

Heterogeneous catalytic reaction in PFTR





- 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 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





- 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

$$U \frac{\partial u}{\partial z} = D_u \frac{\partial^2 u}{\partial z^2} - j_u(u, \tilde{u})$$
$$U \frac{\partial v}{\partial z} = D_v \frac{\partial^2 v}{\partial z^2} - j_v(v, \tilde{v})$$
$$U \frac{\partial w}{\partial z} = D_w \frac{\partial^2 w}{\partial z^2} - j_w(w, \tilde{v})$$





The fluxes j take the traditional mass transfer coefficient form $i = \kappa (u - \tilde{u})$

$$J_{u} = \kappa_{u} (u - u),$$

$$j_{v} = \kappa_{v} (v - \tilde{v}),$$

$$j_{w} = \kappa_{w} (w - \tilde{w}),$$

$$j_u = j_v = -j_w$$

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







(a) Bulk concentrations decay

(b) Surface concentrations exhibit crossover

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





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

a	variables	Fix unit				
9	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				





- 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 was specified, so entering zero Neumann conditions is a nonconstraint (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.





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Model Navigator							
New Model Library Us	er Models Settings						
Space dimension:	1D						
CMLAD ▷ 💼 Chemical Engine ▷ 💼 Diffusion	ering Module	General Form					
PDE Modes PDE Coeffic PDE, Coeffic PDE, Gener	DEs cient Form al Form		$d_a \frac{\partial u}{\partial t} + \nabla \cdot \Gamma = F$				
Weak Form Weak Form	, Subdomain , Boundary		Description:				
			Model using a system of one or more partial differential equations on general form.				
Dependent variables:	u v w us vs ws]					
Application mode name:	g						
Element:	Lagrange - Quadratic	•	Multiphysics				
			OK Cancel				

1. Select 1-D space dimension.

2

4.

CIICK OK.

- 2. Select PDE modes-PDE general.
 - Set dependant variables : U V W US VS WS.





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





Constants		X
Name	Expression	Value
uO	1	1
v0	0.4	0.4
Du	1	1
Dv	1	1
Dw	0.001	0.001
u	0.5	0.5
К	1e-5	1e-5
ku	0.2	0.2
kv	1	1
kw	100	100 🗸
		OK Cancel Apply

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





1. Physics Menu – Select boundary setting

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. Flick OK.

Subdomain Settings - PDE, General Form (g)	Chungnam National University
Equation マ・Г=F	
Subdomain selection F G Select by group Active in this domain F C </th <th></th>	
OK Cancel Apply	ral Form (g) : [Untitled] sics <u>M</u> esh <u>Solve</u> Postproce
 Physics Menu – Select domain setting Select boundary 1. Γ Tab – Set 	Boundary Settings Boundary Settings Scalar Variables Properties Equation System Periodic Conditions Model Settings Selection Mode
$\Gamma_1 = -D_u \times U_x; \Gamma_2 = -D_v \times V_x; \Gamma_3 = -D_w \times W_x; \Gamma_4 = -D_w$	$\Gamma 5 = \Gamma 6 = 0$
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Equation ⊽·Γ = F	
1. Setting F tab. 2. Setting d_a tab. 3. Setting Init tab. 4. Crick OK.	ply

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Active in this domain							

Subdomain selection	Г F d _a	Init Element Weak
	Initial value	
	V(t ₀)	
	vV(t ₀)	0
-	US(t ₀)	0
Select by group	VS(t₀)	0
Active in this domain	WS(t _o)	0



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Mesh Parameters					×	<u>е</u>	Chungnam National Universit
Global Subdomain I	Boundary						
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- 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 Remest and OK.



FEMLAB - Geom1/PDE, General Form (g) : [Untitled]											
<u>F</u> ile	Edit	<u>Options</u>	<u>D</u> raw	Physics	<u>M</u> esh	Solve	Postprocessing	M <u>u</u> lti	physics		
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- 1. Select stationary Nonlinear solver.
- 2. Nonlinear tab : Check "highly nonlinear problem"
- 3 Click OK.
- 4. Click Solve Problem.













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

