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Research Note

Numerical study of the agglomerates dispersion behavior in shear and elongational flow fields in viscous media using Population Balance Modeling (PBM)

A. Afshar[a], M. Salami Hosseini[a,*] and E. Behzadfar[b]

a. *Institute of Polymeric Materials, Department of Polymer Engineering, Sahand University of Technology, Tabriz, P.O. Box 51335-1996, Iran.*
b. *Department of Polymer Engineering, Amirkabir University of Technology, Tehran, Iran.*

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Abstract. In particulate systems, formation and fragmentation of agglomerates/aggregates are the major phenomena in the case of dynamic processing of suspensions. In the present work, the dispersion of the agglomerates has been studied in Shear Flow Fields (SFF) and Elongational Flow Fields (EFF) using population balance Method. Since there is no direct data on EFF, predicted data obtained through Discrete Element Method has been used to obtain a proper breakup kernel for EFF. So, a power-law breakup kernel is proposed for EFF and an exponential one is considered for SFF. It has been shown that increasing the intensity of deformation rate in both flow fields, speeds up the breakup process and the mean aggregate/agglomerate sizes shift toward the finer flocs. This effect is more pronounced for SFF showing more sensitivity to the deformation rate. It has been concluded that because of the ability of EFF in agglomerate breakup, it would break the agglomerates even in lower deformation rate. Since agglomerate could rotate in SFF, the final agglomerate size would show more dependency on the deformation rate. Results depict that EFF leads to broader agglomerate size distribution in comparison with SFF. The final fragment size shows more dependency to the agglomerates structure in SFF compared to EFF.

1. Introduction

Flocculation and fragmentation are two mostly encountered phenomena in particulate systems. These phenomena gain importance in many applications, such as chemical engineering and pharmaceutical industries upon affecting the final product properties. For many years, significant research works have been devoted to this subject. Bos et al. [1] studied the kinetics of breakup and aggregation in continuous and batch mixers and showed that because of the complex nature of these two processes data on batch mixers could not be used in continuous one. They stated that there was a dynamic equilibrium between these two processes that could be regarded as the source of complexity of the system. Shiga and Furuta [2] studied the dispersion of carbon black agglomerates and observed that the particles detached from the mother agglomerate layer by layer leading to propose the "onion model" for dispersion of the carbon black agglomerates. Feke and Manas-Zlockzower [3] proposed a model for the rupture probability of spherical clusters in shear flow fields. Xie et al. [4] investigated the nano-particle dispersion in a stirred tank and showed that particle size distribution

*. *Corresponding author. Tel.: +98 411 3459082; Fax: +98 412 344431*
E-mail address: salami@sut.ac.ir (M. Salami Hosseini)

exhibited a bimodal distribution due to the prevailing of the shattering mechanism in high shear devices. Hasegawa et al. [5] proposed a model for dispersion of fine particles in a Newtonian melt and showed that the model was capable of estimating the steady state values of the slurry viscosity and the mean particle numbers in a cluster.

