

CFD Analysis of Mixing in Polymerization Reactor

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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

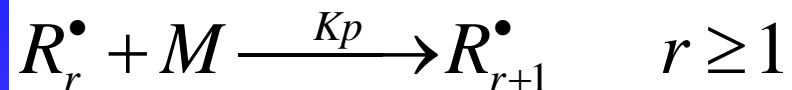
- Styrene can be polymerized in absence of Initiator.



- Steady-state hypothesis

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

Kinetic Model



- 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))

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

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

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

- Cp=1880 J/kg.k
 - K =0.126 J/m.s.k
 - Dm=2.0 x 10⁻⁹ m²/s
- } (Soliman et.al.(1994))

Reactor Geometry

Tank diameter = 14 cm

Liquid level = 26 cm

Impeller type = pitched blade

No. of blades = 4

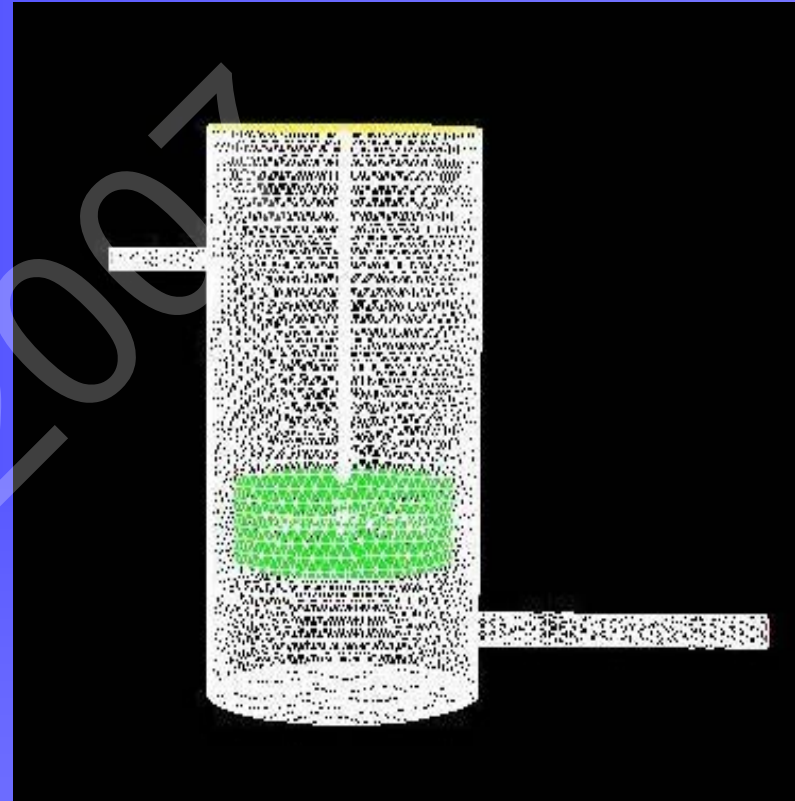
Impeller diameter = 8.4 cm

Impeller speed = 100 to 1000 rpm

Inlet diameter = 1 cm

Outlet diameter = 1.5 cm

Reactor temperature = 140°C



- Discretised domain of a reactor
- 372,000 cells

Governing equations

- Continuity Eq.

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

- Momentum

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

where

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

Governing equations

- Energy

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

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

$$h = \sum_j Y_j h_j$$

$$h_j = \int_{T_{ref}}^T c_{p_j} dT$$

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

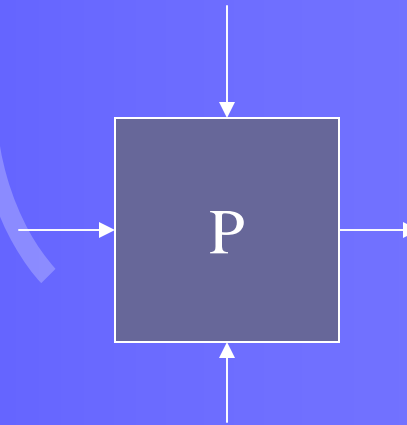
$$\frac{\partial \rho \phi}{\partial t} v + \sum_f^{N_{faces}} \rho_f \vec{v}_f \phi_f \cdot \vec{A}_f = \sum_f^{N_{faces}} \Gamma_\phi \nabla \phi_f \cdot \vec{A}_f + S_\phi V$$

