Indian Journal of Chemical Technology
Vol. 23, March 2016, pp. 114-120

Study on residence time distribution of CSTR using CFD

Akhilesh Khapre*, Divya Rajavathsavai & Basudeb Munshi

Department of Chemical Engineering, National Institute of Technology, Rourkela 769 008, Odisha, India

E-mail: akhilesh_khapre@yahoo.co.in

Received 12 December 2013; accepted 9 June 2014

The mixing of fluid in a CSTR in presence/absence of impeller and baffles is investigated numerically using Computational fluid dynamics software package, Ansys Fluent. At the inlet of the CSTR, tracer (KCl) is injected by step change and the tracer concentration at the exit is noted with time to determine the age distribution function $I(\theta)$. The study helps to understand the residence time distribution (RTD) of CSTR. The CFD simulated predictions are compared with the literature data and a good agreement is found. The mixing performance of CSTR is studied using system parameters like tank Reynolds number and impeller rotation. The mixing characteristics such as Holdback, Segregation, mean residence time, variance and number of ideal CSTR in series equivalent to single actual CSTR are also determined and all these study ensures that the flow behaviour changes from dispersion to ideal mixing with increasing the tank Reynolds number and impeller speed.

Keywords: Age distribution function, CFD, Residence time distribution, CSTR, Tracer injection method

The residence time distribution (RTD) is a characteristic of mixing of the chemical reactor. It gives information on how long the various elements have been in the reactor. The quantitative knowledge of liquid RTD is very much important for a number of reasons[1], develop accurate kinetic modelling of the system, and design reactor with the desired flow pattern[2]. Also, it is a tool in successful process scale-up.

An extensive experimental and theoretical works on RTD of CSTR have been carried out in the past. Recently, Arratia *et al.*[3] have investigated the effect of presence of inlet and outlet condition and agitation speed on the efficiency of mixing process using RTD. Ochieng & Onyango[4] carried out mixing studies in stirred tank at low impeller clearance. They have reported, by adding a draft tube in the tank, a significant improvement in mixing performance can be achieved. Saravanathamizhan *et al.*[5] has developed RTD models for single tank and two/three tanks in series for the parallel plate electrochemical reactor. The exit age distribution curves and the electrolyte flow behavior in reactor are studied with the help of tracer distribution.

The recent development of Computational Fluid Dynamics has improved the understanding and prediction of the complete velocity distribution in a vessel which is an alternative and simpler mean of determining the RTD[6]. The computed velocity distributions of stirred tank using CFD tools are extensively available in literature. Choi *et al.*[7] has done both the experimental and theoretical study on RTD of a CSTR. The experimental results of the baffled tank are compared with CFD predicted RTD using k-ε model for transitional flow regime. All the qualitative aspects of the CFD predicted RTDs were found similar to those measured experimentally. Javed *et al.*[8] has carried out mixing studies both numerically and experimentally to find concentration of tracer at eight different locations in bulk and impeller region. Ghirelli *et al.*[9] has analyzed the residence time distribution of the fluid using Eulerian particle tracking and Lagrangian particle tracking method and have concluded that the Eulerian approach is superior to Lagrangian approach. Liu[10] has studied the effect of inlet and outlet locations, flow rates, the ratio of mean residence time to the batch blend time on the mixing performance of continuous flow stirred tank reactor at fully turbulent regime.

Burghardt and Lipowska[11] have studied the mixing behaviour of CSTR measuring KCl (tracer) concentration at the exit stream followed by the calculation of age distribution function, $I(\theta)$. The study was carried out in absence/presence of impeller and baffles. The hydrodynamic behaviour of fluid has a strong effect on the mixing. It can be studied in terms of RTD of CSTR. A through search of literature finds that no one yet predicted numerically the RTD in terms of $I(\theta)$ of Burghardt and Lipowska[11]. Therefore, the objective of the present work is to employ CFD tools in order to predict the effect of tank Reynolds number and impeller rotation on the mixing performance of the CSTR by computing $I(\theta)$. The effects of crucial parameters like tanks Reynolds number, rotational speed of the impeller and the viscosity of water-glycerin solution on the nature of mixing are demonstrated here. The nature of flow, ideal or dispersion flow, are determined using computed parameters like mean residence time, variance, holdback, segregation and N_{CSTR}.