Along with the experimental and analytical studies, statistical methods were also employed to predict the final state of aggregates dispersion. Among these methods, Population Balance Method (PBM) is the most widely used one which is based on "addition" and "division" of agglomerated particles, as the fluid effects and aggregate size distribution are predictable by use of this method [6]. Many works have been devoted to improve PBM to adapt it for using in particulate systems. Kim and Kramer [7,8] examined various techniques and proposed an improved model for discretization scheme to be used in population balance modeling. Autunes et al. [9] considered the polymer bridging effect and its characteristics on PCC flocculation through integrating it into the population balance framework. They also achieved a good accordance between the experimental floc size distribution and their predicted results. Selomulya et al. [10] studied the effect of shear on floc properties with considering the role of restructuring through population balance method. It is found that denser flocs were formed when structural deformation dominated, while rather tenuous ones were observed when formation and breakup kinetics were the governing mechanisms. Soos et al. [11] investigated the aggregation, breakage and restructuring kinetics of colloidal dispersions in turbulent flows by use of population balance modeling and static light scattering. They discussed the effect of agglomerate structure and mass distribution on the average structure factor and the apparent fractal dimension measured by the static light scattering. A theoretical development and experimental validation of a novel mechanistic breakup kernel were examined by Ramachandran et al. [12] which was incorporated within the three-dimensional population balance equations. Through performing qualitative validation of breakup kernel and trends of lumped and distributed properties as well, they achieved good agreement with the expected behavior of the mixing process. Diemer and Olson [13] employed the bivariate moment methods for modeling simultaneous coagulation and breakup of agglomerates and exhibited the reconstructed steady-state distributions formed when the rate kernels are size independent. It is noted that for solving PBEs, different methods were proposed [14]. Bove et al. [15] developed a novel numerical method, known as "Parallel Parent and Daughter Classes (PPDC) technique", for solving Population Balance Equations (PBEs) that can be applied for solving a wide class of problems such as polymerization, aerosol dynamics, bubble columns, etc. This method was shown to be as accurate as Quadrature Method Of Moments (QMOM) [16]. Among the operative factors of the agglomerate fragmentation and formation of final floc size distribution in suspensions, the kind of flow fields has a significant impact. Quantitative studies of agglomerate breakup in simple shear and elongational flow fields [17-19] have shown that elongational flow field is more effective than simple shear one. Higashitani et al. [18] have adopted this method to develop a method, referred to as the modified DEM, to predict the response of agglomerate in simple flow fields. Cundall [19] introduced a numerical method called as Discrete Element Method (DEM) in which the displacement of each particle was predicted according to the balance of forces applied on it. Hosseini et al. [20] employed this approach to investigate the effect of different flow fields on dispersion process. These studies have been verified by the experimental results reported by Powell and Mason [21] and the theoretical calculations of Manas-Zloczower and Feke [22] who pointed out that elongational flow fields enhance the process of agglomerate dispersion in comparison to simple shear flows. It is worth noting that analytical methods have widely been applied to model the dispersion process of agglomerates in the last few years. Fanelli et al. [23] used this method to study the dispersion of aggregates in nano-scale in steady and oscillating shear flow fields. Eggersdorfer et al. [24] applied this method to study the restructuring and fragmentation of soft-agglomerates in a simple shear flow.

The main objective of this work is to employ population balance method to model the agglomerate breakup behavior based on the results obtained through 2D discrete element method to predict and study the dispersion process of agglomerates in different flow such as simple shear and elongational flow fields in suspensions.

2. Theory and method

2.1. Population balance model

Population balance modeling is used to demonstrate the effect of processing parameters on aggregate structure size distribution. Majority of available coagulation models are based on Smolochoweski's researches in 1917 [25] as follow:

$$\frac{dn_k}{dt} = \frac{1}{2} \sum_{i=1, j=k-1}^{i=k-1} \alpha_{i,j} \beta(r_i, r_j) n_i n_j - n_k \sum_{i=1}^{i=\infty} \alpha_{i,j} \beta(r_i, r_k) n_i, \qquad (1)$$

where n_k, α, β_i, j, r and t are number concentration of flocs of size k, collision efficiency, collision frequency for particles of size class i and j with characteristic radius r_i and r_j, radius of particles and mixing time, respectively. The indices of i, j and k denote the class of particles consist of i, j and k primary mono particles. The first term in the right hand side of the equation indicates the formation of aggregates in kth class by collision of two lower class particles, and the second term is attributed to the loss of the particles in kth class by collisions of kth class particles with other classes of the particles. In later studies and by evaluation of complicated systems in various processing conditions, Eq. (1) has been corrected and modified to comply with the experimental results.

As it is known, aggregates breakup process is controlled by inter-particle forces within an aggregate and external exerted stresses by the fluid, as competitive forces. Therefore, it seems necessary to apply some other functions to Population Balance Equations (PBEs) which state the aggregates breakup in suspensions [26]. So, Eq. (1) can be rewritten as

$$\frac{dn_k}{dt} = \frac{1}{2}\sum_{i=1,j=k-1}^{i=k-1}\alpha_{i,j}\beta(r_i,r_j)n_in_j - n_k\sum_{i=1}^{i=\max}\alpha_{i,k}\beta(r_i,r_k)n_i - s_k + \sum_{j=k+1}^{j=\max}\Gamma_{k,j}s_jn_j, \tag{2}$$

where S_k is the fragmentation rate of agglomerates of size k and Γ_k, j is the breakage distribution function defining the volume fraction of the fragments of size k coming from j-sized particles. The third term on right hand side of Eq. (2) describes the loss of aggregates with size k by fragmentation, and the fourth term expresses the formation of flocs of size k through fragmentation of larger agglomerates.

