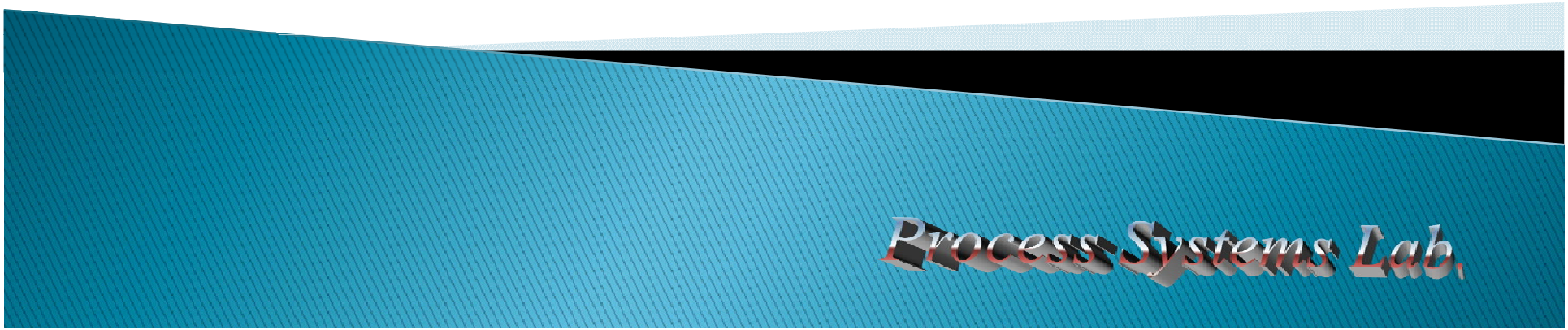
Heterogeneous catalytic reaction in PFTR



Theory

- The **plug flow reactor** (**PFR**) model is used to describe chemical reactions in continuous, flowing systems.
- Fluid going through a PFR may be modeled as flowing through the reactor as a series of infinitely thin coherent "plugs", each with a uniform composition, traveling in the axial direction of the reactor, with each plug having a different composition from the ones before and after it.

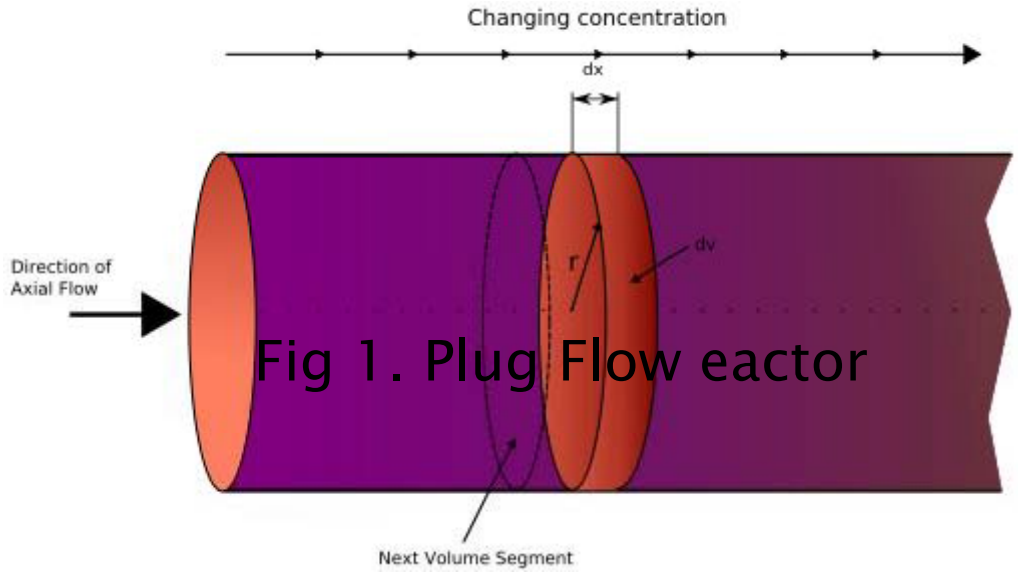


Fig 1. Plug Flow eactor

Theory

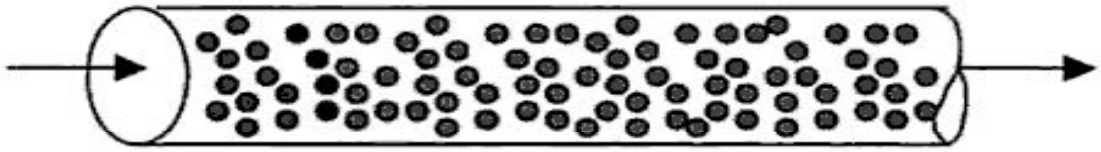


Fig 2. Schemetic of a fixed bed with reaction largely localized

- Mchedlov proposed a general parameter model for heterogeneous reaction in a dispersed phase.
- The model focuses on situations where mass transfer is asymmetric.
- Some species have greater mass transfer coefficients with the dispersed phase than others.
- Turbulence usually leads to equal mass transfer coefficients for each species

Theory

- Consider the reaction $u + v \leftrightarrow w$

- Mass transfer coefficient
  The mass transfer coefficient is a diffusion rate constant that relates the
  mass transfer rate, mass transfer area, and concentration gradient as
  driving force.
- The reaction only occurs in the dispersed phase. The lumped parameter model gives three convection-diffusion-mass transfer equations in the bulk
  phase.

Reaction equations

$$U\frac{\partial u}{\partial z} = D_u\frac{\partial^2 u}{\partial z^2} - j_u(u,\tilde{u})$$

$$U\frac{\partial v}{\partial z} = D_v\frac{\partial^2 v}{\partial z^2} - j_v(v,\tilde{v})$$

$$U\frac{\partial w}{\partial z} = D_w\frac{\partial^2 w}{\partial z^2} - j_w(w,\tilde{w})$$

Theory

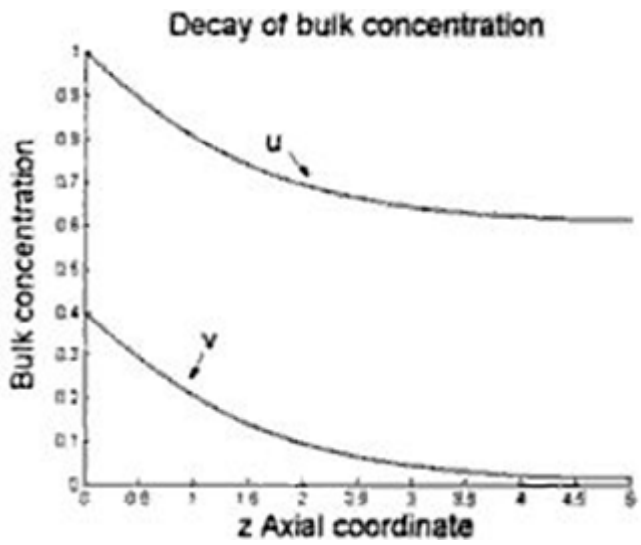
- The fluxes j take the traditional mass transfer coefficient form

$$j_u = \kappa_u (u - \tilde{u}),$$
$$j_v = \kappa_v (v - \tilde{v}),$$
$$j_w = \kappa_w (w - \tilde{w}),$$

