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Research note

CFD Investigation of Hydrodynamics in an Industrial Suspension Polymerization Mixing Reactor

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Abstract
Turbulent flow field in a 200 m^3 industrial suspension polymerization reactor, which is a baffled agitated vessel, was simulated using CFD. Multi-reference frame (MRF) methods and k-ε turbulence model were used to solve turbulent flow equations. It was found that turbulent flow field in reactor is non-homogenous. This non-homogeneity is especially common among three compartments of a reactor based on turbulent kinetic energy (TKE) dissipation rate. A compartment around the impeller with very high rate of TKE dissipation (impeller zone), a compartment around the baffles with a relatively high rate of TKE dissipation (baffle zone) and a relatively big compartment in bulk of flow with low TKE dissipation rate (circulation flow). Therefore a three-compartment model was used to explain the non-homogeneity of turbulent flow field. The parameters of this model are compartment volume ratios (μ_i and μ_b), compartment energy dissipation ratios (λ_b and λ_i) and exchange flow rates (Q_i and Q_b), which were obtained from simulations for different agitation rates.

Keywords: *CFD, Suspension Polymerization, Turbulent Flow, Three-compartments*

1. Introduction

One of the most important tasks in suspension polymerization is achievement of desirable particle size distribution (PSD) of final product.

The effects of parameters such as the design of the stirrer [1], the type [2] and concentration of stabilizer [3,4], the stirring rate [4-6], the design of internal elements of the reactor [7], water to monomer weight ratio and suspending agent concentration [8] on PSD were studied experimentally in the past.

Forming of the final PSD depends on two basic phenomena, namely, breakage of a droplet and coalescence of a pair of droplets. Population balance equation is a model, which is used to predict particle size distribution of droplet in suspension systems. In the population balance formulation, dispersed phase is considered as a group of droplets which are continuously destroying and forming by breakage and coalescence. The population balance equation for a single droplet with diameter of *a*, can be written as [9]:

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$$\frac{dY_i}{dt} = Y_{i,in} + \sum_{j=i+1}^{n_c} \nu(a_j)\beta(a_i,a_j)g(a_j)Y_j$$
$$+ \sum_{j=1}^{\#(\vartheta_i/2)} F((a_i^3 - a_j^3)^{1/3}, a_j)Y_i Y_j - Y_{i,out} - g(a_i)Y_i - Y_i$$
$$\sum_{j=1}^{\#(\vartheta_{nc} - \vartheta_i)} F(a_i, a_j)Y_j \qquad (1)$$

Wherein Y_i is the number concentration of drop class i, and a_i and a_j the characteristic diameter of the class i and j, respectively. F (a_i, a_j) is the binary coalescence rate between droplets a_i and a_j in unit volume, and $g(a_j)$ is breakage rate of a droplet with diameter a_j.

Rate of these processes depends on reactor stirrer geometry, stirrer speed, type and concentration of stabilizing agent and turbulent flow field properties [9]. Fundamental studies on these parameters, combined with Computational Fluid Dynamics (CFD) can play an important role in predicting PSD.

Therefore analyzing the turbulent flow pattern and its properties in stirred vessels may be a beneficial tool to predict PSD in suspension polymerization processes. The suspension polymerization reactor is usually a stirred tank reactor.

Turbulent kinetic energy (TKE) dissipation rate in the stirred tank reactor has a direct effect on the coalescence and breakage rates. Application of local turbulent kinetic energy dissipation in the population balance models is difficult. So, it is commonly considered that turbulent flow field is homogenous and energy dissipation rate in the entire tank is assumed constant for simulation purposes. However, experimental measurements and CFD simulations showed that turbulent flow field is far from homogeneity. This non-homogeneity is represented based on energy dissipation rate that varies by orders of magnitude in different locations of the reactor. Two-compartment population balance model was developed for taking into account the non-homogeneity of turbulent field and order-of-magnitude variation of TKE dissipation rate at different locations of the reactor [10]. The stirred tank was divided into eleven subregions and each subregion was assumed to be completely mixed. The time variation of drop size distribution in the tank was investigated and tested in a parameter fitting procedure [11]. Single block and multiblock population balance models were used for simulations, both showing good agreement with experimental data.

