LARGE EDDY SIMULATION OF PARTICLE-PARTICLE INTERACTIONS IN TURBULENT FLOW: COLLISION, AGGLOMERATION AND BREAK-UP EVENTS

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Abstract

A numerical study of particle-particle interactions in a turbulent flow is performed using an Eulerian-Lagrangian particle tracking code with a hard-sphere collision model extended to take into account coalescence between the colliding particles and break-up of agglomerates. The effect of the agglomerate fractal dimension on the break-up events, and eventually on collision and agglomeration, is presented. The computational domain was seeded with primary particles (calcite, a nuclear waste simulant) of size 60 micron and allowed to run until steady state before the particle-particle interactions were activated. Break-up events reduce as the agglomerate fractal dimension (d_f = 2.0, 2.5, 2.8 and 3.0) increases, and with no break-up event as the control, the effect of break-up on particle-particle interactions is presented. The results show an increase in the number of collisions, and the number of collisions leading to agglomeration, with a decrease in the agglomeration rate and agglomerate size with increasing hydrodynamic stress, as a consequence of break-up.

1 Introduction

Particle agglomeration is likely to occur during some stages of the waste management process (retrieval and transport) of UK legacy nuclear waste, resulting in unwanted effects such as the formation of deposits and plugging of transfer and process pipes. Agglomerates also affect the viscosity, solid settling rate, and other waste characteristics that affect pumping. The rate of agglomeration in pumps and in pipe flow are important characteristics that feed into transport prediction models used in the industry. Rector and Bunker (1995) have shown that the primary particle size, agglomerate diameter and the fractal dimension of the agglomerate have a significant effect on two important sedimentation parameters, namely the settling rate and gel point. Previous studies (e.g. Balakin et al, 2012; Breuer and Almohammed, 2015; Ho and Sommerfeld, 2002; Njobuenwu and Fairweather, 2015; Njobuenwu and Fairweather, 2016b) have considered the effect of particle size, flow turbulence, particle restitution coefficient, gravity and the structure model of the arising agglomerate (volume-equivalent sphere model, inertia-equivalent sphere model, and closely-packed sphere model) on the number of particle collisions, and those that lead to agglomeration. The number of collisions leading to agglomeration was determined by the sticking potential due to the van der Waals forces. Whilst Ho and Sommerfeld (2002) adopted a stochastic collision model, Balakin et al (2012), Njobuenwu and Fairweather (2015) and Breuer and Almohammed (2015) applied a deterministic approach based on the hard-sphere collision model.

In most studies, agglomeration is considered alone, without accounting for the effect of break-up of agglomerates in studying the stability of colloidal suspensions. In suspensions populated with solid agglomerates, these agglomerates might break up either from inter-agglomerate collisions, through impact with a wall or due to hydrodynamic shear forces in the flow (Ammar et al, 2012). In this paper, we will restrict our efforts to investigating agglomerate break-up in turbulent flow due to hydrodynamic shear stress in the flow. Accounting for break-up events in agglomeration processes is important as break-up is one of the two main mechanisms that can interrupt the growth of an agglomerate in a destabilised suspension of infinite extent, with the other mechanism being sedimentation which removes large aggregates from the suspension (Babler et al, 2015). Therefore, simulation of agglomeration and break-up together is important to determine agglomerate size distributions. Agglomerate break-up by turbulent structures has been extensively studied in the context of break-up of droplets in shear flows, e.g. Jones and Lettieri (2010), for which the mechanisms involving droplet deformation are completely different from break-up of solid agglomerates. In contrast, little work seems to have been carried out on the influence of turbulent shear stresses on the break-up of solid agglomerates. Recent work by (Babler et al, 2015) has shown that the hydrodynamic shear stresses in a turbulent flow acting on a single agglomerate act in opposition to the van der Waal's adhesive forces binding the agglomerate together and can break an agglomerate. We adopt the (Babler et al, 2015) break-up model in this work.