It is completely disputable that analytical solution of PBEs is complicated. There exist different ways for discretization of the calculation space [27,28] and by the simplest one, the lengths of the selected intervals are equal (uniform discretization) [29]. However, due to the high volume of the calculations needed for considering the larger number of particle classes in this way, the non-uniform discretization has been usually employed. Thus, in order to model the evolution of the particle size distribution during dispersion, the solution of less number of differential equations would be required via using a suitable discrete model. Each section is represented by a characteristic volume V_i which is the average volume of the sizes included in the section. The overall discretization scheme can be summarized as [30]:

$$v_i = fv_{i-1}, \tag{3}$$

where f is the discretization factor, and in present study $f = 2$ was considered for discretization of the calculation domain [31]. This scheme is shown to be better than the uniform discretization method, because the large fragments can also be taken into account by using fewer equations and the complexity of the equations is reduced to a great deal. Therefore, the rate change of the number concentration of particles through coagulation and fragmentation process in suspensions can be written as [32]:

$$\frac{dN_i}{dt} = \sum_{j=1}^{i-2}2^{j-i+1}\alpha_{i-1,j}\beta_{i-1,j}N_{i-1}N_j + \frac{1}{2}\alpha_{i-1,i-1}\beta_{i-1,i-1}N_{i-1}^2 - N_i\sum_{j=1}^{i-1}2^{j-i}\alpha_{i,j}\beta_{i.j}N_j - N_i\sum_{j=i}^{i=\max}\alpha_{i,j}\beta_{i,j}N_j - S_iN_i + \sum_{j=i}^{i=\max}\Gamma_{i,j}S_jN_j, \tag{4}$$

where N_i is the number concentration of flocs with volume V_i.

2.2. *Agglomeration/coagulation*

Collision frequency is defined by the particles translational motion mechanism. These mechanisms are classified into three categories: Brownian motion, fluid motion and sedimentation. With the assumption that the Peclet number is large enough and the particles are same-sized, the major mechanism that brings the particle to collide together is fluid motion or orthokinetic translation. The collision frequency for turbulent shear-induced coagulation, in the absence of viscous retardation and binary collision of spherical particles and homogeneous, isotropic turbulence, is [33]:

$$\beta_{i,j} = 1.294\left(\frac{\varepsilon}{\nu}\right)^{\frac{1}{2}}\left(R_{c,i}+R_{c,j}\right)^3, \tag{5}$$

where ε shows the homogeneous turbulent energy dissipation rate of the stirred tank, and ν is the kinematic viscosity of the suspending fluid.

The collision radius, R_c, of an aggregate will determine aggregation kinetics and is a function of its fractal dimension (D_f) which can be expressed as:

$$R_{c,i} = R_p \left(\frac{i}{k}\right)^{\frac{i}{D_f}}, \tag{6}$$

where R_p is the radius of primary particles, and k is the lacunarity, a form of packing density; here, $k = 1$ is used [34]. From Eq. (6), it is clear that the smaller the D_f, the more openly and loosely structured the aggregate, and thus the larger its collision profile.

2.3. Viscous retardation

As two spherical particles approach to each other in fluid media, the viscous fluid layer between them suppresses the collision in some cases completely. In the population balance equations, viscous resistance is reflected in the collision efficiency, the ratio of the actual collision frequency, and the collision frequency in the case that every collision is assumed to be successful.

An analogous empirical form of Kusters' model of collision efficiency is thus adopted for this study as [31]:

$$\alpha_{i,j} = \left[\frac{\exp\left(-x\left(1-\frac{i}{j}\right)^2\right)}{(i \times j)^y}\right] \times \alpha_{\max}, \tag{7}$$

where i and j indicate the sections where the colliding aggregates are located. This function allows higher values of α_{ij} for aggregates of comparable sizes (i.e. when $i = j$), and lower values otherwise, with x and y as the fitting parameters and $\alpha_{\max}$ denoting the upper limit of α_{ij} $(0 \leq \alpha_{\max} \leq 1)$.

2.4. Fragmentation

The rupture and breakage of agglomerates in suspension can be caused mainly by hydrodynamic forces. The greater an aggregate becomes, the more susceptible to break will be. Different functions for breakup of agglomerates in suspensions, S_i, have been employed in the literature. Nevertheless, all of these functions have been brought into discussion in shear flow fields with neglecting the elongational flow field. In the present study, considering the elongational flow field and applying it in the S_i as ε'_e, the effect of the elongational flow field on aggregates breakup process would be evaluated.

