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Development of a generalized criterion for selecting optimal MRF rotation zone for CFD simulation of stirred tank reactors

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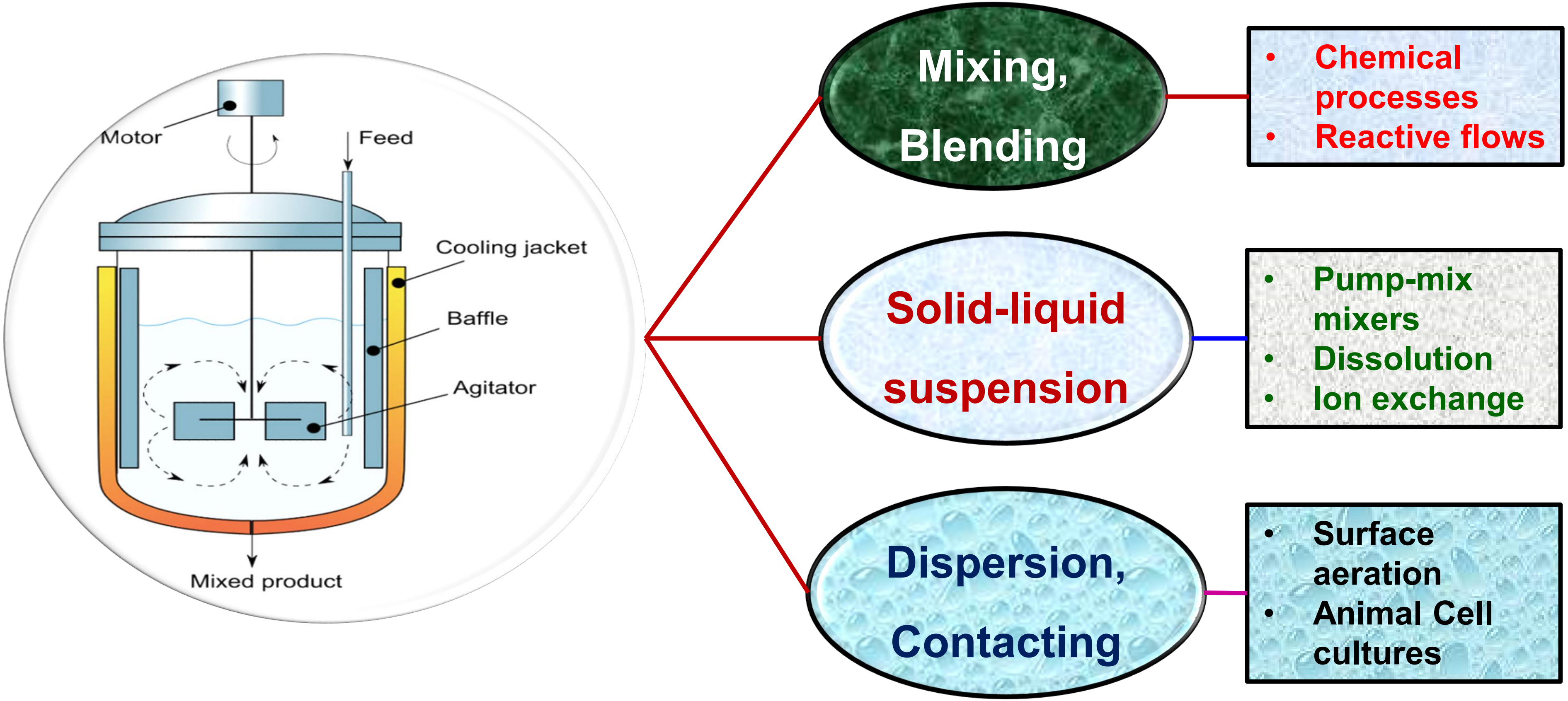
OUTLINE OF PRESENTATION

- Introduction
- MRF approach
- MRF boundary
- Stirred tank configuration
- Computational Methodology
- Governing equations
- Computational grid
- Convergence of CFD simulation
- Grid independence study
- Position of MRF boundary
- Conclusions
- Acknowledgements
- References