The overall aim of this study is, therefore, to perform a fully coupled simulation of particle-

particle interaction in a dense suspension, accounting for particle-fluid interactions and particle-particle interactions (collisions, agglomeration and break-up). These phenomena must all be accounted for in developing a framework for the modelling and simulation of solid-liquid separation using computational fluid dynamics techniques, enabling the prediction of sludge settling efficiency. This paper, therefore, studies particle-particle interactions to understand particle agglomeration and break-up in turbulent flow using nuclear waste simulant properties.

2 Mathematical formulation

A four-way coupled Eulerian-Lagrangian approach is adopted since the suspension is dense with high particle volume fractions. In large eddy simulation (LES), the continuity and Navier-Stokes equations are spatially filtered so that the energy-containing large-scale turbulent motions are directly solved for. On the other hand, the scales smaller than the filter width, the subgrid scales (SGS), are modelled. The filtered governing equations with the influence of the dispersed phase can be expressed as:

$$\frac{\partial \overline{u}_j}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\overline{\sigma}_{ij} - \tau_{ij}\right) + \frac{\Pi}{\rho} + \frac{S_{m,i}}{\rho} \tag{2}$$

where $\overline{\sigma}_{ij} = -2\nu\overline{s}_{ij}$ represents the viscous stress, $\overline{s}_{ij} = \frac{1}{2}(\partial\overline{u}_i/\partial x_j + \partial\overline{u}_j/\partial x_i)$ is the filtered strain-rate tensor, ν is the kinematic viscosity, $\tau_{ij} = \overline{u_i u_j} - \overline{u}_i\overline{u}_j$ is the SGS tensor which represents the effect of the SGS motions on the resolved motions, t is time, x_j is the spatial co-ordinate directions, u_j is the velocity vector, p is the pressure, and ρ is the density. The SGS tensor is computed using the dynamic version of the Smagorinsky model proposed by Piomelli and Liu (1995). Its specific implementation has been presented in a recent paper (Njobuenwu and Fairweather, 2016a). $\Pi = -\rho u_\tau^2/h$ is the mean pressure constant imposed along the streamwise direction (z-axis) that drives the flow. $S_{m,i}$ is a source term and accounts for the action on the fluid of the particles, given by the sum of all hydrodynamic forces in the momentum equation due to all particles in a fluid computational cell.

The BOFFIN-LES code was used to solve the LES equations. The shear Reynolds number of the channel flow was $Re_\tau = u_\tau h/\nu = 590$ based on the shear velocity, u_τ, the channel half height, h, and the kinematic viscosity, $\nu = 10^{-6}$ m^2 s^{-1}, with the density $\rho = 10^3$ kg m^{-3}. The computational domain was discretised using grid nodes of 129×129×129 in the wall normal, spanwise and streamwise directions, respectively.

The motion of a particle in an LES predicted turbulent flow field can be viewed as a random process with its position determined by a deterministic part, evaluated in terms of filtered values, and a stochastic component, arising from the SGS turbulent motions of the fluid phase. For a solid-liquid flow, hydrodynamic forces (drag, shear lift, pressure gradient and added mass) are considered and a stochastic Markov model (Bini and Jones, 2007; Bini and Jones, 2008) is used to represent the influence of the unresolved carrier fluid velocity fluctuations experienced by a stochastic particle over a time interval dt which is added to the deterministic contribution.

An Adams 4th-order predictor-corrector method is used for the particle equation of motion integration in a Lagrangian particle tracking (LPT) code, with a trilinear interpolation scheme employed for the fluid dynamic properties at the particle position and the non-linear Schiller and Naumann correction used for the drag coefficient. Other forces accounted for are the shear-lift, added mass and pressure gradient, and the fluid SGS velocity fluctuations. The particle momentum was fed-back to the fluid momentum equation as a source term. The time step used was set equal to that of the LES, while particle initial velocities were equal to those of the fluid at the particle position. For particle-particle interactions, the deterministic hard sphere frictionless collision model (Rani et al, 2004; Sundaram and Collins, 1996) is used subject to the following assumptions:

- particles and agglomerates are modelled as spheres; interaction between particles is due to binary collisions;
- only van der Waals' forces are responsible for post-collision adhesion;
- only small deformations of particles are allowed post-collision; and
- agglomeration is based on the pre-collision energy momentum balance and van der Waals' interactions (Breuer and Almohammed, 2015).