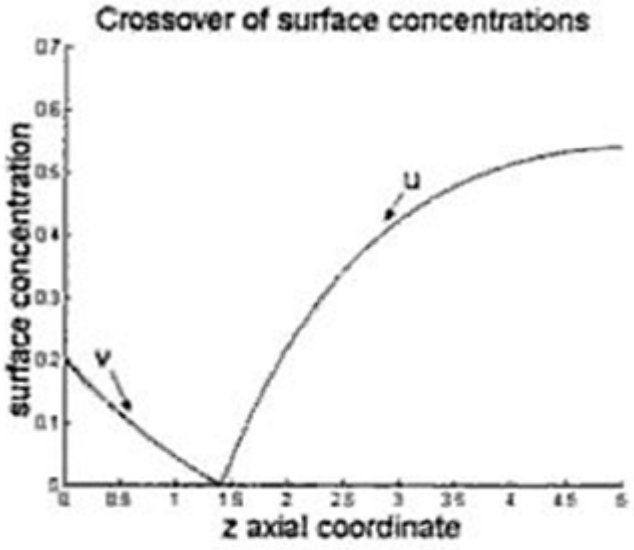
$$j_u = j_v = -j_w$$

- At steady state, these fluxes $\tilde{u}\tilde{v} - K\tilde{w} = 0$ are all equal due to stoichiometry and thus give two constraints on the bulk variables u, v, w and on the disperse phase concentrations u, v, w

Theory



(a) Bulk concentrations decay



(b) Surface concentrations exhibit crossover

Fig 3. Crossover in a tubular, heterogenous catalytic reactor.

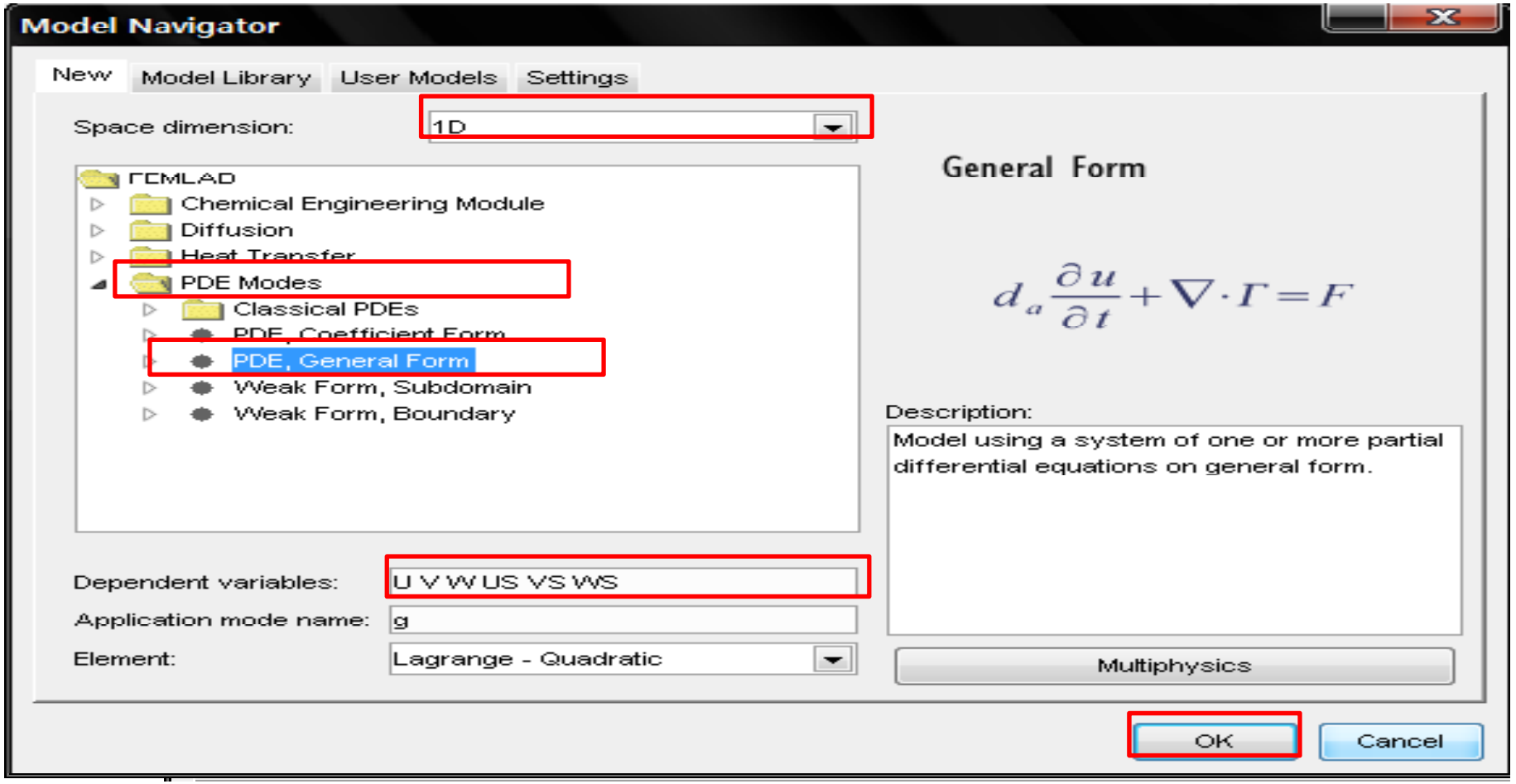
Theory

- The boundary conditions will be taken as fixed concentrations of u and v at the inlet, no w, and outlet conditions with convection much g

