CFD Analysis of Mixing in Polymerization Reactor

By

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Outline

- Introduction
- Model development
- Simulation
- Model Setup for Fluent
- Results and discussion
- Conclusions
- Future work
- Questions

Introduction

- CFD is a simulation tool to analyze a system having transport equations of mass, momentum and energy.
- Originally developed for aerospace and now it is being expanded to other fields.
- Flow domain is divided into large number of small cells and one equation is written for each cell for each transport equation and then it is solved.

Introduction

- Polymerization is a complex reaction.
- Viscosity increase very rapidly during polymerization.
- Mixing plays an important role in deciding the conversion and the quality of polymer formed.
- Several studies are reported to relate mixing with polymerization but they are of limited use.
- CFD has been used for tubular reactors.
- No attempt has been reported for polymerization in CSTR.

Kinetic Model

- Styrene can be polymerized in absence of Initiator.
- Thermal initiation $3M \xrightarrow{Kth} 2R_1^{\bullet}$
- Propagation $R_r^{\bullet} + M \xrightarrow{Kp} R_{r+1}^{\bullet} \qquad r \geq 1$
- Termination $R_r^{\bullet} + R_s^{\bullet} \xrightarrow{Ktc} P_{r+s} \qquad r,s \geq 1$

- Steady-state hypothesis

$$[R] = \sqrt{\frac{2K_{th}[M]^3}{K_{tc}}}$$

Kinetic Model

$$R_r^{\bullet} + M \xrightarrow{Kp} R_{r+1}^{\bullet} \qquad r \geq 1$$

- Propagation rate

$$R_p = -k_p M[R]$$

where

$K_p = A_p \exp(-E_p / RT)$

Similarly for K_{th} & K_{tc}

•Values of A_{p}, A_{th} , A_{tc} , E_{p} , E_{th} and E_{tc} were taken from Dhib.et.al.(2000).

Physical Properties

- Zero shear viscosity(Kim and Nauman(1992))

$$\ln(\mu_0) = -11.091 + 1109/T + M_w^{0.1413}[12.032 W_p - 19.501 W_p^2 + 2.923 W_p^3 + (-1327 W_p + 1359 W_p^2 + + 3597 W_p^3)/T]$$

- Shear viscosity (Kim and Nauman(1992))

$$\mu = \mu_0 /(1 + \mu_0 \gamma^{1.2} / 35000)^{0.60} \ Pa.s$$

- Density (Soliman et.al.(1994))

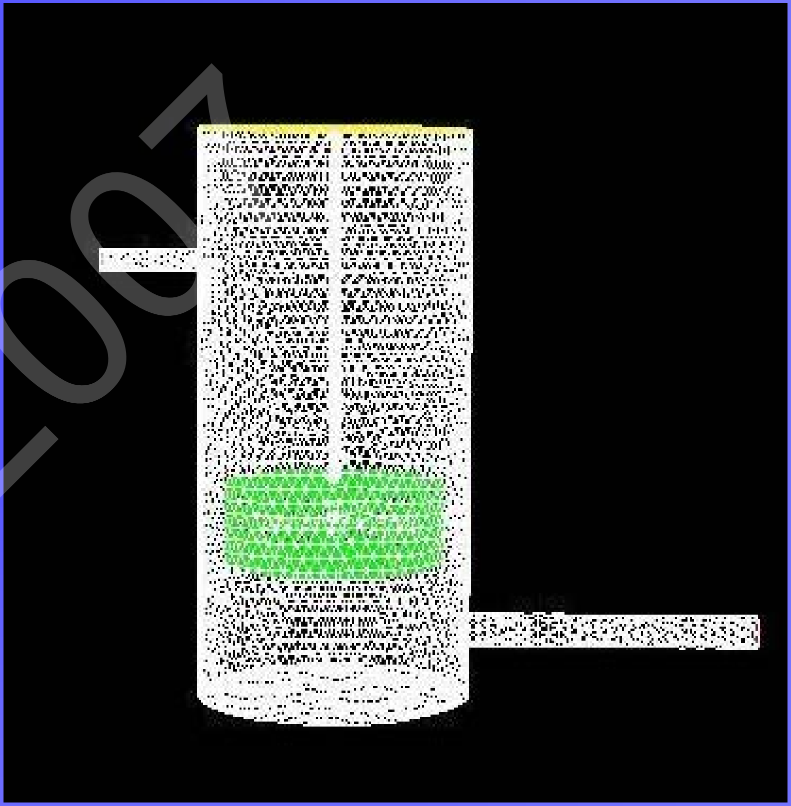
$$\rho = (1174.7 - 0.918T)(1 - W_p) + (1250.0 - 0.605T)W_p \ Kg/m^3$$

- Cp=1880 J/kg.k
- K =0.126 J/m.s.k
- Dm=2.0 x 10^{-9} m^2/s

} (Soliman et.al.(1994))

Reactor Geometry

Tank diameter = 14 cm
Liquid level = 26 cm
Impeller type = pitched blade
No. of blades = 4
Impeller diameter = 8.4 cm
Impeller speed = 100 to 1000 rpm
Inlet diameter = 1 cm
Outlet diameter = 1.5 cm
Reactor temperature = 140^{o}C



- Discretised domain of a reactor
- 372,000 cells

Governing equations

- Continuity Eq.

$$\nabla\cdot(\rho\vec{v})=0$$

- Momentum

$$\frac{\partial}{\partial t}(\rho\vec{v})+\nabla\cdot(\rho\vec{v}\vec{v})=-\nabla p+\nabla\cdot(\bar{\bar{\tau}})+\rho g+\vec{F}$$

where

$$\bar{\bar{\tau}}=\mu[(\nabla\vec{v}+\nabla\vec{v}^{T})-\frac{2}{3}\nabla\cdot\vec{v}\,I]$$

Governing equations

- Energy

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + P)) = \nabla \cdot (K_{eff} \nabla T - \sum h_j \vec{J}_j + (\overline{\overline{\tau}}_{eff} \cdot \vec{v})) + S_h$$

$$E = h + \frac{v^2}{2}$$

$$h = \sum_j Y_j h_j$$

$$h_j = \int_{T_{ref}}^{T} c_{p,j} \, dT$$

Governing equations

- Species

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i$$

$$\vec{J}_i = -\rho D_{i,m} \nabla Y_i$$

- Only monomer species transport equation was solved and polymer mass fraction was obtained by (1- w_m).

Discretisation

- Flow domain was divided into 372,000 small volumes.
  - Integrating on each cell volume

$$\int_v \frac{\partial \rho\phi}{\partial t} dv + \oint \rho\phi \vec{v} \cdot d\vec{A} = \oint \Gamma \nabla \phi \cdot d\vec{A} + \int_v S_\phi dv$$

  - Discretisation

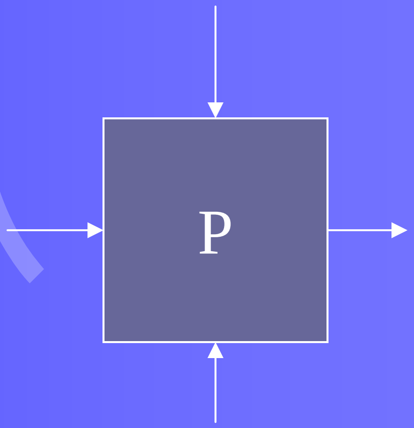
$$\frac{\partial \rho\phi}{\partial t} v + \sum_f^{N_{faces}} \rho_f \vec{v}_f \phi_f \cdot \vec{A}_f = \sum_f^{N_{faces}} \Gamma_\phi \nabla_{\phi_f} \cdot \vec{A}_f + S_\phi V$$

  - For steady state, Above equations result in algebraic equations.