Break-up is defined as a singular event in time, i.e. there is an exact moment in time when an agglomerate turns from being intact into being broken. We assume that this happens when the local hydrodynamic stress ($\sigma \sim \mu(\varepsilon/\nu)^{1/2}$) at the agglomerate position, acting on the agglomerate, exceeds a critical stress, σ_{cr} (Babler et al, 2015; Babler et al, 2012; Babler et al, 2008); where ε is the turbulence energy dissipation rate at the position of the agglomerate, and μ and ν are the dynamic and kinematic viscosities. The critical stress σ_{cr} is a characteristic of the considered agglomerate, that is, σ_{cr} is a function of the aggregate properties such as size, structure, type of the constituting particles, and the chemical environment. Among these variables, the size of the aggregate is most crucial. A large body of experimental, numerical and theoretical studies, see Babler

et al (2015) and cited references, suggest a power law dependency of the form:

$$\sigma_{cr} \sim r^{-q} = N_{pp}^{-q/d_f} \qquad (3)$$

where $N_{pp} \sim r^{d_f}$ is the number of primary particles constituting the agglomerate, d_f is the agglomerate fractal dimension, r is the radius of the primary particle, and q is a scaling exponent that depends on the agglomerate structure. For dense but non-compact agglomerates, Zaccone et al (2009) obtained $q = [9.2(3 - d_f) + 1]/2$, which has been shown to perform well when compared with experimental data (Harshe et al, 2011). There are no exact models to effect break-up, and recent research (Babler et al, 2015; Babler et al, 2012; Babler et al, 2008) has been limited to detecting the moment break-up events are likely to occur. We adopt this model for detecting break-up events for small agglomerates and subsequently break-up the parent agglomerate into two daughter particles. This method of breaking an agglomerate into two parts is a popular modelling assumption mainly because of the lack of data for other types of break-up modes.

3 Results and discussion

The channel was laden with N_0 = 2,747,570 spherical calcite particles (d_p =60 µm), a simulant for UK legacy waste sludge, at volume fraction α_p=10^{-3}, with the mechanical properties for this simulation listed in Table 1 (Ho and Sommerfeld, 2002; Tomas, 2007).

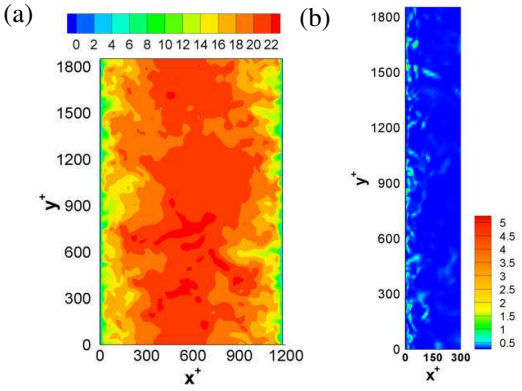

Figure 1: Instantaneous contour profiles at the plane z^+=3678, (a) streamwise fluid velocity (w^+), and (b) turbulence kinetic energy dissipation rate, (ε^+).

Simulations were carried out for agglomeration without break-up events as a control (no break-up) and then with break-up of agglomerates formed from the injected primary particles by varying the fractal dimension, d_f = 2.0-3.0. Turbulence in the suspending fluid, with strong non-homogeneity and the presence of a mean shear in the channel flow, shown in Figure 1(a) for $Re_\tau = 590$, has a distinct influence on the agglomeration process by facilitating collisions amongst particles (Njobuenwu and Fairweather, 2015) and inducing break-up of the formed aggregates (Babler et al, 2015). Break-up occurred mostly in the near-wall region where the hydrodynamic stresses, $\sigma \sim \varepsilon^{1/2}$, resulting from the local energy dissipation rate, ε, are largest, as shown in the contour map of Figure 1(b).