INTRODUCTION



Mixing, Blending

- Chemical processes
- Reactive flows

Solid-liquid suspension

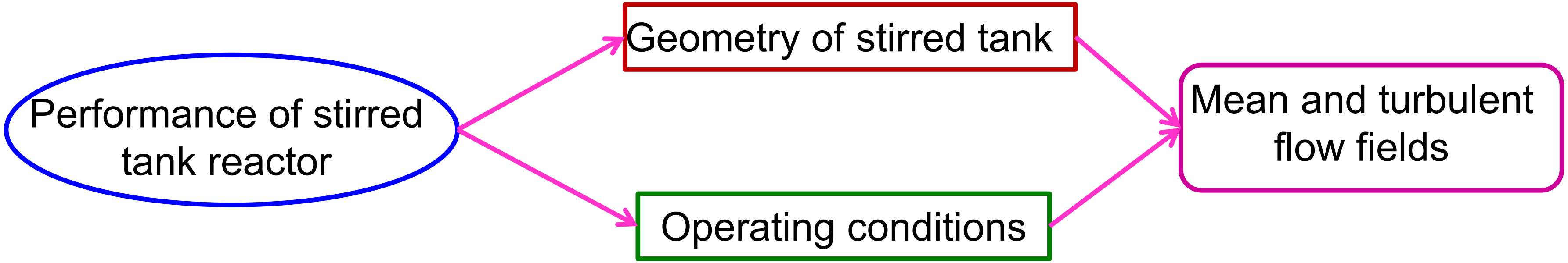
- Pump-mix mixers
- Dissolution
- Ion exchange

Dispersion, Contacting

- Surface aeration
- Animal Cell cultures

Fig. 1: Stirred tank reactor and its applications (Source: https//www.comsol.com)

INTRODUCTION Contd.


Performance of stirred tank reactor

Geometry of stirred tank

Operating conditions

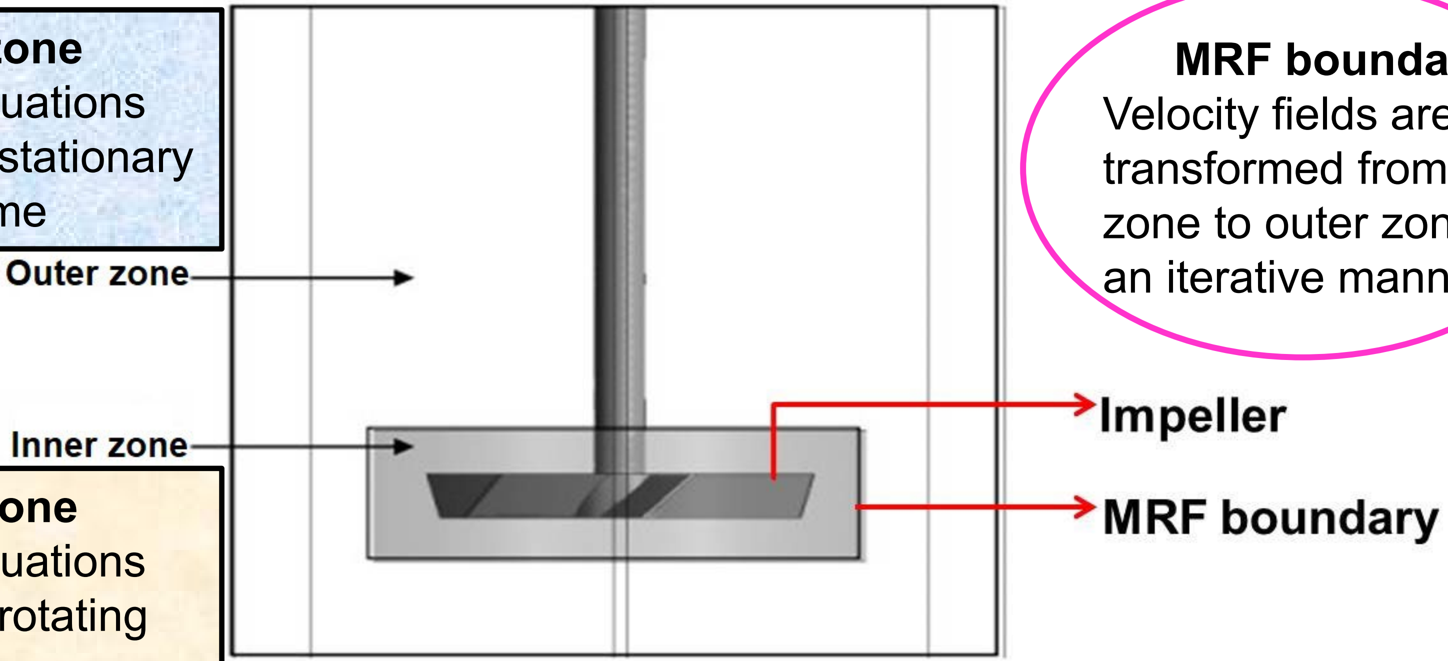
Mean and turbulent flow fields

- Proper design requires detailed knowledge of stirred tank hydrodynamics
- Computational Fluid Dynamics (CFD) → Popular tool for predicting tank hydrodynamics
- Modelling of impeller rotation is a major challenge
- Multiple Reference Frame (MRF) approach → Popular model for impeller rotation

MRF APPROACH

Outer zone
Governing equations are solved in stationary reference frame

MRF boundary
Velocity fields are transformed from inner zone to outer zone in an iterative manner