Simulation Methodology

Description of System

A schematic representation of a CSTR used by Burghardt and Lipowska[11] with four baffles at 90° interval and a six blades disk turbine along with a single inlet and outlet streams is shown in Fig. 1. The diameter of tank (D) is 0.17 m. The impeller diameter (d_m) is 1/3rd of D. The length (a) and height (b) of impeller blade is $d_m/4$ and $d_m/5$ respectively. The baffles width (b_w) is equal to $D/12$. The diameter (d) of both the inlet and outlet tube is 0.0066 m. The height of tank is taken equal to the diameter of tank (D). The working fluid is water-glycerin solution whose properties are given in Tables 1 and 2.

Governing Equations and Solution Method

The general form of conservation of mass or continuity equation is[12]:

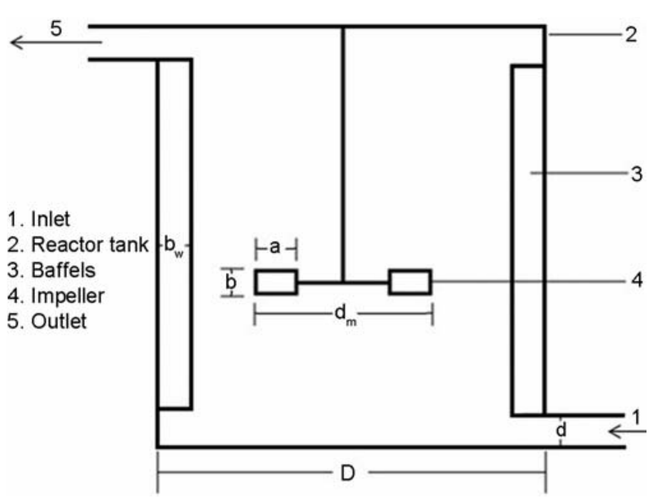

Fig. 1 — Schematic diagram of CSTR system

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho \vec{v}) = 0 \qquad \dots (1)$$

where, $\vec{v}$ is the velocity vectors.

The conservation of momentum equation for calculating velocity is given by[12]:

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla.(\rho \vec{v}\vec{v}) = -\nabla P + \nabla.(\bar{\bar{\tau}}) + \rho \vec{g} \qquad \dots (2)$$

where, P is the static pressure and $\bar{\bar{\tau}}$ is the stress tensor; $\vec{g}$ is the gravitational body force. The stress tensor $\bar{\bar{\tau}}$ is

$$\bar{\bar{\tau}} = \mu\left[\left(\nabla \vec{v} + \nabla \vec{v}^{T}\right) - \frac{2}{3}\nabla.\vec{v}I\right] \qquad \dots (3)$$

where, μ is the molecular viscosity, I is the unit tensor, and the second term on the right hand side is the effect of volume dilation.

To compute the distribution of tracer in CSTR the equation of mass transfer for species k in absence of reaction is solved and it is expressed as[12]:

Table 1 — Parameters for CSTR without impeller and baffles case

Sr. No.	μ	ρ	V^*	τ	Re	Type of Flow
1	1	1000	105	1.85	218.4	Ideal Flow
2	1	1000	75	2.66	156.0	Ideal Flow
3	1	1000	55	3.74	114.4	Ideal Flow
4	1	1000	14.3	13.75	29.3	Ideal Flow
5	1	1000	10	19.32	20.8	Ideal Flow
6	1.0	1141	8	87.40	4.7	Dispersion Flow
7	4.2	1110	20.25	10.64	11.1	Dispersion Flow
8	6.2	1130	24.75	8.62	9.5	Dispersion Flow
9	8	1144	41.40	5.14	12.2	Dispersion Flow