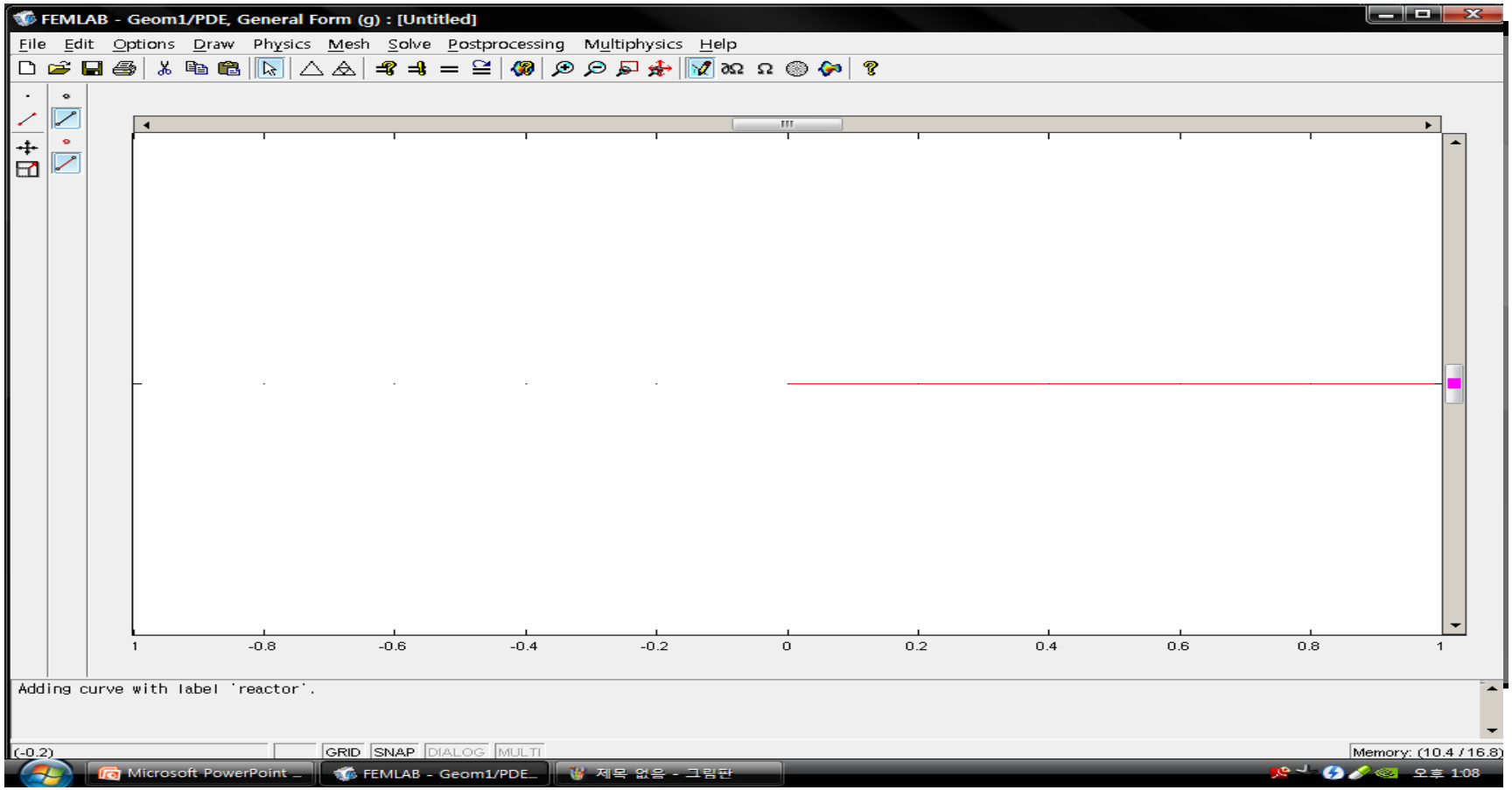
variables	Fix unit
diffusivities	$D_u=D_v=1$
Mobile product	$K_w=100$, $D_w=0.001$
mass transfer coefficient	$K_v=1$
Irreversible reaction	$K=10^{-5}$
Reactor of length	$L=5$
Velocity	$u=0.5$
Mass transfer asymmetry	$K_u=0.2$
The inlet conditions	$U_0=1$, $V_0=0.4$

Theory

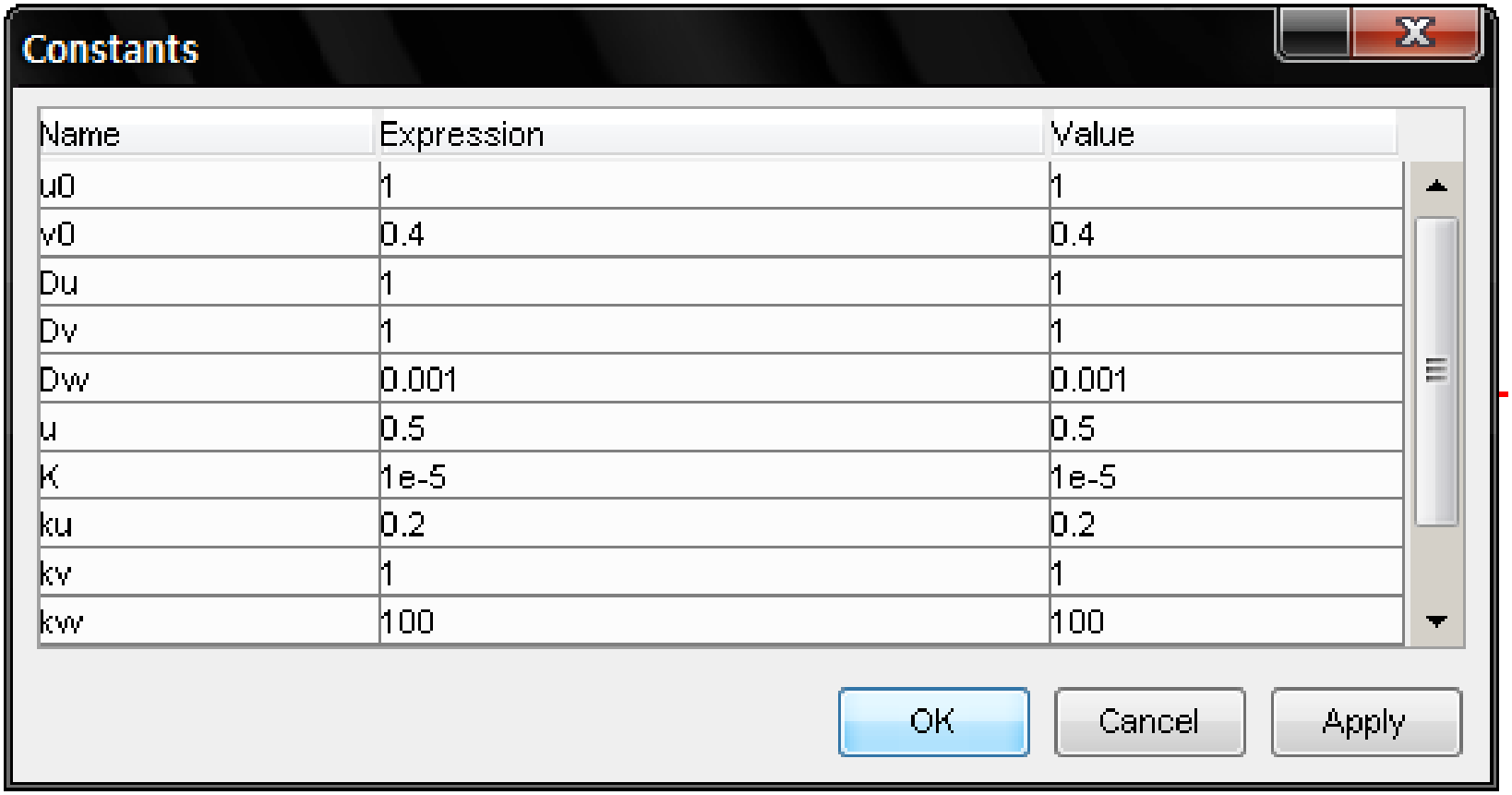
- Now to set up the COMSOL multiphysics model.
- The differential variables U, V, W have Dirichlet boundary conditions at the reactor entry (boundary 1) and Neumann conditions at the outlet.
- For the surface variables $\Gamma = 0$ was specified, so entering zero Neumann conditions is a non-constraint (0=0).
- This model turns out to be highly nonlinear. The reason for difficulty in convergence is that this model mixes differential equations for the bulk variables with algebraic constraints for the surface variables.



