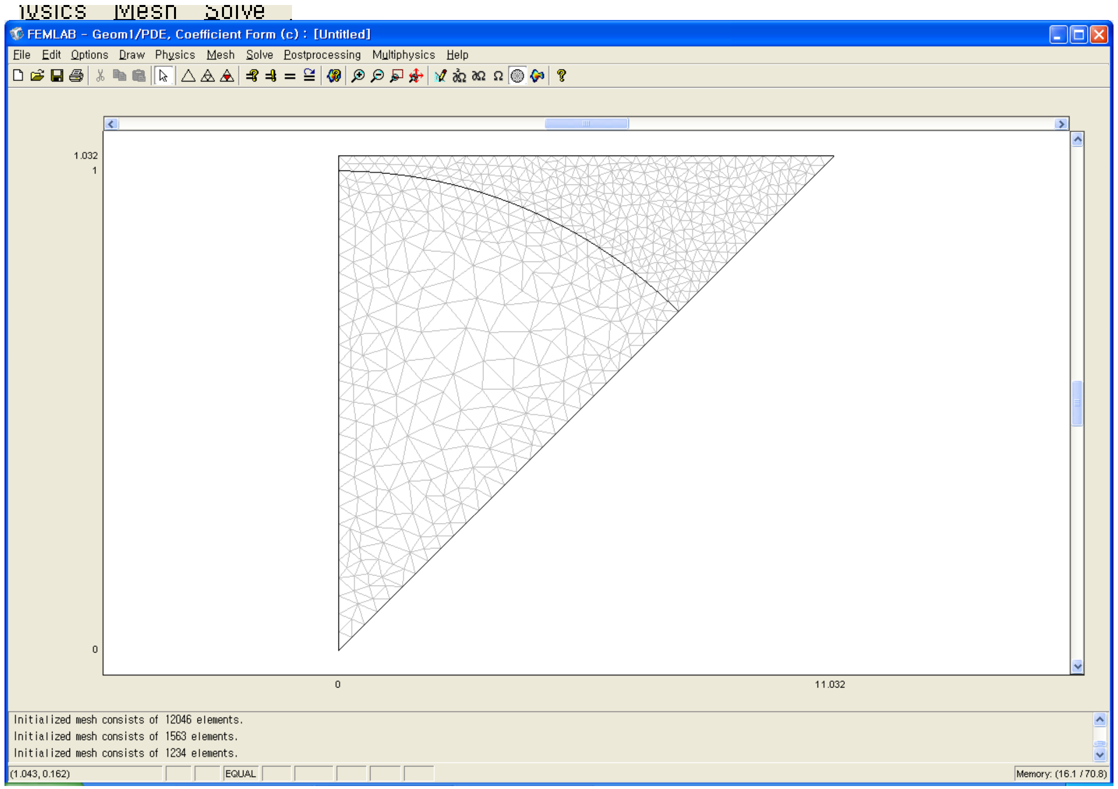
1. Enter boundary coefficients according to the following figure.

Physics settings (subdomain)



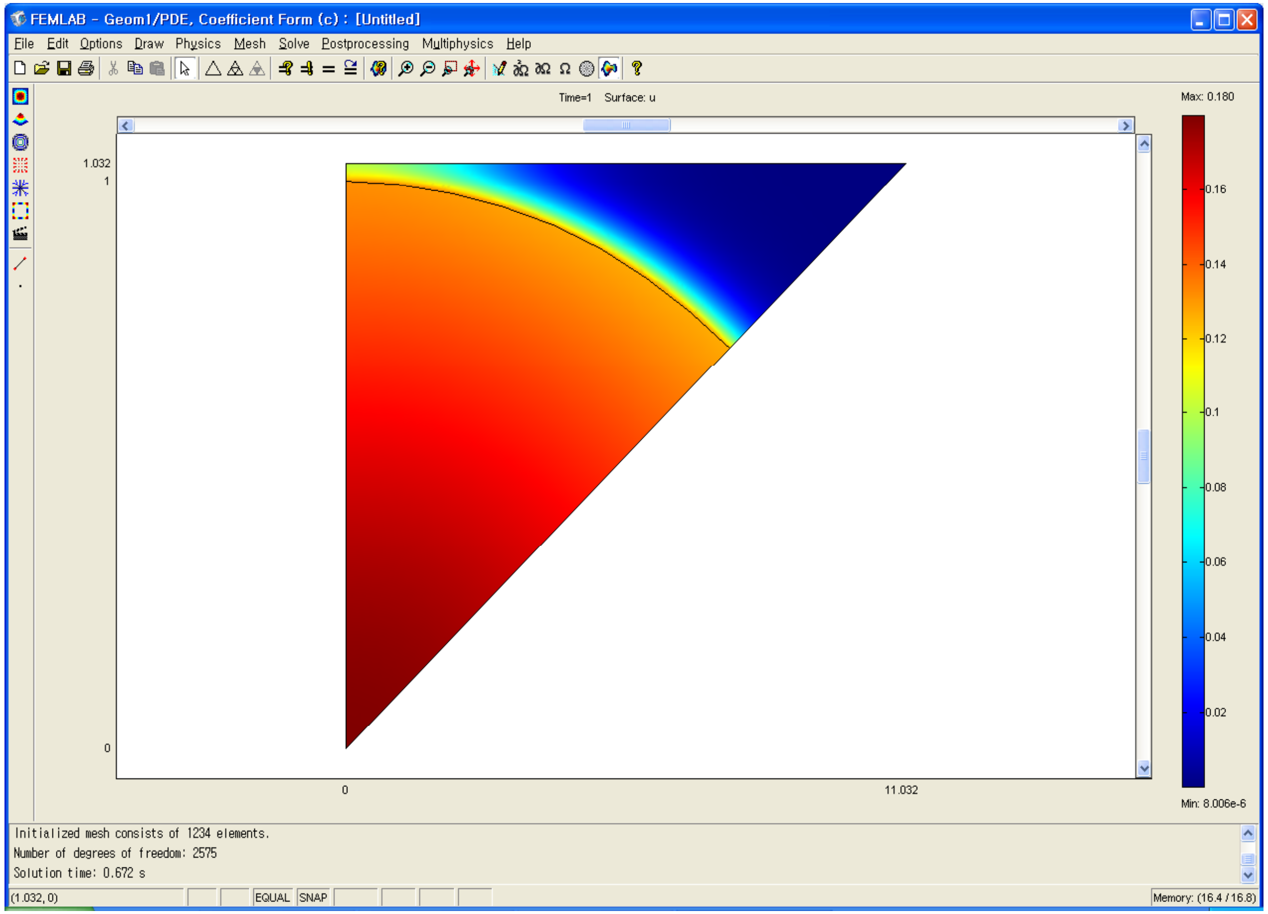
1. Enter PDE coefficients according to the following figure.
2. Set the initial condition to 1 for both subdomains.

