FINITE ELEMENT STUDY OF THE MASS TRANSFER IN ANNULAR REACTOR

COMSOL CONFERENCE
2014 CURITIBA

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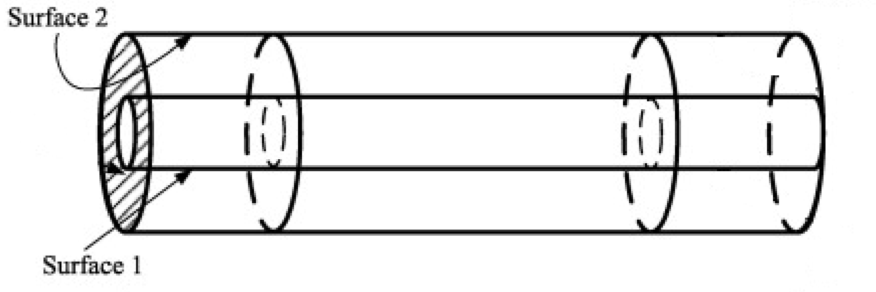
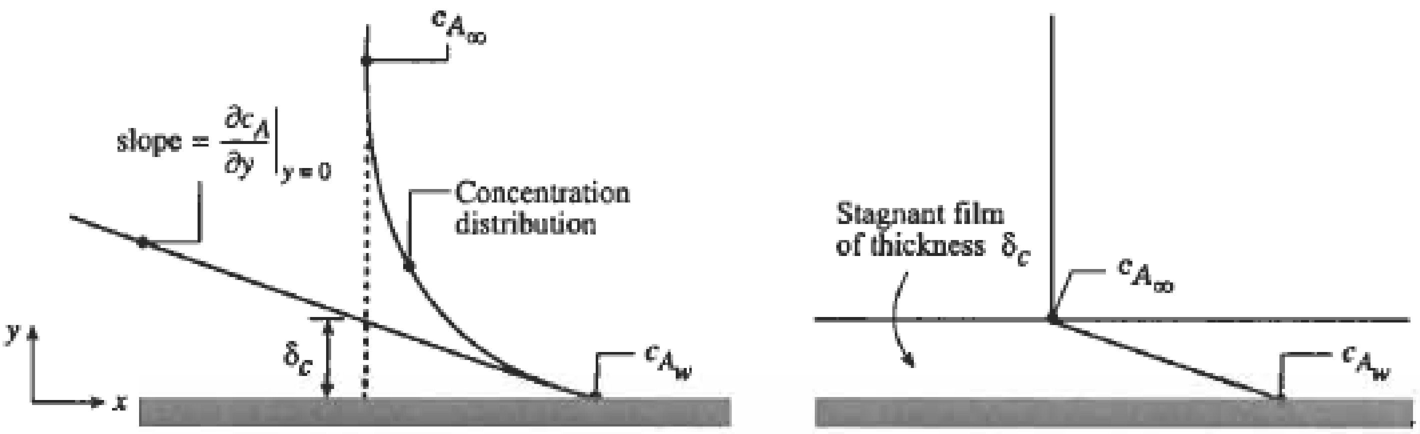
ANNULAR REACTOR

- Low pressure drop
- Easy temperature control
- Lower Diffusion path
- Higher surface to volume ratio
- Photocatalytic reactions



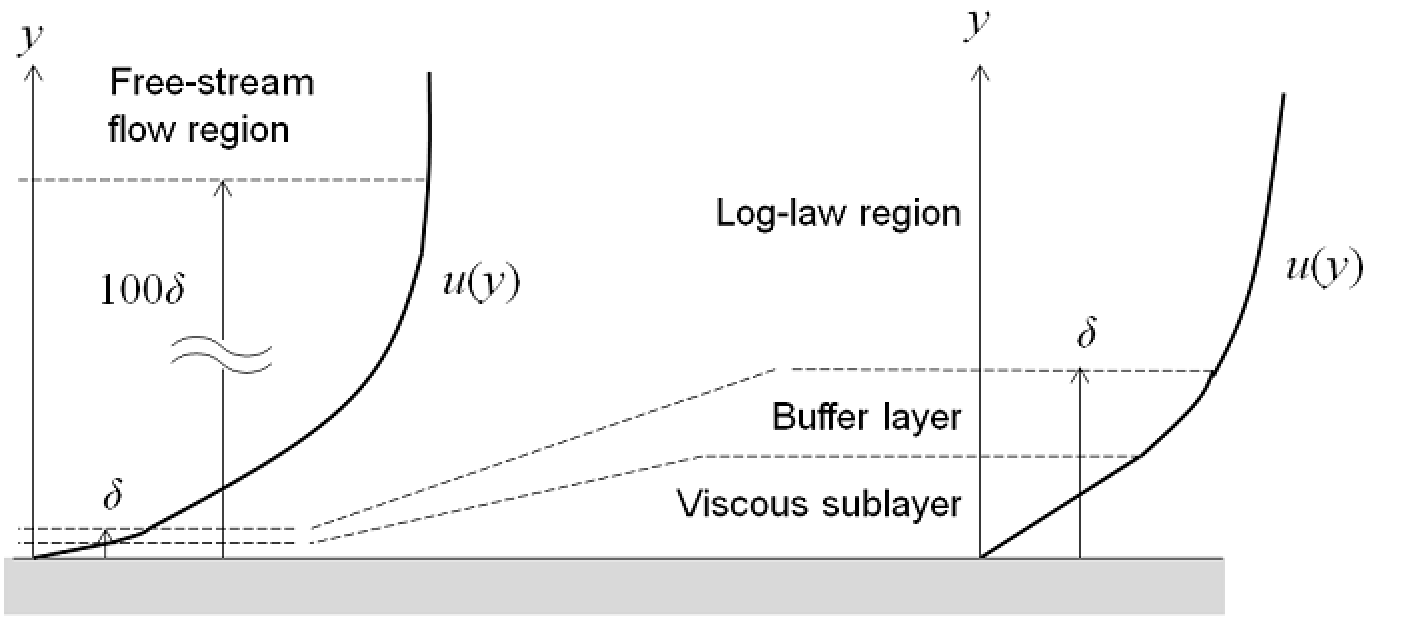
MODELING MASS TRANSFER RATE

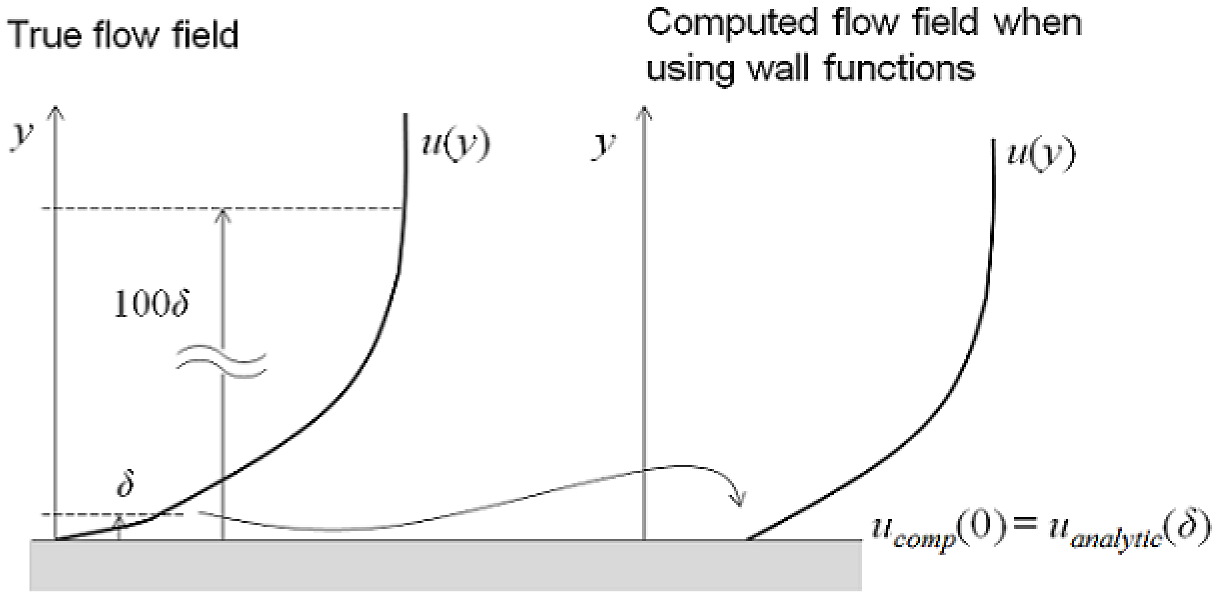
- Diffusion Controlled Reaction
- Corrosion (Diffusion Controlled Corrosion)



a) Actual case

b) Idealized case


y
Free-stream
flow region
100δ
u(y)
δ
y
Log-law region
u(y)
δ
Buffer layer
Viscous sublayer


True flow field
Computed flow field when using wall functions
y
u(y)
100δ
δ
y
u(y)
$u_{comp}(0) = u_{analytic}(\delta)$

Hydrodynamic Condition	Source	Correlation	Equation number
Laminar Flow Fully developed	(Ross & Wragg) [1]	$Sh_{av} = 1.614\ (Re.Sc.\varphi d_e/l)^{\frac{1}{3}}$	(i)
Developing	(Mobarak et al) [2]	$Sh_{av} = 1.029\ Re^{0.55}.Sc^{\frac{1}{3}}.(d_e/l)^{0.472}$	(ii)
	(Ghosh & Upadhyay) [3]	$Sh_{av} = 2.703\ (Re.Sc.\varphi d_e/l)^{\frac{1}{3}}$	(iii)
Turbulent Flow Fully developed	(Ross & Wragg) [1]	$Sh_{av} = 0.023\ Re^{0.8}.Sc^{\frac{1}{3}}$	(iv)
	(Rai et al.) [4]	$Sh_{av} = 0.027\ Re^{0.8}.Sc^{\frac{1}{3}}.(d_2/d_1)^{0.53}$	(v)
	(Pickette) [5]	$Sh_{av} = 0.145\ Re^{2/3}.Sc^{\frac{1}{3}}.(d_e/l)^{0.25}$	(vi)
Developing	(Mobarak et al) [2]	$Sh_{av} = 0.095\ Re^{0.85}.Sc^{\frac{1}{3}}.(d_e/l)^{0.472}$	(vii)
	(Ghosh & Upadhyay) [3]	$Sh_{av} = 0.305\ Re^{\frac{2}{3}}.Sc^{\frac{1}{3}}.(\varphi d_e/l)^{\frac{1}{3}}$	(viii)
	(Rai et al.) [4]	$Sh_{av} = 0.032\ Re^{0.8}.Sc^{\frac{1}{3}}.\left[1 + (d_e/l)^{\frac{2}{3}}\right](d_2/(d_1)^{0.53}$	(ix)

1. Ross T., W.A., *Electrochemical mass transfer studies in annuli.* Electrochimica Acta, 1965. 10: p. 1093 - 1106.
2. Mobarak A. A., F.H.A., & Sedahmed G. H. , *Mass transfer in smooth and rough annular ducts under developing flow conditions.* Journal of Applied Electrochemistry, 1997. 27: p. 201 - 207.
3. Ghosh U., U.S., *Mass Transfer to Newtonian and Non-Newtonian Fluids in Short Annuli.* AIChE Journal 1985. 31(10): p. 1721 - 1724.
4. Rai B., S.A., Ghosh U., Gupta S., & Upadhyay S. , *Force convective mass transfer in annuli.* Chemical Engineering Communications, 1988. 68: p. 15 - 30
5. Pickett, D.J., *Electrochemical Reactor Design*. 1979, Elsevier Scientific Publishing Company: Amsterdam.

