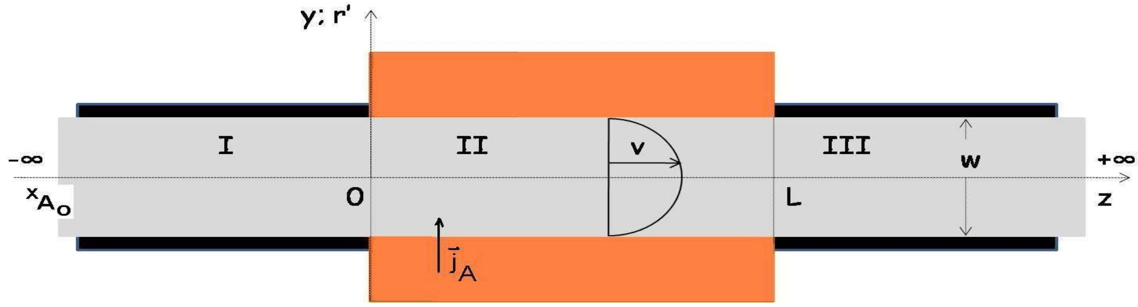
NOME :

ESCOLA POLITECNICA DA UNIVERSIDADE DE SÃO PAULO

PQI-5776-Fenômenos de Transporte I

TAREFA:	4	distribuída:		entregar:			
h	*g*	*f*	*e*	*d*	*c*	*b*	*a*

NUSP:



a) Para o reator acima operando com um fluido diluído, escreva o sistema de equações diferenciais que rege o fenômeno, com o mínimo pertinente de simplificações.

$$\frac{\partial \rho \varphi}{\partial t} + \operatorname{div} \rho \vec{v} \varphi = -\operatorname{div} \vec{j}_{\Phi} + \dot{\sigma}_{\forall \Phi}$$

Considere as conservações de momentum, energia, massa total e da espécie química A

Se *a* < 3 reator cilíndrico, se não placas planas infinitas.

b) Considerando as hipóteses listadas abaixo, simplifique as equações, justificando.

- **regime permanente**
- **escoamento incompressivel, laminar e desenvolvido**
- **dissipação viscosa desprezível**
- **entalpia de reação nula**
- **propriedades físicas (ρ, cp,...) e coeficientes de transporte (ν, $\mathcal{D}_A$, ...) constantes**
- **sistema isotérmico**
- **reação química de consumo de A de ordem zero, irreversivel, homogênea e apenas no meio II**

c) apresente as condições de contorno

d) Preencha o gabarito abaixo, utilizando seu número USP para obter os parâmetros

	densidade	difusividade	reatividade	velocidade	Damkholer
meio	$\rho(kg/m^3)$	$\mathcal{D}_A(10^{-5}m^2/s)$	$K_{reação}$ (kg/m^3s)	$v_m(m/s)$	$Da = K_{reaç}L/v_m\rho x_{Ao}$
I	1,0	(*b*+1)/5=	0	(*d*+1)/100=	0
II	1,0	(*b*+1)/5=	(*c*+1)/1000=	(*d*+1)/100=	
III	1,0	(*b*+1)/5=	0	(*d*+1)/100=	0

L(m)	w(m)	$x_A\|_{-oo}$ (kg_A/kg_{total})
(*d*+1)/20=	(*g*+1)/200=	(*f*+5)/100=

e) calcule os Peclets mássicos radial/normal e o axial e, se for o caso, simplifique as equações

$Pe_{radial/normal} = v_m w/\mathcal{D}_A =$	$Pe_{axial} = v_m L/\mathcal{D}_A =$

f) apresente as novas condições de contorno

g) considerando que para Pe superior a 10 a difusividade pode ser desprezada em relação à convecção e considerando j_A = 0, calcule o perfil de composição de A em L e a composição média 'bulk" de A em L.

$x_{AIII}\|_L =$	kg_A/kg_{total}

h) compare com o resultado obtido pelo balanço global na região II.