Mesh generation



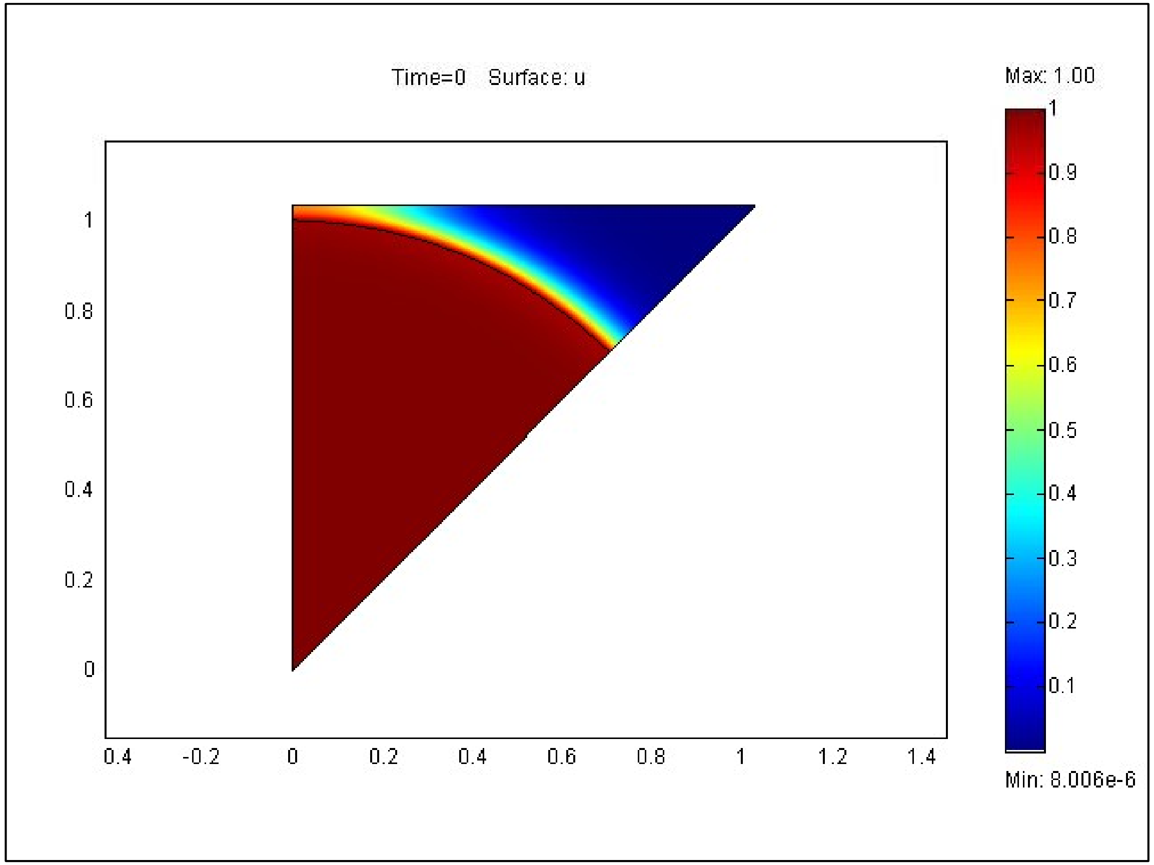
1. In the **Mesh Parameters** dialog box, enter 1 0.2 2 0.03 as **Max element size for subdomains**.
2. Initialize the mesh.

Solving the model



1. In the **Solver Parameters** dialog box, verify that **Output** times is 0:0.1:1 and set **Relative Tolerance** to 0.001.
2. Solve the problem.

Postprocessing and visualization



1. To see the concentration along the whole channel, press the **Animation** button.

Conclusions

- Concentration in the solid-phase drops rapidly towards zero close to the monolith wall. This is because the reaction in this model is quite rapid and the reacting gas is consumed near the outer surface.
- It would therefore be enough to coat the channels with a smaller amount of washcoat.