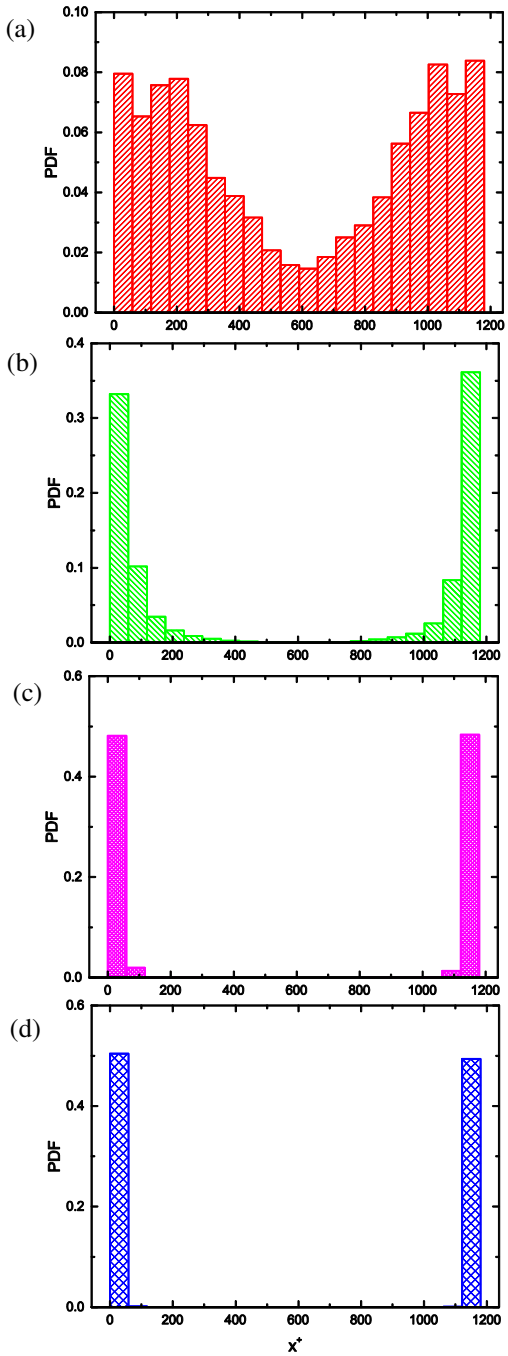

Figure 2: Influence of fractal dimension, d_f, of the agglomerate structure on the probability density function, PDF(x^+), of the non-dimensional position in the wall-normal direction where break-up events occur; d_f = (a) 2.0, (b) 2.5, (c) 2.8 and (d) 3.0.

The effect of the fractal dimension on the location where break-up events occur, irrespective of the size of the agglomerates involved, is shown in Figure 2. It has been shown in Soos et al (2006) that agglomeration of solid primary particles in a typically random process results in agglomerate structures with fractal dimensions around 2.0, while under flow conditions the value of the fractal dimension can be significantly larger, even up to its threshold value of 3.0 due to the restructuring and breakage processes. Hence, in this work, we have limited our studies on the sensitivity of agglomerate break-up to the fractal dimension to the range d_f = 2.0 to 3.0. With respect to the high kinetic energy dissipation rates shown in Figure 1(b), it is clear in Figure 2 that the fractal dimension has a large effect on the probability of where along the wall-normal direction, x^+, an agglomerate break-up occurs. For fractal dimension d_f = 2.0, Figure 2(a) shows agglomerate break-up occurring across all positions between the two parallel walls bounding the channel flow, most of which occur in the near-wall region. This observation is significantly different compared to all other cases where d_f > 2.0. In particular, for d_f = 2.8 and 3.0, agglomerate break-up occurs at the plane closest to the both walls where the stresses are at a maximum.

Table 1: Simulation and properties of calcite.