Table 2 — Parameters for CSTR with impeller and baffles case

Sr. No.	μ	ρ	V^*	τ	Re	N	Type of flow
1	11	1152	3.50	60.43	0.753	10	Dispersion flow
2	11	1152	3.45	63.30	0.753	20	Dispersion flow
3	11	1152	3.45	60.70	0.753	30	Dispersion flow
4	11	1152	3.45	63.91	0.753	40	Ideal flow
5	21	1180	4.42	53.76	0.516	12	Dispersion flow
6	21	1180	4.34	54.74	0.508	25	Dispersion flow
7	21	1180	4.46	53.27	0.520	50	Dispersion flow
8	21	1180	4.35	54.64	0.508	70	Ideal flow
9	43	1200	13.95	16.12	0.788	25	Dispersion flow
10	43	1200	12.75	16.52	0.741	50	Dispersion flow
11	43	1200	13.50	15.60	0.784	80	Dispersion flow
12	43	1200	16.80	12.54	0.974	100	Dispersion flow
13	43	1200	13.95	15.10	0.811	150	Ideal flow
14	43	1200	13.65	15.40	0.792	200	Ideal flow

$$\frac{\partial}{\partial t}(\rho\omega_k)+\frac{\partial}{\partial x_j}(\rho u_j\omega_k)=\frac{\partial}{\partial x_j}\left(\rho D_{eff}\frac{\partial\omega_k}{\partial x_j}\right) \quad \ldots (4)$$

where, ω_k is the mass fraction of k^{th} species, D_{eff} is the effective diffusivity of the species in the mixture.

In mixing process, the normalized step tracer input at the inlet can be evaluated by the following equation

$$F(t)=\frac{C(t)-C_0^-}{C_0^+-C_0^-} \quad \ldots (5)$$

The age distribution function $I(\theta)$ for the step change of tracer concentration is obtained by[11]:

$$I(\theta)=\tau I(t)=1-F(t)=\frac{C_0^+-C(t)}{C_0^+-C_0^-} \quad \ldots (6)$$

where, tracer concentration at the inlet changes by step from C_0^- to C_0^+, and C(t) is the concentration in the outlet at any time, t. The dimensionless time is $\theta = t/\tau$. The residence time or holdup time, τ is defined as:

$$\tau=\frac{V}{V^*} \quad \ldots (7)$$

where, liquid enters the reactor with volumetric flow rate, $V^*$and the reactor has liquid volume capacity of V.

The RTD of CSTR is studied using the tank Reynolds number, *Re*, as the parameter of the system and it is defined as:

$$\mathrm{Re}=\frac{4V^*\rho}{\pi D\mu} \quad \ldots (8)$$

where, D is a diameter of CSTR.

The mean residence time, τ_m, is given by the first moment of the residence time distribution function, $E(t)$ and computed by[1]:

$$\tau_m=\int_0^\infty tE(t)dt \quad \ldots (9)$$

The variance, σ^2 can be calculated from:

$$\sigma^2=\int_0^\infty (t-\tau_m)E(t)dt \quad \ldots (10)$$

The $E(t)$ is calculated by

$$E(t)=\frac{1}{C_0^+-C_0^-}\frac{dC(t)}{dt} \quad \ldots (11)$$

To understand the relative efficiency of the real reactor over ideal reactor it is required to calculate the number of ideal CSTR in series giving equivalent performance of the actual CSTR and it is calculated by:

$$N_{CSTR}=\frac{\tau_m^2}{\sigma^2} \quad \ldots (12)$$

The holdback is defined as the average spending time of the fluid inside the reactor compared to the hydraulic residence time, τ and mathematically, it can be defined as[13]:

$$Holdback=\frac{1}{\tau}\int_0^\tau F(t)dt \quad \ldots (13)$$

Holdback varies from 0 for plug flow to 1 when most of the space in the vessel is dead zone. For completely mixed flow, $Holdback = 1/e$.

The efficiency of mixing in a vessel can be given by a single quantity, *S* called Segregation, which is defined as[13]:

$$S=\int_0^\tau (F_{Ideal}(t)-F(t))dt \quad \ldots (14)$$

S varies from + 1/*e* for piston flow to values approaching -1 when most of the space in the system is dead zone.

where

$$F_{Ideal}(t)=1-e^{-V^*t/V}=1-e^{-\theta} \quad \ldots (15)$$

The state of flow depends on both the tank and impeller Reynolds numbers. The ranges of impeller Reynolds number are: Re_i < 10 for laminar flow, 10 < $\mathrm{Re_i}$ < 10,000 for transition flow and Re_i > 10, 000 for turbulent flow. The maximum impeller Reynolds number is found 300 in the present study and thus, the flow is very close to laminar. It is well accepted fact that turbulent models are much more computation intensive than laminar models and hence, the laminar models are used in the present study. The well predicted results using laminar models have justified the use of laminar models.