$x_{AIII}\|_L =$	kg_A/kg_{total}

TABLE E3.2-1 MODELS USED TO DESCRIBE A TUBULAR CHEMICAL REACTOR WITH STEADY-STATE TURBULENT FLOW*

$A + B + \cdots \rightarrow R + S + \cdots$

Form of Balance Relation	Boundary Conditions
1. Multiple gradient, with velocity profile and radially variable axial and radial dispersion coefficients.	
$v_z(r)\frac{\partial c_i}{\partial z} = D_z(r)\frac{\partial^2 c_i}{\partial z^2} + \frac{1}{r}\left(\frac{\partial}{\partial r} r D_R(r)\frac{\partial c_i}{\partial r}\right) + R_i$	$v_z(r)c_{i0} = v_z(r)c_i(0,r) - D_z(r)\frac{\partial c_i(0,r)}{\partial z}$ $\frac{\partial c_i}{\partial z}(L,r) = 0$ $\frac{\partial c_i}{\partial r}(z,0) = 0$ $\frac{\partial c_i}{\partial r}(z,R) = 0$
$\rho C_p\left[v_z(r)\frac{\partial T}{\partial z}\right] - k_z(r)\frac{\partial^2 T}{\partial z^2} + \frac{1}{r}\left(\frac{\partial}{\partial r} r k_R(r)\frac{\partial T}{\partial r}\right) + \Delta H_r R_A$	$v_z(r)T_0 = v_z(r)T(0,r) - \frac{k_z(r)}{\rho C_p}\frac{\partial T(0,r)}{\partial z}$ $\frac{\partial T}{\partial z}(L,r) = 0$ $\frac{\partial T}{\partial r}(z,0) = 0$ $\frac{\partial T}{\partial r}(z,R) = \frac{U}{k_R}[T_s - T(z,R)]$
2. Multiple gradient, with velocity profile and constant axial and radial dispersion coefficients.	
$v_z(r)\frac{\partial c_i}{\partial z} = D_z\frac{\partial^2 c_i}{\partial z^2} + \frac{D_R}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_i}{\partial r}\right) + R_i$	$D_z(r) \rightarrow D_z$ Same form as in 1 with
$\rho C_p\left[v_z(r)\frac{\partial T}{\partial z}\right] - k_z\frac{\partial^2 T}{\partial z^2} + \frac{k_R}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \Delta H_r R_A$	$k_z(r) \rightarrow k_z$
3. Multiple gradient, with constant velocity.	
$v_z\frac{\partial c_i}{\partial z} = D_z\frac{\partial^2 c_i}{\partial z^2} + \frac{D_R}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_i}{\partial r}\right) + R_i$	$v_z(r) \rightarrow v_z$ Same form as in 2 with $D_z \rightarrow D_L$
$\rho C_p\left[v_z\frac{\partial T}{\partial z}\right] - k_z\frac{\partial^2 T}{\partial z^2} + \frac{k_R}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \Delta H_r R_A$	$k_z \rightarrow k_L$
4. Multiple gradient, ignoring radial gradients.	
$v_z\frac{dc_i}{dz} = D_L\frac{d^2 c_i}{dz^2} + R_i$	$v_z c_{i0} = v_z c_i(0) - D_L\frac{dc_i(0)}{dz}$ $\frac{dc_i}{dz}(L) = 0$
$\rho C_p\left[v_z\frac{dT}{dz}\right] = k_L\frac{d^2 T}{dz^2} + \Delta H_r R_A + U\frac{P}{S}(T_s - T)$	$v_z T_0 = v_z T(0) - \frac{k_L}{\rho C_p}\frac{dT(0)}{dz}$ $\frac{dT(L)}{dz} = 0$
5. Maximum gradient, ignoring all dispersion.	
$v_z\frac{dc_i}{dz} = R_i$	$c_{i,0} = c_i(0)$
$\rho C_p\left[v_z\frac{dT}{dz}\right] = \mp\Delta H_r R_A + U\frac{P}{S}(T_s - T)$	$T_0 = T(0)$
6. Macroscopic material and heat balances assuming conversion known.	
$\Delta(c_i v_z S) = R_{i,av}V_{tot}$	
$\Delta(\rho C_p T v_z S) = \mp\Delta H_r R_{i,av}V_{tot} + UA_{tot}(T_s - T)$	None

* Special Symbols:

U = overall heat transfer coefficient at wall

$\frac{P}{S} = \frac{\text{reactor perimeter}}{\text{cross-sectional area}} = \frac{\text{surface area}}{\text{volume}} = \frac{2}{R}$ for cylinder

V_{tot} = total volume of reactor

A_{tot} = total surface area of reactor

ΔH_r = net heat of reaction per mole of $A = \Sigma(\nu H)_{products} - \Sigma(\nu H)_{reactants}$ on the basis of component A, where ν is the stoichiometric coefficient.