Discretisation

- Finally all equations can be written as

$$a_p \phi = \sum_{nb} a_{nb} \phi_{nb} + b$$



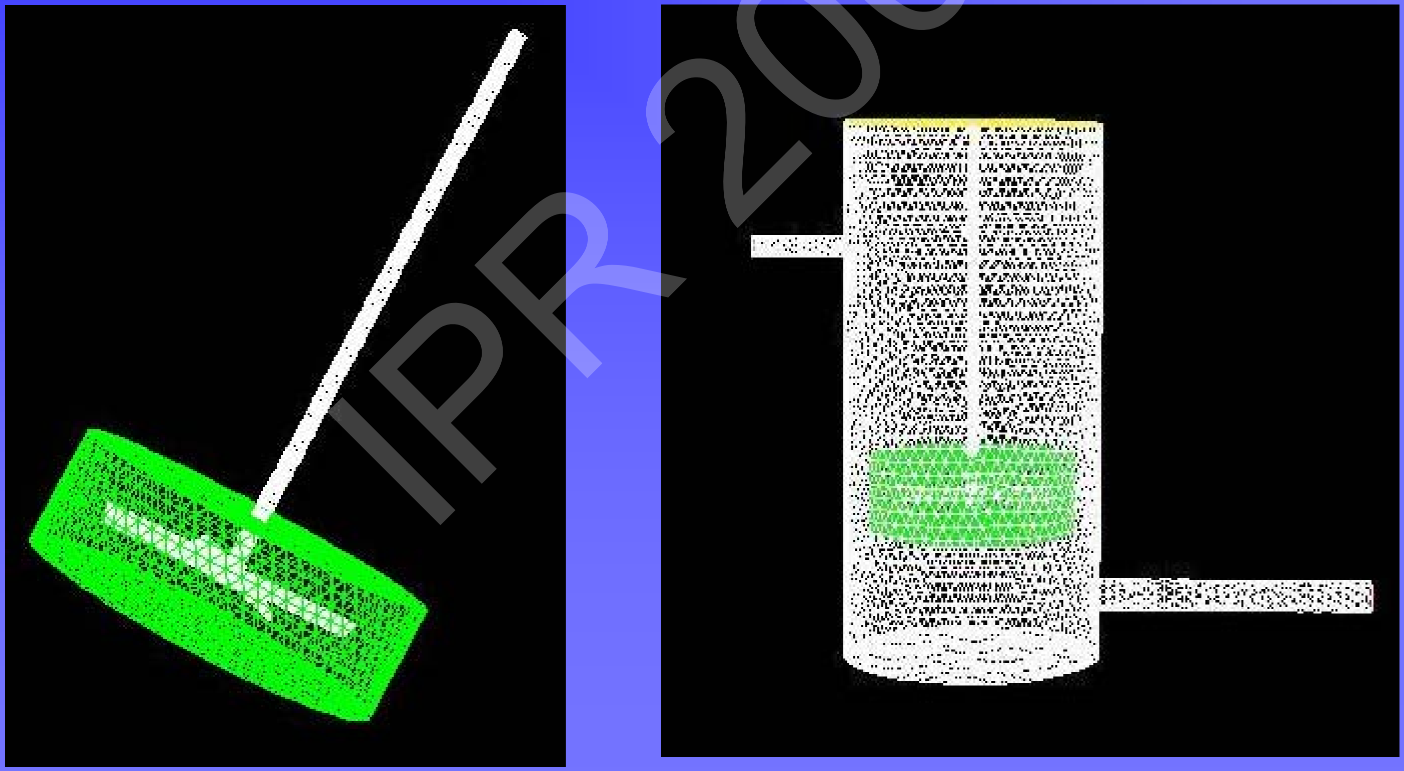
- This algebraic equations were solved using Gauss-Seidel with algebraic multigrid (AMG) method.

Model set-up for Fluent

- Grid generation in MixSim
- Define in Fluent
    - Material properties
    - Boundary conditions
    - Selecting discretisation techniques
    - Select under-relaxation factor
    - Modify Code by hooking UDF
    - Turn on monitors to check Convergence
    - Turn on equations to solve
    - Run Program to solve

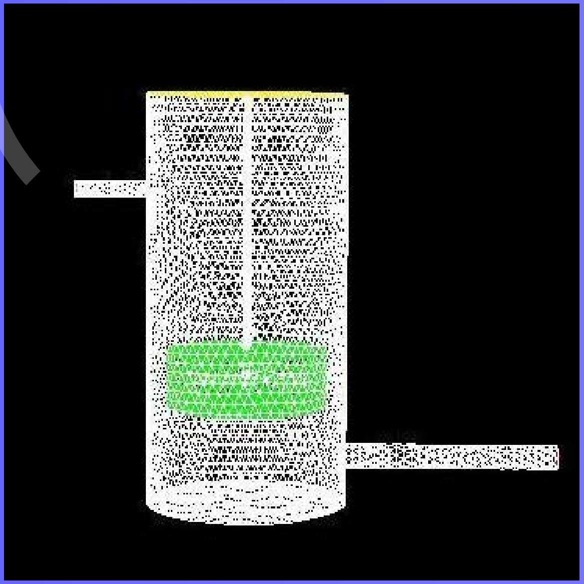
Boundary conditions

- Divide flow domain in two regions(for MRF)
  - -Impeller region(solved in rotating frame)
  - -Far region(solved in stationary frame)



Boundary conditions

- Tank Inlet
  - -Specified Normal velocity
  - -Species mass fraction of styrene=1.0
  - -Inlet temperature=140^o C
- Tank Wall
  - -No slip boundary for momentum
  - -Zero diffusive flux
  - -Fixed temperature=140^o C
- Tank Outlet
  - -Zero normal gradient for all the variables
- Liquid level
  - -Symmetry, No normal gradient



Case set up

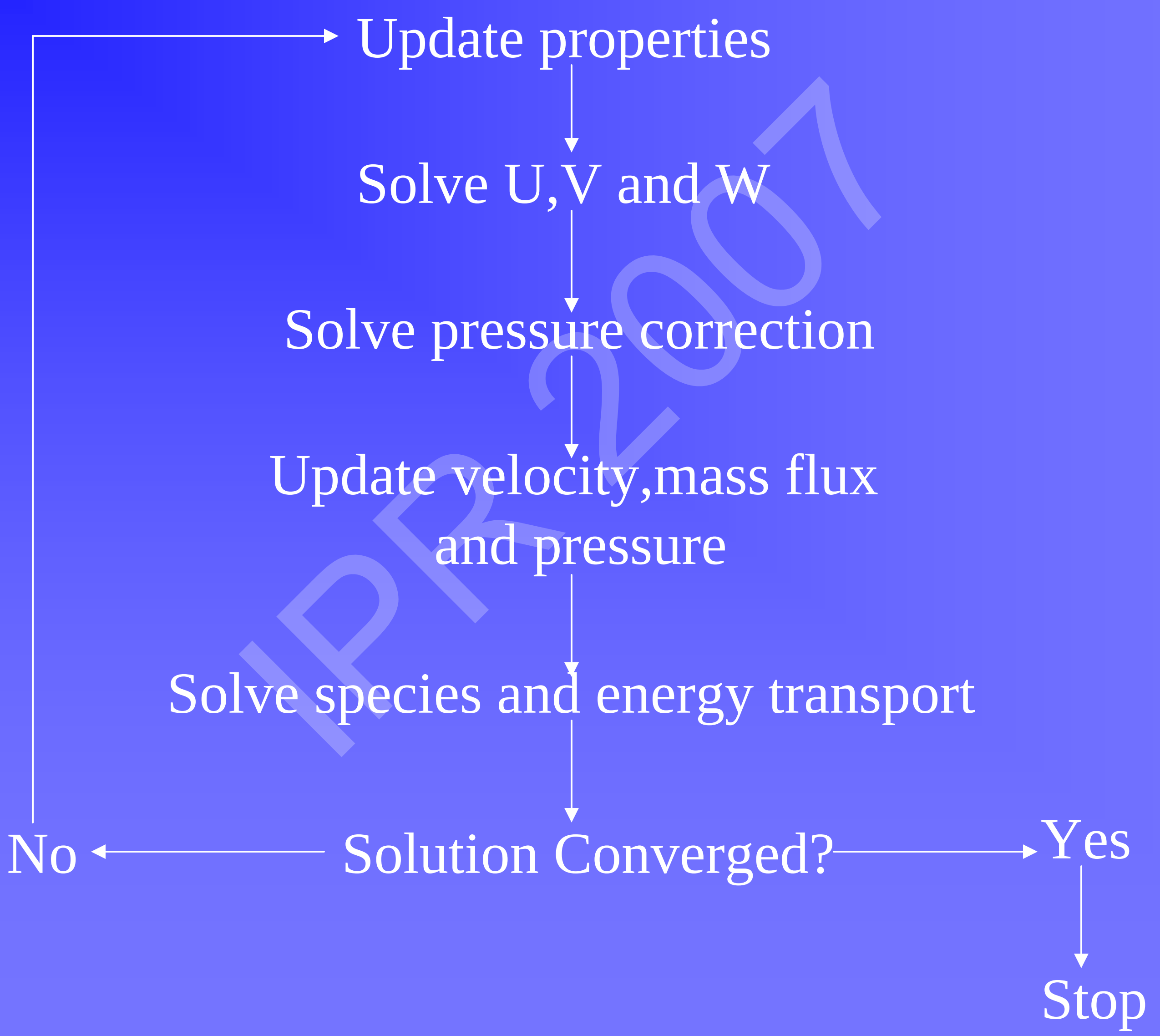
- Discretisation
    - Second-order Upwind for all equations
- Pressure-Velocity Coupling
    - SIMPLEC algorithm
- Under-relaxation to control change in variable
    - Most imp. for species
    - Started with 0.8 for species