To perform the simulation, Commercial CFD package Ansys Fluent is used in the present work. The computational domain is discretized into 600000 unstructured tetrahedral meshes with denser mesh near the impeller to capture the high velocity gradient. Multiple reference frame (MRF) where the computational domain is divided into moving and stationary zones with interfaces between the zones is used. Velocity, pressure etc. are exchanged across the interface between the zones. The transient behavior of moving part systems is captured by sliding mesh approach under MRF model. The moving zone includes impeller, and it rotates with the same speed of the impeller. The stationary zone includes rest of the control volume.

The governing transport equations are discretized using the finite volume method. The convective terms and the transient terms of the governing equations are discretized using first order upwind differencing scheme and first order implicit scheme respectively. A no-slip boundary condition is applied on all the solid bodies. A velocity boundary condition at the inlet and a pressure boundary condition at the outlet of the CSTR are used. The rotating boundary condition is specified for the impeller and shaft. The operating temperature and pressure of the system are 293 K and 101325 Pa respectively. The discretized Navier–Stokes equations coupled with a pressure correction equation are finally solved together with the discretized equations for species component balance equation using SIMPLE (Semi-Implicit Method for Pressure-Linked Equation) algorithm and Gauss-Seidel iterative method[12].

The hydrodynamics equations of CSTR without tracer are solved by steady state solver to achieve an initial hydrodynamic condition for the transient solver. Then the tracer, KCl is introduced in the tank by a step change. The molecular diffusivity of KCl in the solution is taken as 1.95×10^{-9} (m^2/s)[14]. The transient transport equations for tracer along with the hydrodynamic equations are solved. The time increment is taken as 0.001 second and 30 iterations per time increment is found enough to achieve converged solution at each time step. All dependent variables are modified by under relaxation method, and used in the next iteration until the solutions are converged. The convergence criteria i.e. residual of all the discretized transport equations are satisfactorily taken as 10^{-3}, and no further changes in the results are observed with further reduction of the residual value. An overall mass balance is also checked at each time step.

Results and Discussion

The inlet flow energy is only responsible for mixing of liquid inside the tank without impeller and baffles. The inlet flow transmits its energy to the liquid in the tank and causes generation of convective streams and eddy which give rise to the mixing of the contents of the tank. The flow energy increases with inlet Reynolds number. Simulation is carried out using the parameters given in Table 1 to get insight on the hydrodynamics and mixing flow condition in tank as well as to predict the required tank Reynolds number for achieving the ideal mixing condition for the CSTR without impeller and baffles.

The simulation results are compared with the experimental[11] results in Fig 2. Figure 2(a) shows that $I(\theta)$ curve moves away from the ideal mixing line i.e. it becomes dispersed flow with decreasing Reynolds number. At relatively low Reynolds number (4.3-12.2), Fig. 2(b) shows that the computational values are predicting well the experimental data and all the curves are away from the ideal mixing line. An important observation in the figure is made that all the computed values in both the figures follow the flow conditions given in Table 1.