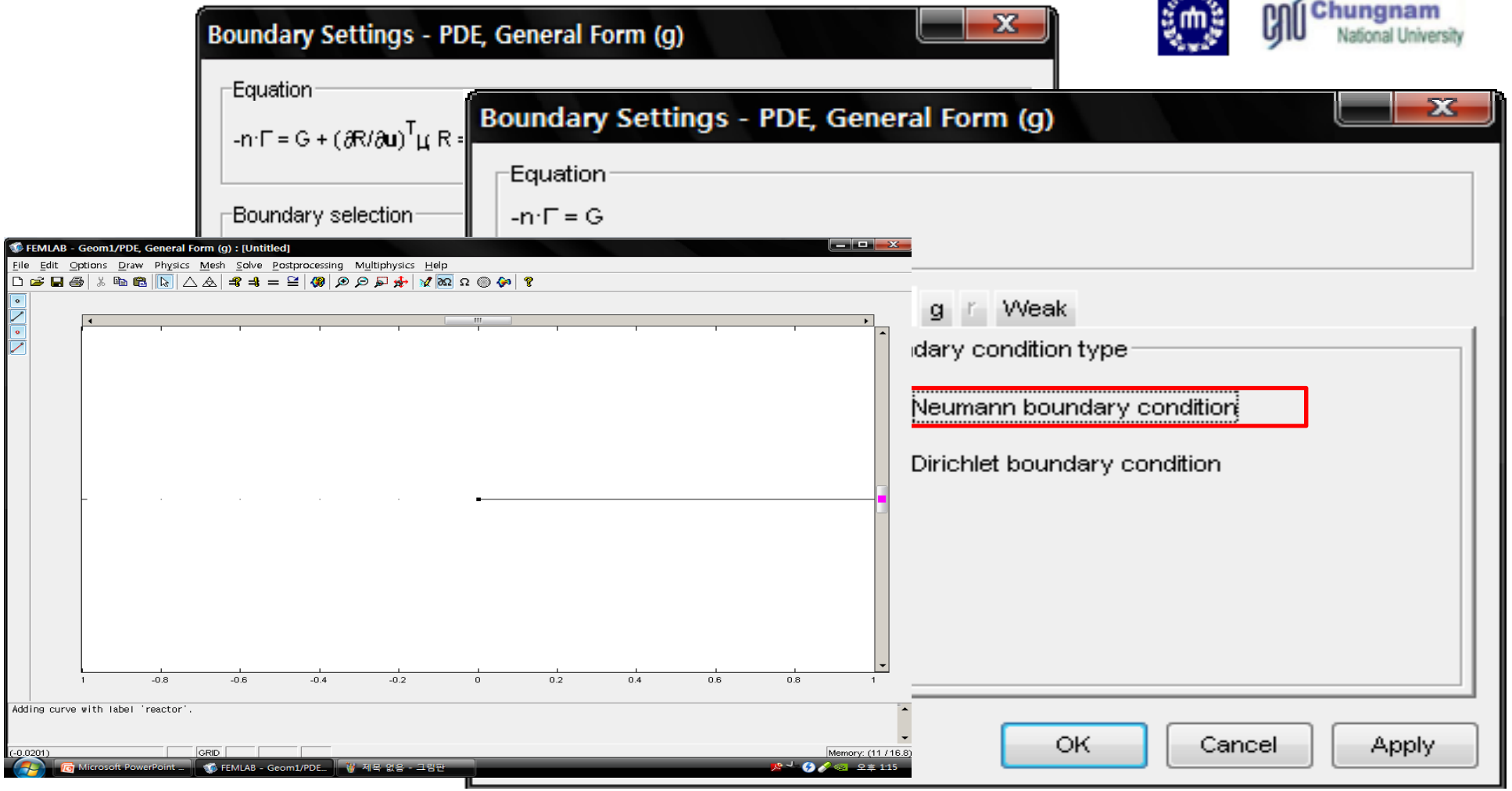
1. Select 1-D space dimension.
2. Select PDE modes-PDE general.
3. Set dependant variables : U V W US VS WS.
4. Click OK.



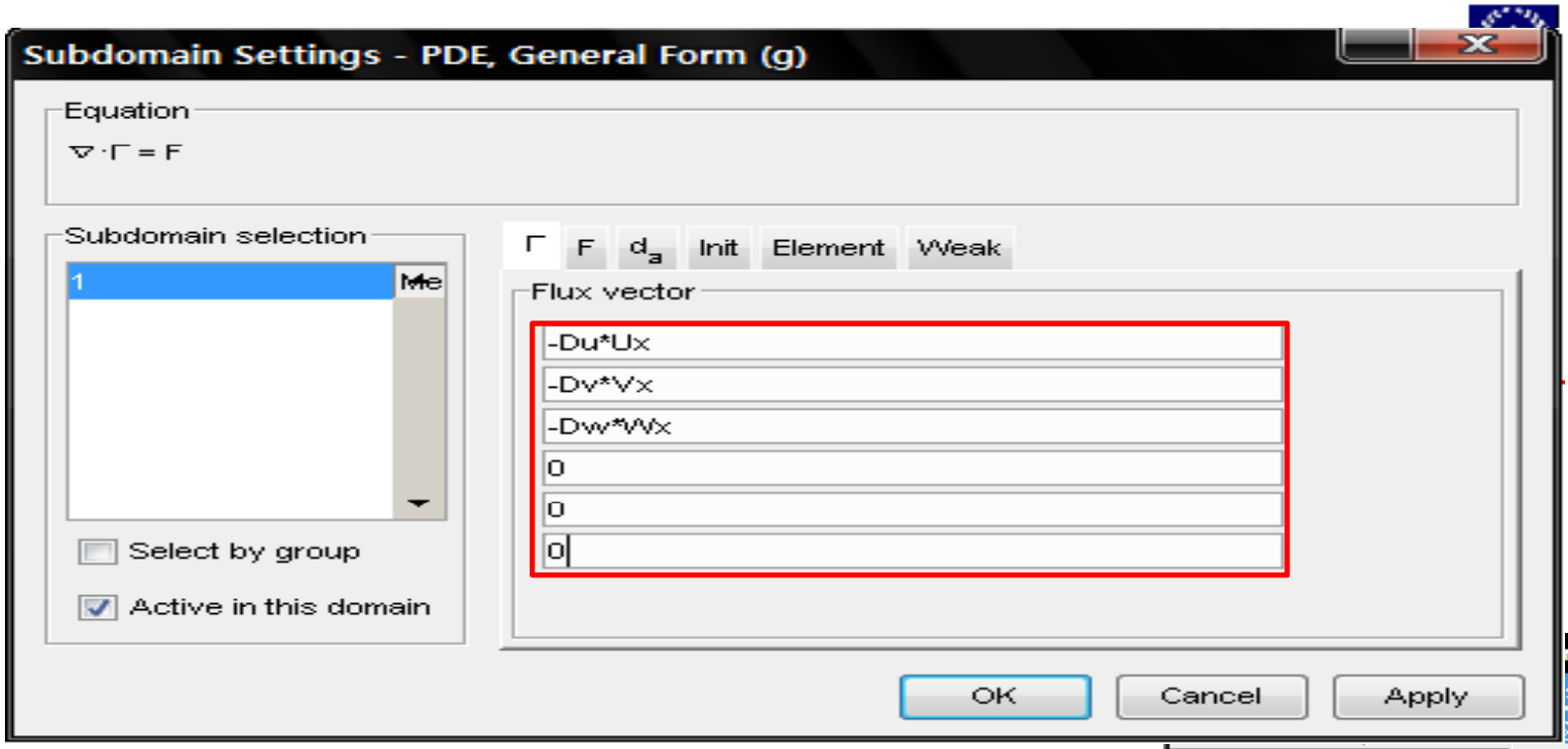
1. Specify objects – Line. Set x : 0.5
2. Set name : reactor. OK.
3. Appear a Flowsheet.