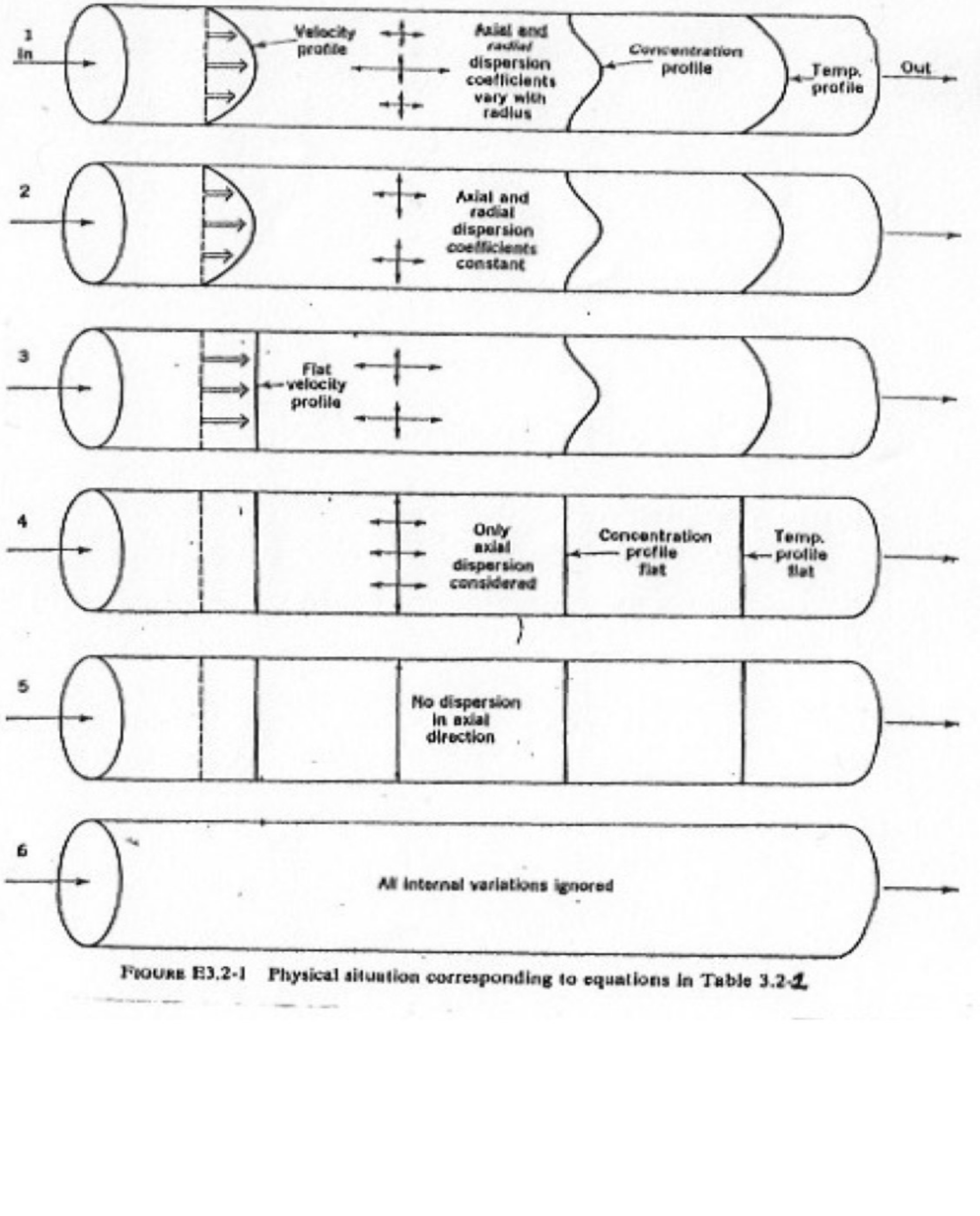


FIGURE E3.2-1 Physical situation corresponding to equations in Table 3.2-1