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

Discretisation

- Finally all equations can be written as

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



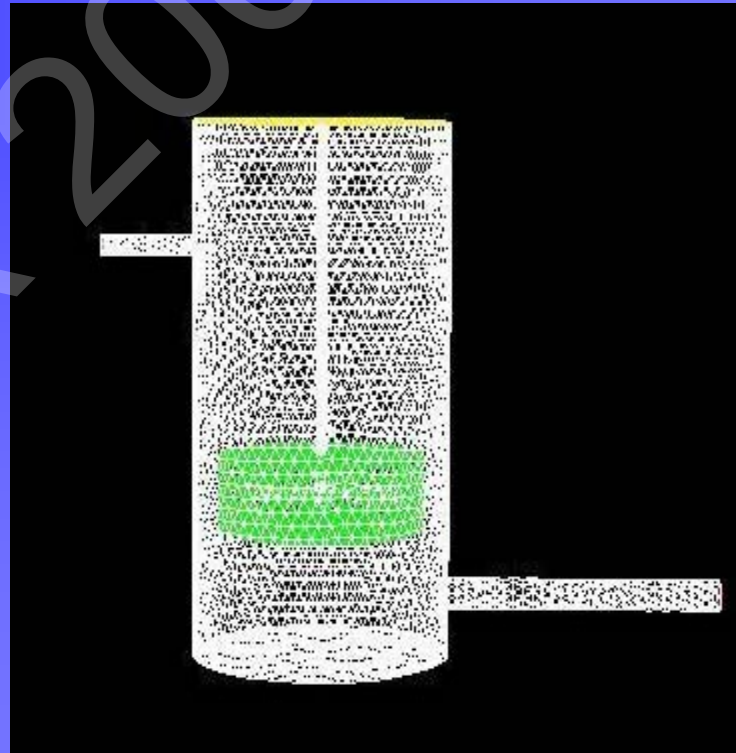
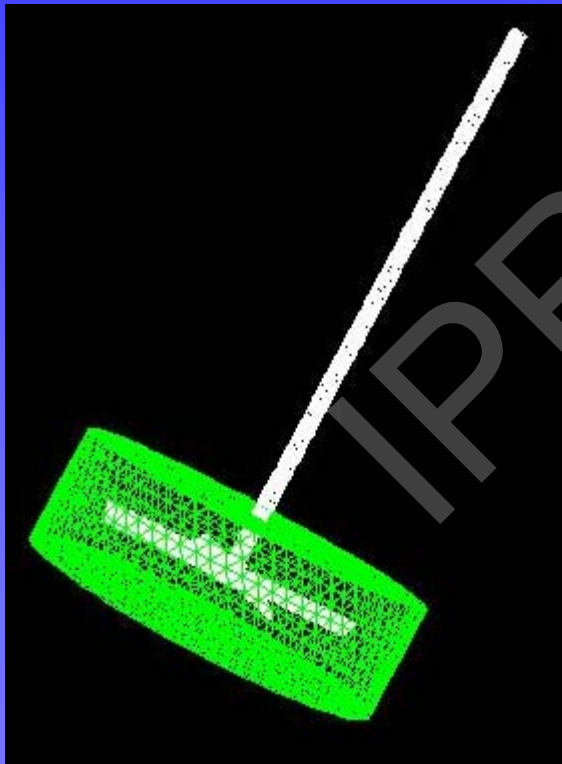
- These algebraic equations were solved using Gauss-Seidel with algebraic multigrid (AMG) method.

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

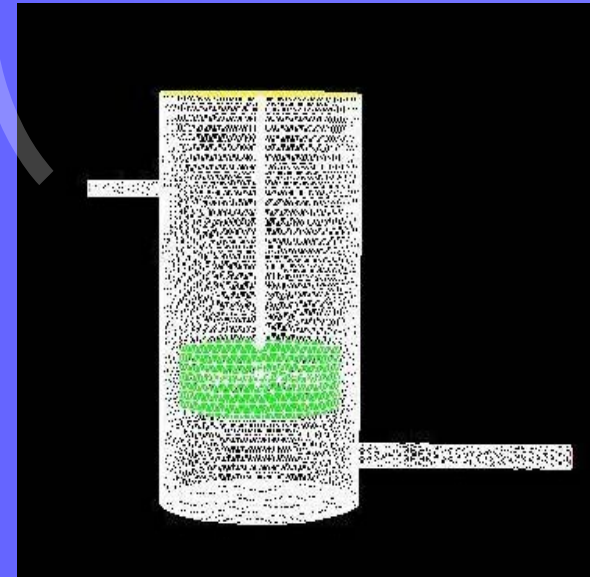
Boundary conditions

- 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° C
- Tank Wall
 - No slip boundary for momentum
 - Zero diffusive flux
 - Fixed temperature = 140° C
- Tank Outlet
 - Zero normal gradient for all the variables
- Liquid level
 - Symmetry, No normal gradient