$$\phi = \phi_{old} + \alpha \Delta \phi$$

- User-Define function(UDF) was written in C programming language for reaction source term and attached to Fluent.
- Monitored

  -Surface integral of the outflow of styrene
  -Residuals for each transport equation
  -Sum of velocity magnitude on symmetry

Solver



Update properties

Solve U,V and W

Solve pressure correction

Update velocity,mass flux
and pressure

Solve species and energy transport

Solution Converged?

No

Yes

Stop

Results and Discussion

- **Computational time**

  - Computational time is directly related to no. of cells, no. of equations and no. of iterations.

  - Our model consists of
    - approx. 372,000 cells
    - momentum, energy, species, pressure correction equations and some other interpolation calculations
    - approx. 240,000 iterations for each equation

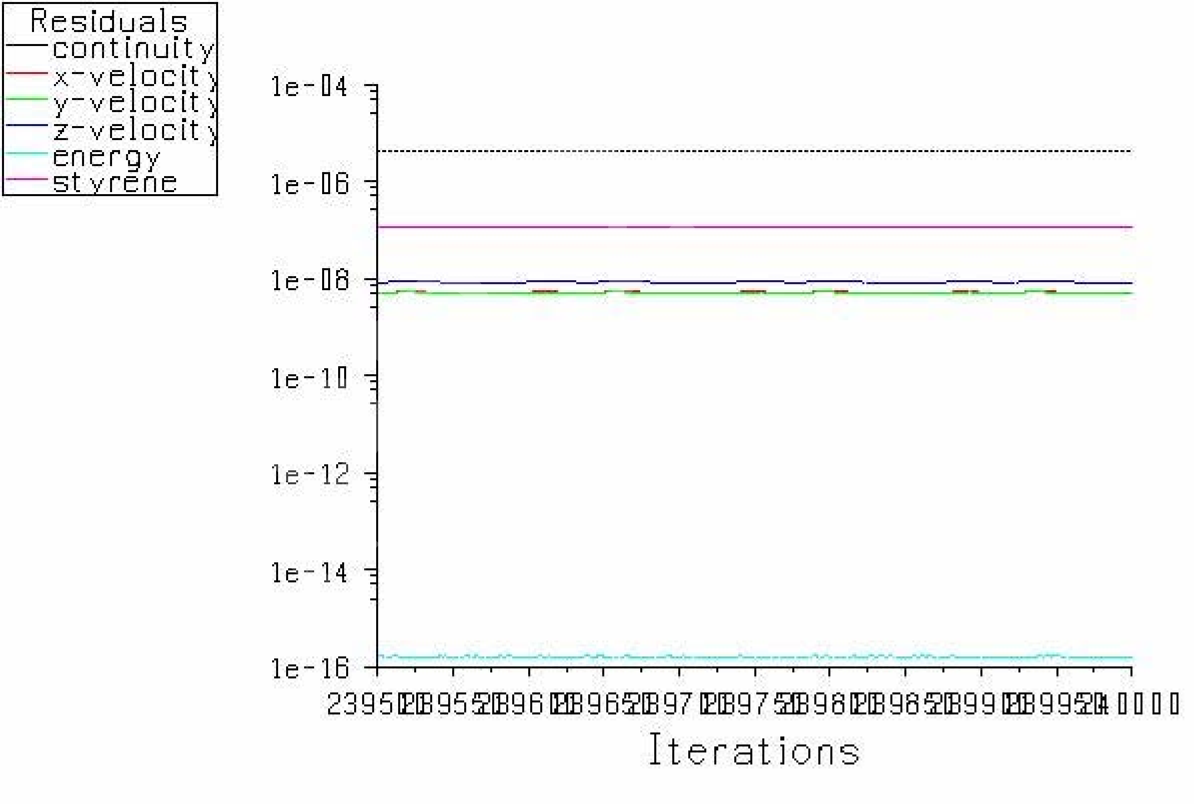
Results and Discussion

- **Computational time**
  - Steady state simulations were run on super-computing facility of HPCVL
    - Flow domain was divided into no. of partitions equal to no. of CPUs available. Each CPU was assigned one grid.
    - 24 to 35 CPUs were used for each simulation
    - It took 4 to 5 days for each run.