Inner zone
Governing equations are solved in rotating reference frame

Fig. 2: Rotating and stationary zones associated with the stirred tank reactor (Source: Joshi et al. (2011))

- ✓ Improper position of MRF boundary increases round-off errors and decreases accuracy and numerical convergence of simulations

MRF BOUNDARY

Position of MRF boundary

- Engineering assumptions
  - Extent of vortex activity (Coroneo et al. (2011))
  - Minimum spatial and temporal flow field variations (Luo et al. (1994))
- Skill of modeller
  - By experience
- Optimization problem
  - Varying radial extent (D_r) and axial extent (H_r) in a trial and error manner

Challenges in determining position of MRF boundary

- Dependency on tank geometry
- Large number of CFD simulations
- Analysis on limited tank configurations

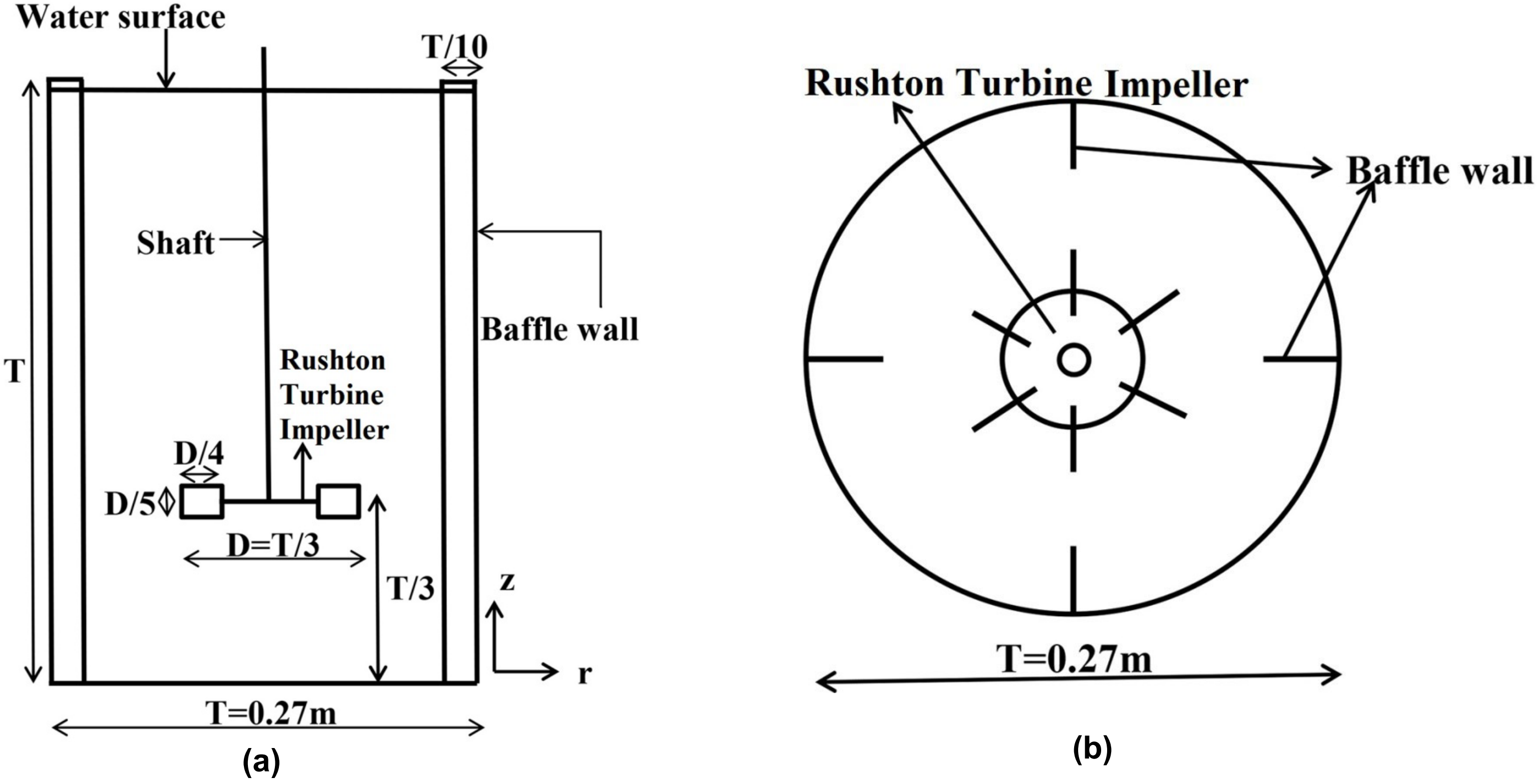
Generalized criterion?

MRF BOUNDARY Contd.

