RYERSON UNIVERSITY

Use of CFD for Exploring the Effect of Mixing on MMA Solution Polymerization in a CSTR

Sh. Fathi Roudsari, F. Ein Mozaffari, R. Dhib

Department of Chemical Engineering, Ryerson University
Toronto, Canada

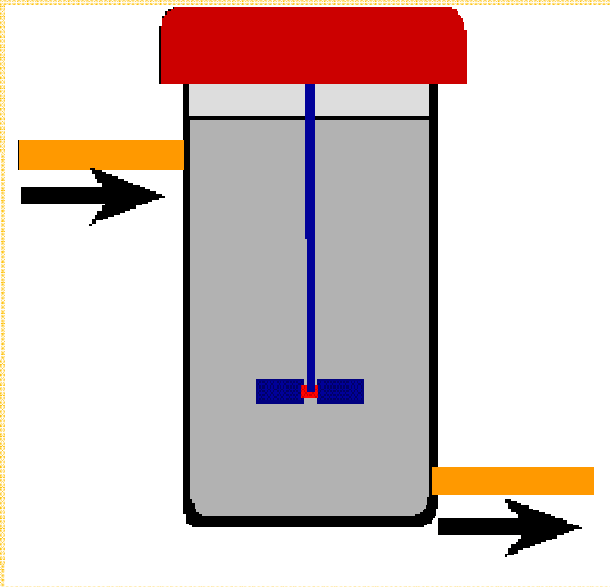
May 2011

Outline

- Introduction
- Objectives
- Reactor Specifications
- CFD Model
- Results and Discussion
- Concluding Remarks

Considerations:

- ❑ Good Mixing ?
- ❑ No Effect of Mixing in Conventional Kinetic models (rarely)
- ❑ Conversion/Mw Dependent on Mixing?
- ❑ Influence of Dead Zones



Computer Simulation Tool involves:

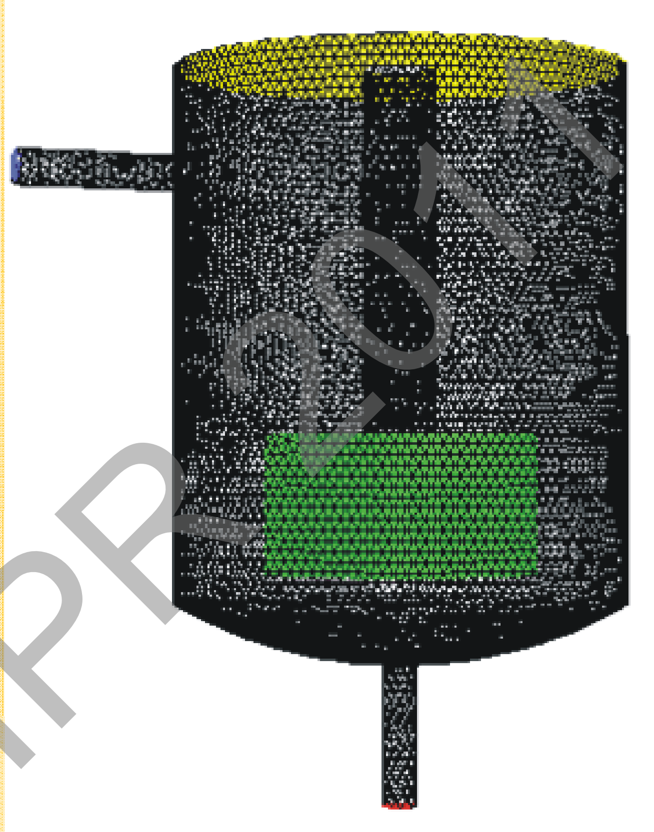
- ❑ Transport phenomena (Reaction)
- ❑ Flow pattern
- ❑ Trial and error analysis (Time/Cost)
- ❑ CFD modeling → Improve reactor performance, Safety issues