Results and Discussion

- Convergence Monitor

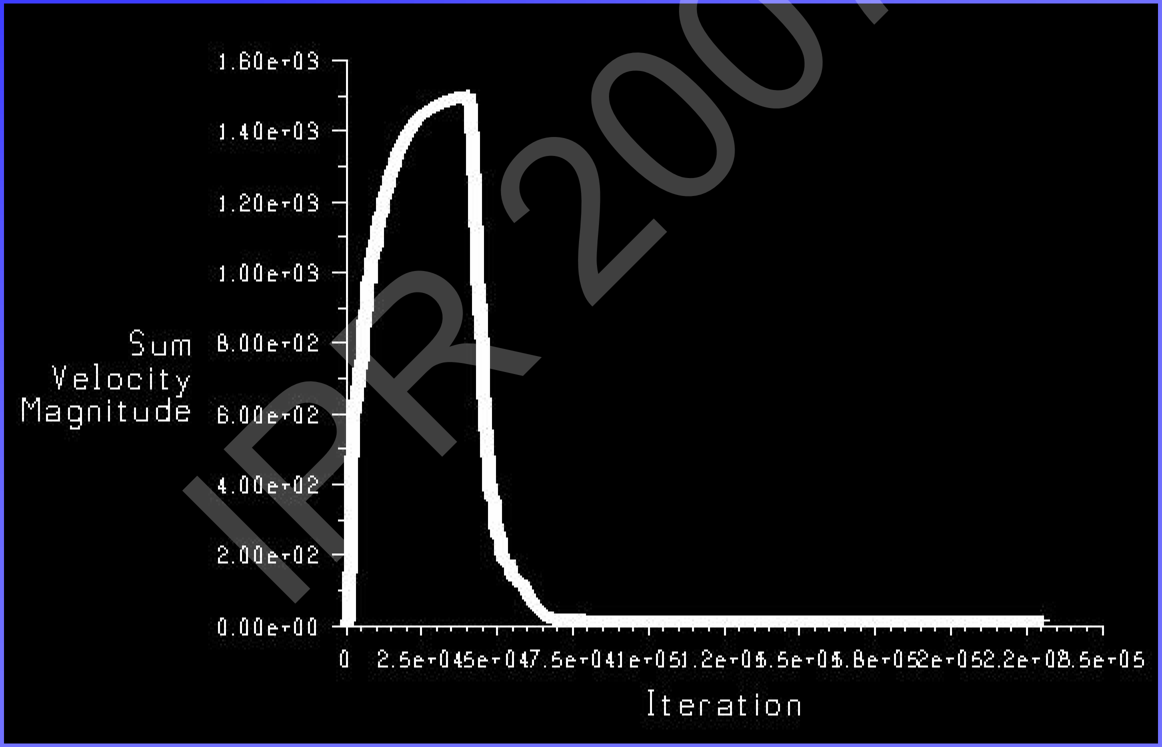
•Residual monitoring



Results and Discussion

- Convergence Monitor

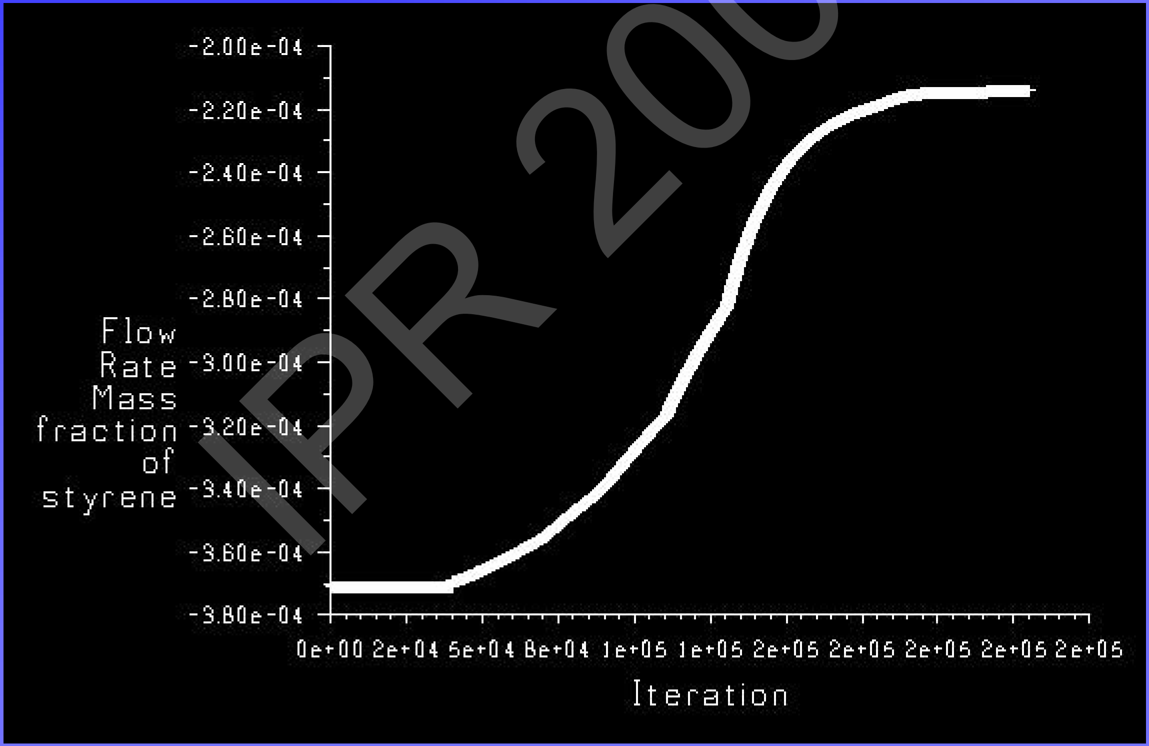
•Sum of Velocity magnitude on symmetry



Results and Discussion

- Convergence Monitor

•Styrene Outflow (kg/h)



Results and Discussion

- **Simulations Scenario**
  - **Effect of impeller speed**

    -100, 500 and 1000 rpm

    - Conversion analysis and comparison
  - **Effect of residence time**

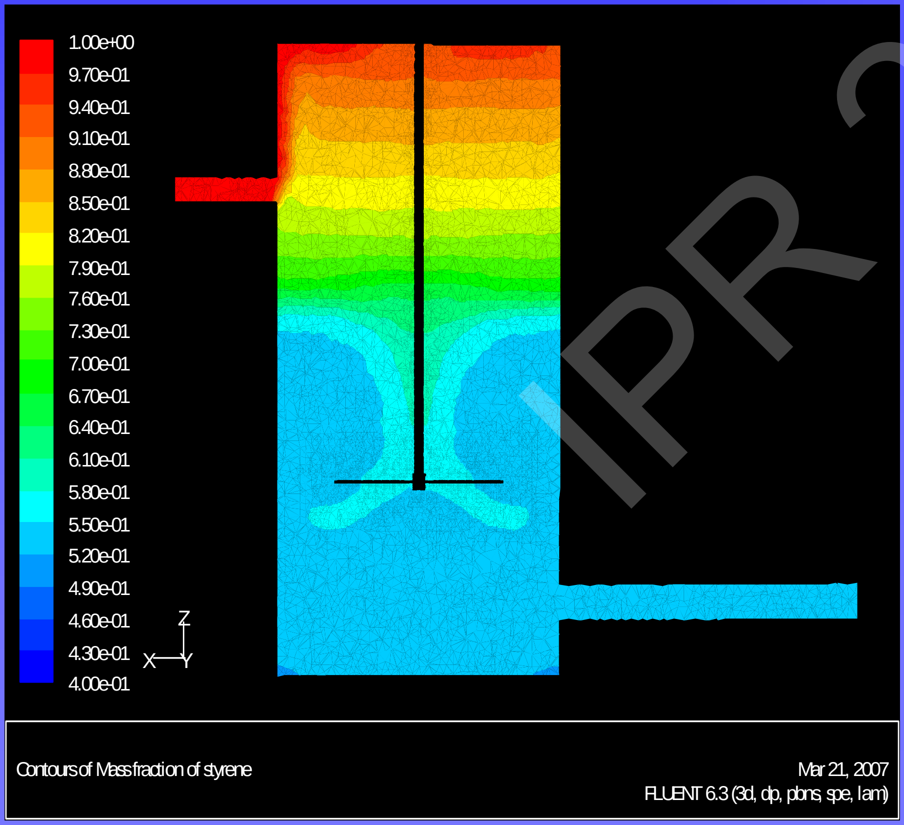
    - 4 different residence time
  - **Effect of input-output location**