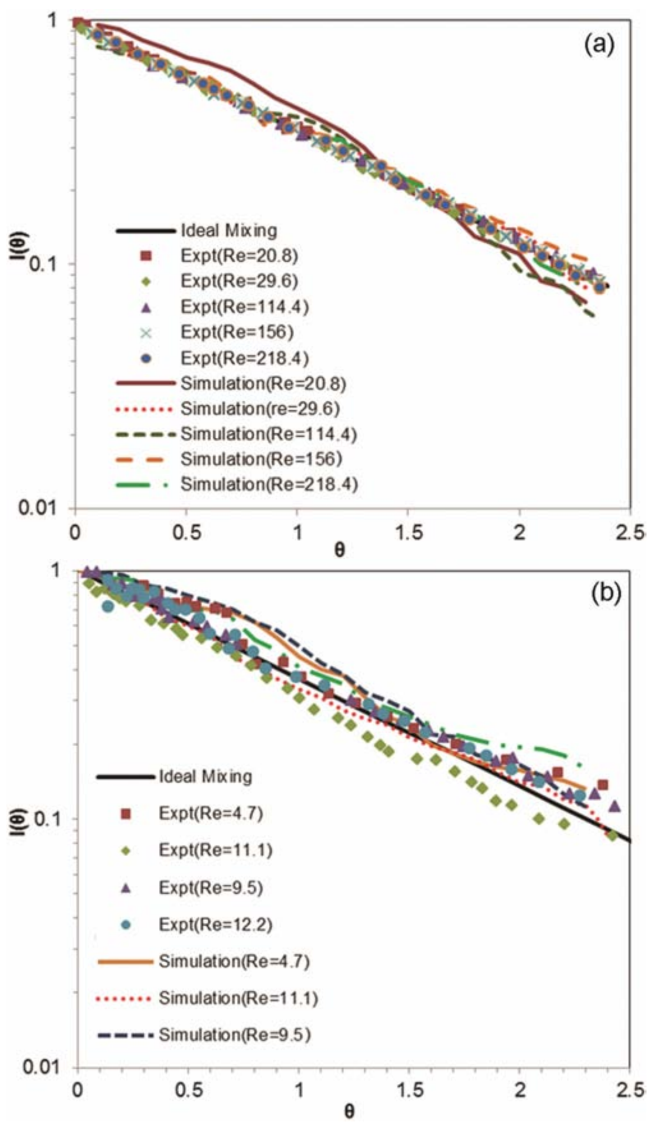

Fig. 2 — Plot of $I(\theta)$ vs θ for a CSTR without impeller and baffles

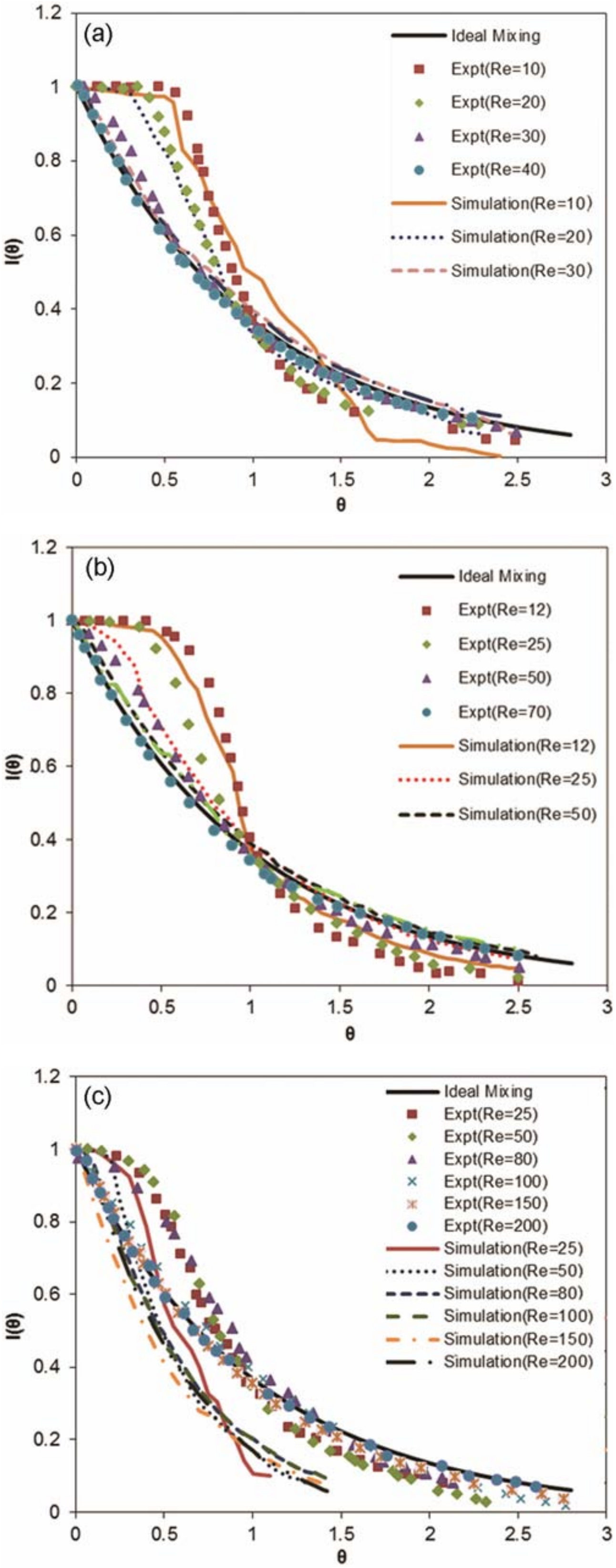

Fig. 3 — Plot of $I(\theta)$ vs θ for a CSTR with impeller and baffles.

In case of tank with impeller and baffles, the computed values of age distribution function $I(\theta)$ are compared with the experimental data[11] in Fig. 3 and the observed types of flow are mentioned in Table 2. The tank Reynolds number is kept low here. The observation finds a good agreement between present predicted values and the experimental data. The figures depict that the computed $I(\theta)$ approaches the ideal mixing line with increasing the impeller rotation, *N*. It happens due to increase of rate of mixing with the impeller rotation. The extent of mixing also depends on viscosity. As viscosity increases more amount of mechanical force is required for mixing. The figures show that the required rotation of the impeller to reach ideal mixing state increases with increasing the viscosity of the liquid.

Effect of tank Reynolds number and speed of impeller on the mixing of CSTR with impeller and baffles