- **Mass conservative equation:** $$\frac{\partial U_j}{\partial x_j} = 0.$$
- **Momentum conservation equation:**

$$\rho \left[\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} \right] = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}[T_{ij}^{(v)} + \sigma_{ij}],$$

$$T_{ij}^{(v)} = \mu \left[\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right], \quad \sigma_{ij} = \mu_T \left[\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right].$$

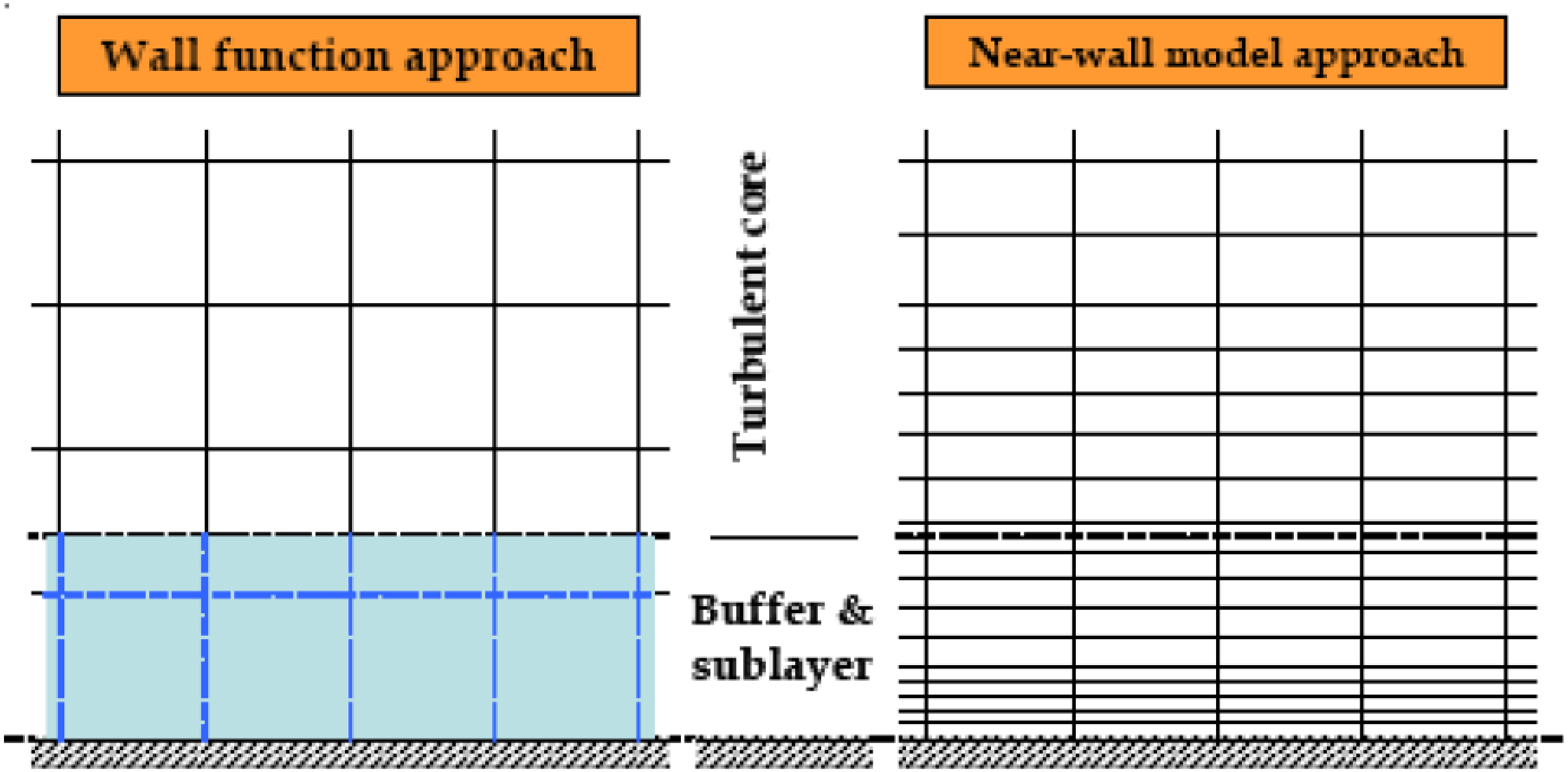
- **Turbulent energy equation:**

$$\rho \frac{\partial k}{\partial t} + \rho U_j \frac{\partial k}{\partial x_j} = \sigma_{ij} \frac{\partial U_i}{\partial x_j} - \rho \epsilon + \frac{\partial}{\partial x_j} \left[(\mu + \frac{\mu_T}{\sigma_k}) \frac{\partial k}{\partial x_j} \right]$$

- **Turbulent dissipation equation:**

$$\rho \frac{\partial \epsilon}{\partial t} + \rho U_j \frac{\partial \epsilon}{\partial x_j} = C_{\epsilon 1} \frac{\epsilon}{k} \sigma_{ij} \frac{\partial U_i}{\partial x_j} - C_{\epsilon 2} \rho \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_T}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right]$$

- **The turbulent viscosity is modeled by:** $$\mu_T = \rho C_\mu \frac{k^2}{\varepsilon}$$



Standard k – ε turbulence model

Semi empirical wall functions are used to bridge the viscosity affected region.

Low Reynolds number k – ε model

Standard turbulent model is modified to model the viscosity affected region with a mesh all the way to the wall.

- **Conservation of species A**

$$\frac{\partial C_A}{\partial t} + \frac{\partial}{\partial x_j}\left(u_j C_A\right) = \frac{\partial}{\partial x_j}\left(D_m \frac{\partial C_A}{\partial x_j}\right)$$

- **Reynolds averaging form**

$$\frac{\partial \overline{C_A}}{\partial t} + \frac{\partial}{\partial x_j}\left(U_j \overline{C_A}\right) = \frac{\partial}{\partial x_j}\left(D_m \frac{\partial \overline{C_A}}{\partial x_j}\right) - \frac{\partial}{\partial x_j}\left(\overline{u_j{}' C_A{}'}\right)$$

- **Turbulent Schmidt number**

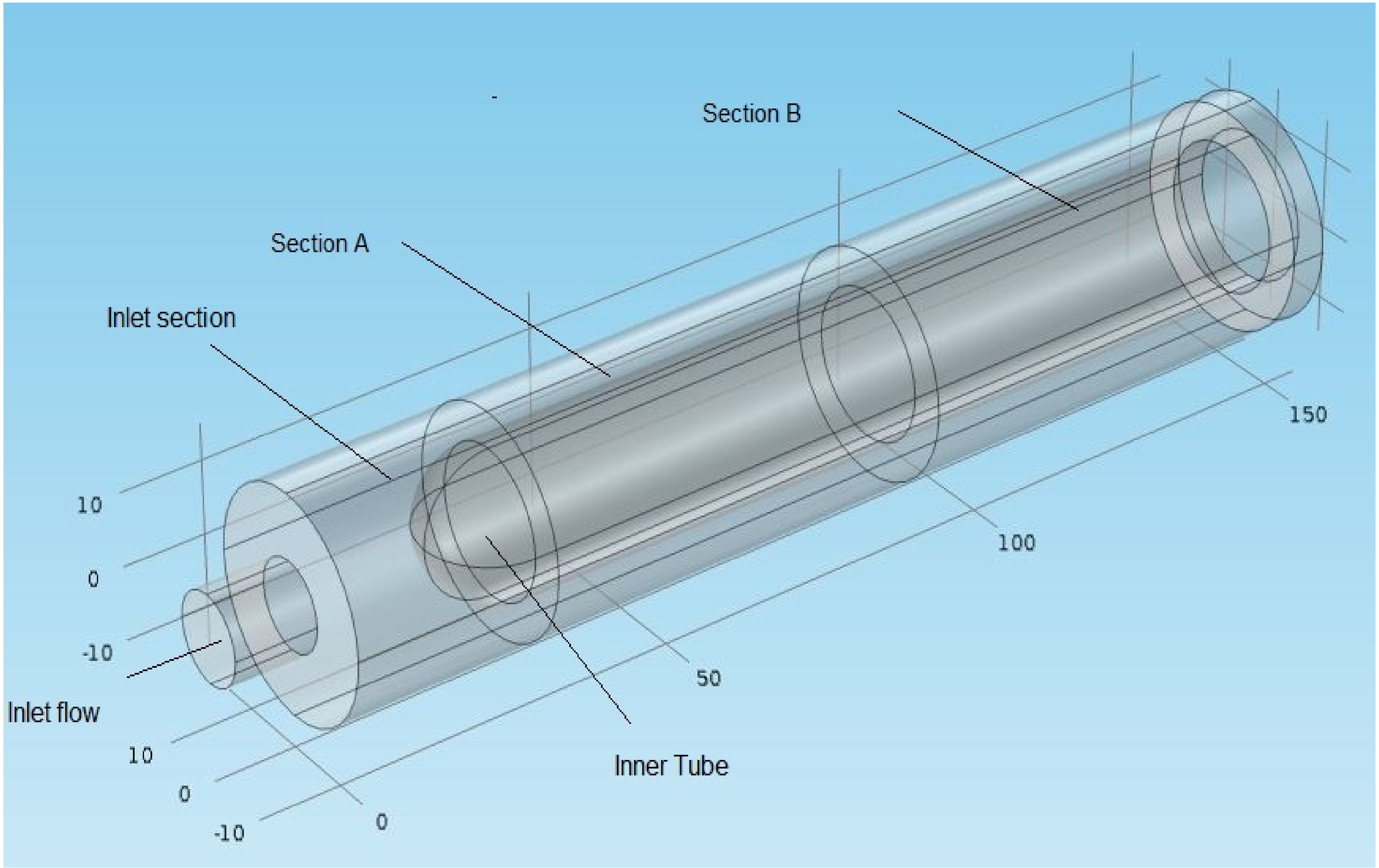
$$\left(\overline{u_j{}' C_A{}'}\right) = J_A^t = -D^t \nabla \overline{C_A}$$

$$Sc^{(t)} = \frac{\mu^{(t)}}{\rho D^{(t)}}$$

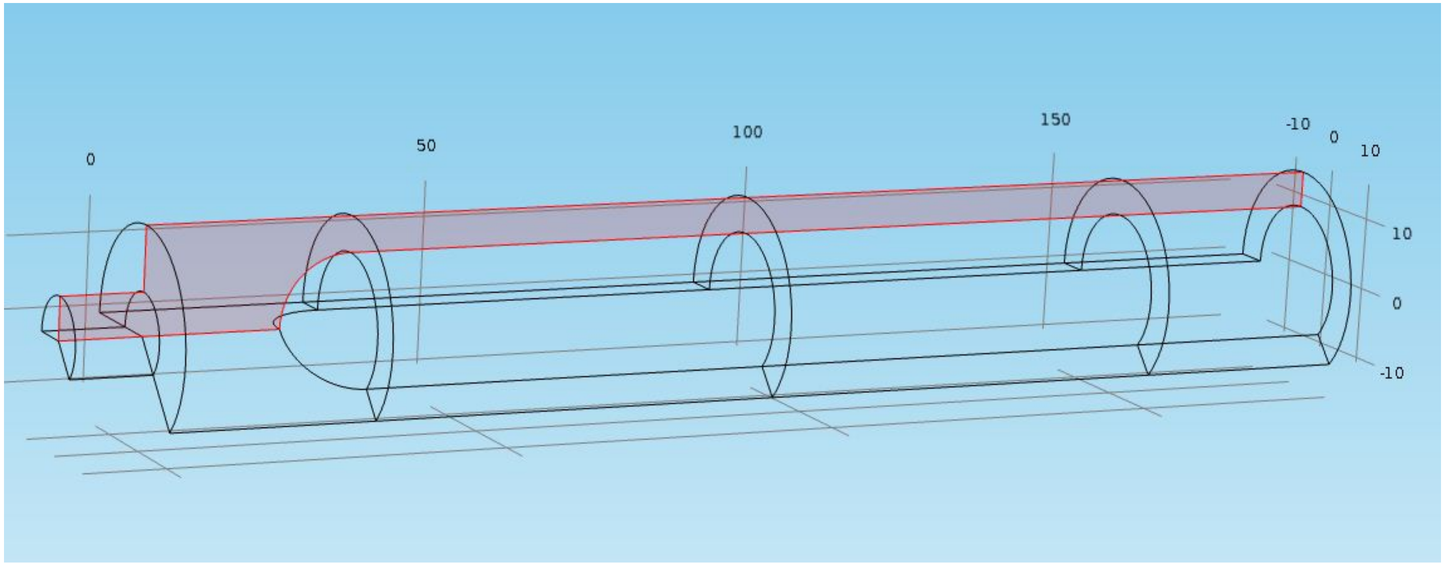
AIM OF WORK

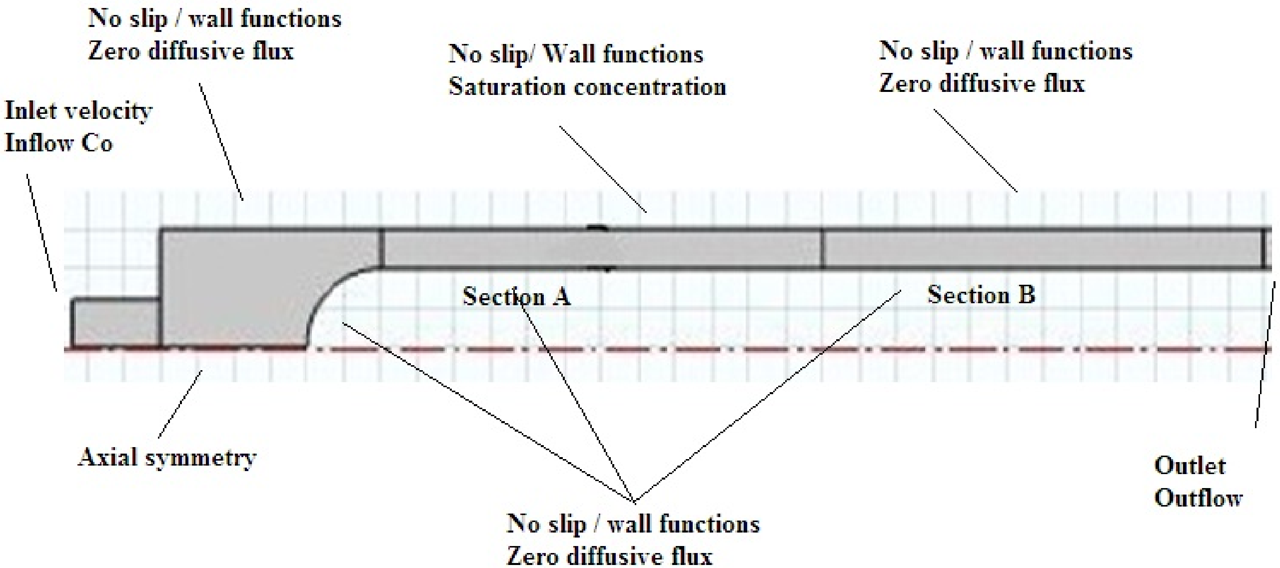
- **To carry out a comprehensive CFD study for modeling single – phase liquid fluid flow and mass transfer phenomena in annular reactors.**
- **To evaluate the simulation results in comparison with available measurements of mass transfer in annular reactors reported in the literature.**
- **To provide a better understanding of the design factors that affects the rate of mass transfer in annular reactors.**