Computational fluid dynamics (CFD) is a proper tool for simulating turbulent flow field in stirred tanks, which was used by several researchers in the past [12-16]. The study of turbulent flow field and its properties in stirred tanks has been the subject of numerous theoretical and numerical investigations. Harris et al. (1996) applied both experimental and numerical methods to predict flow field in baffled stirred tank reactors using time-dependent sliding mesh techniques [17]. It was clearly shown that the comparison between the experimental findings and the numerical predictions was generally satisfactory, especially in regions far away from the impeller. Sahu et al. (1998) have attempted to improve the CFD predictions by means of zonal modeling [18]. They divided the vessel into several zones. In each zone, different sets of values for 'k-ε' model parameters were specified. Based on their work, predictions of 'k' were significantly improved by using zonal modeling. Montante et al. (2001) simulated the flow and turbulence field in a fully baffled vessel stirred by a turbine, using the sliding-grid and inner-outer methods [13]. They investigated dependency of flow pattern on impeller clearance in stirred vessels. Deglon and Meyer (2006) investigated the effect of grid resolution and discretization scheme on the CFD simulation of fluid flow in a baffled mixing tank stirred by a rushton turbine, using the MRF impeller rotation model and the standard k-ε turbulence model [14]. Simulations have also been performed in a rotating frame of reference where the impeller was assumed to be stationary by Alexopoulos, et al. (2002) [19]. This method is especially suitable for unbaffled vessels, where the outer-wall boundary condition is easily defined. Alexopoulos, et al. (2002) applied a two-compartment model, which is comprised of two mixing zones. An impeller zone of high local energy dissipation rate and a circulation zone of low energy dissipation rate formed the compartments. They applied their simulation results to determine drop size distribution of non-homogenous liquid-liquid dispersion.

In this paper, we present CFD simulations for flow field in an industrial suspension polymerization reactor of vinyl chloride. The reactor is a baffled stirred tank. Therefore, a three-compartment model has been applied. Three mixing zones, namely an impeller zone of high local TKE dissipation rate, a baffle zone of relatively high TKE dissipation rate and a relatively large circulation zone of low TKE dissipation rate were the compartments considered. Multiple reference frame (MRF) method is used for simulations. The model parameters (volume ratios of impeller and baffle zones, ratio of the average TKE dissipation rate at impeller and baffle zones and the exchange flow rates between impeller-circulation and baffle-circulation zones) were determined. The effect of agitation rate on the above mentioned parameters was investigated.

2. Model geometry

The reactor is an 8m high, 5.37m diameter tank with 181.2m^3 volume. The tank is equipped with two 1.66m high baffles that are set at the 7.1m height from the bottom of the reactor as shown in Fig. 1. Reactor is filled to the middle of baffles, with water as continuous phase. The reactor content was stirred with a particular three blade impeller with 3.7m diameter located at the bottom of the tank as shown in Fig. 2.