    - bottom inlet location
    - 100 rpm & 500 rpm

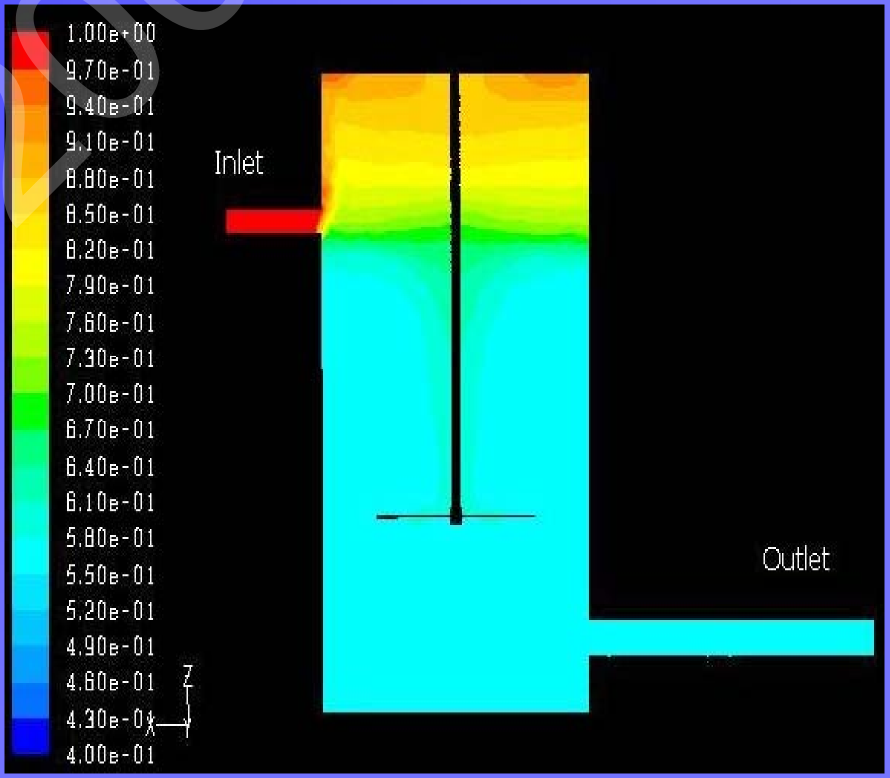
Results and Discussion

- Contours for Styrene mass fraction for 144 min. residence time

At 100 rpm

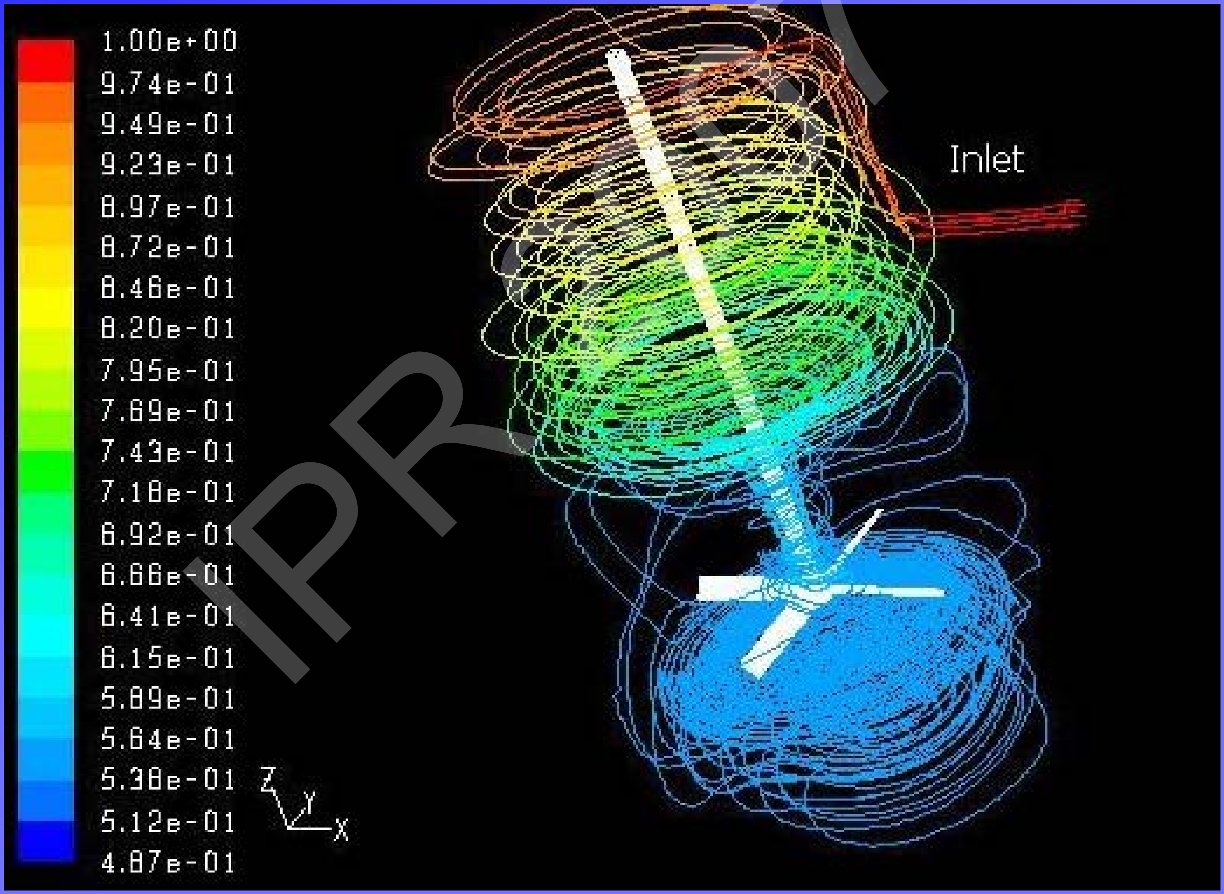


At 500 RPM



Results and Discussion

- Path lines for the particles entering at inlet (colored by styrene mass fraction)