GEOMETRY

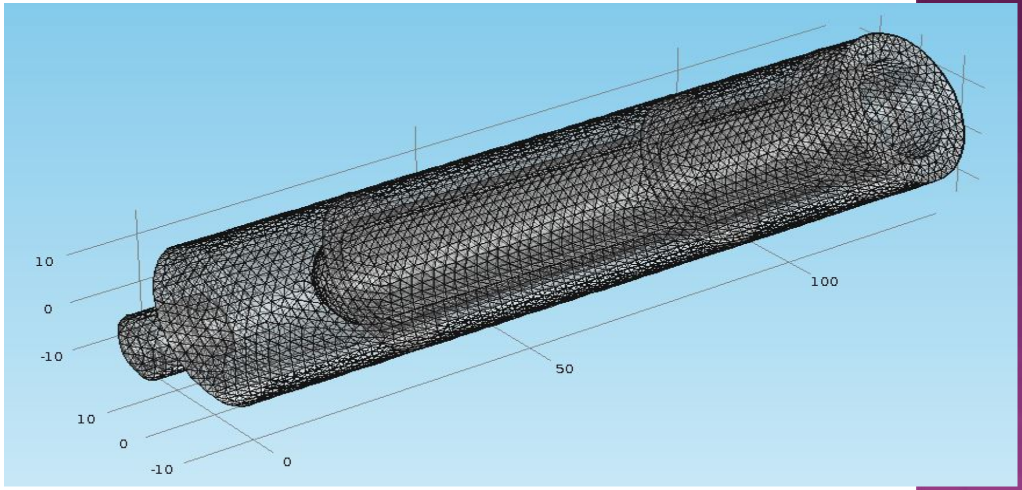


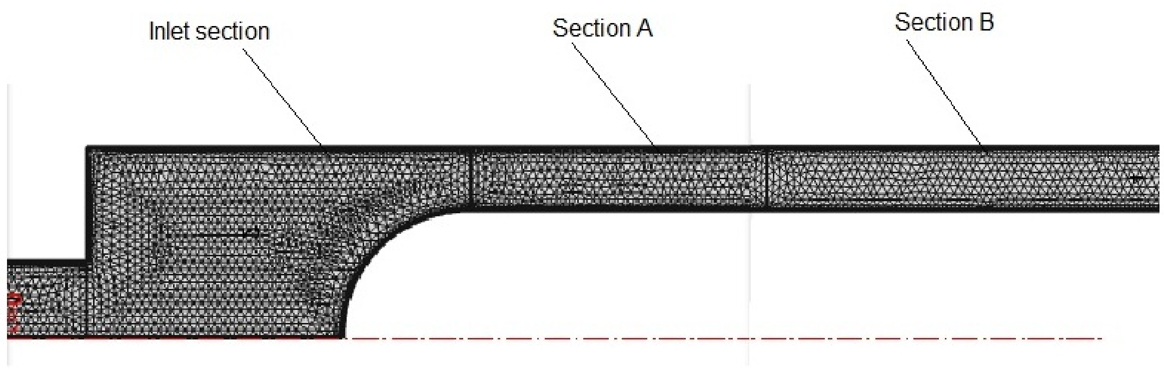
Section B
Section A
Inlet section
10
0
-10
Inlet flow
10
0
-10
0
50
100
150
Inner Tube


0
50
100
150
-10
0
10
10
0
-10


No slip / wall functions
Zero diffusive flux
No slip/ Wall functions
Saturation concentration
No slip / wall functions
Zero diffusive flux
Inlet velocity
Inflow Co
Section A
Section B
Axial symmetry
No slip / wall functions
Zero diffusive flux
Outlet
Outflow

- Complete mesh consisted of 146579 elements
  - 78591 tetrahedral elements
  - 548 pyramid elements
  - 67340 prism elements
  - 100 hexahedral elements.
- Average element quality 0.3729
- Minimum element quality 0.002502





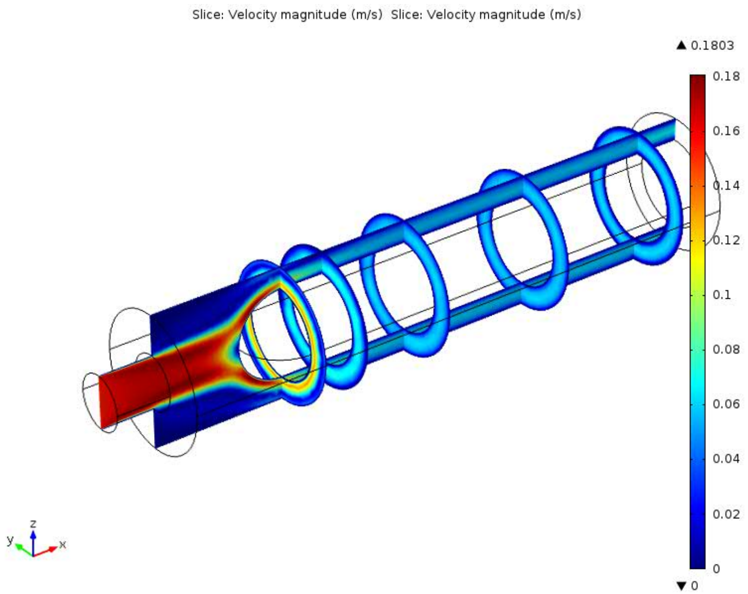
- Complete mesh consisted of 16631 elements
  - 8388 triangular elements
  - 8243 quadrilateral elements
- Average element quality 0.4621
- Minimum element quality 0.001733

-

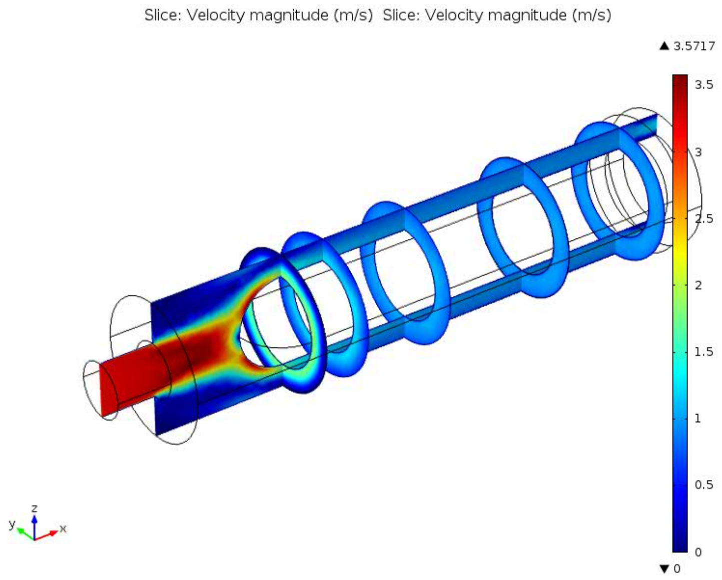
Percentage difference in the average mass transfer coefficient predicted by the empirical correlation of the results of (Mobarak et al.) equation (vii) and the CFD simulation results for several mesh refinement.

Mesh	Percentage Difference
Extra coarse (4317 elements)	12.97
Coarser (6742 elements)	4.43
Coarse (9331 elements)	1.89
Normal (16631 elements)	1.31
Fine (23610 elements)	1.31

CFD HYDRODYNAMIC SIMULATIONS

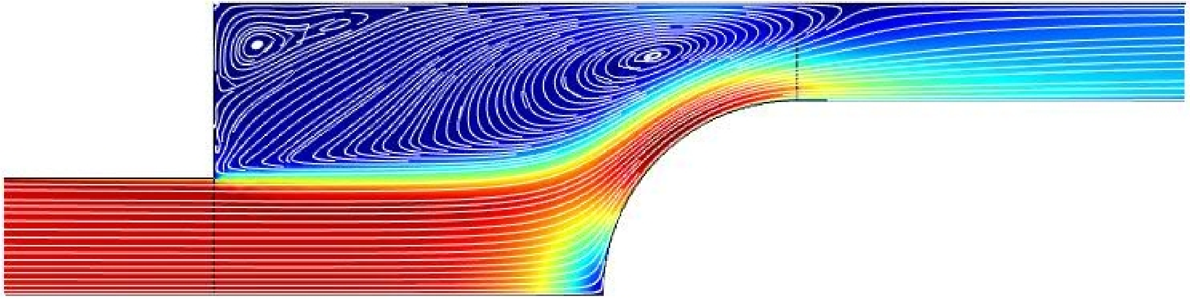


Velocity profile at the longitudinal center plane and transversal planes. Laminar flow (Re = 500)

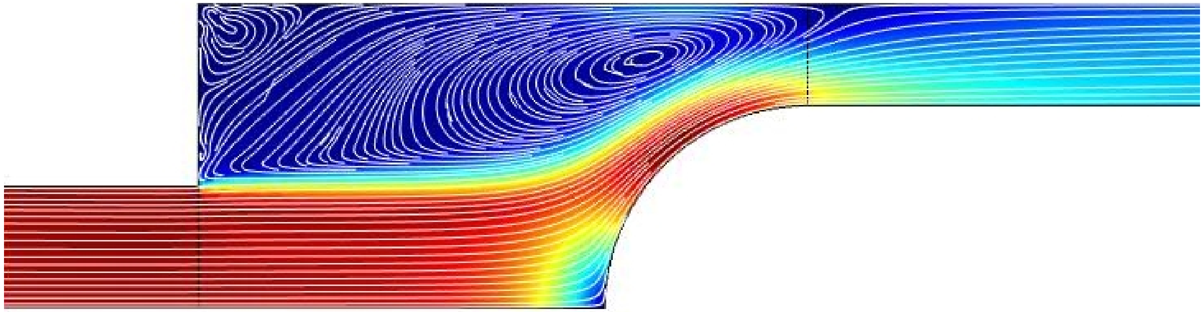


Velocity profile at the longitudinal center plane and transversal planes. Turbulent flow (Re = 10000)