Authors	Optimal MRF boundary	Remarks
Oshinowo et al. (2000)	D_r : $2.05D$ H_r: $\pm 0.5D$	Optimal axial extent was determined while radial extent was kept constant
Zadravec et al. (2007)	D_r : $1.43D$ H_r: $0.63D$	Larger extents of MRF boundary are suitable for modelling reactor vessels
Shi and Rzehak (2017)	D_r : $1.66D$ H_r: $\pm 1.452D$	Optimal radial extent was determined while axial extent was kept constant
Patil et al. (2021)	D_r : $2D$ H_r: $0.62D$	Optimal extents were determined from mean velocity predictions
Mittal and Kikugawa (2021)	D_r : $1.4D$ H_r: $0.42D$	MRF boundary near impeller or baffle walls generate unsteady effects in tank

- ✓ Objective: Development of a generalized criterion for determining optimal extents of MRF boundary for any configuration of stirred tank reactor

STIRRED TANK CONFIGURATION



(a)

(b)

Fig. 3: (a) Sectional elevation and (b) Plan of the standard configuration of stirred tank reactor adopted for the present study (Impeller speed: 200 rpm; Reynolds number: 29,000) (Source: Wu and Patterson (1989))

COMPUTATIONAL METHODOLOGY

Parameter	Approach adopted for CFD simulations
Modelling approach	Steady state three dimensional Reynolds Averaged Navier Stokes (RANS) equations
Turbulence model	Standard $k-\varepsilon$ turbulence model
Impeller rotation model	Multiple Reference Frame (MRF) impeller modelling scheme
Boundary conditions	Tank periphery, tank bottom, impeller: No-slip boundary condition Tank top surface: Symmetry boundary condition
Pressure-Velocity coupling scheme	SIMPLE scheme
Discretization scheme	Second order upwind scheme
Convergence criteria	10^{-6}
Workstation	Double precision 64 bit Intel (R) Xeon (R) E5-1620 3.6 GHz processor with 12 cores
Software	ANSYS 17.0 version

GOVERNING EQUATIONS

Continuity equation:

$$\nabla.(\rho\vec{\mathbf{u}}) = 0 \qquad (1)$$

Momentum equation:

$$\nabla.(\rho\vec{u}\vec{\mathbf{u}}) = -\nabla P + \nabla.\left(\bar{\bar{\tau}} + \overline{\overline{\tau^R}}\right) + \rho\vec{g} + \overrightarrow{F^{MRF}} \qquad (2)$$

Turbulent viscosity (μ_t) from standard $k - \varepsilon$ model:

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \qquad (3)$$

Transport equations of k and ε:

$$\nabla.(\rho\vec{\mathbf{u}}k) = \nabla.\left(\frac{\mu_t}{\sigma_k}\nabla k\right) + G_k - \rho\varepsilon \qquad (4)$$

$$\nabla.(\rho\vec{\mathbf{u}}\varepsilon) = \nabla.\left(\frac{\mu_t}{\sigma_\varepsilon}\nabla\varepsilon\right) + \frac{\varepsilon}{k}(C_{1\varepsilon}G_k - C_{2\varepsilon}\rho\varepsilon) \qquad (5)$$

GOVERNING EQUATIONS Contd.

Performance goals

Power number based on impeller torque (N_{pt}): $N_{pt} = \frac{2\pi N\tau}{\rho N^3 D^5}$ (6)

Power number based on turbulence dissipation rate $(N_{p\varepsilon})$: $N_{p\varepsilon} = \frac{\iiint \rho\varepsilon \, dV}{\rho N^3 D^5}$ (7)

Energy imbalance = $\frac{N_{pt} - N_{p\varepsilon}}{Npt}$ (8)