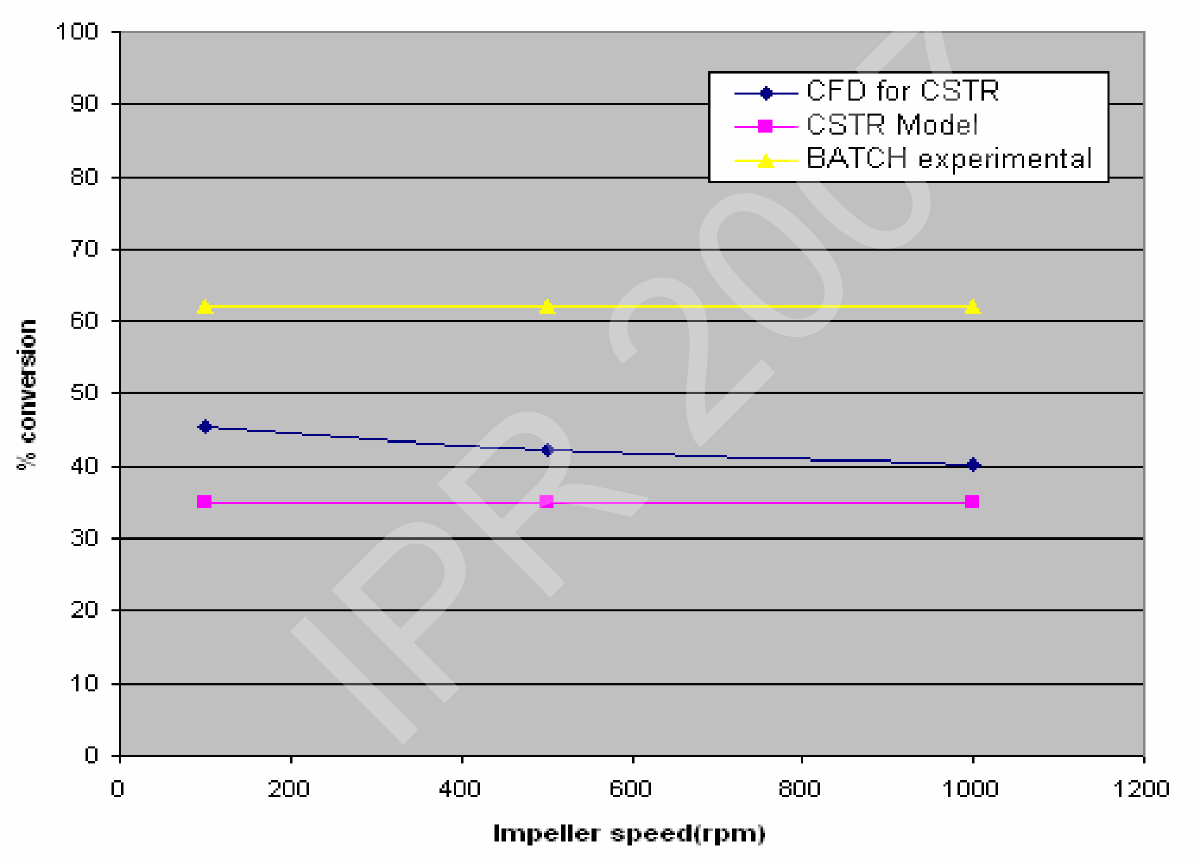


Results and Discussion

- Styrene mass fraction contours for 1000rpm and 144 min. residence time

Results and Discussion

- **Conversion Analysis and Comparison**

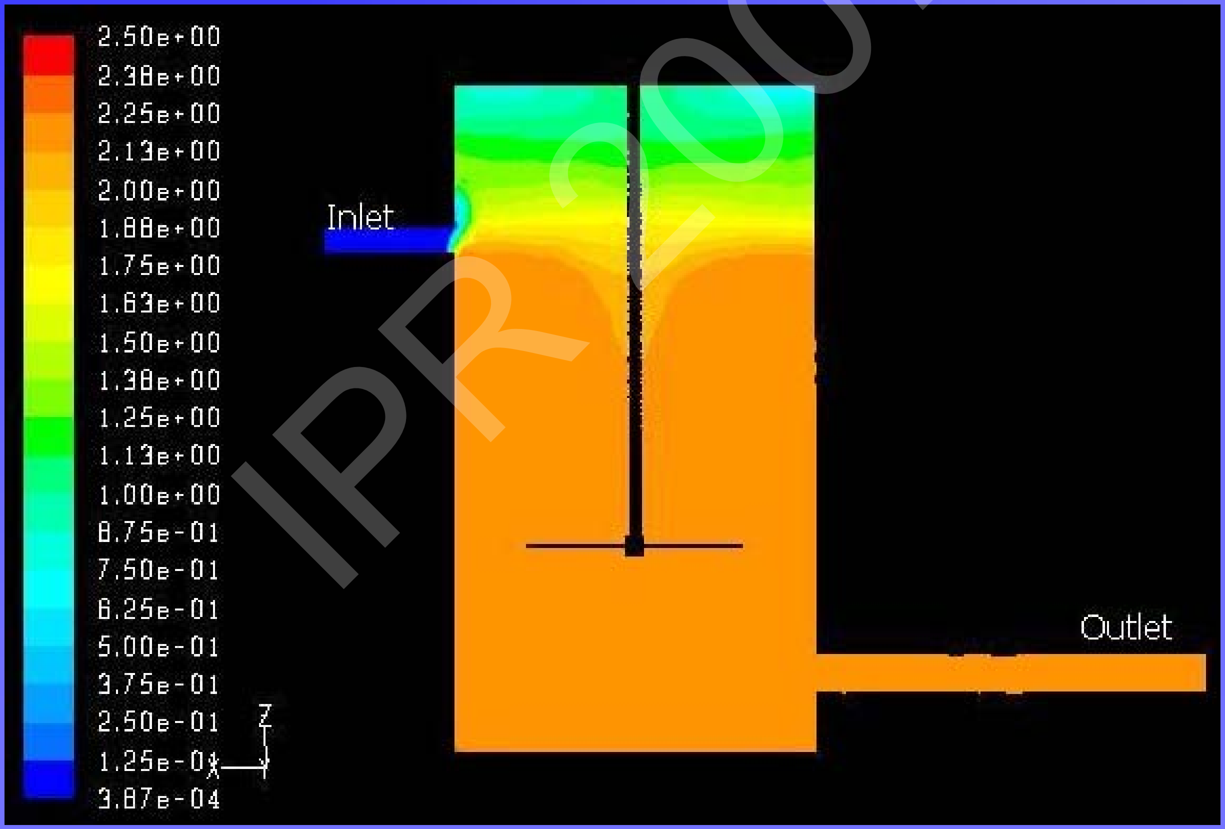


$$R_p = -k_p M[R]$$

$$[R] = \sqrt{\frac{2K_{th}[M]^3}{K_{tc}}}$$

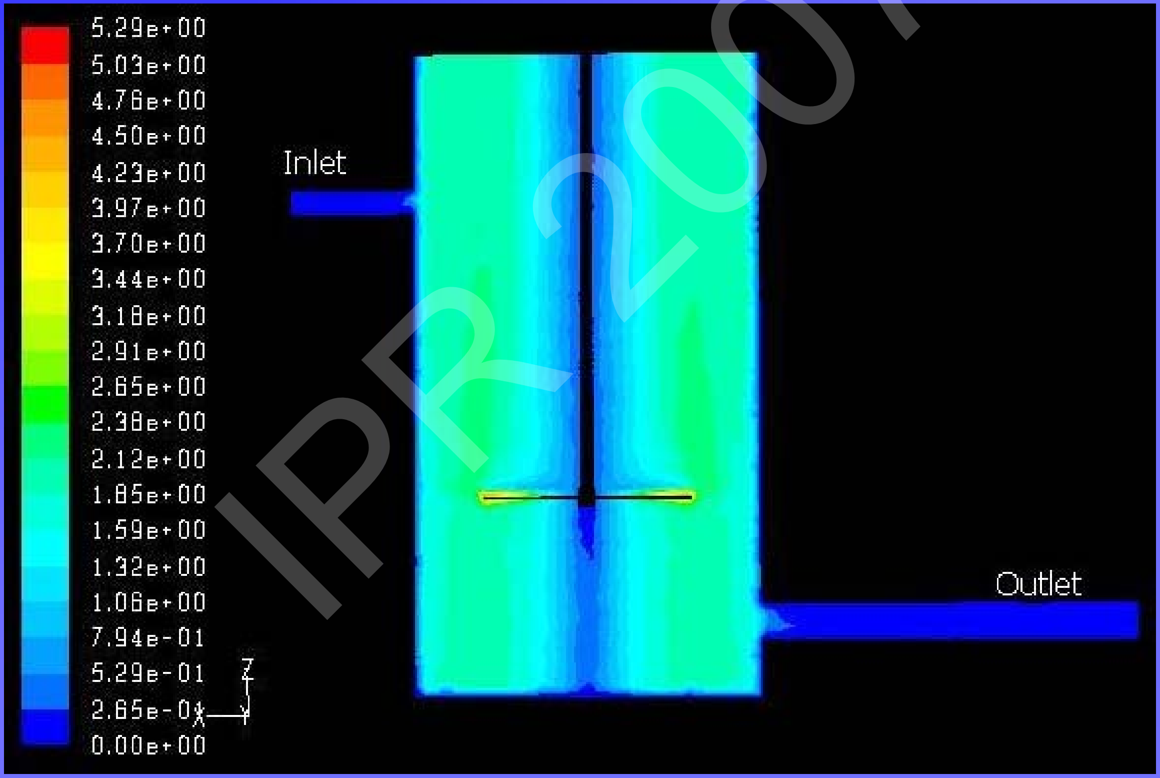
Results and Discussion

- **Reactive flow vs. Non reactive flow**
  - viscosity rises to approximately 10,000 times the viscosity of styrene