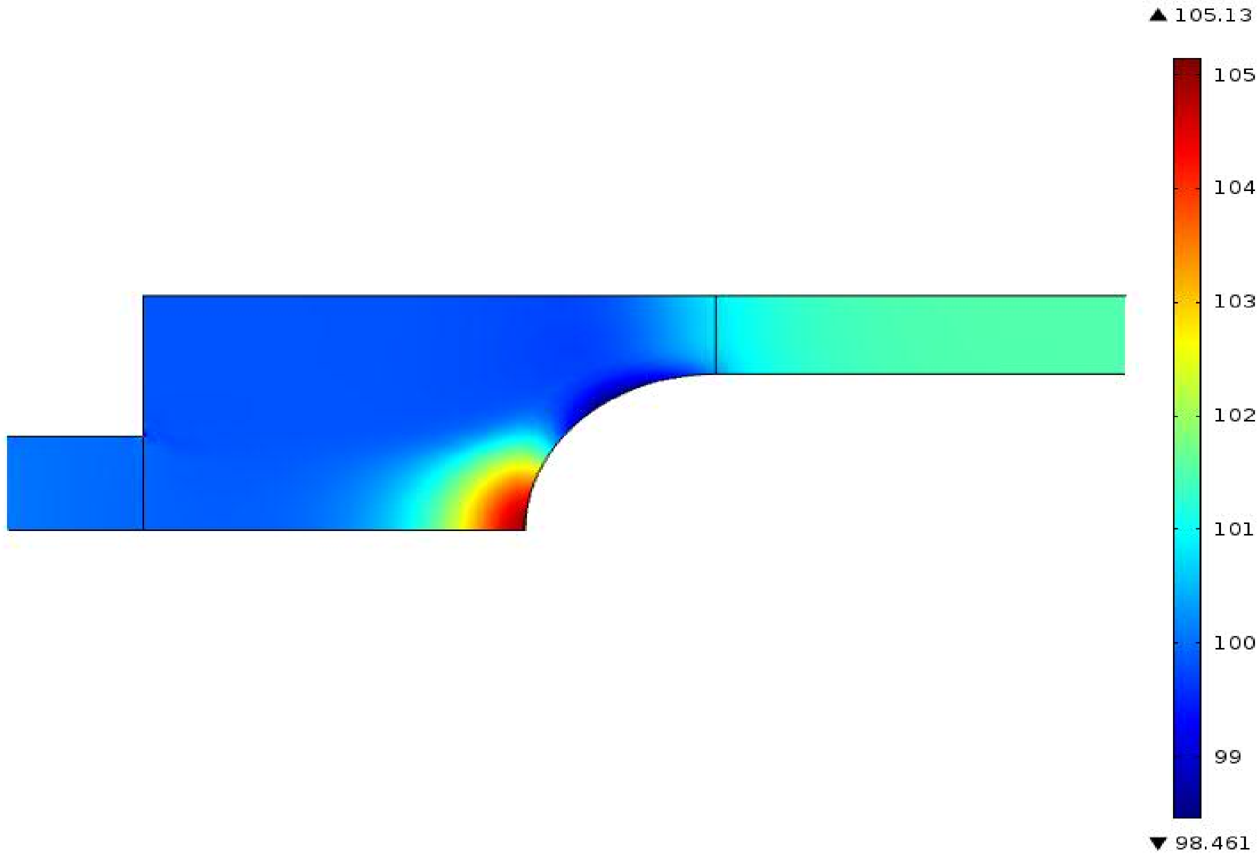
RESULTS



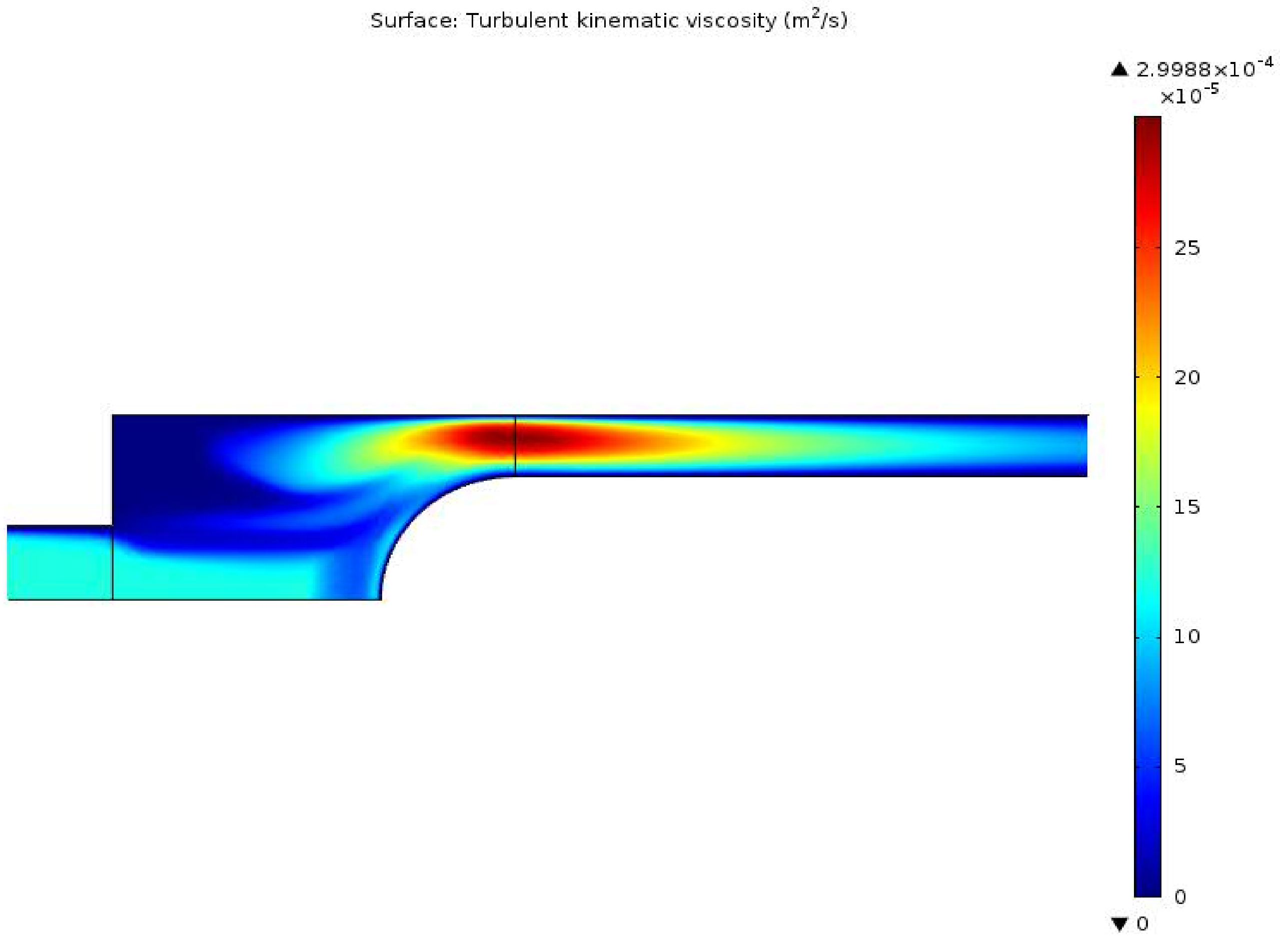
Streamlines of velocity field using Low Reynolds k – ε turbulence model (Re = 10000)



Streamlines of velocity field using k – ε turbulence model (Re = 10000)

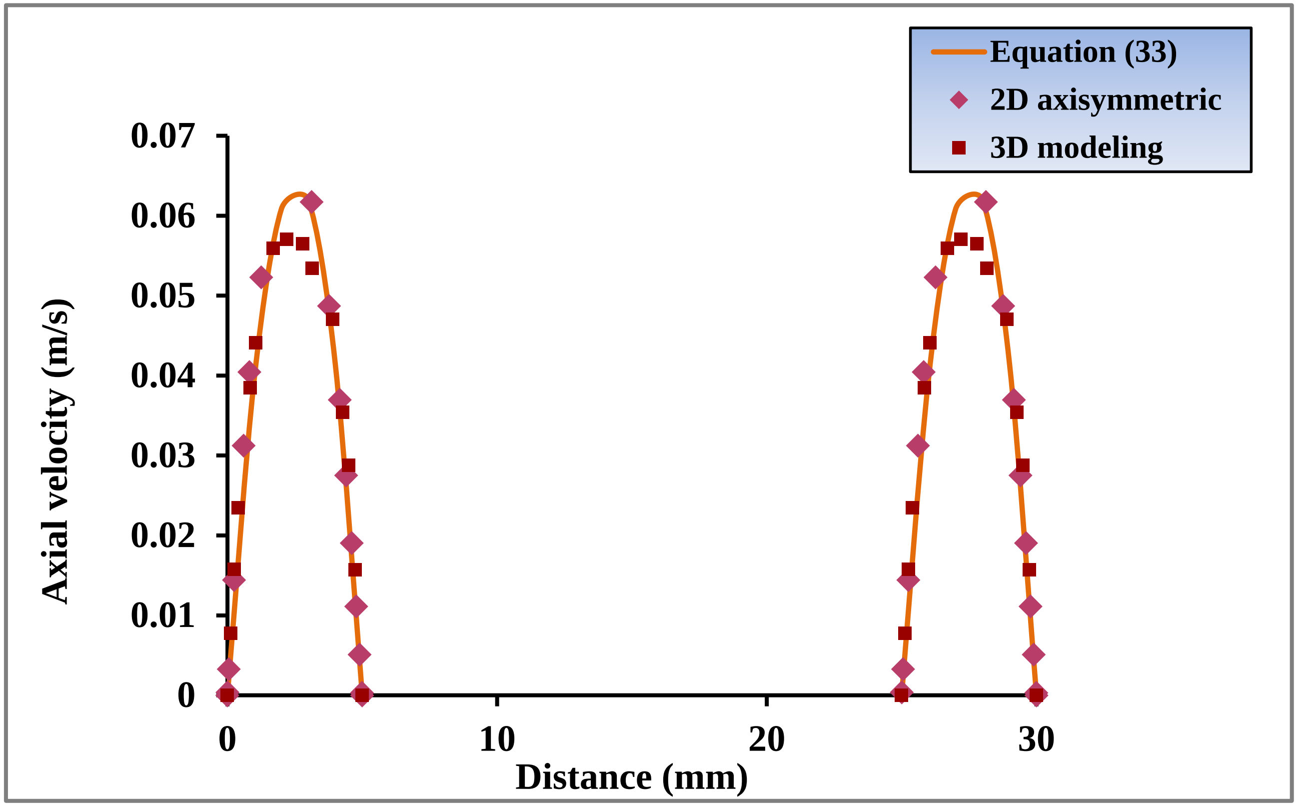


Pressure profile (kPa) on the longitudinal center plane at the inlet region for flow rate corresponding to Re = 10000



Turbulent eddy viscosity profile (m2/s) on the longitudinal center plane for flow rate corresponding to Re = 10000

$$v_z = \frac{\Delta P \times r_o^2}{4\mu l}\left[1 - \left(\frac{r}{r_o}\right)^2 + \left(\frac{1 - \left(\frac{r_i}{r_o}\right)^2}{\ln\left(\left(\frac{r_o}{r_i}\right)\right)}\right)\ln\left(\frac{r}{r_o}\right)\right]$$



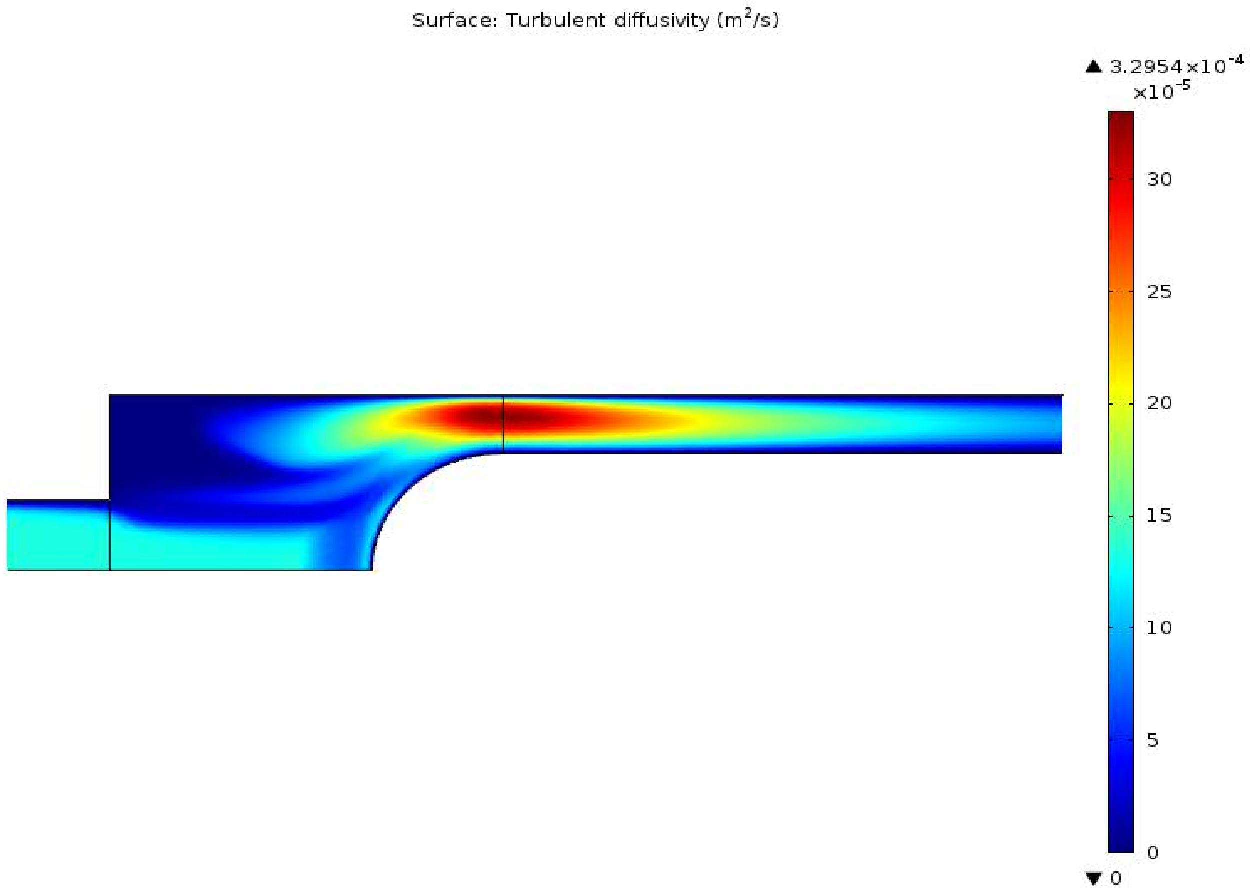
$$K_{av} = \frac{Q}{A} ln\left(\frac{C_{sat} - C_i}{C_{sat} - C_o}\right)$$