Some of researchers [32,35] have reported an exponential relationship for breakup function of agglomerates in shear flow fields. The fragmentation rate, S_i, is:

$$S_i = \left(\frac{4}{15\pi}\right)^{\frac{1}{2}} \left(\frac{\varepsilon}{\nu}\right)^{\frac{1}{2}} \exp\left(\frac{-\varepsilon_{b,i}}{\varepsilon}\right), \tag{8}$$

where $\varepsilon_{b,i}$ is the critical turbulent energy dissipation rate at which the flocs are fragmented. Since larger aggregates are more susceptible to turbulent stresses, the value of it must be related to the agglomerate size inversely as:

$$\varepsilon_{b,i} = \frac{B}{R_{c,i}}, \tag{9}$$

where B is a fitting parameter. Using the results of Discrete Element Method (DEM) [20], a power-law relation for breakup of agglomerates in elongational flow fields can be proposed as:

$$S_i = K_B(\varepsilon_e^-)^p (r_i)^q. \tag{10}$$

In this equation, ε'_e, p and q are elongational rate and appropriate constants, respectively. As mentioned in the above, binary fragment size distribution is used which describes the fragmentation of agglomerate into two equal fragments [30]

$$\Gamma_{i,j} = \frac{V_j}{V_i}, \qquad j = i + 1,$$

$$\Gamma_{i,j} = 0, \qquad j \neq i + 1. \tag{11}$$

3. Results and discussion

In the present work, the dispersion behavior of agglomerates with two different structures, was studied in two different flow fields; shear and elongational flow fields. As there is no direct data available for elongational flow fields, the results obtained from Discrete Element Method (DEM) for shear and elongational flow fields were applied. For detailed information, one may refer to Hosseini et al. [20].

To follow the evolution of agglomerate dispersion process, weighted average fragment size, $< w >$, was defined and used as:

$$w = \frac{\sum_i n_i i^2}{\sum_i n_i i}, \tag{12}$$

where n_i is the number of agglomerate with i particles.

In solving the PBEs, the maximum number of particle classes is considered to be 25. To evaluate the breakup behavior of agglomerates in elongational flow field, the obtained results from DEM were applied through the breakup kernel of agglomerates within the framework of PBM. To do so, a comparison was made between the data obtained from DEM and the predicted ones from PBM, and by adjusting the fitting parameters, the best fitted data were obtained while $KB = 5.4213$, $p = 2.5$ and $q = 3$ (Figures 1 and 2). In addition, the constant parameters depend on operational conditions, material properties and type of the flow field. The material properties used for DEM and PBM calculations are listed in Table 1.

The results predicted for dispersion behavior of the agglomerates with fractal dimension of 2 in different flow fields were evaluated in terms of weighted average

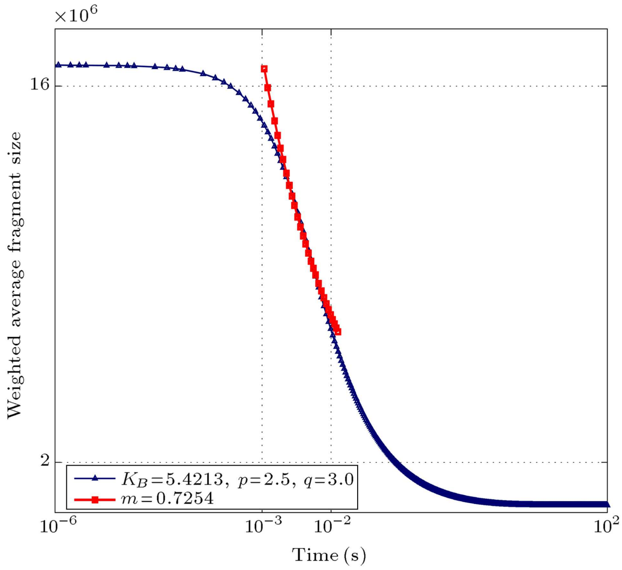

Figure 1. The most appropriate value for breakup kernel (elongational flow field, $\varepsilon_e = 224$ (1/s) and $D_{sf} = 2.00$).