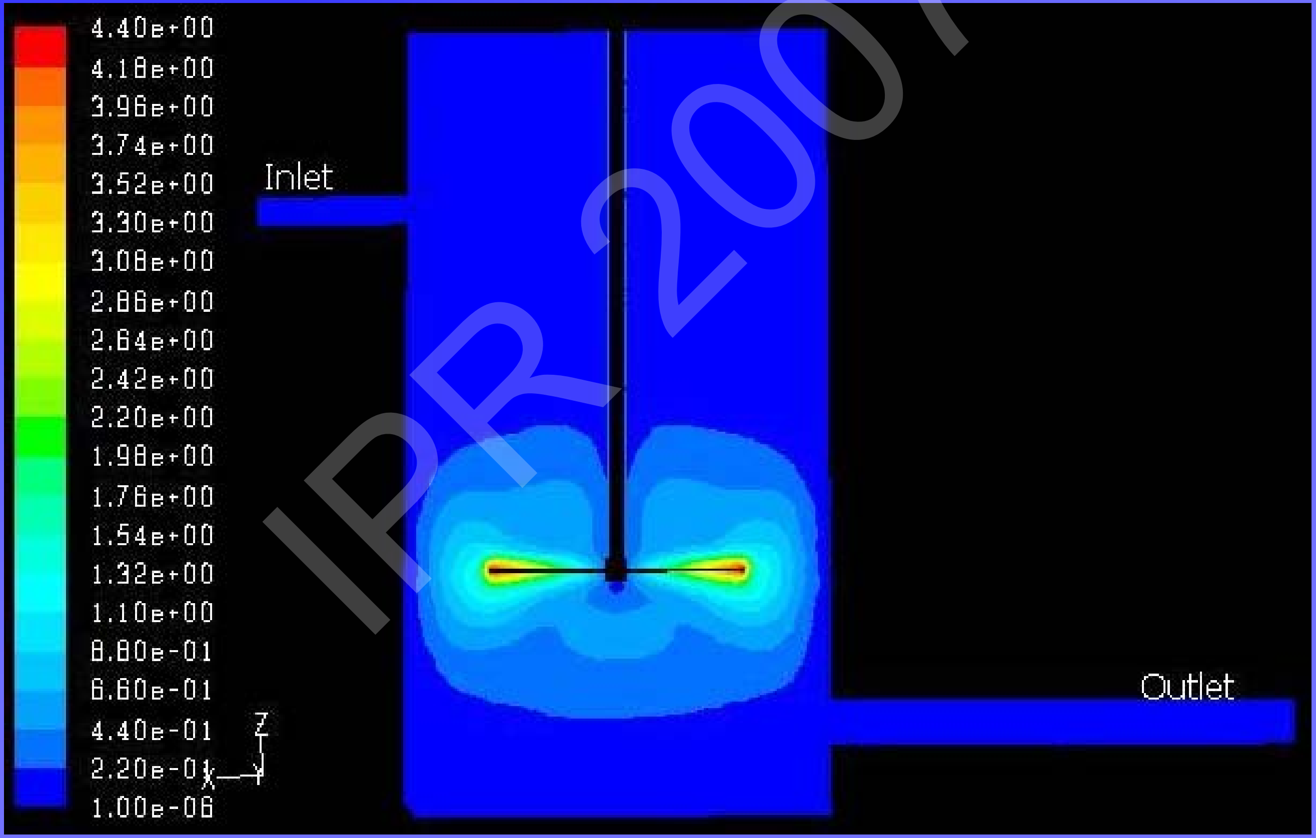
Results and Discussion

- **Reactive flow vs. Non reactive flow**
  - Velocity Magnitudes (m/s) for non-reactive mass



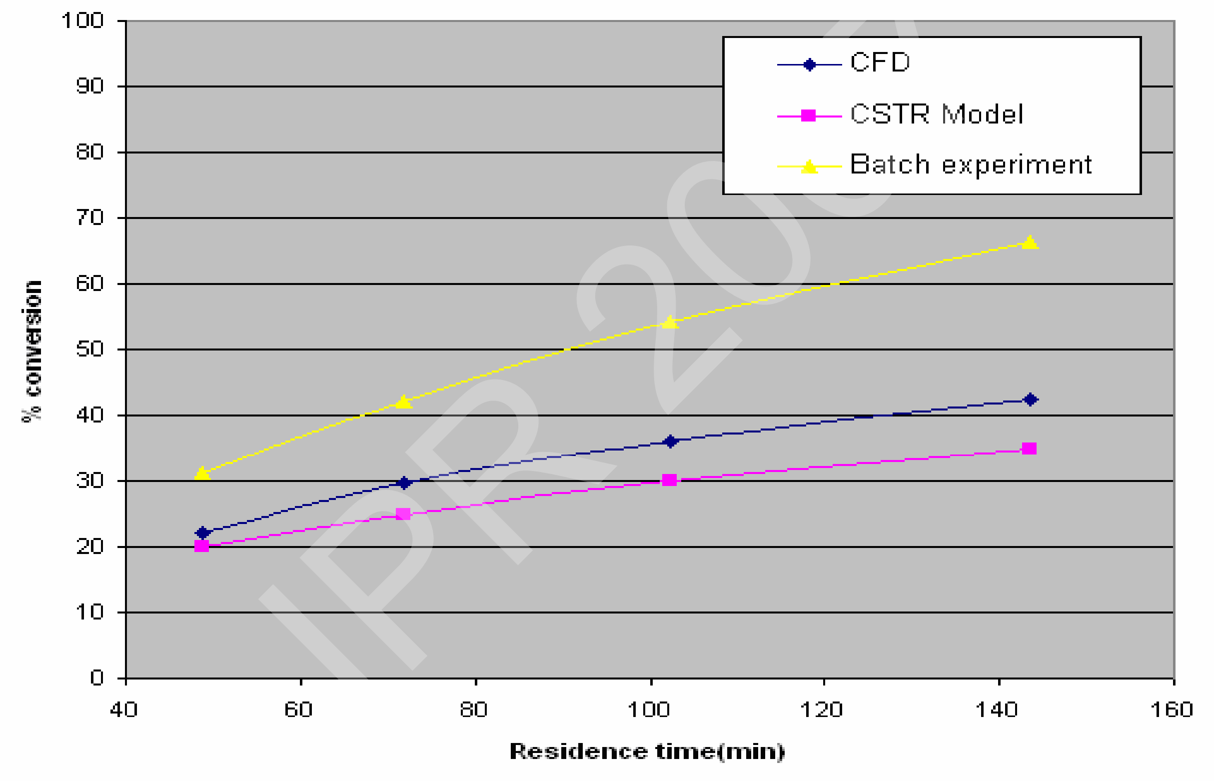
Results and Discussion

- **Reactive flow vs. Non reactive flow**
  - Velocity Magnitudes (m/s) for reactive mass