Q **Flow rate**

Ci **Concentration at the inlet**

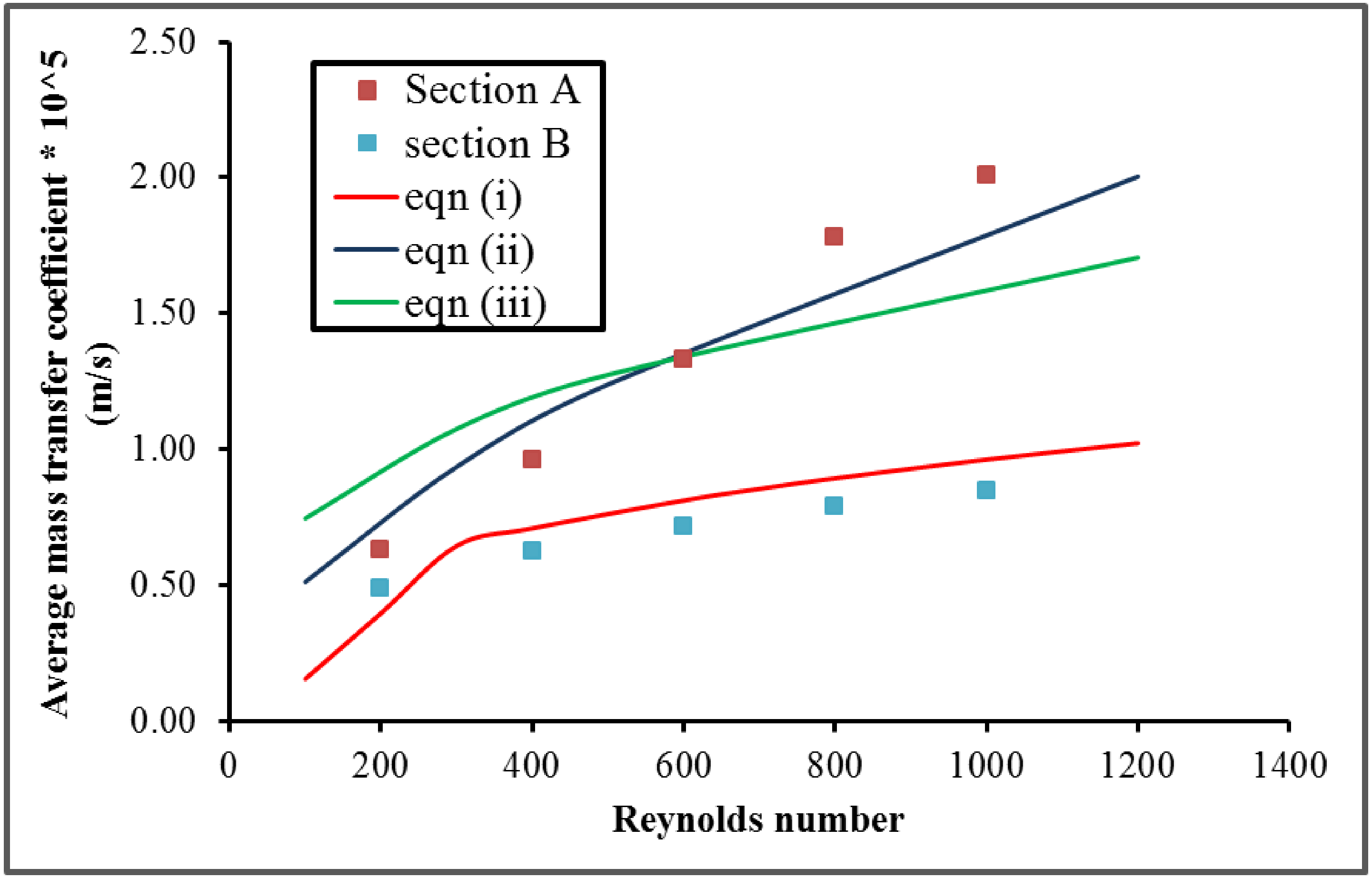
Co **Concentrations at outlet**

Csat Saturation Concentation (at the wall of mass transfer)

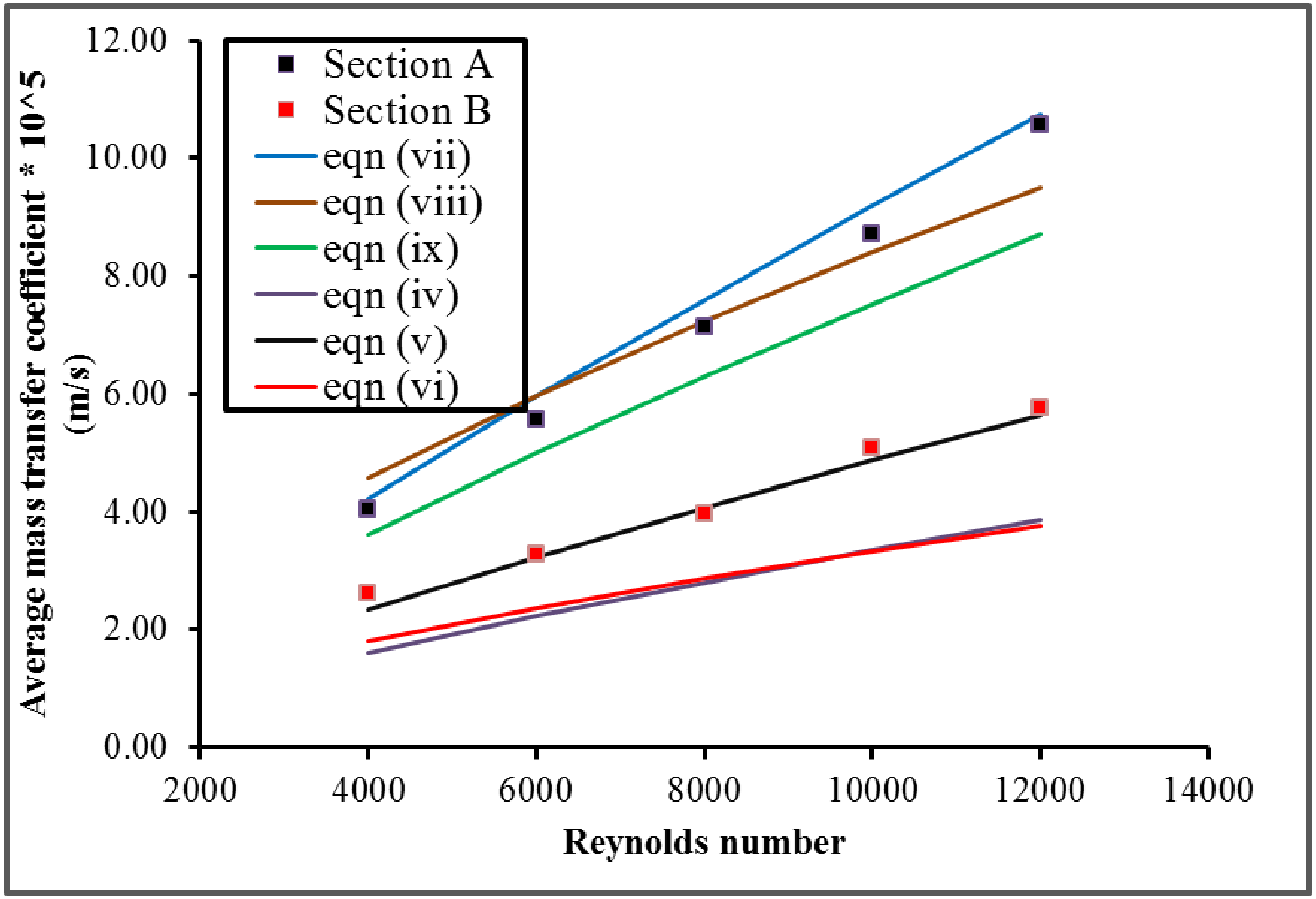


Turbulent diffusivity profile (m^2/s) on the longitudinal center plane for flow rate corresponding to Re = 10000 using low Reynolds k – ε turbulence model.

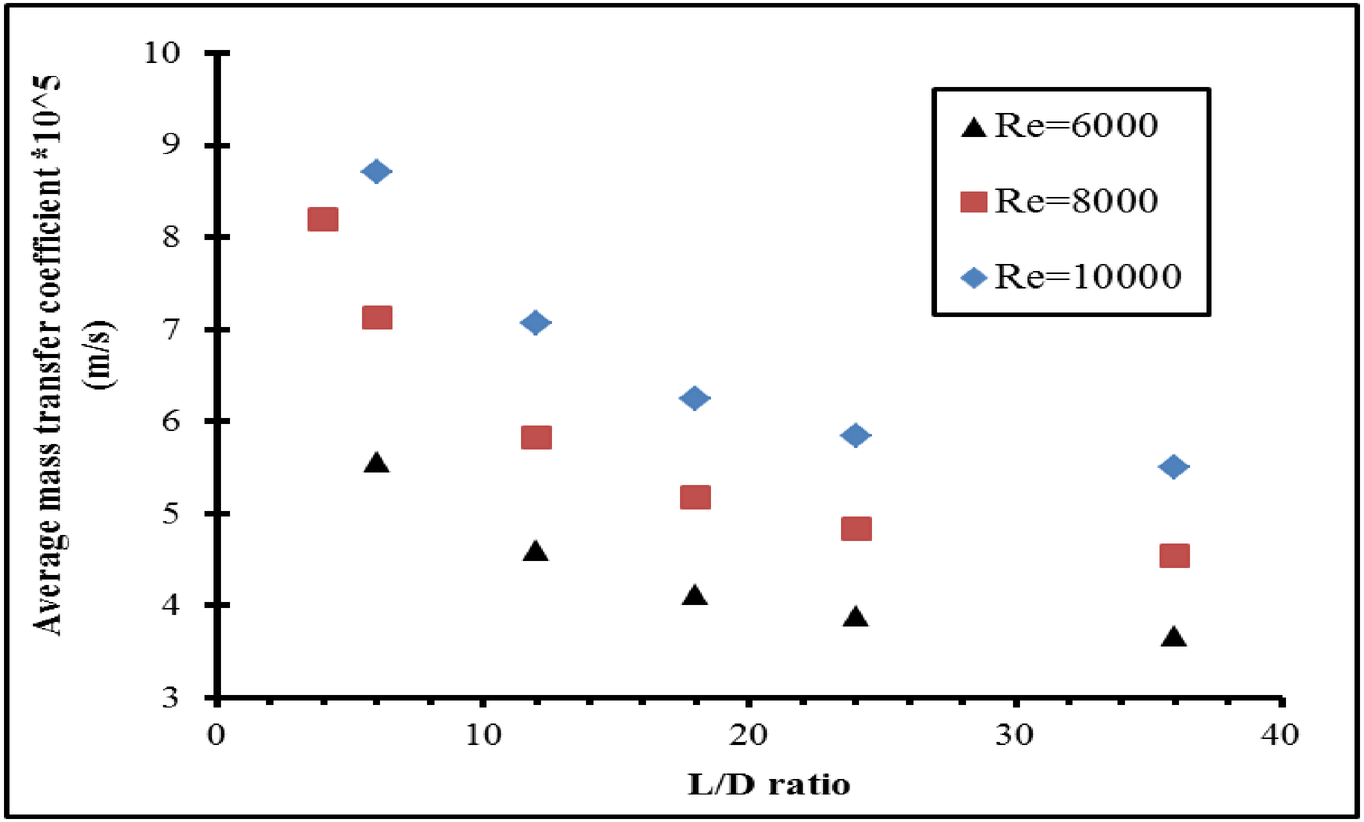
Validation of mass transfer predictions with different correlations reported in literature