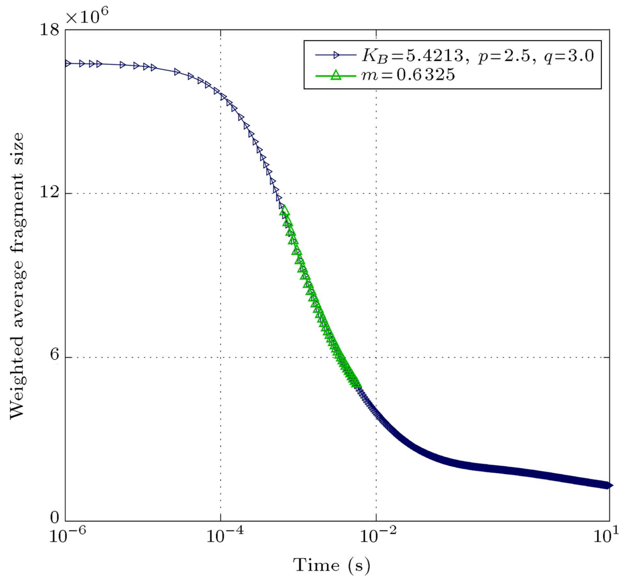

Figure 2. The most appropriate value for breakup kernel (elongational flow field, $\varepsilon_e = 56$ (1/s) and $D_f = 1.66$).

Table 1. The properties of the particles.

Property	Value	Unit
Density	1.05×10^3	kg m^{-3}
Hamaker constant	1.3×10^{-20}	J
Fluid viscosity	8.4×10^{-4}	Pa.s
Radius of particles	100	Nm
Collision Diameter	0.5	Nm

fragment size versus mixing time and were demonstrated in Figures 3 and 4 for shear and elongational flow fields, respectively.

Increasing shear rate, G, increased the level of agglomerate dispersion process, and the values of

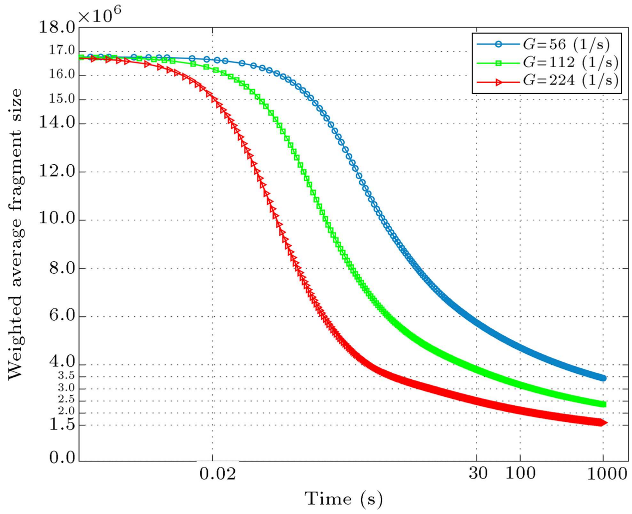

Figure 3. The effect of shear flow field on dispersion process of agglomerate versus time, $D_f = 2.00$.

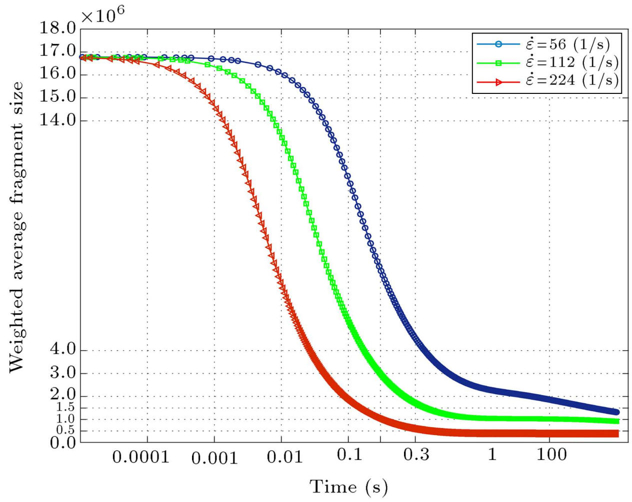

Figure 4. The effect of elongational flow field on dispersion process of agglomerate versus time, $D_f = 2.00$.

weighted average fragment size, $< w >$, decreased during mixing process (Figure 3). Similar trend was obtained for the elongational flow field which is shown in Figure 4. In elongational flow field, increasing the deformation rate would cause the breakup process of the agglomerate to commence at earlier stage of mixing process, and lead to steady state fragment size more quickly than that was achieved for shear flow field which has been verified by the experimental results reported by Powell and Mason [21]. This could be explained in terms of the higher ability of the elongational flow field to breakup agglomerates in comparison to shear one. The predicted results showed that the choice of the breakup kernel for elongational flow field reflected the characteristics of such flow fields. It can be also noted that the same expected trend can be found regarding the shear flow field and the selected breakup kernel for it through