- **Patel et al. (2010) investigated the CFD modeling of styrene bulk polymerization in a CSTR.**
- **Shi and Luo (2010) studied the effects of velocity and solid particle size on the CFD modeling of Propylene Polymerization in a tubular loop.**
- **Cherbanski et al. (2007) used CFD to study the effect of process parameters on temperature behaviour in suspension polymerization .**
- **Serra et al. (2007) investigated the styrene free radical polymerization in a T-junction micro reactor and calculated conversion.**
- **Heath and Koh (2003) applied CFD modeling to calculate aggregation and breakage of solid polymer particles in a tubular pipe.**
- **Maschio & Moutier (1989) studied the effect of solvent fraction on polymer chain mobility in batch and CSTR reactors**

- **Study the effects of solvent content, impeller speed and residence time, on MMA conversion in a CSTR using CFD**

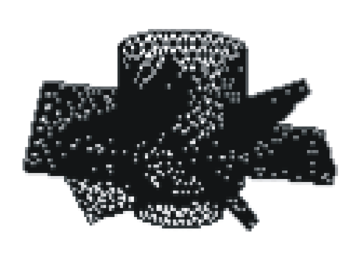
Geometry Grid

Inlet



Outlet

- ❑Gambit 2.4
- ❑Tetrahedral,
- ❑Triangular Faces
- ❑~280,000 cells
- ❑MRF
- ❑1 Litre Reactor
- ❑Six 45° pitched bladed Impeller



Parameter	Value	Parameter	Value
Tank diameter	4 inches	Impeller diameter	2 inches
Liquid level	5.3 inches	Blade width	0.55 inches
Outlet diameter	0.25 inches	Blade thickness	0.8 inches
Inlet diameter	0.25inches	Inlet wall length	1.5 inches
Impeller type	45° six pitched blade	Outlet wall length	1.5 inches

Fluid	Density (kg/m^3)	Viscosity (Pa. s)	Molecular Weight (g/mole)
Methyl Methacrylate (MMA)	895	0.00037	100.12
Azobisisobutyronitrile (AIBN)	1100	0.000278	164
Toluene (Solvent)	866	0.000586	92.07

- ❑ **Transport Equations**
- ❑ **Polymerization Source Equations**
- ❑ **Physical Properties**

Transport equations

$$\frac{\partial \rho}{\partial t} + (\nabla \bullet \rho \vec{\upsilon}) = 0$$

$$\frac{\partial}{\partial t}(\rho \vec{\upsilon}) + \nabla \bullet (\rho \vec{\upsilon} \vec{\upsilon}) = -\nabla P + \left(\nabla \bullet \vec{\vec{\tau}}\right) + \rho g + \vec{F}$$

$$\vec{\vec{\tau}} = \mu \left[\left((\nabla \vec{\upsilon}) + (\nabla \vec{\upsilon})^T \right) - \frac{2}{3} \nabla \bullet \vec{\upsilon} \right]$$

$$\frac{\partial}{\partial t}(\rho W_j) + \nabla \bullet (\rho \vec{\upsilon} W_j) = -\nabla \bullet J_j + R_j + S_j$$

$$\vec{J}_j = -\rho D \nabla W_j$$

Polymerization Source

Assumptions:

- ❑ Steady-state condition
- ❑ Termination: Combination reaction only
- ❑ No gel effect

Polymerization Source

$$[R\cdot] = \sqrt{\frac{2\ f\ K_d\,[I]}{K_{tc}}} \qquad R_p = -K_p\,[M]\sqrt{\frac{2\,f\,K_d\,[I]}{K_{tc}}}$$

$$S_{monomer} = R_P \times M_{w,monomer}$$

$$S_{initiator} = R_P \times M_{w,initiator}$$

$$K = A\ \exp\left(-E / R_g T\right)$$

Parameter	Values [1]	Parameter	Values [1]
A_d	1.33 10^{15}m^3/s	E_d	30700 cal/mol
A_p	4.41 10^{5} m^3/kmol s	E_p	4350 cal/mol
A_{tc}	6.5 10^{7} m3/kmol s	E_{tc}	700 cal/mol
f	0.4		