Terminology

ρ: Time averaged density

P: Static pressure

$\mathbf{u}$: velocity of fluid

$\bar{\bar{\tau}}$: Viscous stress tensor

$\overline{\overline{\tau^R}}$: Reynolds stress tensor

$\rho\vec{g}$: Gravitational body force

$\overrightarrow{F^{MRF}}$: Centrifugal and coriolis forces

k: Turbulent kinetic energy

ε: Turbulent dissipation rate

G_k: Turbulence generation rate

σ_k, σ_ε: Turbulent Prandtl numbers

$C_{1\varepsilon}, C_{2\varepsilon}$: constants

$C_\mu = 0.09, C_{1\varepsilon} = 1.44, C_{2\varepsilon} = 1.92$

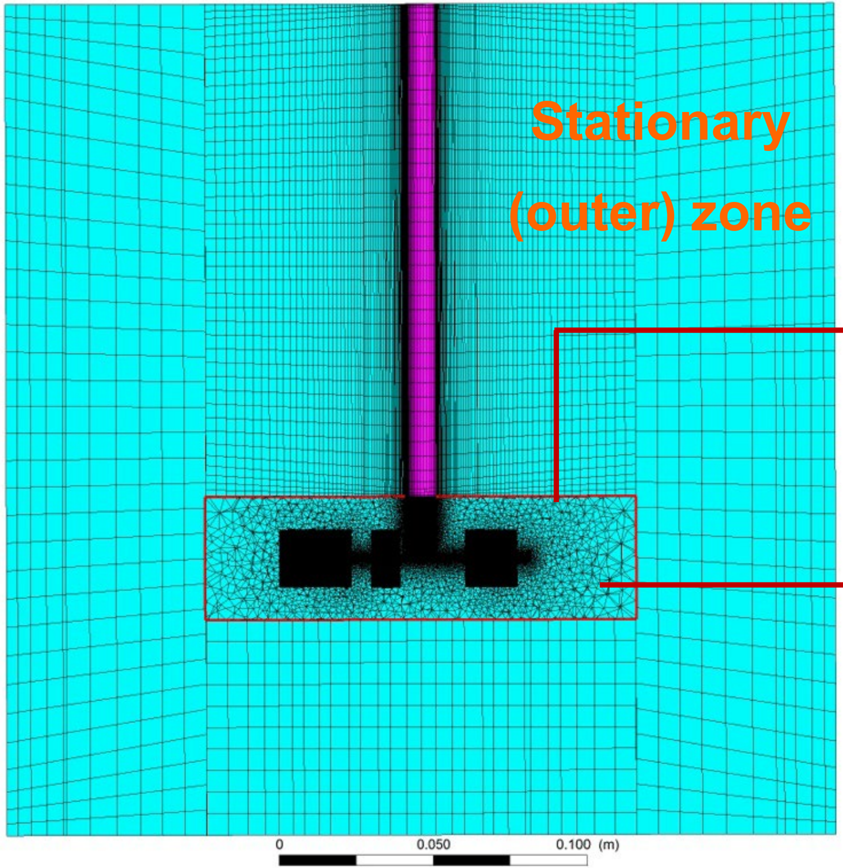
$\sigma_k = 1, \sigma_\varepsilon = 1.3$