Beyond validation of the experimental data it is necessary to know the effect of system parameter on the performance of the mixing phenomena. The effect of tank Reynolds number and impeller rotation speed on the mixing behaviour of CSTR is studied and represented in Fig. 4. It is carried out keeping impeller speed constant at 20 rpm. At Re = 0.5, a dispersion flow occurs and Re = 0.75, the mixing line reaches relatively closer to ideal mixing line and further increase of it to 1.0 makes the mixing line to follow ideal mixing line. The convective energy of the inlet flow increases with V^*, which increases proportionately with Re. This inlet energy helps to mix-up the tracer with liquid. Therefore, $I(\theta)$

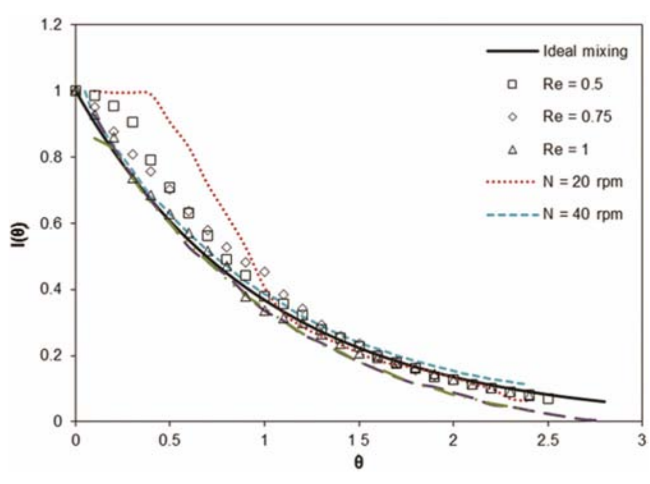

Fig. 4 — Effect of tank Reynolds number (Re) and impeller rotation (N) on $I(\theta)$ for a CSTR with impeller and baffles, μ = 11 cP

approaches ideal mixing line at higher *Re*. It is also observed that the nature of the flow changes from dispersion to ideal mixing state with increasing *N*. To study the effect of impeller rotation on mixing, the tank Reynolds number is kept constant at 0.753. A distinct dispersion flow is depicted at *N* equal to 20. As expected, the figure also shows that the type of mixing is very near to ideal mixing state for *N* in the range of 40 to 60.