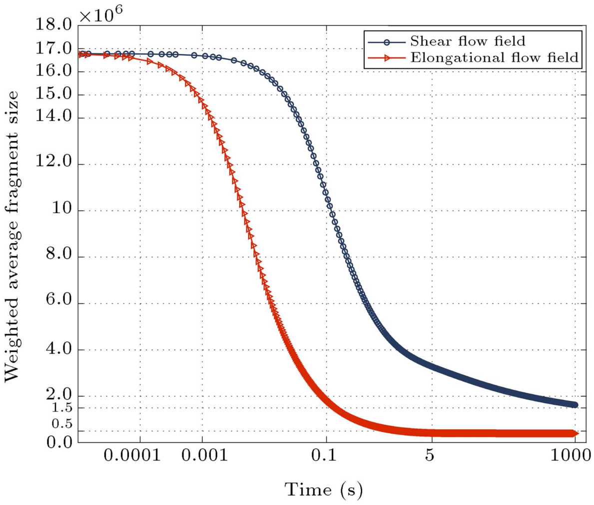

Figure 5. Comparison between shear and elongational flow field at deformation rate of 224 (1/s), $D_f = 2.00$.

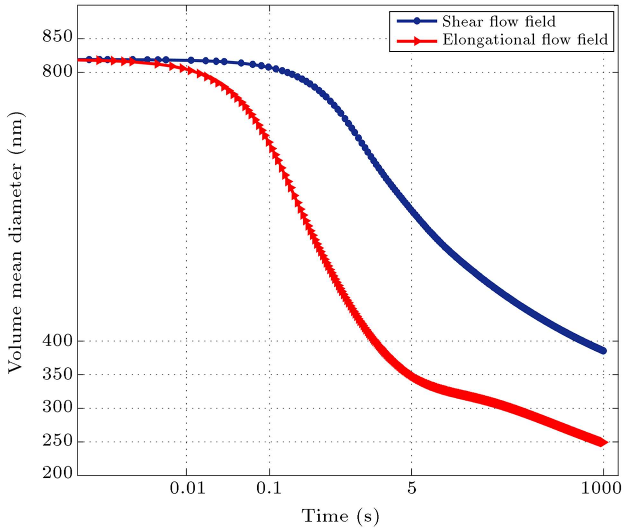

Figure 6. Comparison between volume mean diameter of agglomerate in shear and elongational flow fields at deformation rate of 56 (1/s).

the framework of PBM. Comparing Figures 3 and 4, one may notice that increasing the deformation rate of elongational flow field has less effect on the level of agglomerate dispersion than that of shear one which can be clearly discerned through Figure 5. Since, as mentioned before, the elongational flow field has more capability in breaking up the agglomerates than the shear one, achieving such results through the mixing process within suspensions was expected. Figure 5 compares the dispersion process of the agglomerates in elongational and shear flow fields. As can be noticed, in elongational flow field, the breakup process started at earlier time of mixing and reached to steady state fragment size more quickly than shear flow field. This could be due to the ability of elongational flow field in fragmenting the agglomerates. This is consistent with the results of DEM [20], where it has predicted that the elongational flow field was more efficient in breaking up the agglomerate than shear one. As the earlier studies have shown [18,20], since the rotation tensor in the elongational flow field is zero, there would not be any rotating movement which is proceeded to rearranging the agglomerates structure, as well as aligning in the direction of the flow field, so ensuing to intensify the breakup of the agglomerates. This is while in shear flow fields, rotation tensor is inconceivable to zero, rotating the agglomerates within the flow field occurs and rearranges to more denser, packed and hard-to-break one. It depicts the appropriate accuracy in choosing the breakup kernel as to shear and elongational flow fields.

The evolution of dispersion process was also studied using Volume Mean Diameter (VMD) of agglomerates defined as:

$$\mathrm{VMD} = d[4,3] = \frac{\sum_i n_i d_{c,i}^4}{\sum_i n_i d_{c,i}^3}. \tag{13}$$

Figure 6 shows the changes of Volume Mean Diameter (VMD) during mixing process for shear and elongational flow field. As can be seen, in elongational flow field, breakup process of agglomerates begins at earlier time of mixing than in shear flow, and smaller size of aggregates was achieved at the end of the mixing process.

Table 2. PDI for different flow fields in steady state.