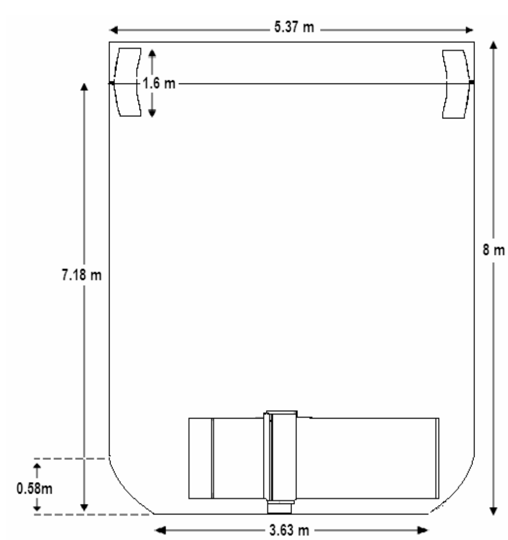

Figure 1. geometry of reactor

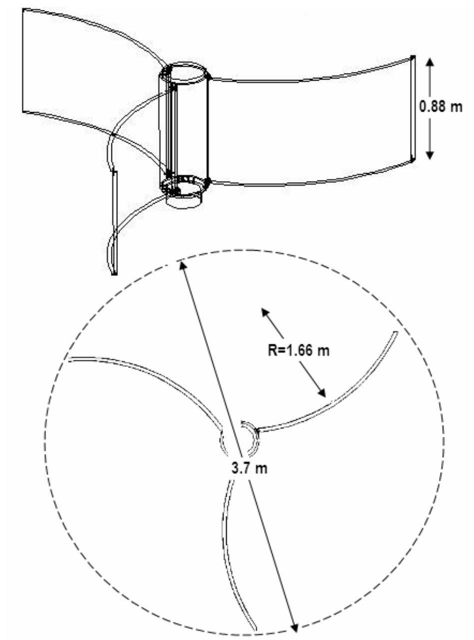

Figure 2. geometry of stirrer

3. Grid generation

Due to the use of MRF method for simulation, the volume of the tank should be divided into two cylindrical zones. The inner zone comprises an impeller and the outer zone includes tank walls and baffles. Gambit 2.0 software was used to credit and mesh the model. A non-uniform grid with tetrahedral elements consisting of about 350000 nodes was used. The grids were refined near the impeller blade and baffles. A finer grid, (about 48800 nodes) was also used to establish mesh independency. Negligible differences were observed between predictions obtained from the two mesh sizes.

4. Governing equation

The flow in suspension polymerization reactor becomes steady state in a short time. Therefore, it can be considered steady state flow in stirred tank. Governing equations for steady state flow in an incompressible fluid are:

Continuity equation: $\frac{\partial \bar{u}_j}{\partial x_j} = 0$ (2)

Motion equation:

$$-\frac{\partial}{\partial x_j}(\rho \bar{u}_j \bar{u}_i) - \frac{\partial}{\partial x_j}(\rho \overline{u'_j u'_i}) + \mu \nabla^2 \bar{u}_i - \frac{\partial \bar{P}}{\partial x_i} + \rho g_i = 0 \quad (3)$$

In equation (3) $-\rho\overline{u'_i u'_j}$, Reynolds stress can be modeled by semi empirical relations. Two-equation k-ε model was used in this work.

Governing equations for turbulent kinetic energy and kinetic energy dissipation rate are:

$$\rho \bar{u}_j \frac{\partial k}{\partial x_j} = \tau_{ij}^{(t)} \frac{\partial \bar{u}_i}{\partial x_j} - \rho\varepsilon + \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu^{(t)}}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] \quad (4)$$

$$\rho \bar{u}_j \frac{\partial \varepsilon}{\partial x_j} = C_{E1}\frac{\varepsilon}{k}\tau_{ij}^{(t)}\frac{\partial \bar{u}_i}{\partial x_j} - C_{E2}\rho\frac{\varepsilon^2}{k} + \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu^{(t)}}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] \quad (5)$$

Where:

$C_{E1} = 1.44$; $C_{E2} = 1.92$; $C_\mu = 0.09$;
$\sigma_k = 1.0$; $\sigma_\varepsilon = 1.3$

5. Fluid properties

For predicting the turbulence field in the tank it was assumed that the reactor was filled with water with properties as shown in Table

1. Turbulence field was then corrected for the real suspension as in the following relation [20]:

$$\frac{\varepsilon_D}{\varepsilon_c} = \left(\frac{\nu_c}{\nu_D} \right)^3 \quad (6)$$

Wherein ε_c and ε_D are TKE dissipation of continuous phase and dispersion, respectively and υ_c and υ_D are kinematic viscosity of continuous phase and dispersion, respectively.