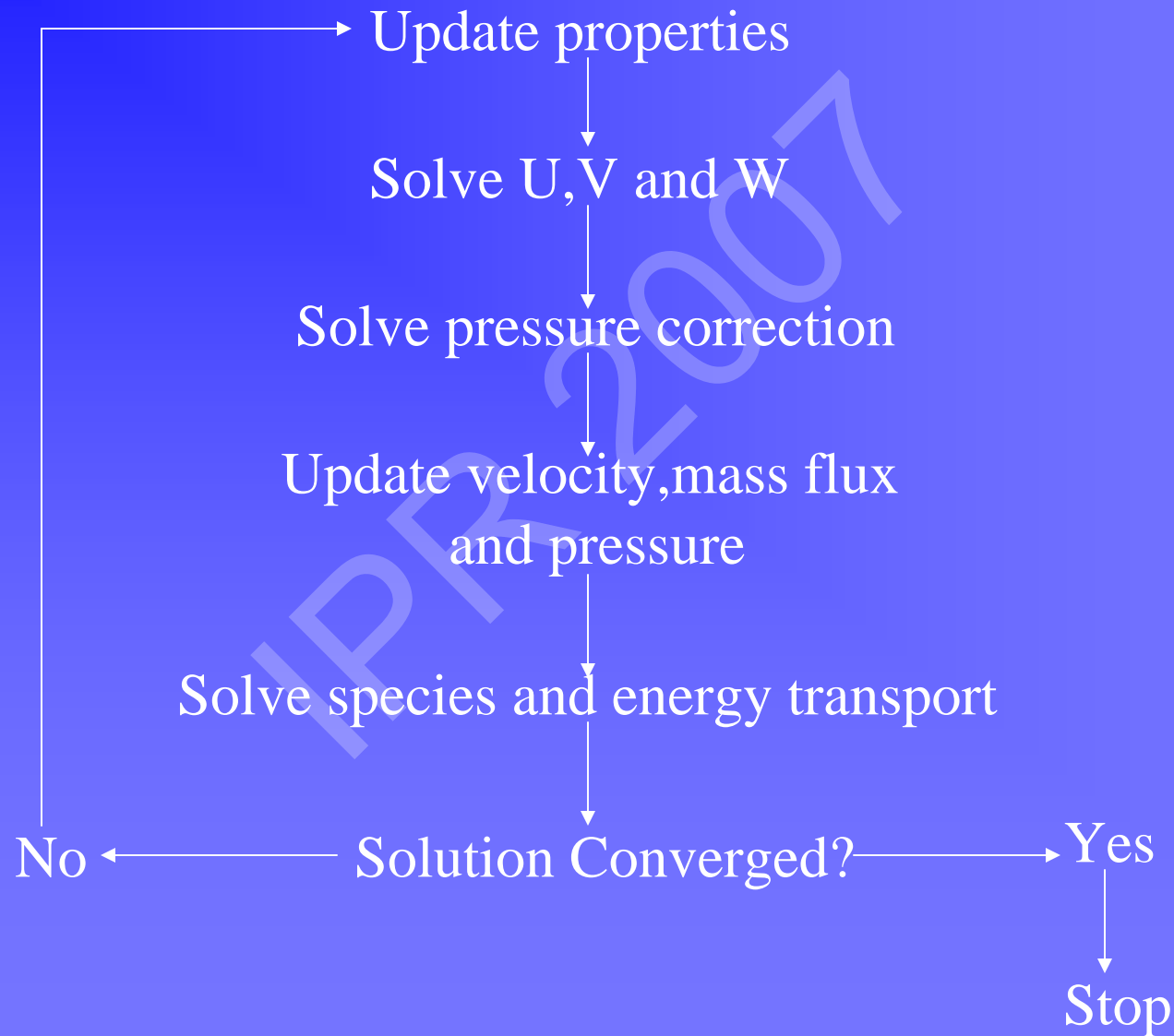


Case set up

- 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
- 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