Kinds of flow field	**Poly dispersity index**
Shear Flow Field	1.3200
Elongational Flow Field	2.0128

The effect of different flow fields on the steady state fragment size distribution of agglomerate is indicated through Figure 7 in terms of particle fraction vs. particle number fraction (Figure 7(a)) and normalized dimensionless floc diameter (Figure 7(b)). As one may notice from Figure 7 and Table 2, the shear flow field showed narrower agglomerate size distribution than that obtained for the elongational flow field. It could be due to the fact that in elongational flow field, more agglomerates will be subjected to breakup and this could lead to have agglomerates with wide range of sizes and classes, making the size distributions broader in comparison to that of shear one. In contrast, in the case of shear flow field, owing to its limited ability through fragmentation of agglomerates and the fact that in shear flow fields, the fragments are more compact than their parents [24,36], the final achievable agglomerate size is limited to larger agglomerates than that for elongational flow field. Accordingly, larger agglomerates will breakup to reach this certain size resulting in narrower size distribution.

Figures 8 and 9 show the evolution of the ag-

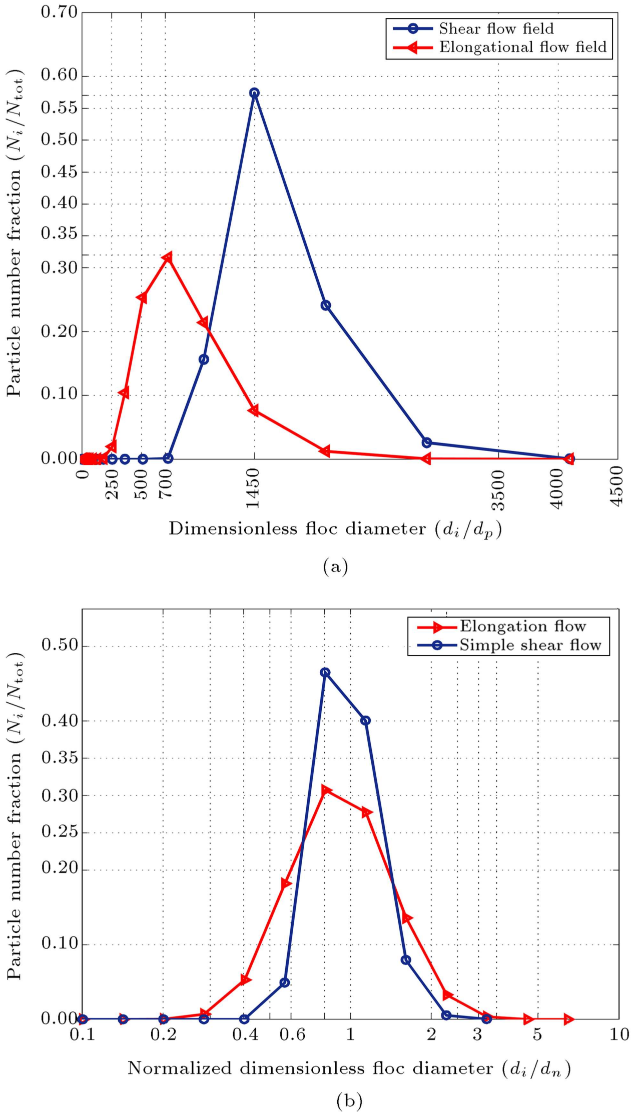

Figure 7. Effect of different flow fields on steady state fragment size distribution in (a) dimensionless floc-size coordinates (scaled by the diameter of the primary particle size, d_1) and (b) normalized dimensionless floc diameter.

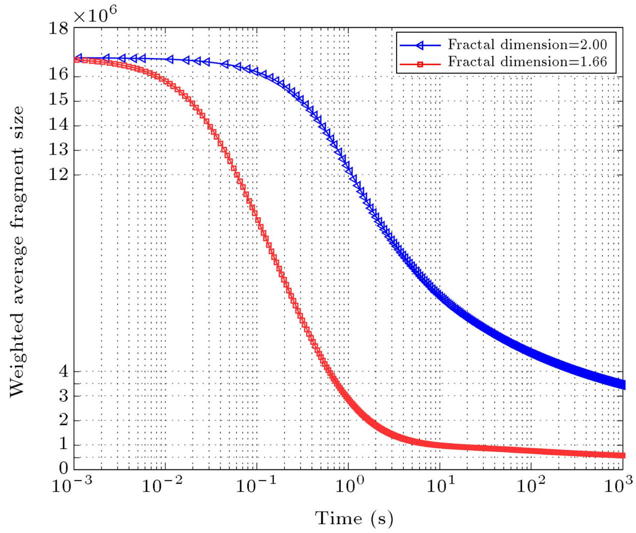

Figure 8. The effect of different agglomerate structure on dispersion process in shear flow fields.