Table 1. fluid properties

Fluid (water) property	**value**
Kinematic viscosity	0.1 cm^2/s
Density	1 g/cm^3
Surface tension	72 dynes/cm

6. Simulation procedures

Simulations were performed using fluent 6.0.12 software. The simulation procedure was explained as shown below:

1. The model was generated and meshed with gambit software and then was exported to fluent software.
2. The fluid was defined for the model. For this purpose, the fluid (water) was selected from a list in software.
3. The k-ε model of turbulence and relative velocity formulation were defined for governing equation.
4. Boundary conditions were defined. Due to using the MRF approach, a rotating coordinate system has been adopted for the inner zone named fluid1. Its rotating rate was set equal to impeller agitation rate, and a non-moving coordinate system has been defined for the outer zone including baffles named fluid2. Angular velocity of impeller has been set to zero with respect to the rotating coordinate system. Zero shear stress was used for free surface. At the interface between the inner and outer zones the velocities and velocity gradients were set to be the same. For liquid in contact with solid surfaces no-slip boundary condition was used.
5. The disccretization scheme was “PRESTO!” for pressure, “SIMPLE” for pressure-velocity coupling and “First order upwind” for momentum, turbulent kinetic energy and energy dissipation rate.
6. To start computations initial guesses should be specified for velocity, pressure and turbulence parameters. The angular velocity of rotating reference frame at the first step of the calculations has been set as 10% of the case under study. After about 1000 time steps, the results were saved and used as initial guess. This procedure prevents the solution from being diverged. Convergence was achieved when residuals on continuity, velocities, kinetic energy and energy dissipation rate all became less than 10^{-5}.

7. Model validation

The CFD simulation was performed for a given case of vinyl chloride suspension polymerization condition. The obtained results were used to predict PSD and compared with experimental data. A good agreement is observed between predicted values and experimental data as shown in Fig. 3.

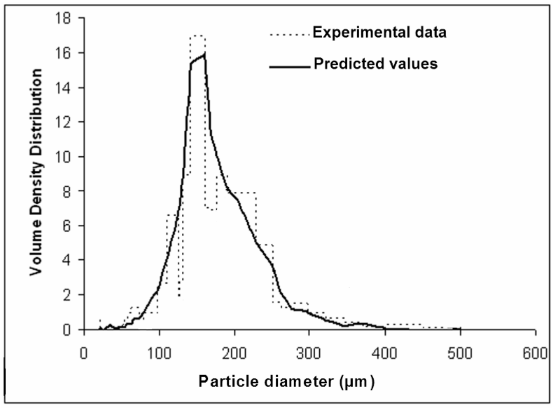

Figure 3. particle size distribution, comparison between experimental data and predicted values

8. Results and discussion

Turbulent flow field in an industrial stirred tank reactor was simulated using CFD. Fig. 4 shows the velocity vectors in a vertical plate passing from the plane 45 degrees between baffles. It is seen that there is a vertical circulating flow in the reactor. The impeller induces a centrifugal force to the fluid that leads it to tend to the tank wall and, after impacting the wall flows up to the top of the reactor. The flow then tends to the center and finally comes down toward the impeller. Zadghaffari et. al. (2010) also found a similar pattern of flow in a baffled mixing tank stirred with a rushton impeller [21]. Of course, the fluid flow pattern in their work consists of an upper and a lower circulating flow from the impeller blade, as the impeller blade clearance from the bottom of the tank was considerable, while it is very low in the present work. Therefore only a circulating flow is formed.

Fig. 5 shows the velocity vectors in a horizontal plate passing from the middle of the baffles. It is seen that there are swirling flows behind the baffle, which lead to generating dead zones there.