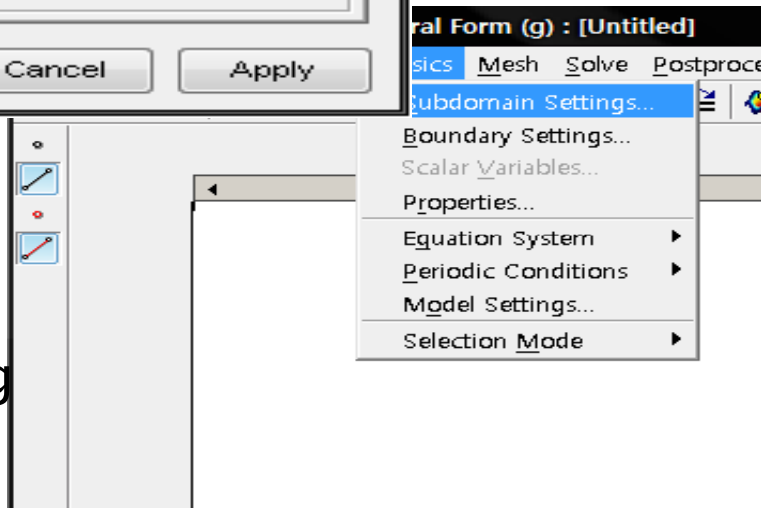


1. Options Menu - Select constants
2. Input constant value



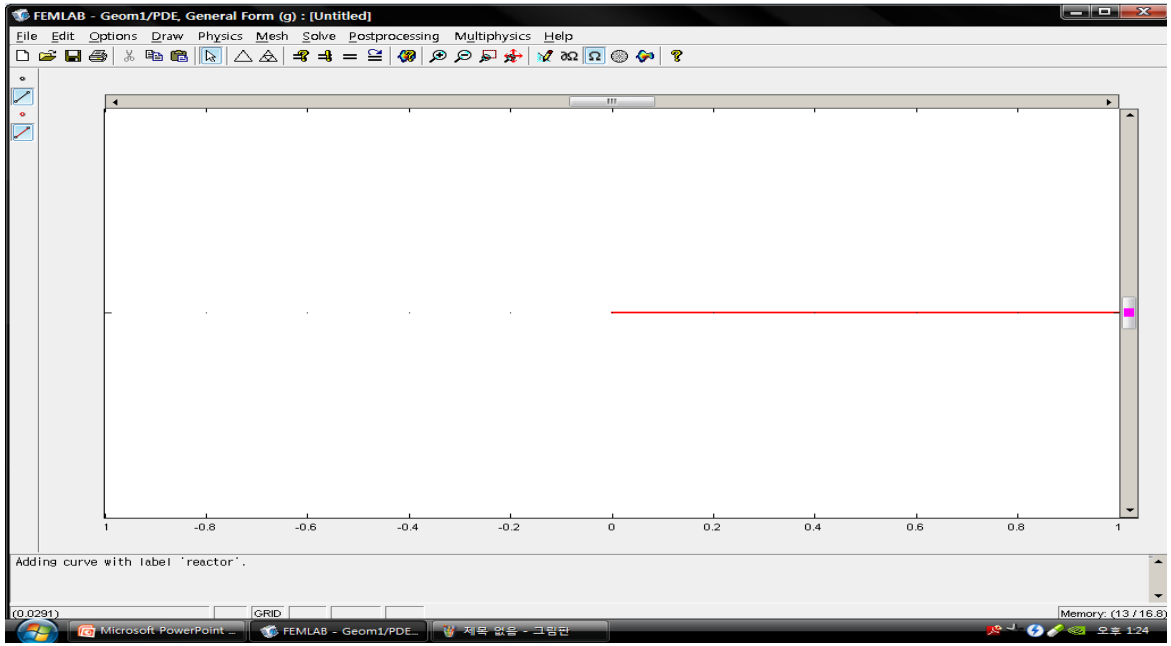
1. Physics Menu – Select boundary setting
2. Select boundary 1. Select Dirchlet type boundary condition
   Setting R tab r1=u0-U r2=v0-V r3=-W r4=r5=r6=0
3. Select boundary 2. Select Neumann boundary type boundary conditions. Click OK.