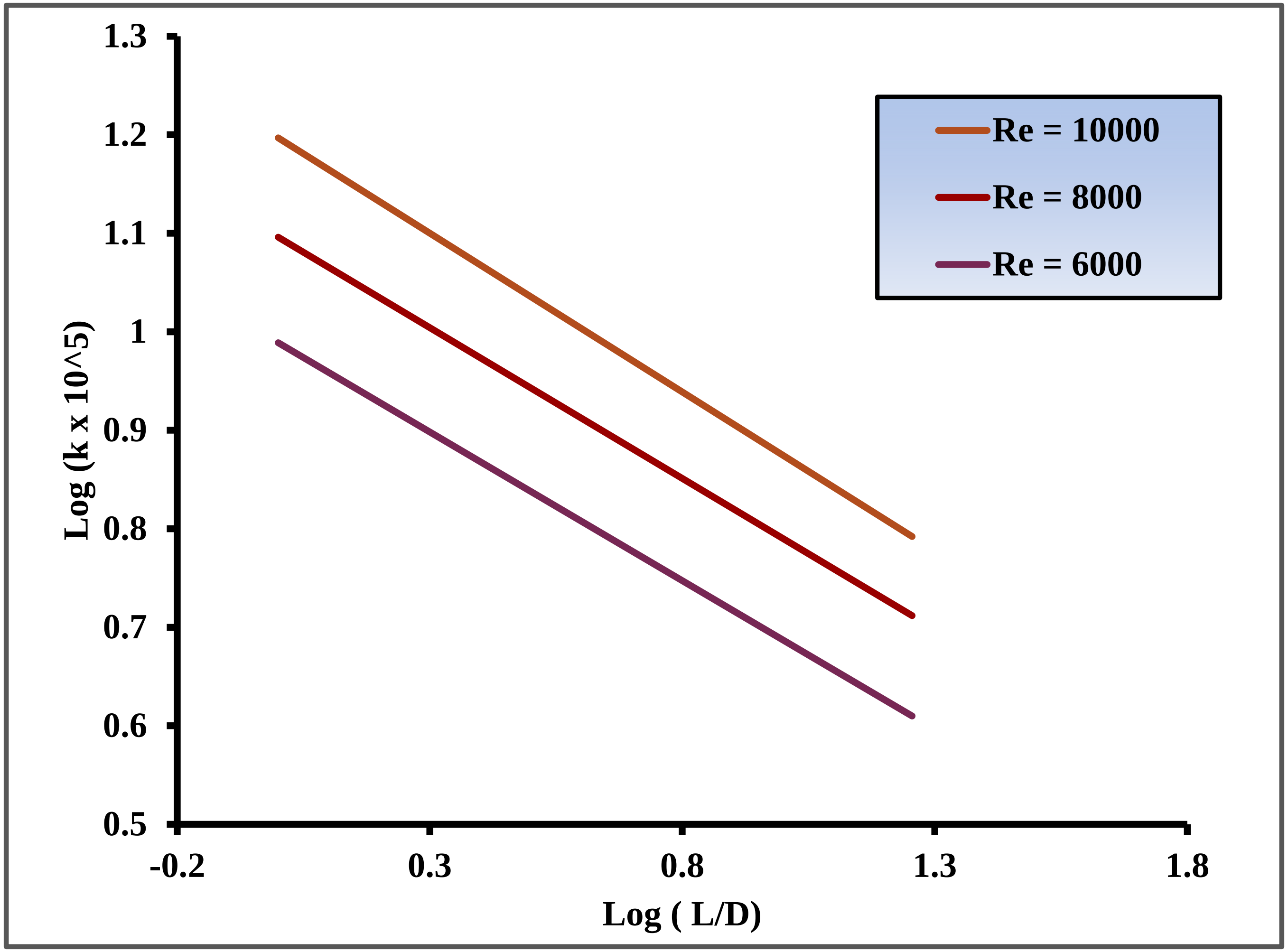
Comparison of the CFD predicted average mass transfer coefficients for laminar flow with the ones estimated using different correlations reported in the literature (Table (1)).



Comparison of the CFD predicted average mass transfer coefficients for turbulent flows with the values estimated using different correlations reported in the literature (Table (1))



Variation of the average mass transfer coefficient with the change in reactor length.

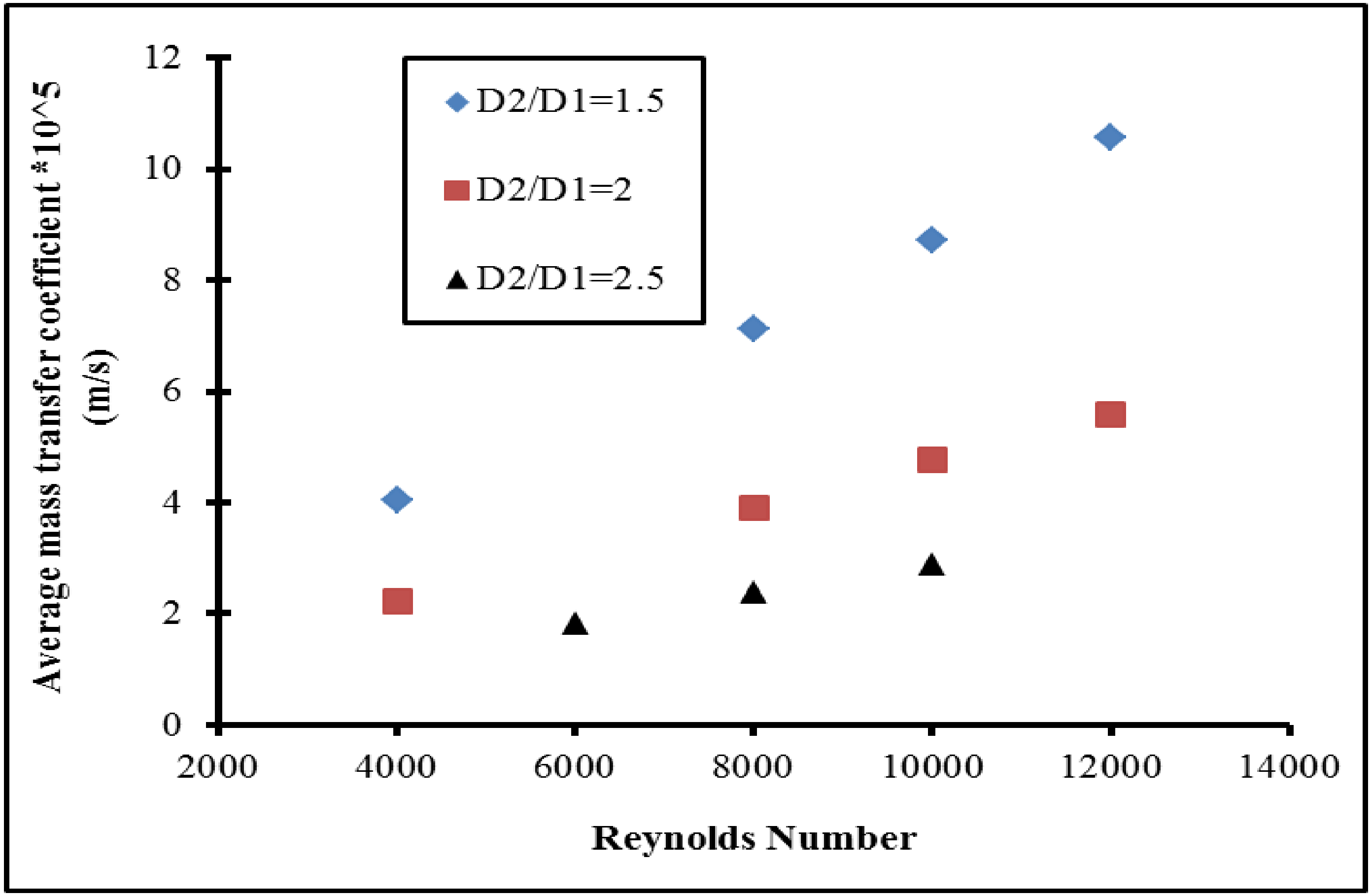


Log (k × 10^5) vs log (L/D) for different Reynolds number.

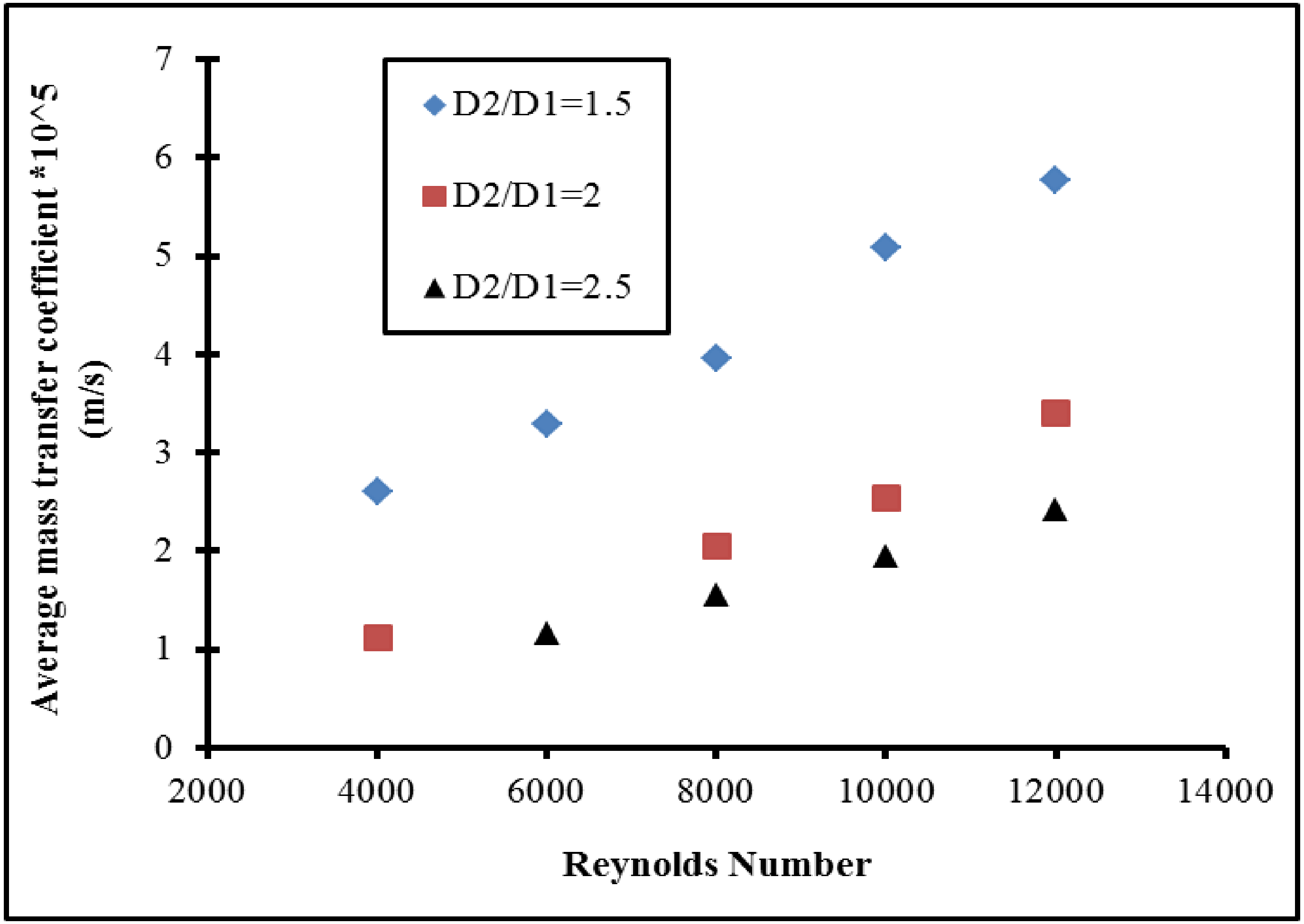
$$k \, \alpha \left(\frac{L}{D}\right)^{-0.322}$$

$$Sh_{av} = 0.305\, Re^{\frac{2}{3}}.Sc^{\frac{1}{3}}.(\varphi d_e/l)^{\frac{1}{3}}$$