[1] Maschio and Moutier, 1989

Physical Properties

$$\log_{10}\mu = J_1 + \frac{J_2}{T} + J_3 T + J_4 T^2$$

$J_1 = -7.7825$

$J_2 = 7.3478 \times 10^{2}$

$J_3 = 1.0258 \times 10^{-2}$

$J_4 = -1.1343 \times 10^{-5}$

Viscosity Correlation with Temperature [1]

$$\log_{10}(\mu) = K' + a\log_{10} X_m + \log_{10} M_w$$

K'= -3.64×10[1]
a=12.8
b=3.4

Viscosity Correlation with Conversion & Molecular Weight [2]

$\rho_m = 966.5 - 1.1(T - 273.15)$

$\rho_p = 1200\ Kg/m^3$

Density Correlation with Temperature [3]

[1] Yaws, 1999
[2] Sangwai et al., 2006
[3] Baillagou & Soong, 1985

Solving Procedure

- ❑ Space: 3D
- ❑ Time: Steady state
- ❑ BC on inlet→ Velocity, Mass Fractions (M, S, I), T= 65° C
- ❑UDF→ Reaction Source
- ❑ HPCVL system→ parallel with 24 CPUs

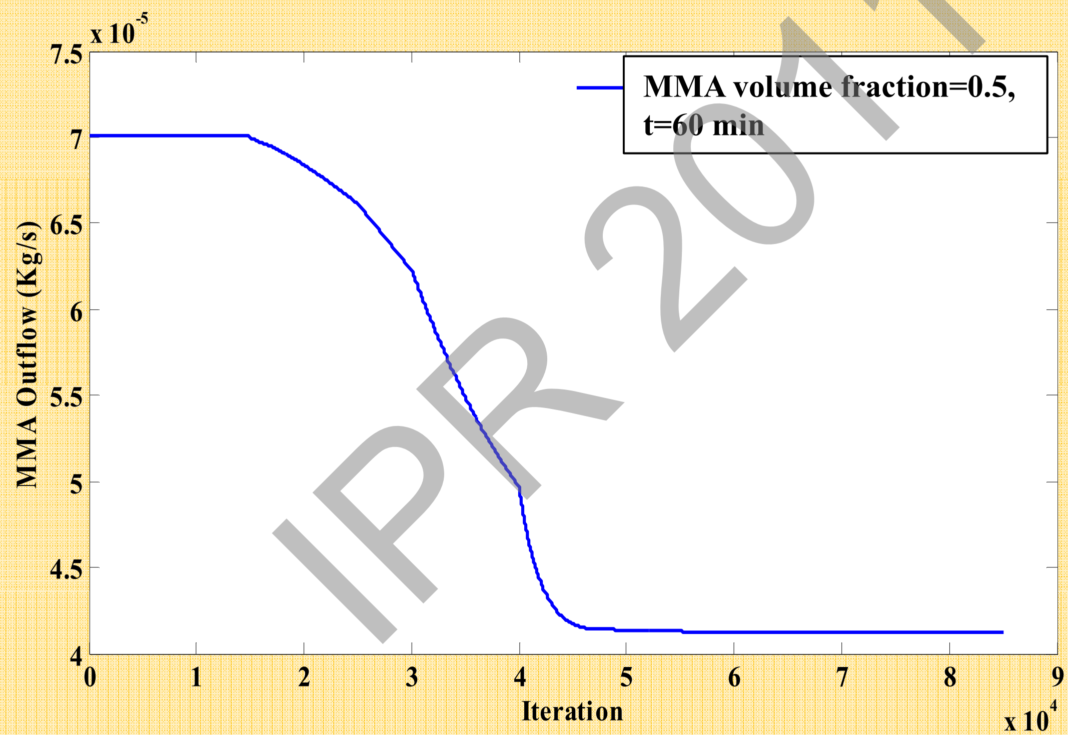
Effects of

- **Solvent Volume Fraction**
- **Residence Time**
- **Impeller Speed**

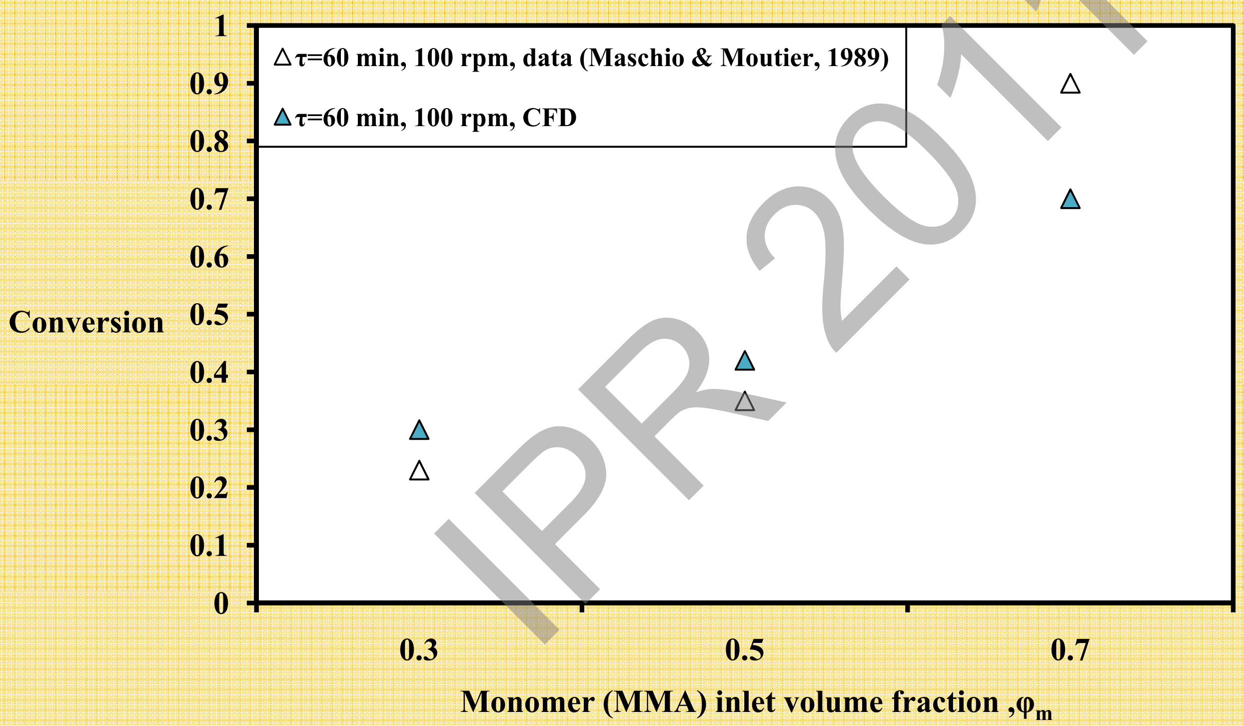
On

- **Conversion of MMA Polymerization**
- **Contour of Monomer Mass Fraction**
- **Medium Viscosity**