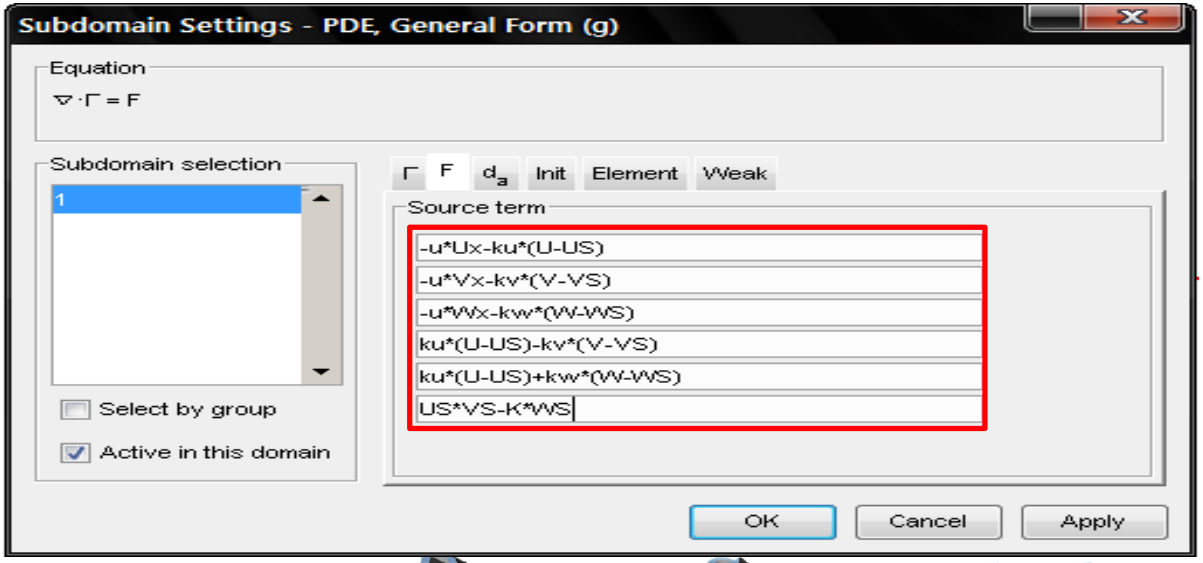




1. Physics Menu – Select domain setting
2. Select boundary 1.
3. Γ Tab – Set

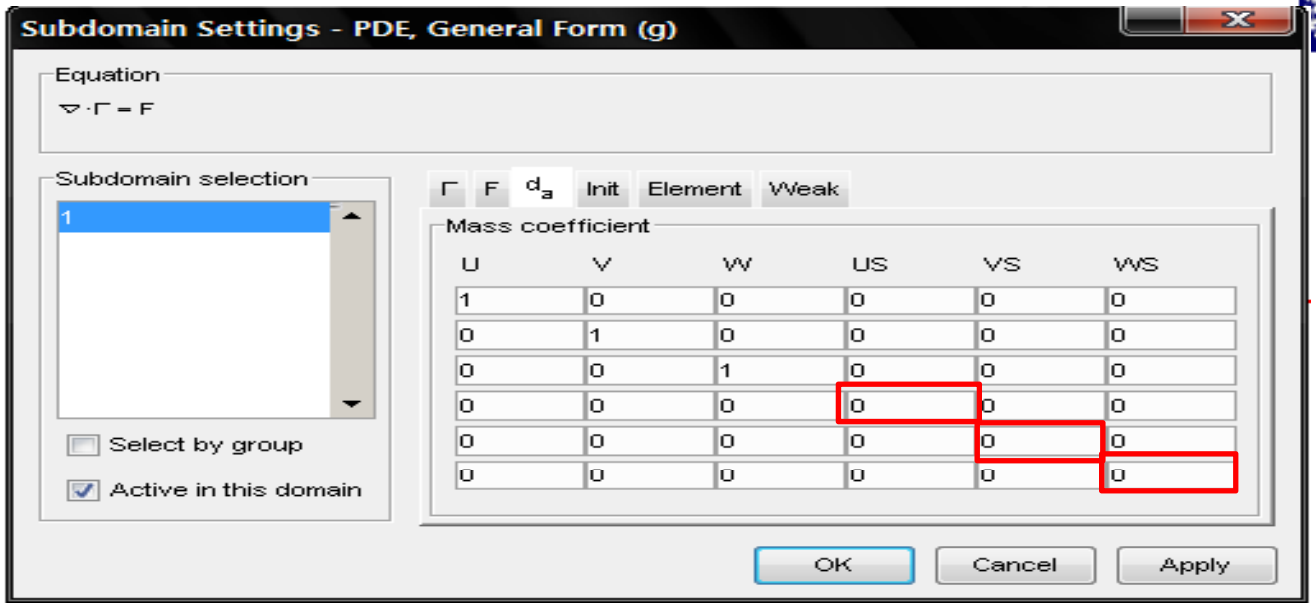
$$\Gamma_1 = -D_u \times U_x ; \Gamma_2 = -D_v \times V_x ; \Gamma_3 = -D_w \times W_x ; \Gamma 4 = \Gamma 5 = \Gamma 6 = 0$$