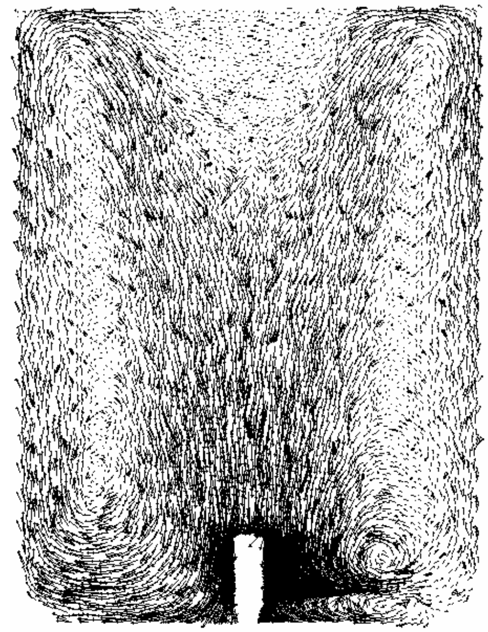

Figure 4. velocity vectors in vertical plane

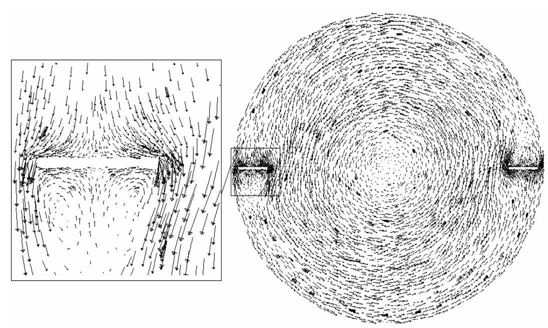

Figure 5. velocity vectors in horizontal plane passing from the middle of baffles

Fig. 6 shows the variation of radial, axial and tangential velocity with distance from the bottom of the reactor. It is seen from Fig. 6-a that radial velocity in the bottom of the reactor is higher than other zones. There is maximum value of radial velocity in the 0.6m distance from the bottom, approximately in the middle of the impeller. Radial velocity decreases with increasing the distance from the bottom and at 1.2m height its sign changes and becomes negative. It means that the direction of radial velocity changes at this point. From 1.5m up to about 6m the radial velocity is approximately constant, and then begins to increase in the negative direction.

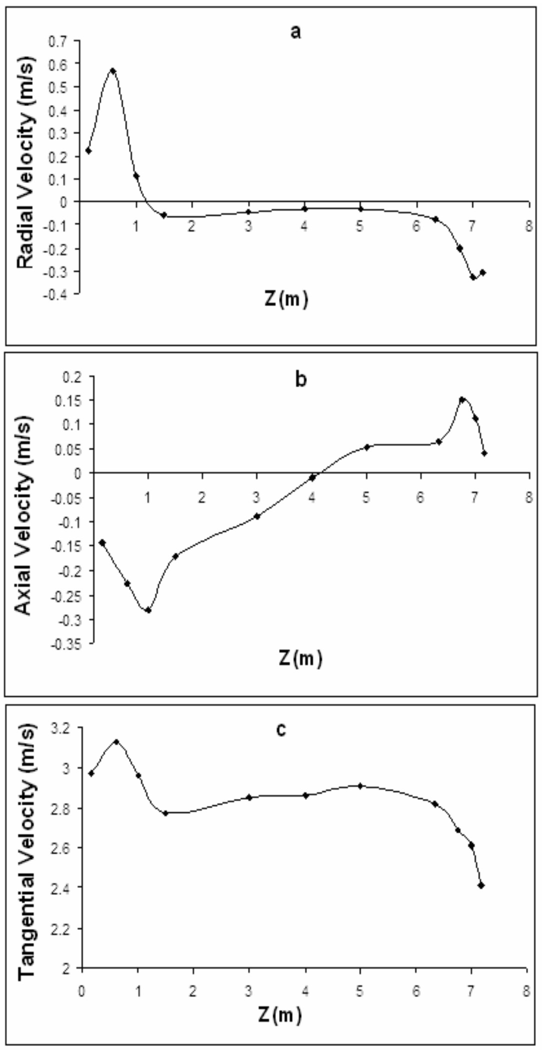

Figure 6. variation of velocity with distance from bottom of reactor, a-radial; b- axial and c-tangential velocity

It is seen from Fig. 6-b that there is a maximum value of axial velocity in the top of the tank (6.8m distance from bottom) and a maximum value (in reverse direction) at about 1m distance from the bottom of the tank. It is also seen from Fig. 6-c that tangential velocity is high at the bottom of the reactor with a maximum at the point around the impeller and is relatively low at the top of the reactor.