Mean residence time, Variance, Holdback and Segregation

For an ideal reactor, variance, σ^2 and mean residence time, τ_m should be equal. The effect of tank Reynolds number on σ^2 and τ_m of the CSTR without impeller and baffles is presented in Fig. 5. The figure shows that at relatively low Reynolds number, 20, there is a substantial difference between the σ^2 and τ_m. It means that the mixing phenomena are non-ideal at lower Reynolds number. As *Re* becomes greater than 20, the mixing process becomes ideal. This is also supported by the profiles in Fig. 2. The distribution of σ^2 and τ_m with impeller rotation *(N)* for CSTR with impeller and baffles are shown in Fig. 5. It shows that σ^2 and τ_m approaches each other with increasing the rotational speed of the impeller. Hence, the mixing process approaches towards ideal mixing condition at higher speed of the impeller.

The distribution of holdback and Segregation with tank Reynolds number for CSTR without impeller is shown in Fig. 6. The figure shows that the value of holdback is close to 0.36 (*1/e*). Hence, based on the holdback distribution, it can be concluded that the mixing is complete at all *Re* values. But the segregation plot as shown in Fig. 6 represents that *S* is negative at lower *Re* values and it increases and tends to 0.36 as *Re* increases. Therefore, it can be concluded from the segregation curve that the mixing becomes complete at only higher *Re* values and at lower *Re* values the liquid in CSTR is mostly dead fluid. Thus the observation from hold back distribution contradicts the observation from segregation distribution. Figure 6 also shows the effect of *Re* on N_{cstr}. The value of N_{cstr} is equal to 1.0 for an ideal reactor. It is observed from the figure that the value of N_{cstr} decreases and then tends to 1.0 at higher *Re*. Therefore, it can be concluded that the CSTR behaves as ideal mixer at higher *Re*.

The holdback distribution of CSTR with impeller and baffles is shown in Fig. 7. It shows that the holdback increases and reaches near about 0.36. Hence, the mixing efficiency increases with increasing the speed of the impeller. The segregation

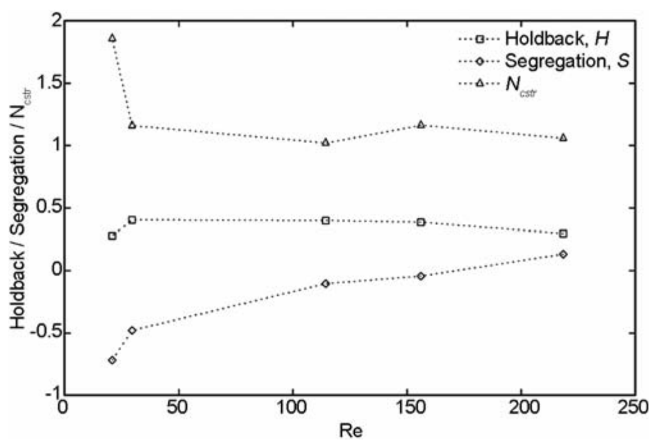

Fig. 6 — Plot of Holdback (*H*) , Segregation (*S*) , N_{CSTR} vs tank Reynolds number for CSTR without impeller and baffles; μ = 1 cP

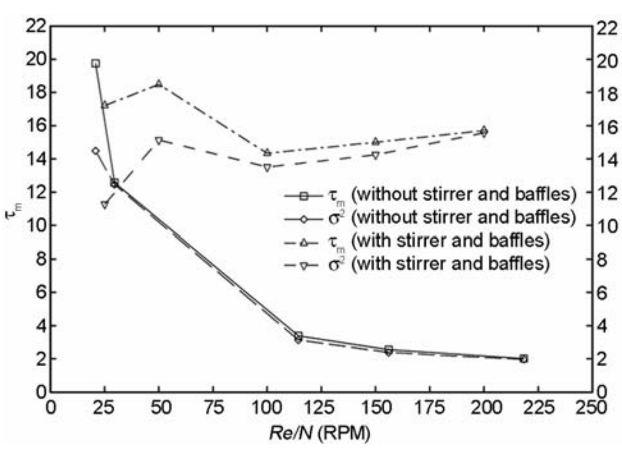

Fig. 5 — Effect of tank Reynolds number (*Re*) and impeller rotation *(N)* on mean residence time (τ_m) and variance (σ^2); for CSTR without impeller and baffles, μ = 1 cP and for CSTR with impeller and baffles, μ = 43 cP