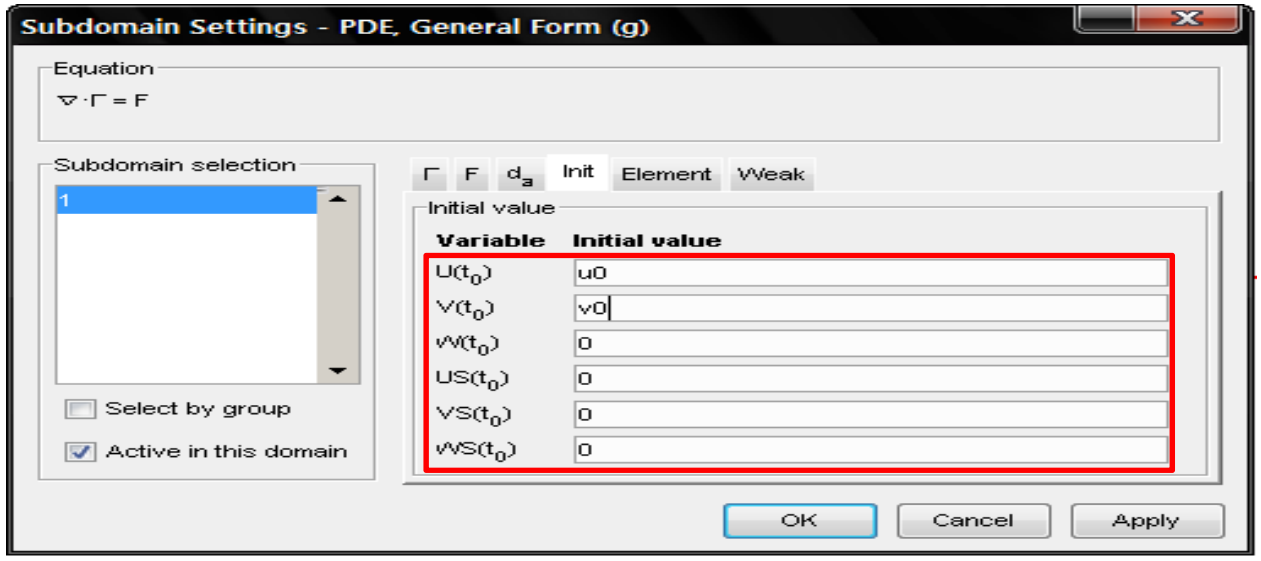


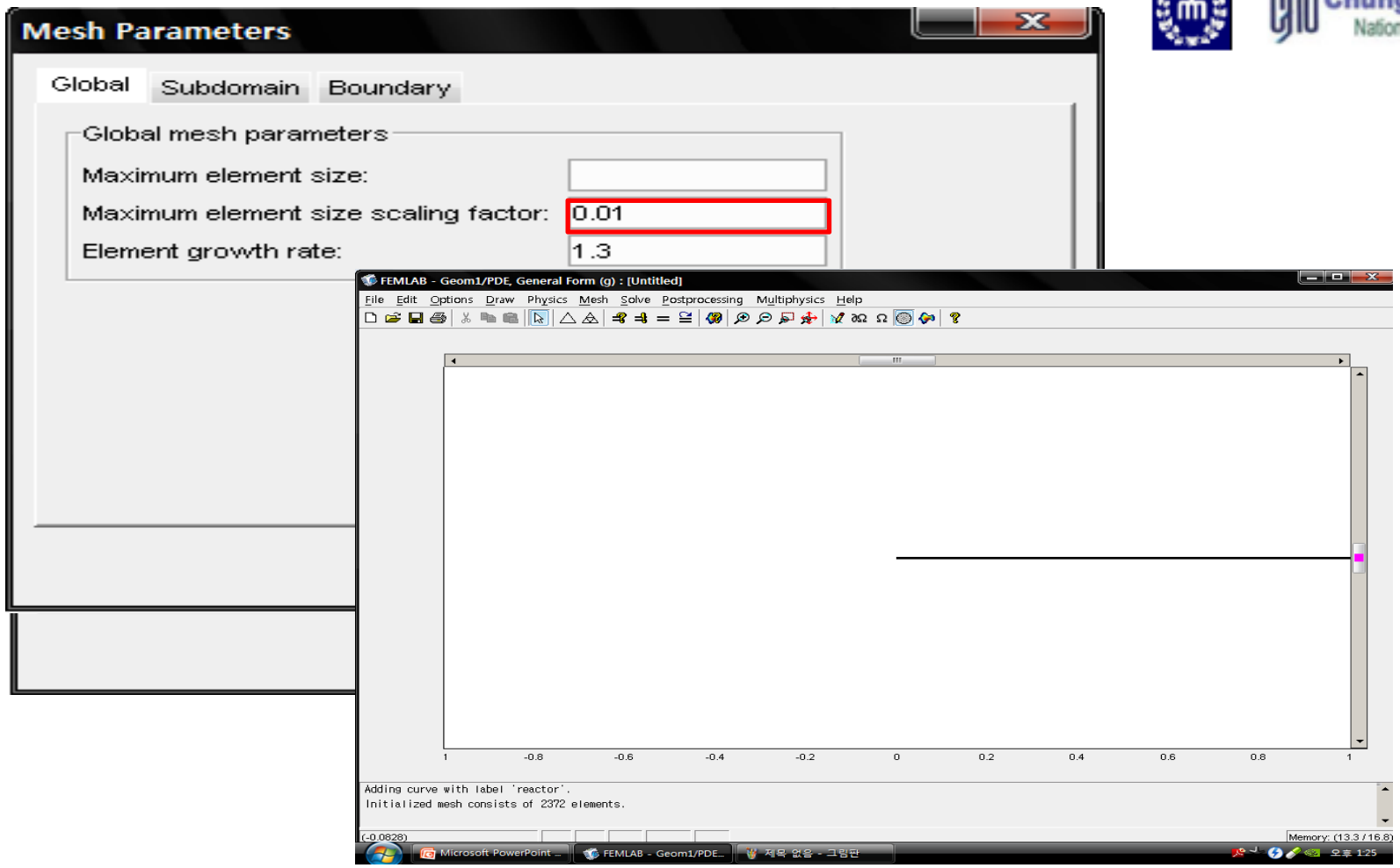


1. Setting F tab.
2. Setting d_a tab.
3. Setting Init tab.
4. Click OK.

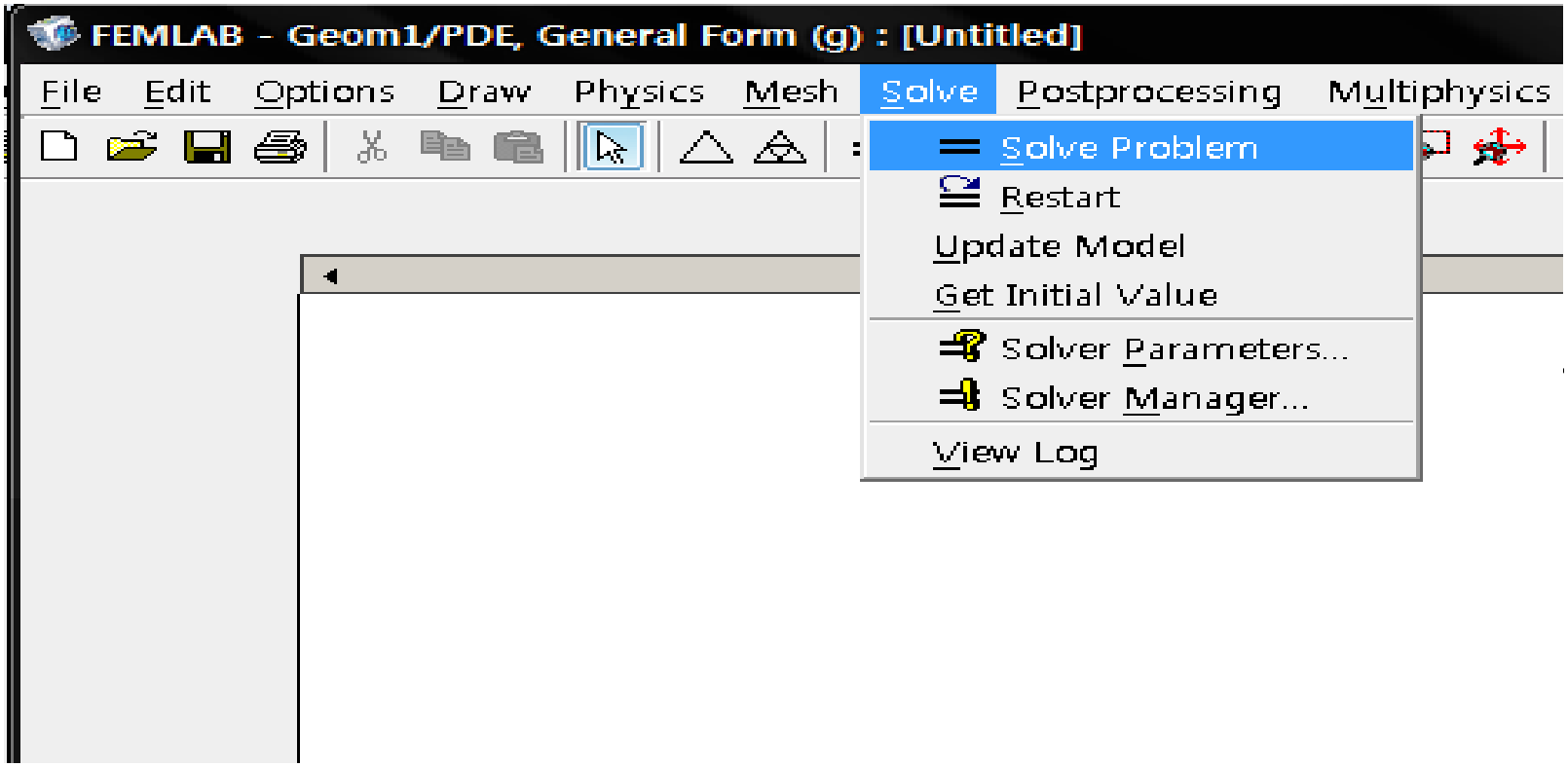
Process Systems Lab.