Figure 7 shows turbulent kinetic energy (TKE) dissipation rate contours in the vertical surface passing from baffles and horizontal surface passing from the middle of the impeller. It is seen from Fig. 7-a and 7-b that turbulent flow field is non-homogenous in the reactor. This non-homogeneity can be seen especially among three zones in the tank: around the impeller, around the baffle and fluid bulk between baffle and impeller. It seems that dividing the volume of the reactor into three homogenous compartments is justified. These compartments are impeller zone with very large value of TKE dissipation rate, baffle zone with relatively large value of TKE dissipation rate and circulation zone which occupies most of the reactor and has a small value of TKE dissipation rate. This nonhomogenity of turbulent flow in mixing tank was also seen by Alexopoulos et. al. (2002) [19]. They simulated the flow in an unbaffled stirred tank and found that TKE dissipation rate is very high around the impeller blade, but very low and relatively homogenous in fluid bulk. So, they used a two compartment model to study flow in unbaffled stirred tank. In this work a baffled stirred tank was simulated. Therefore, there is an extra compartment around the baffle.

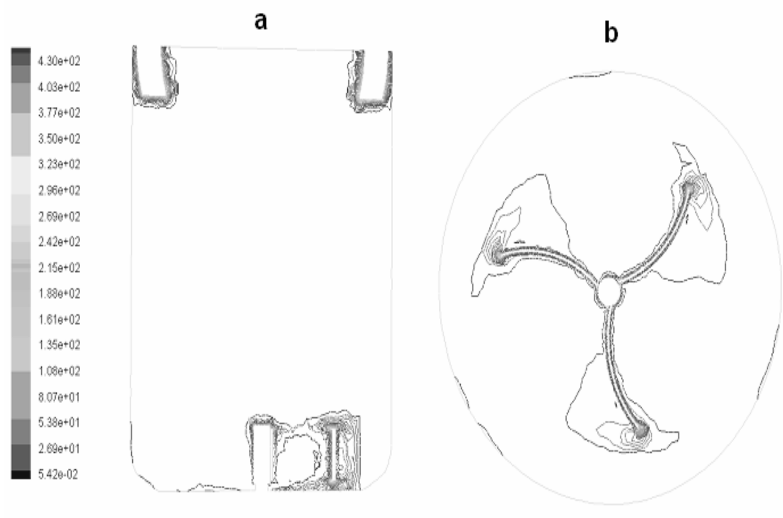

Figure 7. TKE dissipation rate contours in a-vertical plane and b-horizontal plane

Boundaries between zones were determined based on the TKE dissipation rate gradient. Value of TKE dissipation rate at the location where TKE dissipation rate gradient decreases about one order is named energy dissipation rate cut-off, ε_{cut}. Two TKE dissipation rate cut offs exist in the tank determining impeller-circulation and baffle-circulation boundaries. Based on TKE dissipation gradient, impeller zone begins from the impeller tip to the point where TKE dissipation rate gradient begins to decrease. Baffle zone also begins from baffle edge to the point where energy dissipation rate gradient begins to decrease. The remaining fluid is in the circulation zone [22].

The mass-average TKE dissipation rate at the impeller, baffle and circulation zone are 38.54, 26.74 and 0.971 m^2/s^3, respectively for impeller rotating at 36rpm.

Figure 8 shows the variation of TKE dissipation rate with agitation rate in three different zones and the entire tank. It is seen that TKE dissipation rate increases with increasing agitation rate in all zones with a higher slope in the impeller and baffle zones and lower slope in the circulation zone and entire tank.