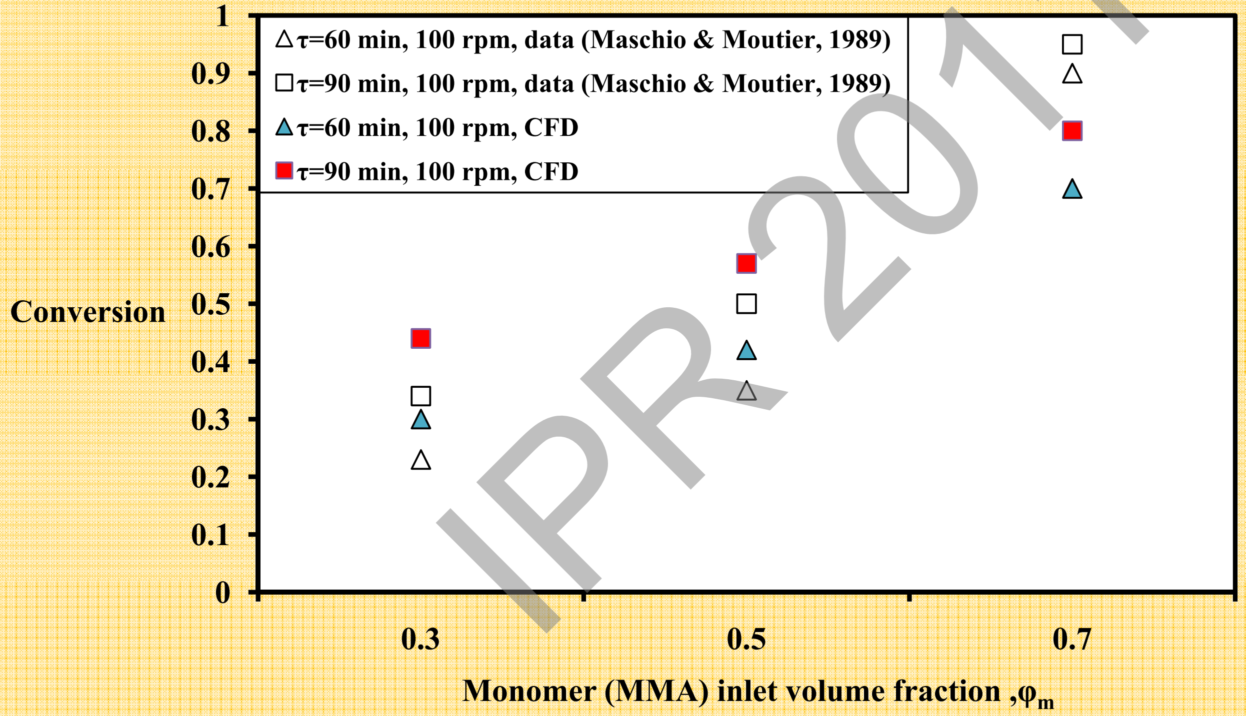
Convergence Monitoring



Effect of Solvent Fraction at 100 rpm

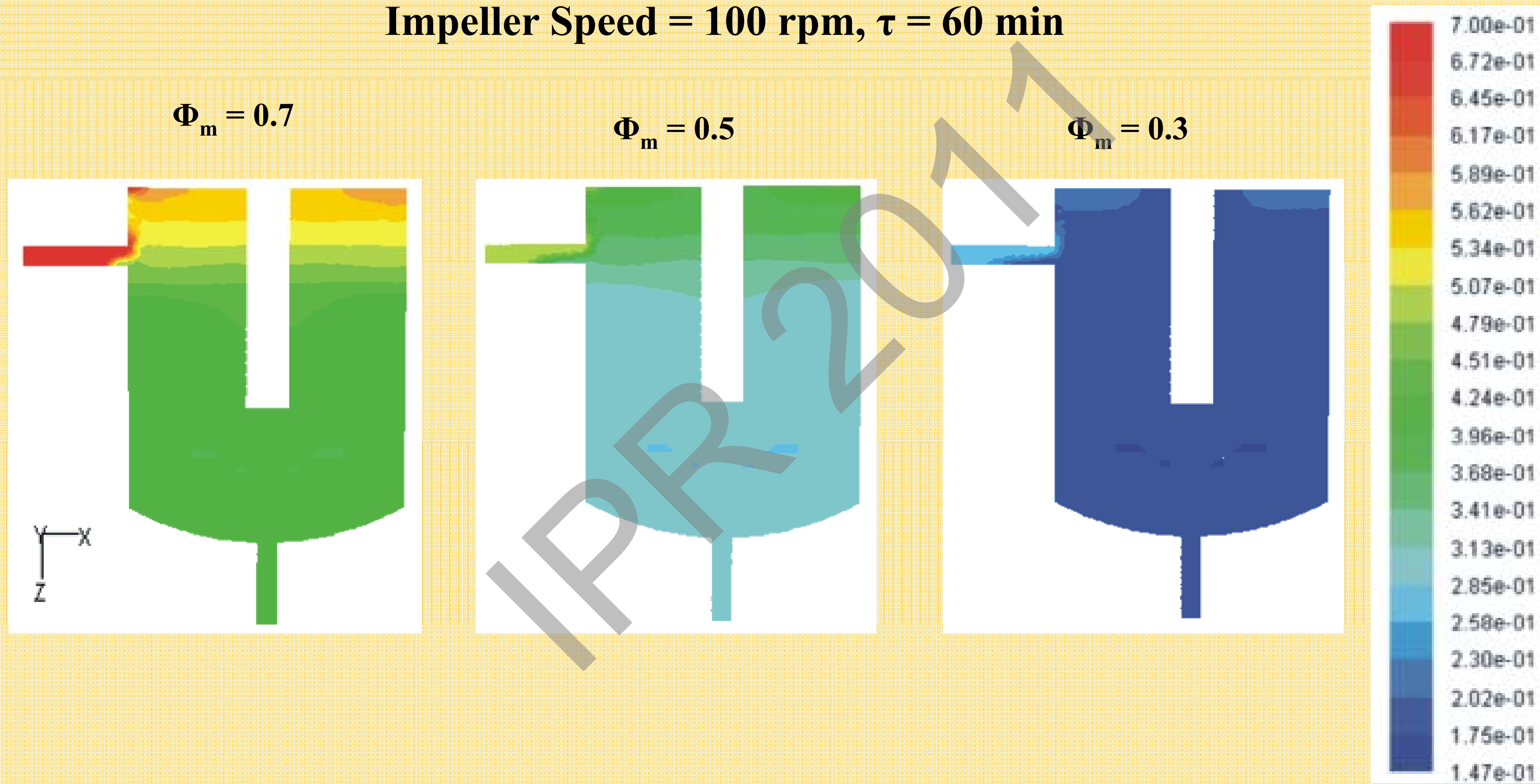


Effect of Solvent Fraction at 100 rpm



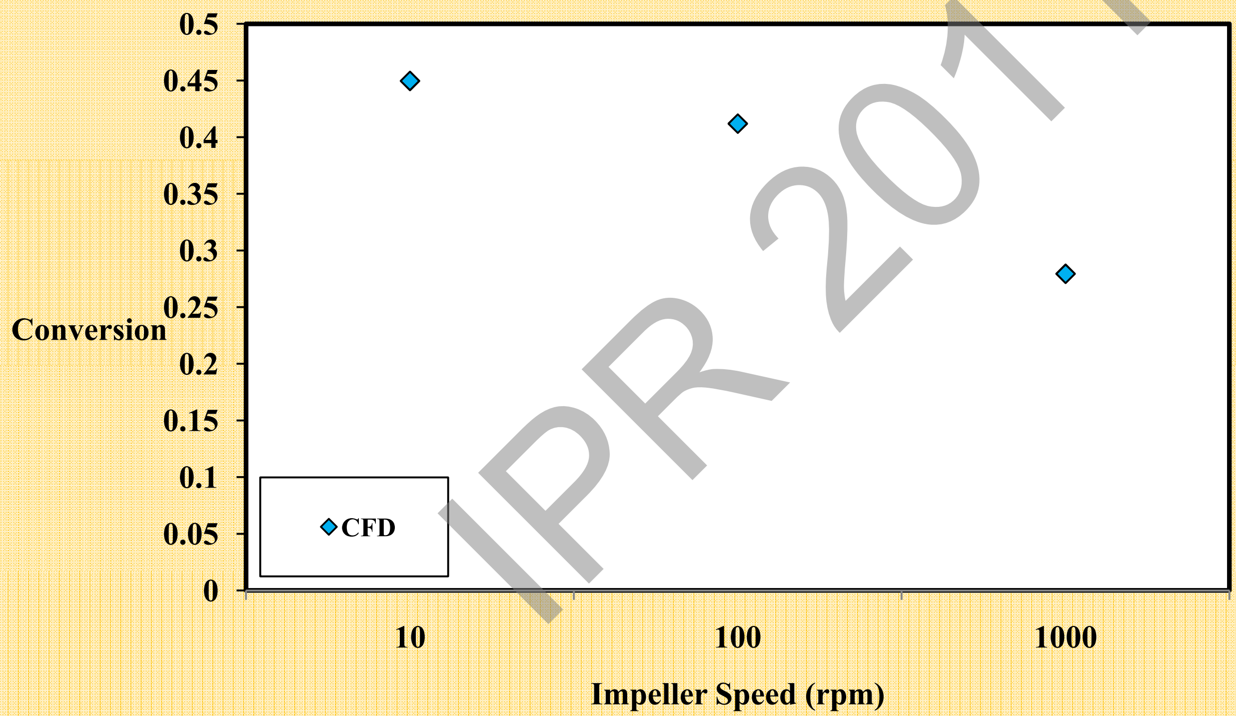
Monomer Mass Fraction Contour