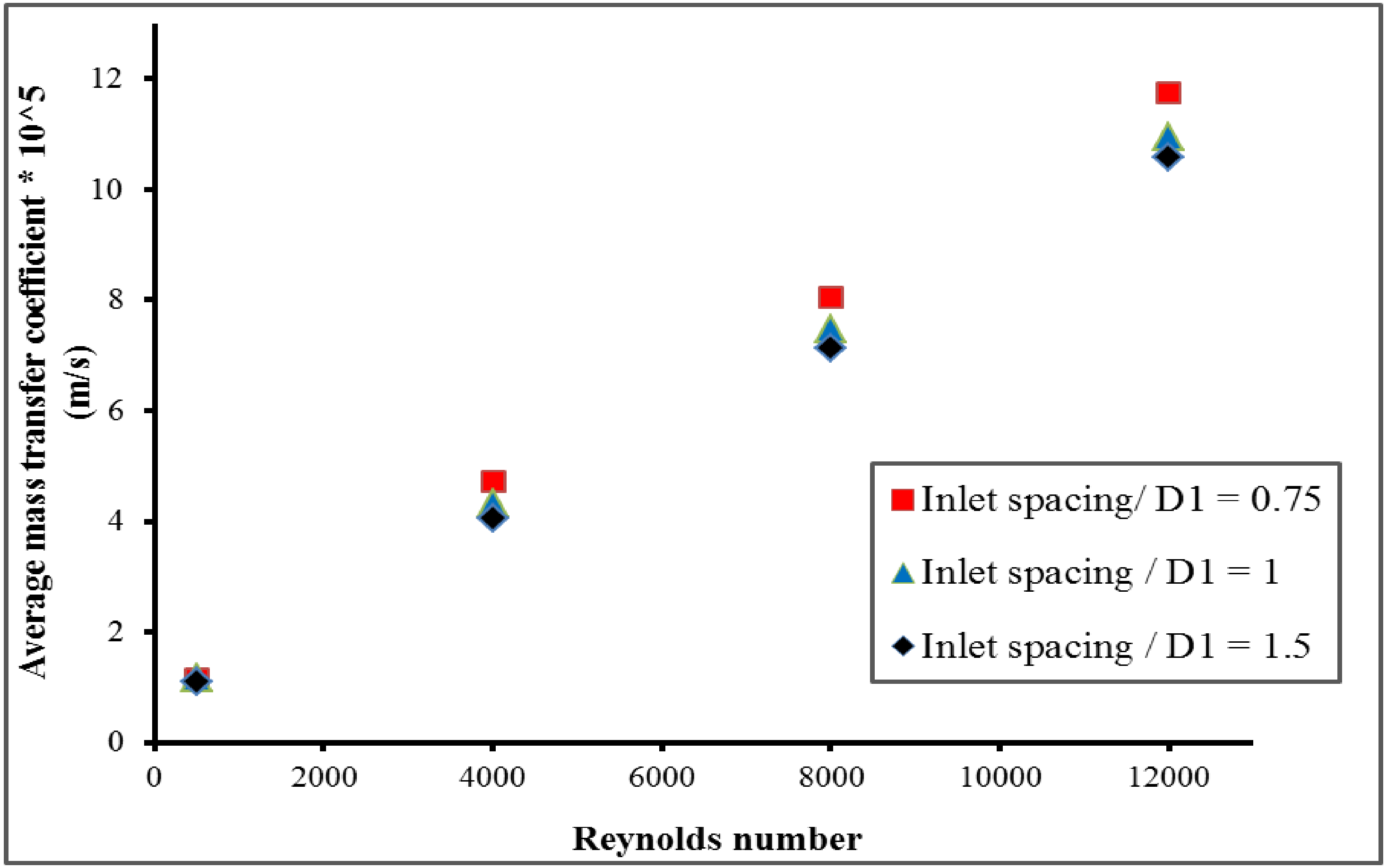
Eq (VIII)



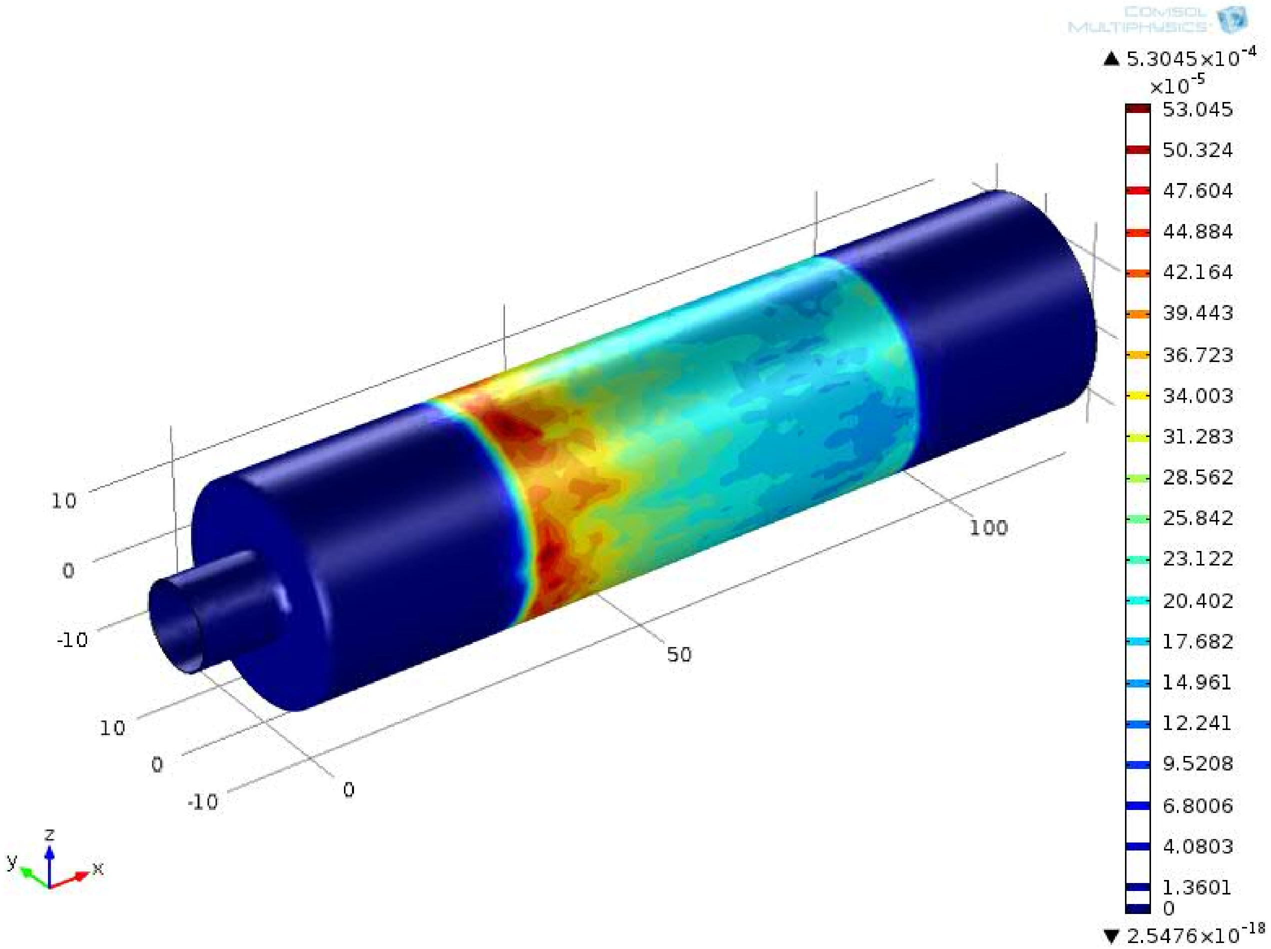
Mass transfer coefficient vs. Reynolds number in section A for three different annulus diameter ratios.



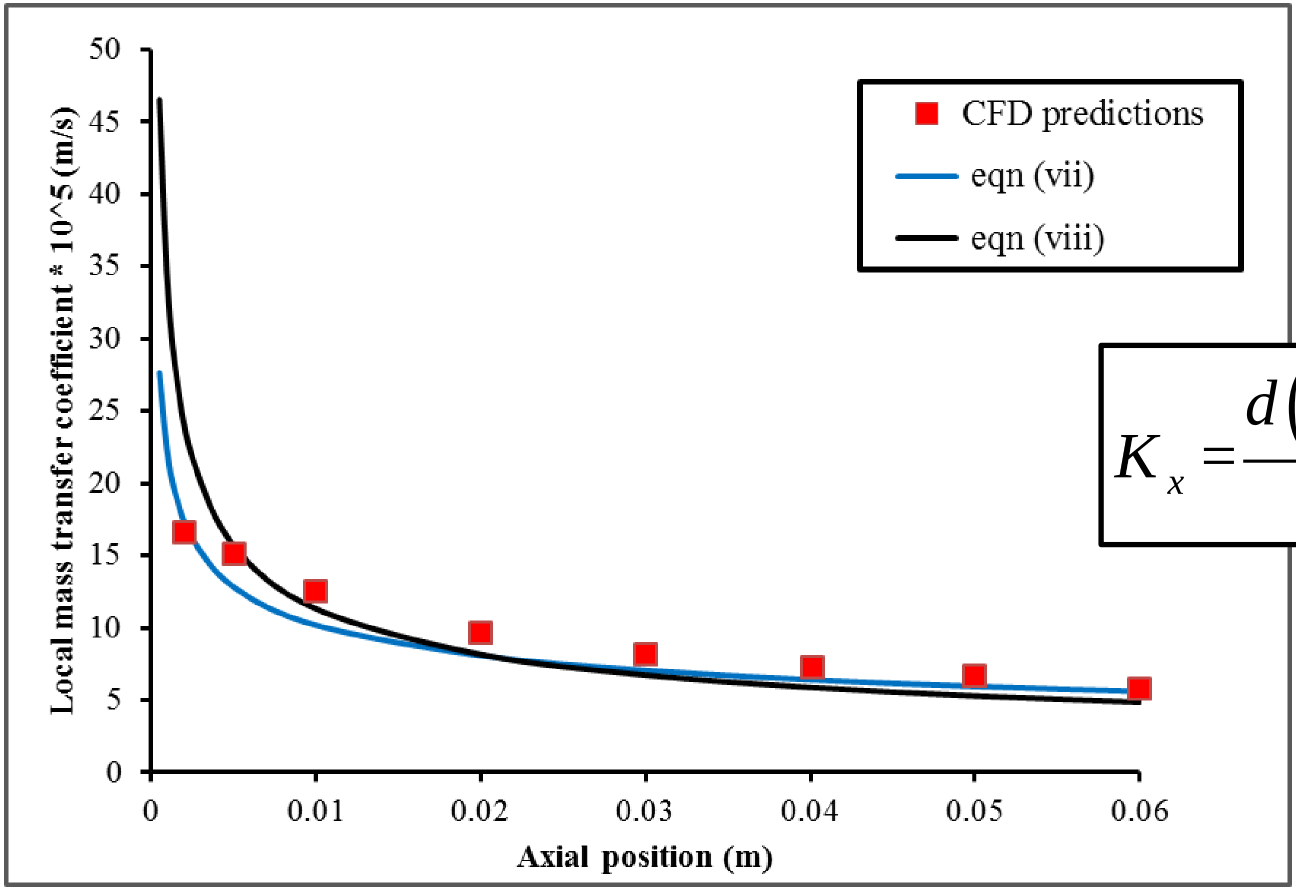
Mass transfer coefficient vs. Reynolds number in section B for three different annulus diameter ratios.



Variation of the average mass transfer coefficient with the change in inlet spacing.



Local mole flux magnitude in section A as computed utilizing the laminar flow model (Re = 500).



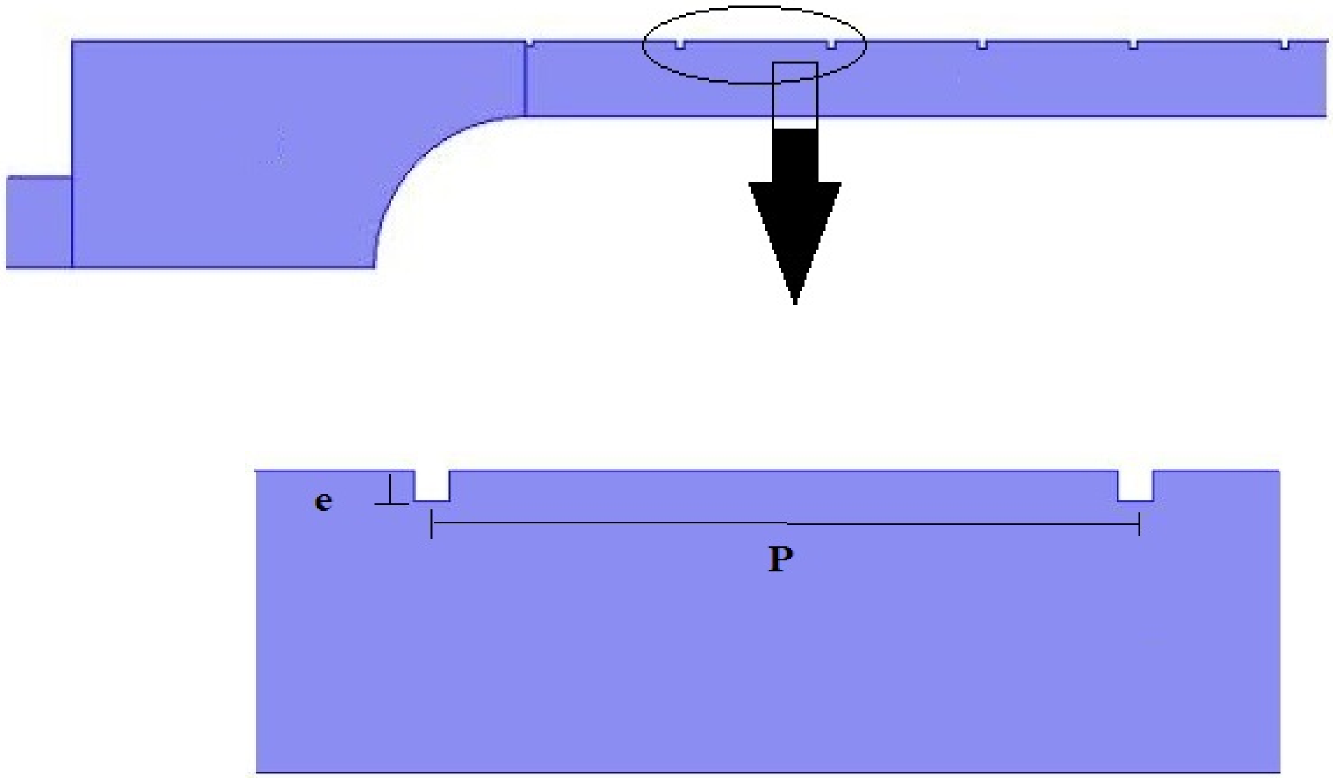
$$K_x = \frac{d\left(K_{av,x}\right)}{dx}$$

CFD predictions of the local mass transfer coefficient along the reactor axis at Re = 10000 compared with values calculated from correlations.