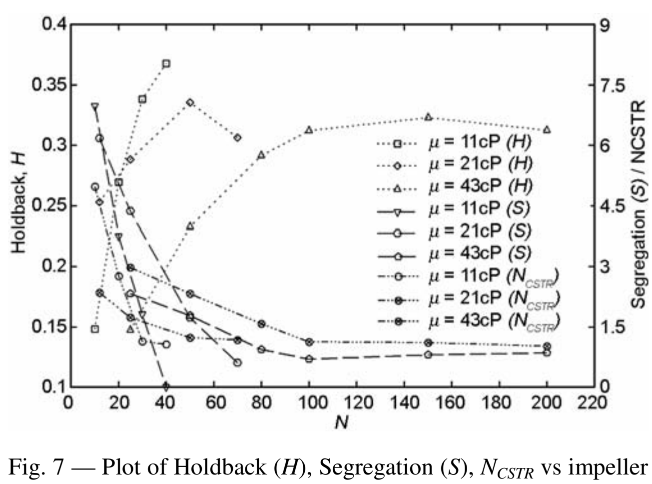

Fig. 7 — Plot of Holdback (*H*), Segregation (*S*), N_{CSTR} vs impeller rotation (*N*) for CSTR with impeller and baffles

of the CSTR with rotating impeller and baffles are found to be out of the theoretical range (-1 to 0.36) (Fig. 7). It also depicts that N_{cstr} tends to 1.0 with increasing the speed of the impeller. Thus mixing in CSTR tends to ideal mixing state at higher N. The figure also depicts that the required rotation of the impeller increases to reach N_{cstr}, 1.0 with the viscosity of the working liquid.

Conclusion

A RTD study of CSTR using CFD simulation by Ansys Fluent has been carried out successfully to predict the mixing behaviour using tracer injection method. The effect of tank Reynolds number and impeller speed are presented and discussed in detail. The CSTR is simulated in absence/presence of impeller and baffles. The simulated age distribution function $I(\theta)$ are found in good agreement with the experimental data of Burghardt and Lipowska[11]. The mixing behaviour is changed from dispersion to ideal mixing state at higher impeller speed and tank Reynolds number. The mixing characteristics study in terms of N_{cstr}, holdback, segregation, mean residence time, τ_m and second moment, σ^2 show that the CSTR behaves as an ideal mixer at higher impeller rotation and tank Reynolds number.

References

1 Fogler H S, *Elements of Chemical Reaction Engineering*, 3rd Edn, (Pearson Education Inc., New York) 1999.
2 Gavrilescu M & Tudose R Z, *Chem Eng Process*, 38 (1999) 225.
3 Arratia P E, Lacombe J P, Shinbrot T & Muzzio F J, *Chem Eng Sci*, 59 (2004) 1481.
4 Ochieng A & Onyango M S, *Chem Eng Process*, 47 (2008) 1853.
5 Saravanathamizhan R, Balasubramanian N & Srinivasakannan C, *J Model Simul Syst*, 1 (2010) 68.
6 Gamba I L, Damiam S M, Estenoz D A, Nigro N, Storti M A & Knoeppel D, *Int J Chem Reactor Eng*, 10 (2012).
7 Choi B S, Wan B, Philyaw S, Dhanasekharan K & Ring T A, *Ind Eng Chem Res,* 43 (2004) 6548.
8 Javed K H, Mahmud T & Zhu J M, *Chem Eng Process*, 45 (2006) 99.
9 Ghirelli F, Hermansson S, Thunman H & Leckner B, *Progr Comput Fluid Dynam Int J*, 6 (2006) 241.
10 Liu M, *Chem Eng Sci*, 69 (2012) 382.
11 Burghardt A & Lipowska L, *Chem Eng Sci*, 27 (1972) 1783.
12 ANSYS FLUENT 12.0 Theory Guide, ANSYS Inc., 2009.
13 Danckwerts P V, *Chem Eng Sci*, 2 (1953) 1.
14 Harned H S & Nuttall R L, *J Am Chem Soc*, 71 (1949) 1460.