Subdomain Settings - PDE, General Form (g)
Equation
∇·Γ = F
Subdomain selection
1
Select by group
Active in this domain
Γ F da Init Element Weak
Mass coefficient
U V W US VS WS
1 0 0 0 0 0
0 1 0 0 0 0
0 0 1 0 0 0
0 0 0 0 0 0
0 0 0 0 0 0
0 0 0 0 0 0
OK Cancel Apply

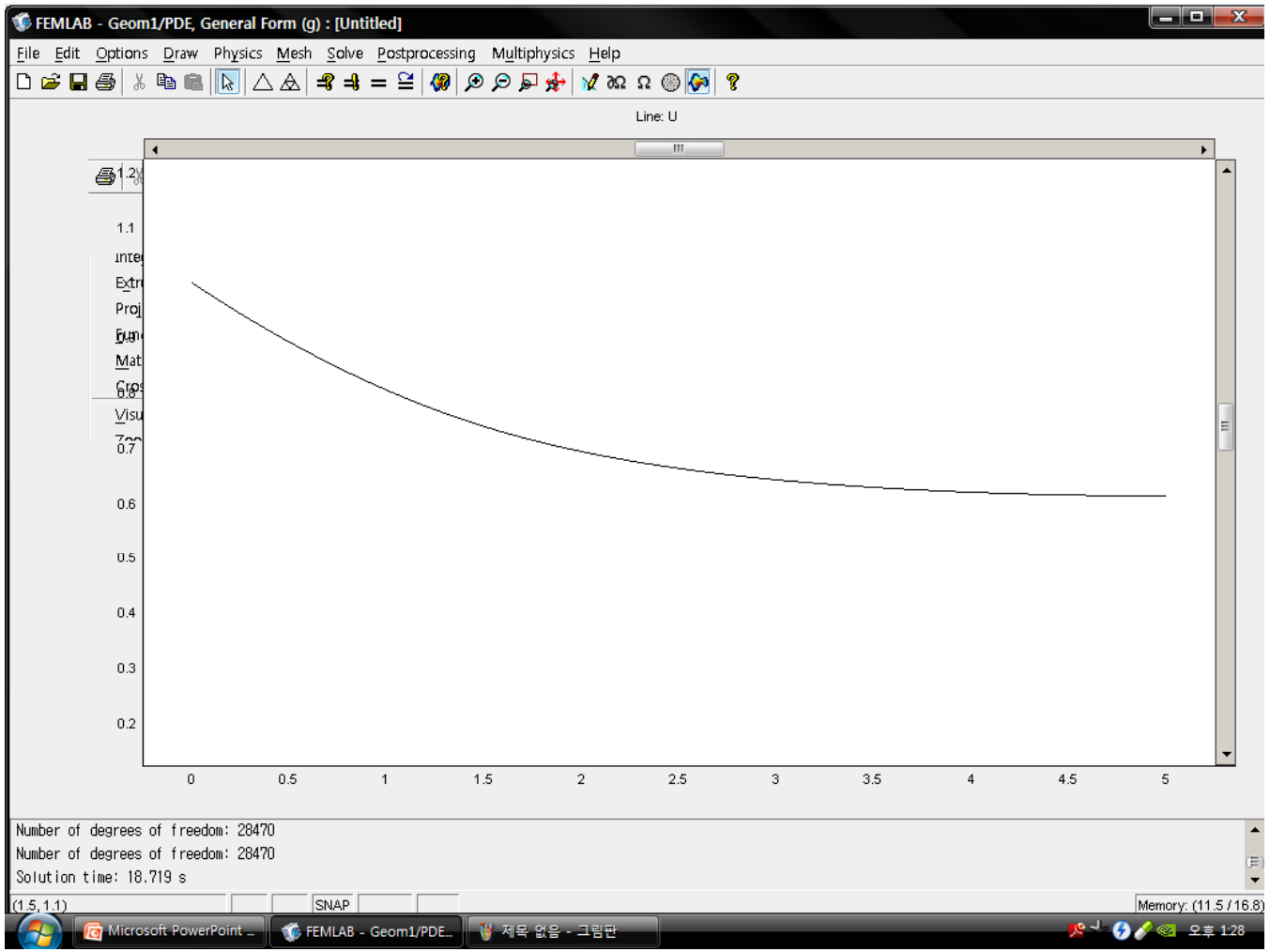

Subdomain Settings - PDE, General Form (g)
Equation
∇·Γ = F
Subdomain selection
1
Select by group
Active in this domain
Γ F da Init Element Weak
Initial value
Variable Initial value
U(t0) u0
V(t0) v0
W(t0) 0
US(t0) 0
VS(t0) 0
WS(t0) 0
OK Cancel Apply



1. Select mesh parameters.
2. Boundary tab. Select boundaries 1 and 2.
3. Enter maximum element size : 0.0001
4. Global tab. Set maximum element size scaling factor : 0.01
5. Click Remesh and OK.



1. Select stationary Nonlinear solver.
2. Nonlinear tab : Check “highly nonlinear problem”
3. Click OK.
4. Click Solve Problem.



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Process Systems Lab.

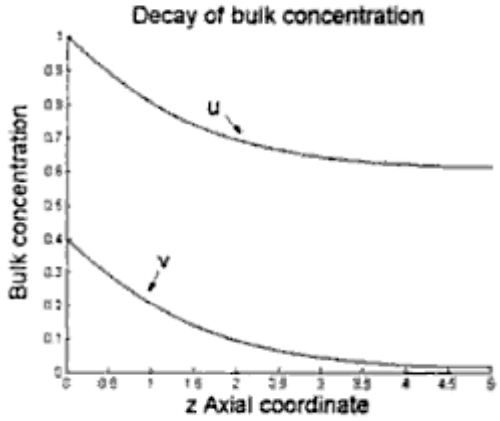

Figure 4.3 Bulk concentrations decay.

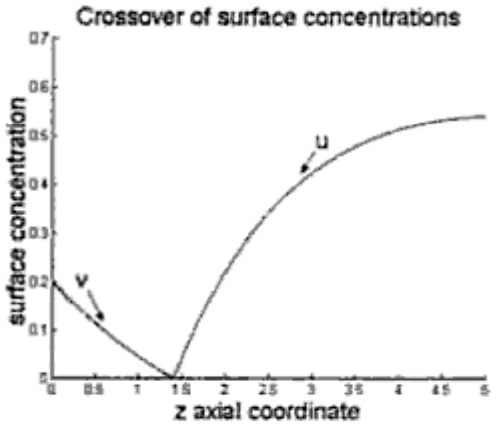

Figure 4.4 Surface concentrations exhibit crossover.

•As time proceeds, the Concentration becomes lower than initial concentration due to reactions is proceeding in the tubular reactor.