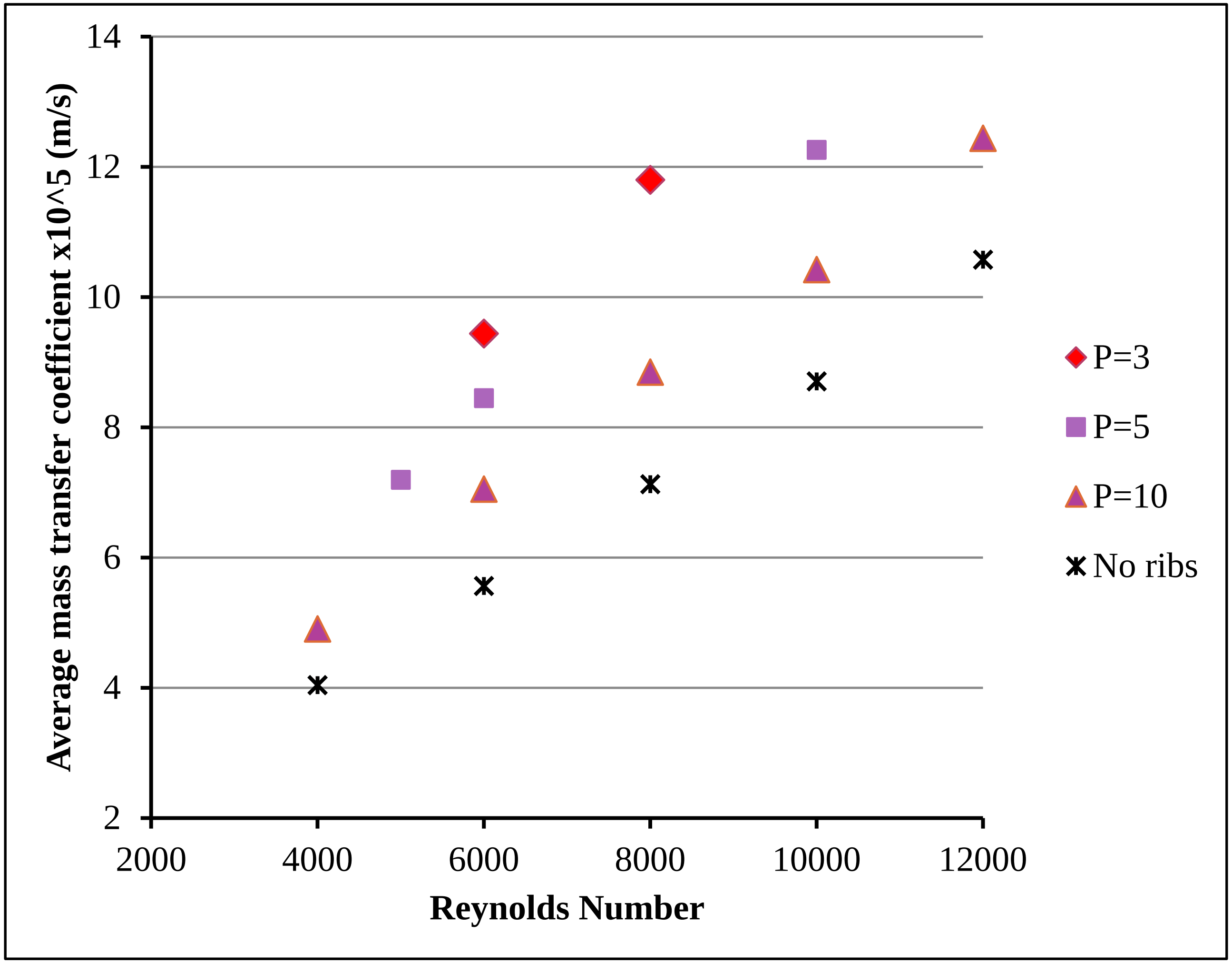
Enhancement in the average mass transfer coefficient in section A due to perturbing flow created by the inlet section

Re (annulus)	**Ratio** $\frac{Kwith}{Kwithout}$	**Percent increase** $\frac{Kwith - Kwithout}{Kwithout}$
4000	1.05	5.22
6000	1.13	12.69
8000	1.20	19.74
10000	1.24	24.46
12000	1.31	30.59

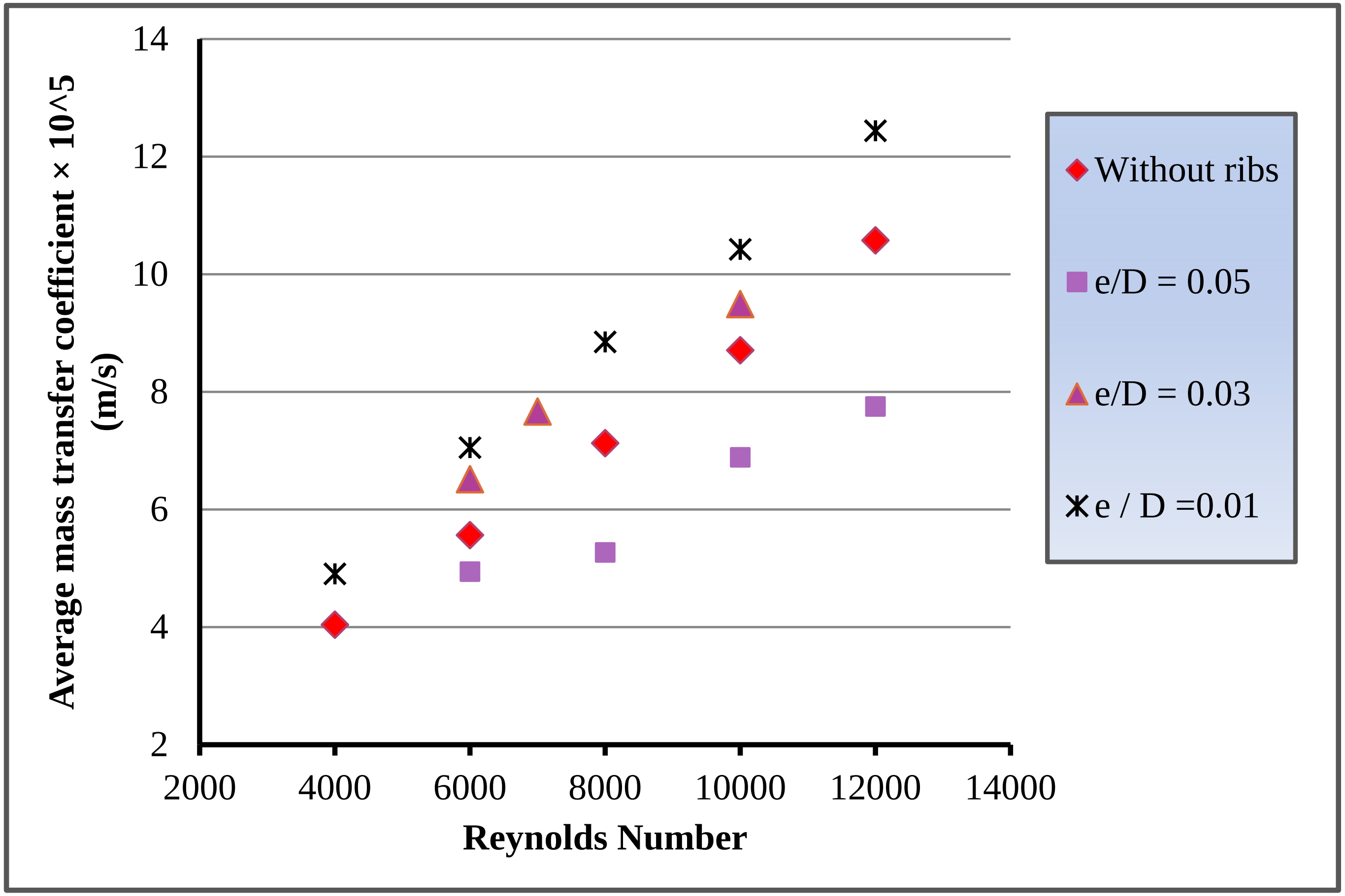
Surface Ribs



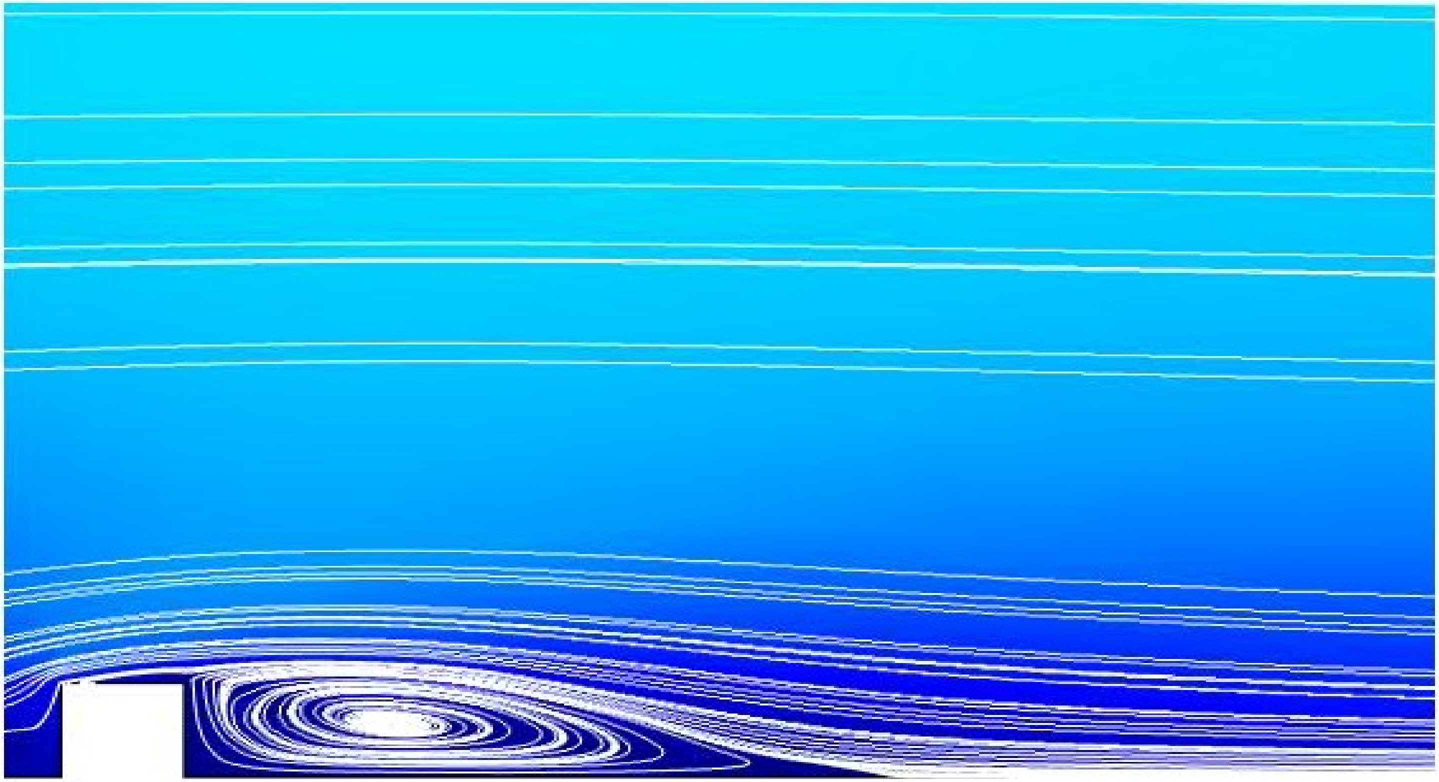
Schematic of the ribs used as external mass transfer enhancement element, the repeated ribs are of height e and separated a distance P



CFD predictions of the variation of the mass transfer coefficient with the rib pitch distance "P" along the reactor coated wall for e/D = 0.01



CFD predictions of the variation of the mass transfer coefficient with the rib height "e" along the reactor coated wall for P = 10 mm



Conclusion

- **The present Comsol model is consistent with the available measurements of mass transfer in annular reactors reported in the literature.**
- **Inlet sections of annular reactors play an important role in the reactor hydrodynamics and consequently on its mass transfer performance.**
- **As the annulus diameter ratio decreases, the mass transfer efficiency of the annular reactor increases.**
- **As the inlet spacing between the inlet port of the reactor and the inner tube rounded front decreases, the mass transfer coefficient increases.**
- **Incorporating squared repeated ribs mass transfer promoters in to the design of such reactors showed better performance which is likely due to the fact that ribs produce turbulence very close to the wall, exactly where mass transfer is taking place.**


Thank You