Impeller Speed = 100 rpm, τ = 60 min



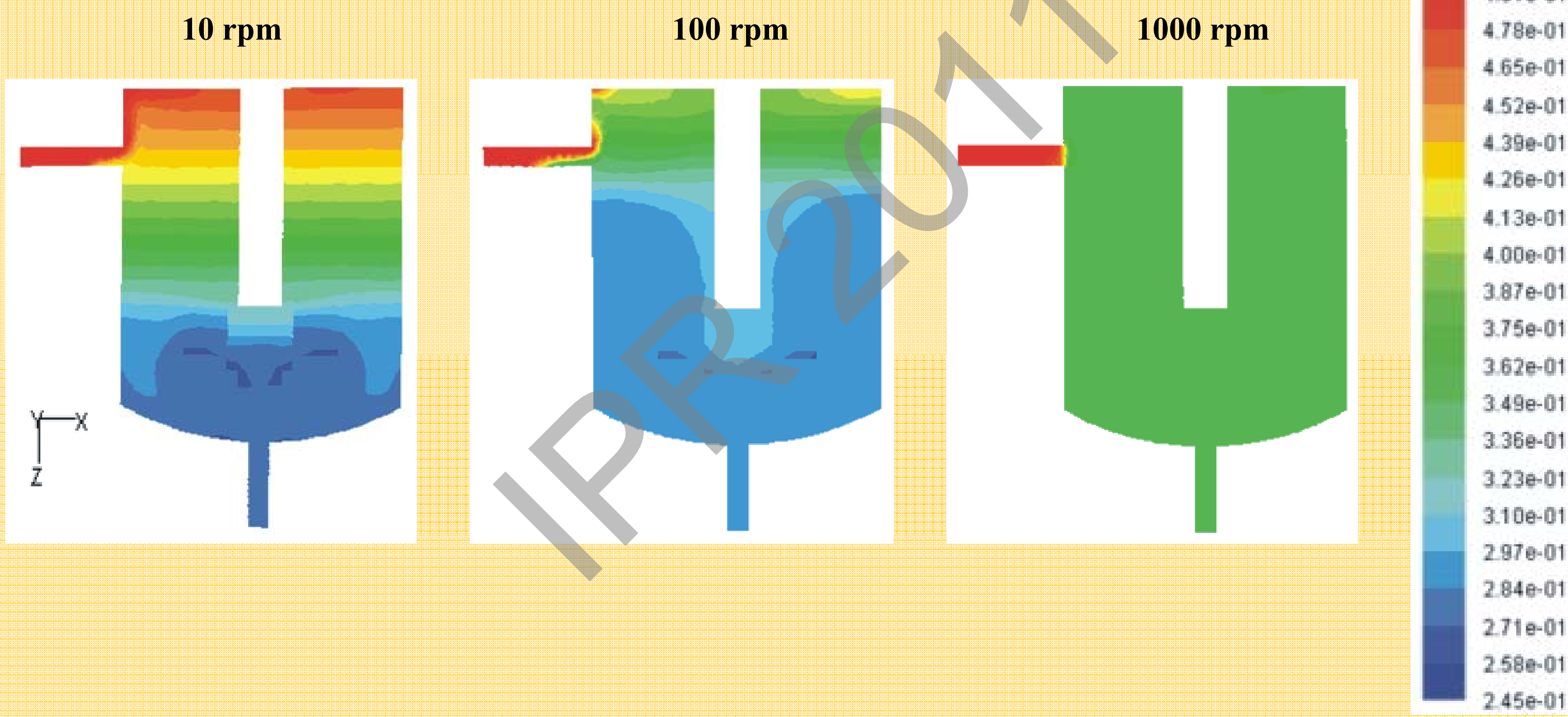
Effect of Impeller Speed

$\Phi_m = 0.5$, $\tau = 60$ min



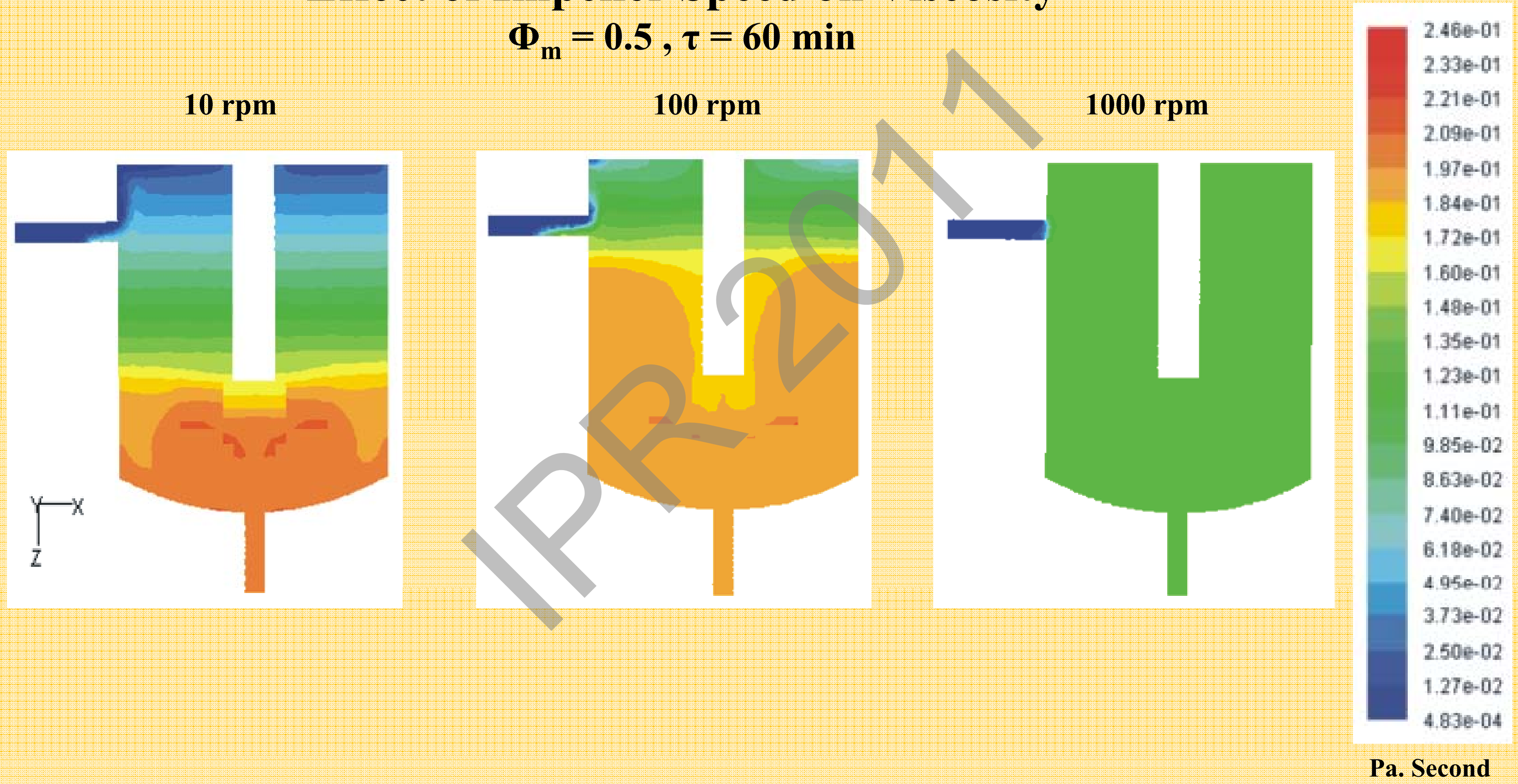
Effect of Impeller Speed on homogeneity

$\Phi_m = 0.5$, $\tau = 60$ min



Effect of Impeller Speed on Viscosity

$\Phi_m = 0.5$, $\tau = 60$ min



- **CFD gave good prediction for conversion at different solvent fractions and different residence times**
- **CFD showed decrease in conversion with increase in impeller speed at fixed solvent fraction and residence time**
- **Homogeneity of medium was improved at higher impeller speeds**

Acknowledgements:

- ❑ NSERC and Ryerson University for financial support
- ❑ Supervisors: Dr. Ein-Mozaffari and Dr. Dhib

Thanks for your attention