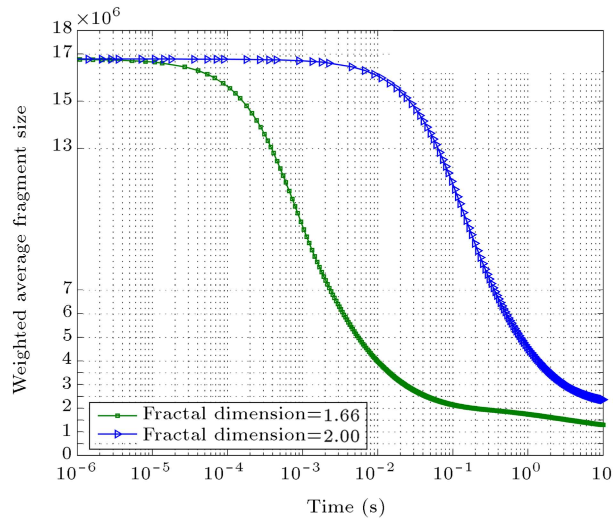

Figure 9. The effect of different agglomerate structures on dispersion process in elongational flow fields.

glomerate dispersion process for the agglomerates with different structure (different fractal dimensions) in shear and elongational flow fields, respectively. As was expected, any decrease in fractal dimension results in increasing the dispersion level of the agglomerate, which is due to the more porous and loose structure of agglomerates with lower fractal dimension. Comparing the results obtained for shear and elongational flow field showed that the final fragment size of the agglomerates, achieved in shear flow field, was more sensitive to variation of fractal dimension. These could be explained as, on one hand, in elongational flow field and regardless of the size and structure of the agglomerate, the breakup process reaches its equilibrium state. On the other hand, in shear flow field, the majority of the agglomerate breakup takes place at the earlier stages of the dispersion process, where the agglomerate strength heavily depends on its structure. In shear flow fields, after a while, the agglomerate will rearrange to form a more packed structure, which will suppress the agglomerate breakup and control the final agglomerate size.

4. Conclusion

The dispersion process of agglomerates in different flow fields was studied by a population balance model, PBM, by using the results predicted from Discrete Element Method (DEM). Employing the results obtained from DEM, a breakup kernel was adopted for elongational flow field to be used in the population balance equations by which the effect of elongational flow field on the breakup of the fragments could be evaluated.

It was shown that in the elongational flow field, the breakup process of agglomerate seems to be much faster than that of shear one and reaches its steady state size at earlier stages of the dispersion process compared to the shear flow field. Moreover, the results depict that the agglomerate breakup process in elongational flow field leads to broader fragment size distribution. It was also indicated that the final fragment size in elongational flow field is almost independent of the agglomerates structure and fractal dimension, while in shear flow field, it depends on the structural variation of agglomerate.

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Biographies

Amir Afshar received his BSc degree in the field of Chemical Engineering, Design of Petroleum Industries Processes, from Technical Faculty of IAU (South-Tehran Branch), Iran, and his MSc Degree in the field of Chemical Engineering, minor in Polymer Engineering from Sahand University of Technology (SUT), Tabriz, Iran, in 2009 and 2011 respectively. From April 2011, he has been working as an E.M. laboratory assistant at University of Tehran, UT. Besides, he is a member of the Iranian Polymer Society, IPS, and National Nanotechnology Laboratory Network, NNLN.

Mahdi Salami Hosseini received his BSc degree in the field of polymer engineering, from Amirkabir University of Technology, in 2001. Afterward, he received his MSc and PhD degrees at Amirkabir University of Technology and graduated in 2004 and 2009, respectively, majoring in the field of simulation and modeling of the polymeric liquids dynamics and suspension rheology. He is now working at Sahand University of Technology as a member faculty in Polymer Engineering Department. His field of interest can be summarized as: Computational rheology, polymeric fluids dynamics, polymer processing, suspension rheology and simulation of transport phenomena in polymeric systems.

Ehsan Behzad Far received his BSc and MSc degree in the Polymer Engineering at Amirkabir University of Technology, in 2006 and 2008, respectively. His research interests in both of these courses were focused on the suspension rheology and modeling of suspension behavior especially the agglomerate breakup process. He is now doing his Ph.D. at University of British Colombia in the field of suspension rheology.