τ: Net impeller torque

D: Diameter of impeller

N: Impeller speed

COMPUTATIONAL GRID



MRF boundary

Rotating (inner) zone

Fig. 4: Computational grid (Hybrid grid type) developed for the present study

CONVERGENCE OF CFD SIMULATION

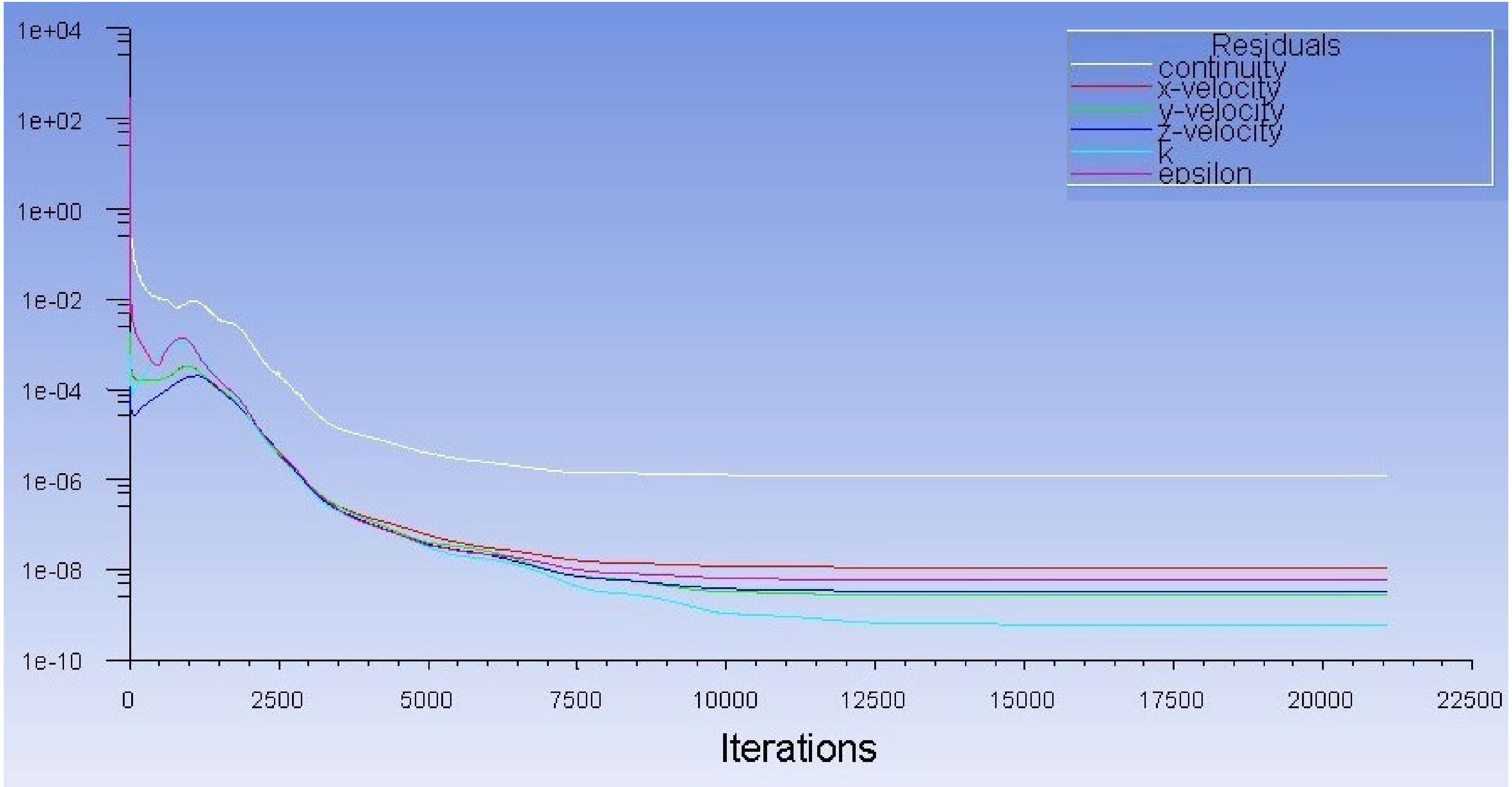


Fig. 5: Typical convergence curve from the CFD model with optimal MRF boundary

GRID INDEPENDENCE STUDY

- Grid independence study was performed for all computational trials
- Size of tetrahedral elements comprising the impeller was successively reduced
- Normalized radial velocity $\left(\frac{u_r}{u_{tip}}\right)$ was monitored for assessing the grid convergence of the CFD model

Table 1: Details of grids used for the grid independence study (D_r×H_r of 14 cm×4 cm)

Grid	Element size of impeller (m)	Number of elements
Grid-1	0.004	300573
Grid-2	0.0008	996072
Grid-3	0.00035	4497937
Grid-4	0.000258	7418360
Grid-5	0.00024	8451837

GRID INDEPENDENCE STUDY Contd.