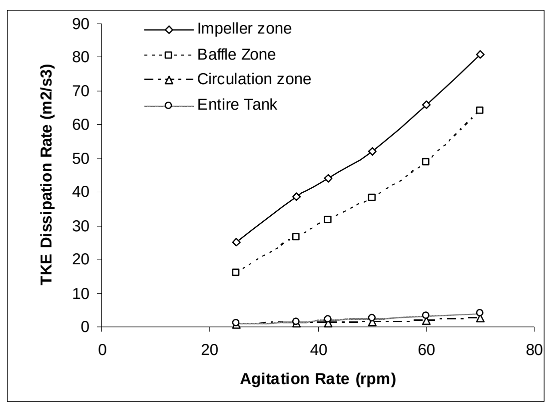

Figure 8. TKE dissipation rate variation with agitation rate at different zones

9. Model parameters

As mentioned above, a three-compartment model can be used to explain the non-homogeneity of turbulent flow field in the tank. Therefore, a three-compartment population balance model can be used to obtain PSD data. In this model, equations were solved in three different zones (impeller, baffle and circulation zones) and PSD was obtained for individual compartments. Then PSD was achieved for the entire reactor by combining the obtained PSD for each compartment by using the following equation:

$$Y_{i,t} = \mu_i Y_{i,I} + \mu_b Y_{i,b} + \left(1 - \mu_i - \mu_b\right) Y_{i,c} \qquad (7)$$

Wherein $Y_{i,t}$, $Y_{i,I}$, $Y_{i,b}$ and $Y_{i,c}$ are number concentration of drop class i per unit volume for the entire tank, impeller zone, baffle zone and circulation zone, respectively.

The parameters of this model are baffle volume ratio μ_b and impeller volume ratio μ_i, that are (baffle zone volume/total volume) and (impeller zone volume/ total volume), respectively. Baffle energy dissipation ratio λ_b and impeller energy dissipation ratio λ_i are other parameters defined as (impeller zone average TKE dissipation rate/ total average TKE dissipation rate) and (baffle zone average TKE dissipation rate/ total average TKE dissipation rate), respectively. Q_i and Q_b are other model parameters that are exchange flow rates between impeller - circulation zones and baffle-circulation zones, respectively. Table 2 shows three-compartment parameters obtained from CFD simulations for different impeller agitation rates.

10. Conclusions

Turbulent flow field in an industrial suspension polymerization reactor was simulated using CFD. It was found from the results that there is a vertical circulating flow in the reactor. The impeller induces a centrifugal force to the fluid leading it to tend to the tank wall and after impacting to the wall, flows up to the top of the reactor. The flow then tends to the center and finally comes down toward the impeller. It was also found that there is a non- homogeneity of turbulent flow field in the reactor. This non-homogeneity can be seen especially among three zones in the tank: around the impeller, around the baffle and fluid bulk between baffle and impeller. Therefore a three-compartment model can be used to explain the non-homogeneity of turbulent flow field in the tank. These compartments are impeller zone with very large value of TKE dissipation rate, baffle zone with relatively large value of TKE dissipation rate and circulation zone which occupies most of the reactor and has a small value of TKE dissipation rate.

Table 2. three- compartment parameters obtained from CFD simulations for different agitation rate

Agitation rate (rpm)	λ_i	λ_b	μ_i	μ_b	$Q_i \times 10^4$ (m^3/s)	$Q_b \times 10^4$ (m^3/s)
25	23.97	15.34	0.0023	0.0013	2.88	16.31
36	28.76	19.96	0.0028	0.0011	5.88	36.33
42	21.1	15.21	0.0034	0.0021	9.04	55.72
50	20.59	15.12	0.0031	0.0016	11.91	73.08
60	20.53	15.21	0.0019	0.0009	19.97	88.27
70	20.21	15.96	0.0025	0.0014	25.83	98.65

The variation of TKE dissipation rate with agitation rate was also studied. It was found that the TKE dissipation rate increases with increasing agitation rate in all zones with a higher slope in the impeller and baffle zones and a lower slope in the circulation zone and entire tank.

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