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

Solver



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

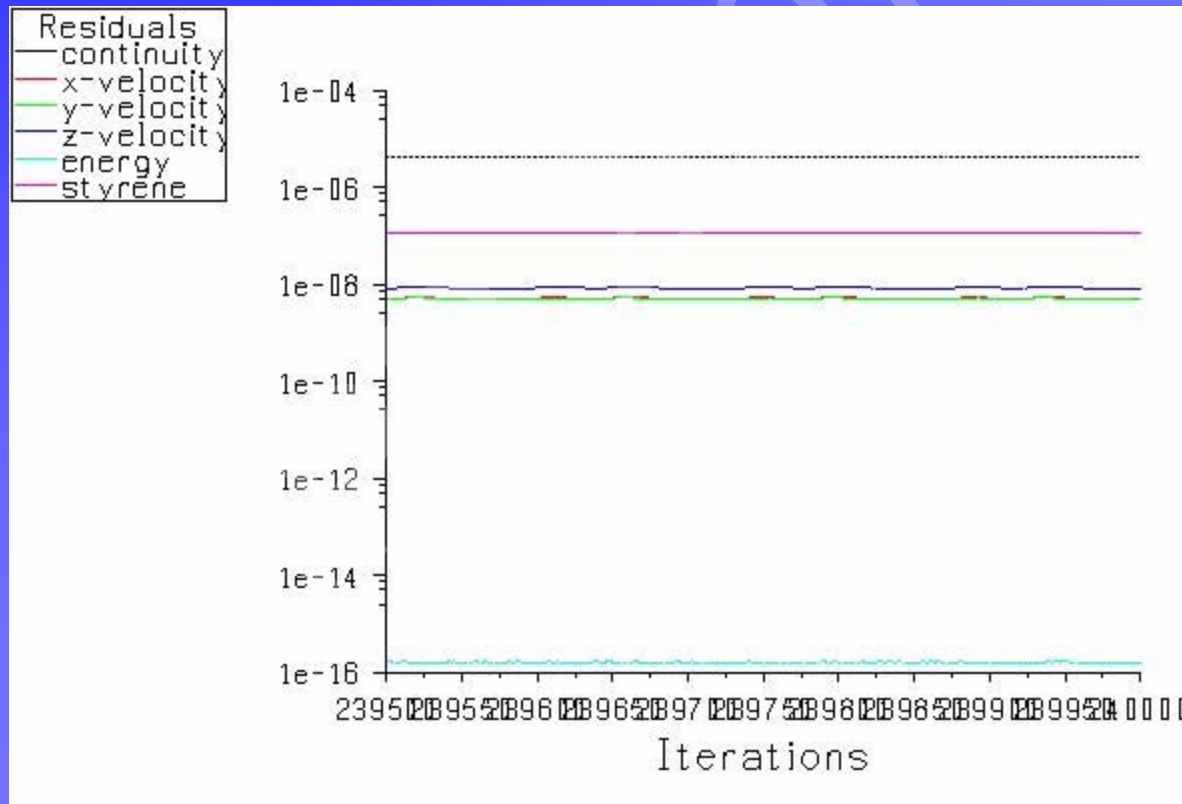
Results and Discussion

- **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