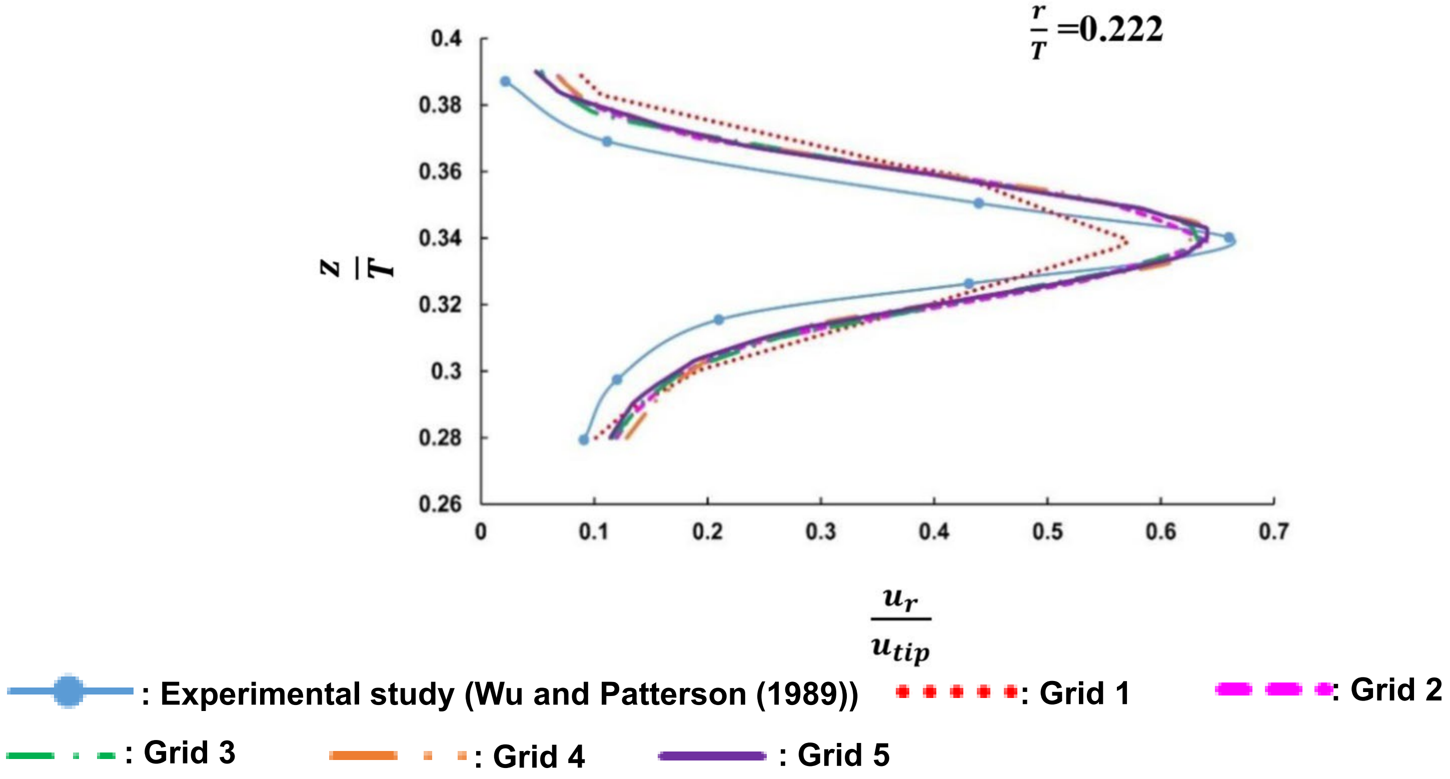


Fig. 6: Variation of axial profile of $\frac{u_r}{u_{tip}}$ close to the impeller with grid resolution

GRID INDEPENDENCE STUDY Contd.

- Verification process:
    - $\frac{u_r}{u_{tip}}$ increases from Grid-1 to Grid-3 and becomes constant thereafter
    - Predictions from Grid-4 were found to be independent of grid resolution
    - Grid convergence Index of peak $\frac{u_r}{u_{tip}}$ is only 1.27%
- Validation process:
    - Accurate prediction of magnitude and location of peak $\frac{u_r}{u_{tip}}$
    - Predictions of $\frac{u_r}{u_{tip}}$ from Grid-4 are in excellent agreement with experimental results of Wu and Patterson (1989)
    - Present CFD model accurately predicts flow behaviour of standard stirred tank reactor

POSITION OF MRF BOUNDARY

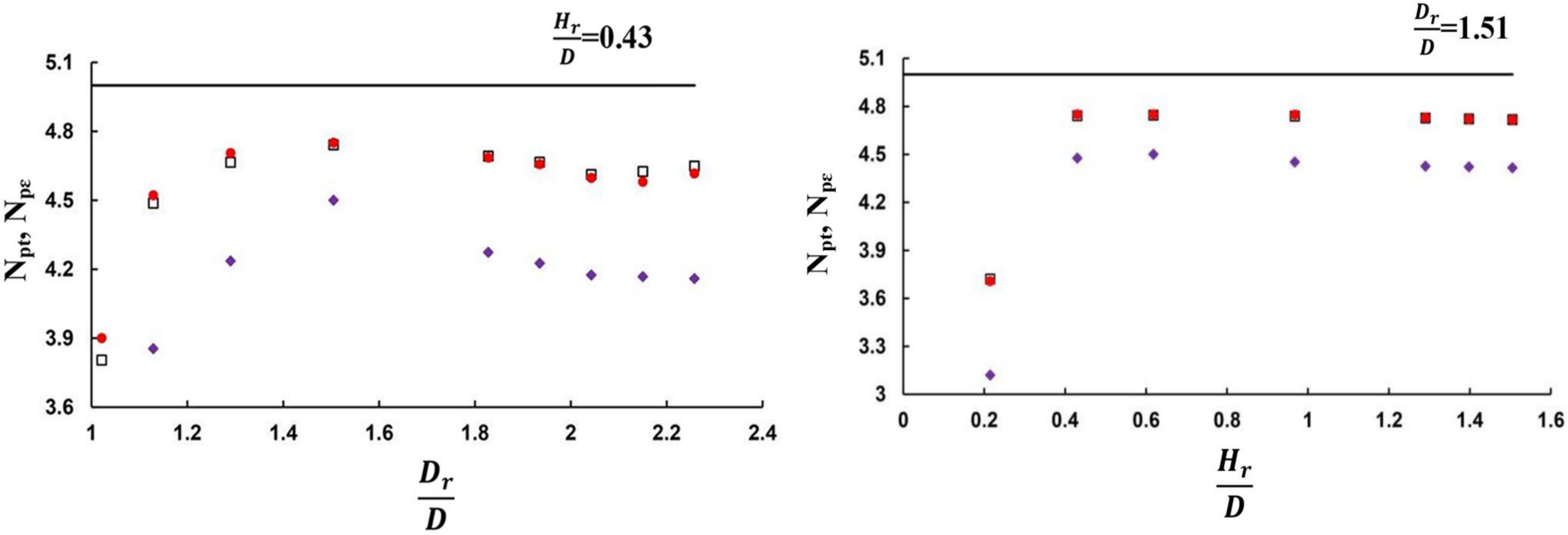
- $\frac{D_r}{D}$ and $\frac{H_r}{D}$ were varied from near impeller region to the periphery of the stirred tank
- Effect of $\frac{D_r}{D}$ and $\frac{H_r}{D}$ on N_{pt} and $N_{p\varepsilon}$ were analysed
- Optimal $\frac{D_r}{D}$ and $\frac{H_r}{D}$ were selected by comparing the predictions of N_{pt} and $N_{p\varepsilon}$ with experimental results