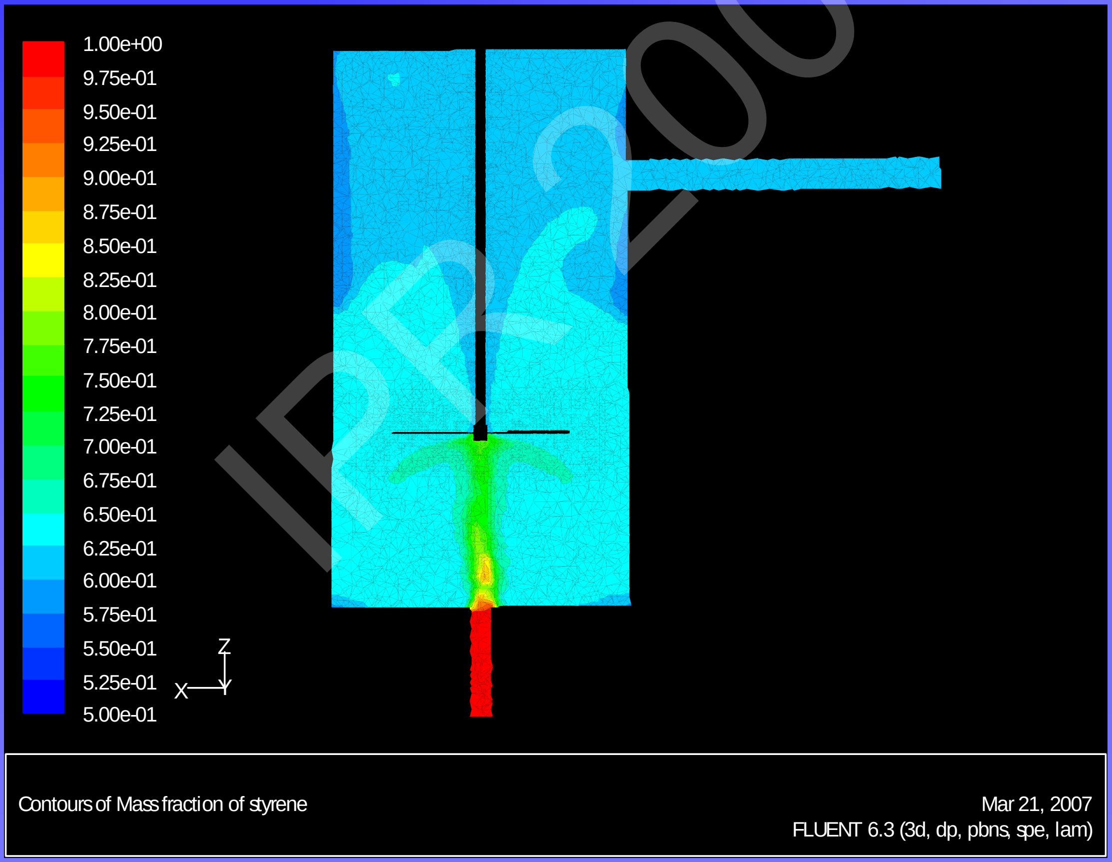
Results and Discussion

- Effect of Residence time at 500 rpm



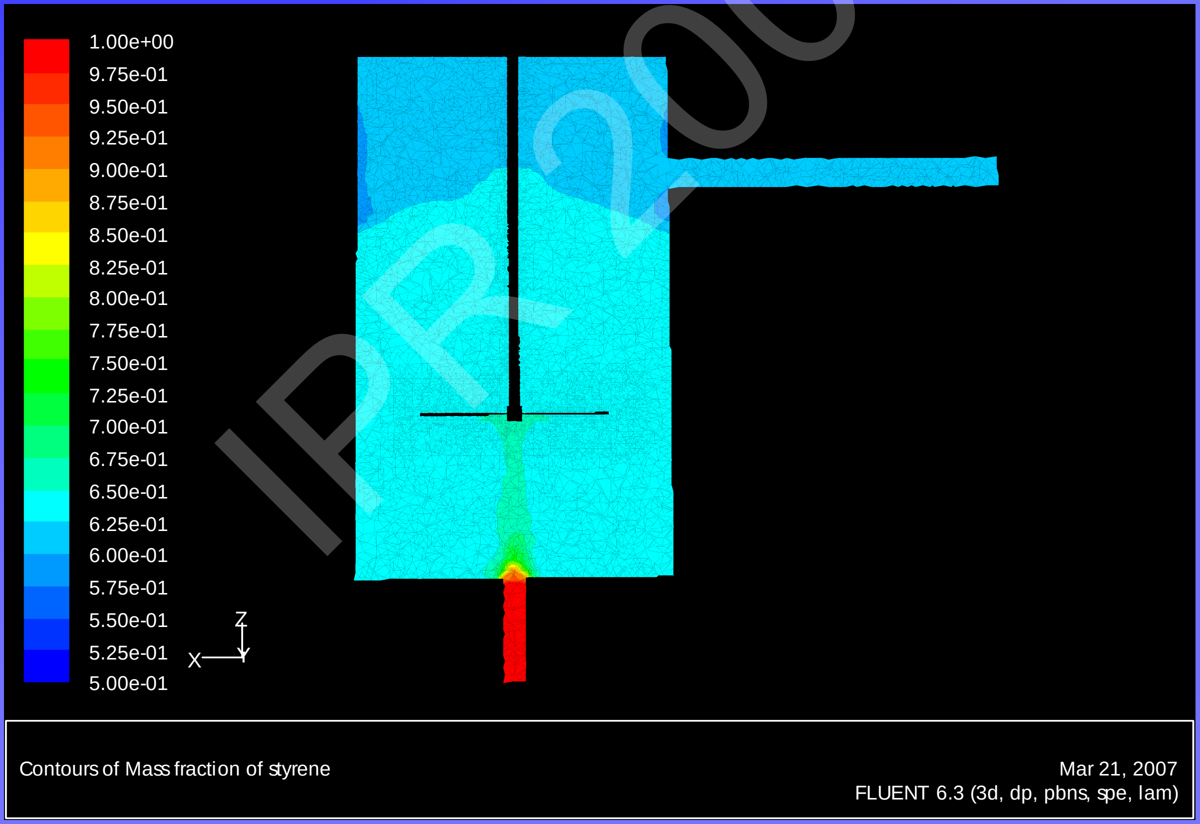
Results and Discussion

- Effect of Bottom inlet
  - Contours of Species mass fraction for100rpm and 144 min. residence time



Results and Discussion

- Effect of Bottom inlet
  - Contours of Species mass fraction for500rpm and 144min residence time

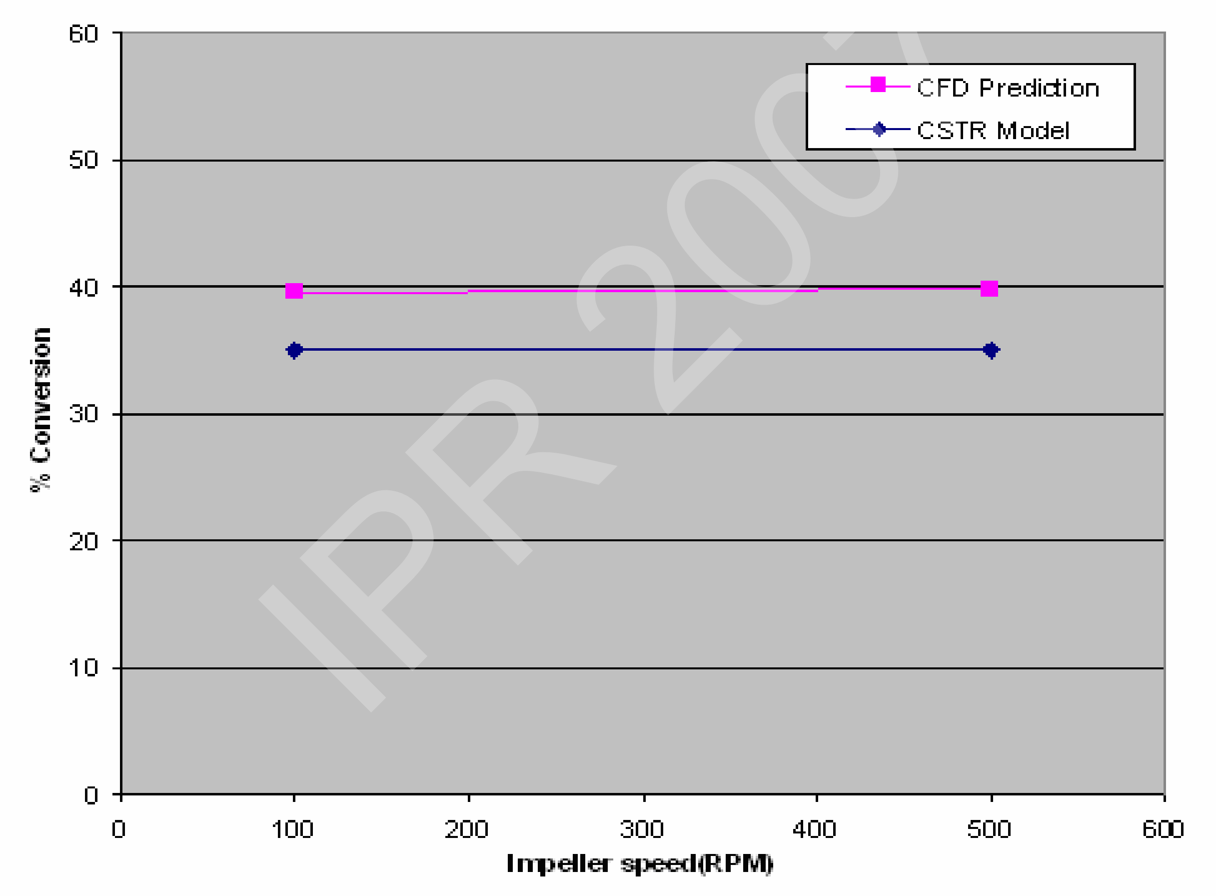


Contours of Mass fraction of styrene

Mar 21, 2007
FLUENT 6.3 (3d, dp, pbns, spe, lam)

Results and Discussion

- Conversion Analysis for bottom inlet



Conclusions

- CFD was proved to be a good tool to analyze polymerization reactor.
- Conversion predicted by CFD was better than CSTR model.
- Detailed flow visualization was made possible.

Future work

- To extend the model to analyze initiator polymerization in CSTR.

Thanks

Questions?