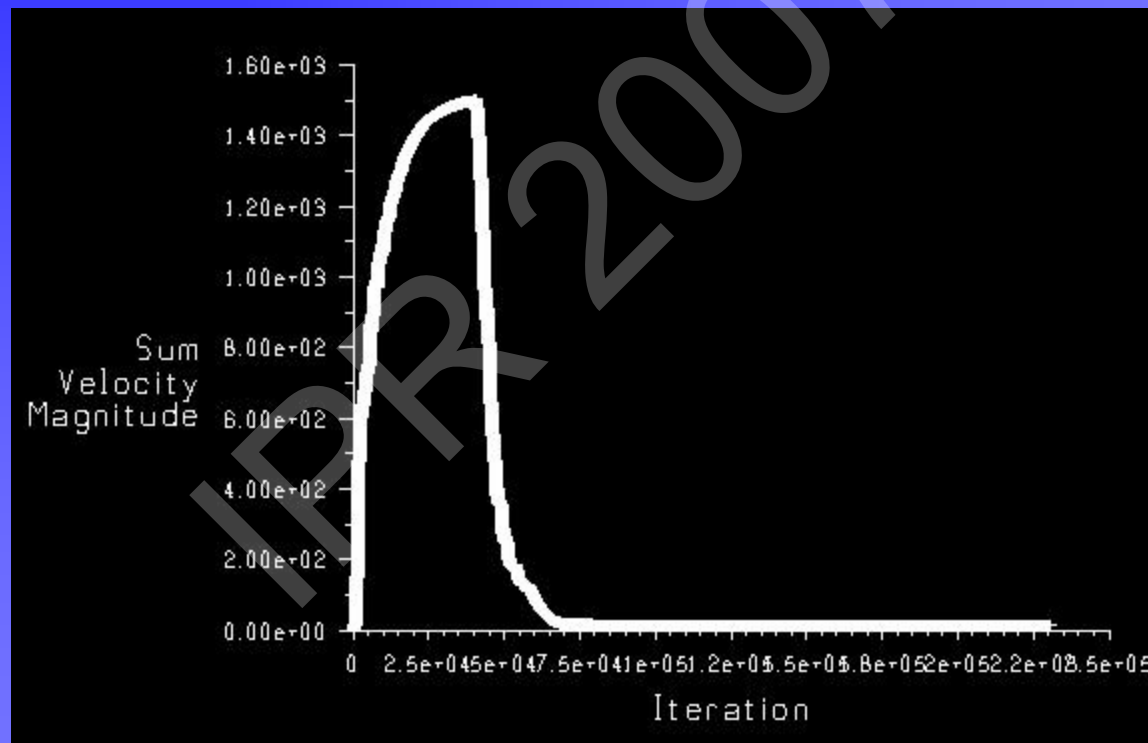
- Residual monitoring



Results and Discussion

- Convergence Monitor

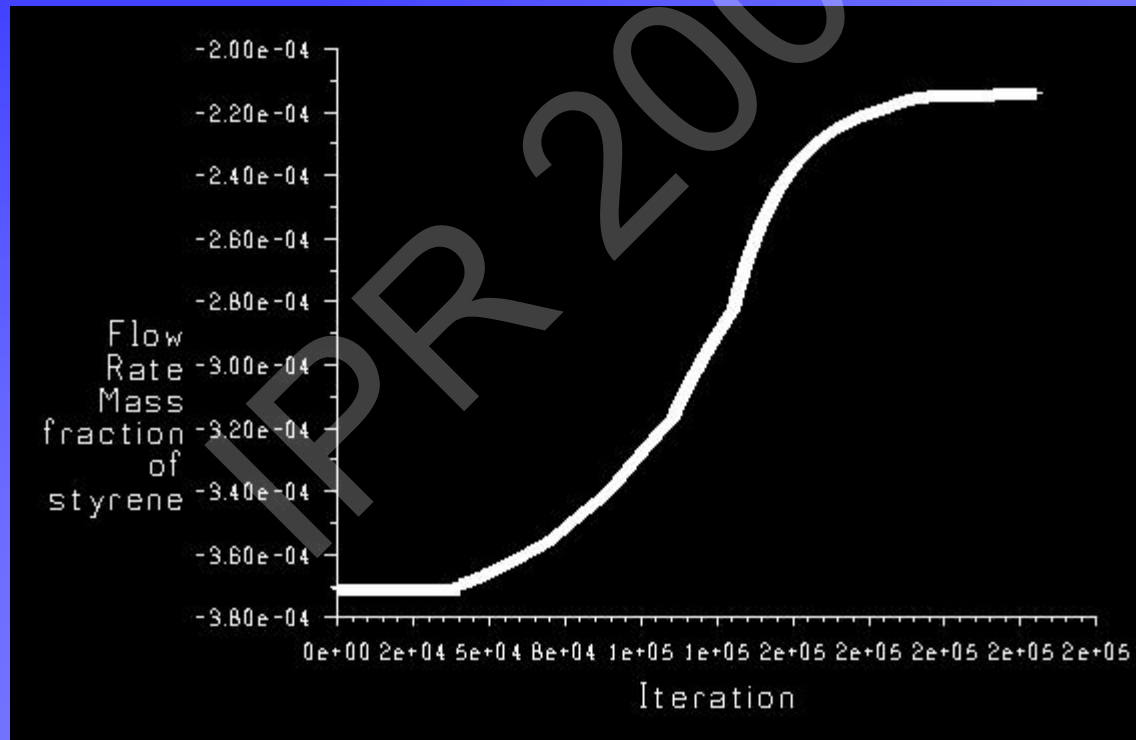
- Sum of Velocity magnitude on symmetry



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