Table 2: Upper and lower limits of D_r and H_r adopted for the computational trials

MRF boundary extent	General limits for any geometry	Possible limits for the present study
D_r	$D < D_r < (T - 2B)$	9.3 cm < D_r < 21.6 cm
H_r	$h < H_r < 2h$	1.86 cm < H_r < 18 cm

Where $B = \frac{T}{10}, h = \frac{T}{3}$

POSITION OF MRF BOUNDARY Contd.



━: Experimental study (Bates et al. (1963))

●: N_{pt} computed from the torque on the impeller (N_{pt}-imp)

□: N_{pt} computed from the torque on the tank and baffle walls (N_{pt}-baff)

◆: $N_{p\varepsilon}$

Fig. 7: Variation of N_{pt} and $N_{p\varepsilon}$ with (a) $\frac{D_r}{D}$ and (b) $\frac{H_r}{D}$

POSITION OF MRF BOUNDARY Contd.

- ❑ Medium $\frac{D_r}{D}$ (1.51-1.94) and larger $\frac{H_r}{D}$ (>±0.22):
  - ❖ Provides superior matching between N_{pt}-imp and N_{pt}-baff
  - ❖ Proper transfer of impeller power towards tank periphery
  - ❖ Produces accurate prediction of $N_{p\varepsilon}$
  - ❖ Optimal MRF boundary
- ❑ Smaller $\frac{D_r}{D}$ (1.05-1.29), smaller $\frac{H_r}{D}$ (0.22) and larger $\frac{D_r}{D}$ (2.04-2.26):
  - ❖ Provides inadequate matching between N_{pt}-imp and N_{pt}-baff
  - ❖ Improper transfer of impeller power towards tank periphery
  - ❖ Inaccurate predictions of $N_{p\varepsilon}$
- ❑ Higher sensitivity of $\frac{D_r}{D}$ as compared to $\frac{H_r}{D}$

POSITION OF MRF BOUNDARY Contd.

- ❑ Medium $\frac{D_r}{D}$ and larger $\frac{H_r}{D}$ exist at suitable distance from the impeller which results in proper transformation of velocity fields at MRF boundary and accurate prediction of various flow field quantities
- ❑ Generalized criterion for selecting optimal MRF boundary:
  - ❖ Proper balance between N_{pt}-imp and N_{pt}-baff
  - ❖ Based on principle of conservation of angular momentum
  - ❖ Applied to any configuration of stirred tank reactor
- ❑ Optimal range of MRF extents from this study includes the MRF extents provided by Patil et al. (2021) and Zadravec et al. (2007)

POSITION OF MRF BOUNDARY Contd.

Table 3: Comparison of errors related with N_{pt} and $N_{p\varepsilon}$ from the present study and that from other literature

Authors	Turbulence model	Error related with N_{pt} (%)	Error related with $N_{p\varepsilon}$ (%)	Energy imbalance
Singh et al. (2011)	Standard $k-\varepsilon$ model	14.00	2.00	10.53
	SAS-SST	38.00	4.00	24.64
	SSG-RSM	30.00	10.00	15.38
	SST-CC	32.00	10.00	31.82
Murthy and Joshi (2008)	Standard $k-\varepsilon$ model	3.92	23.53	20.41
	RSM	1.96	19.61	18.00
	LES	1.96	7.84	9.62
Present study	**Standard $k-\varepsilon$ model**	**5.00**	**10.00**	**5.26**

- ✓ CFD model with optimal MRF boundary significantly improves the predictive capability of standard $k-\varepsilon$ turbulence model

CONCLUSIONS

- A generalized criterion for determining the optimal position of MRF boundary was developed
- $\frac{D_r}{D}$ and $\frac{H_r}{D}$ were varied in the entire domain of stirred tank reactor
- $\frac{D_r}{D}$ and $\frac{H_r}{D}$ close to the impeller and tank periphery were found to be unsuitable for modelling the stirred tank reactors
- Medium $\frac{D_r}{D}$ and larger $\frac{H_r}{D}$ were found to be appropriate for modelling the stirred tank reactors
- Balance between N_{pt}-imp and N_{pt}-baff was determined as the generalized criterion
- CFD model with optimal MRF boundary significantly improves the predictive capability of standard $k - \varepsilon$ turbulence model

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THANK YOU