Density	ρ_p [kg m^{-3}]	2710
Minium distance	δ_0 [m]	3.36×10^{-10}
Resitution coefficient	e_n [-]	0.4
Youngs's modulus	E [Pa]	2.0×10^{8}
Hamaker constant	H [J]	3.8×10^{-20}

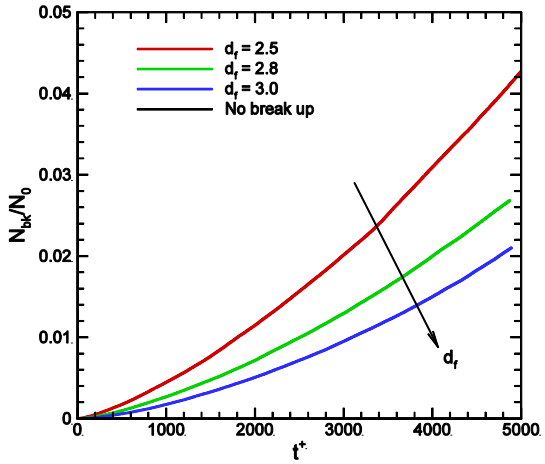

Figure 3: Influence of fractal dimension d_f of the agglomerate structure on the time history of break-up events, N_{bk}, normalised by the initial number of primary particles, N_0 (no break-up is zero).

We further investigated the impact of variations of the agglomerate fractal dimension, d_f, as a constant in the range 2.0-3.0. The results in Figure 3 show, as expected, that the break-up rate decreases with increasing the fractal dimension from 2.5 to 3.0. In terms of the number of collision events shown in Figure 4, these events are in line with the break-up events as more collisions occur with increasing numbers of break-up events and with time. Break-up events populate the flow with agglomerates with a smaller number of primary particles which have a higher propensity to collision and subsequent agglomeration (Balakin et al, 2012; Breuer and Almohammed, 2015; Njobuenwu and Fairweather, 2015). Figure 5 shows the population of collisions that result in agglomeration, N_{agg}, hereafter called agglomeration events, and the population of agglomerates, N_a, as a consequence of agglomeration and break-up events. Initially, both populations are similar, but differences grow with time as more events take place. The number of agglomeration events with time is similar for the four cases of break-up processes considered, but slightly different at longer simulation times. The agglomeration events decrease as the break-up event is increased from 'no break-up' through d_f = 3.0 to d_f = 2.5. The case with d_f = 2.5 has the highest number of agglomeration events consistent with the highest number of inter-particle collisions, see Figure 4, as well as the highest number of break-up events, see Figure 3. The high number of inter-particle collisions is a prerequisite for a large number of agglomeration processes, assuming that the sticking force is large enough (Breuer and Almohammed, 2015), while break-up events populate agglomerates with fewer numbers of primary particles, a precursor to a high collision rate (Njobuenwu and Fairweather, 2015).

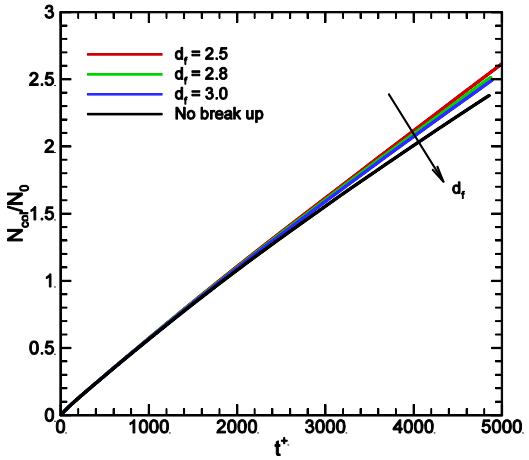

Figure 4: Influence of fractal dimension d_f of the agglomerate structure on the time history of the total number of the particle collisions, N_{col}, normalised by initial number of primary particles, N_0.

As expected, the number of agglomerates of any number of primary particles in the system at any time has a trend directly opposite to the agglomeration and break-up events, as these two events depopulate agglomerates with time. Interestingly, the agglomeration rate (also known as the collision efficiency), defined as the total number of particle–particle colli-

sions leading to agglomeration to the total number of collisions (i.e. N_{agg}/N_{col}), shown in Figure 6, differs only slightly between the no break-up case and those cases with three fractal dimensions. In addition, based on the effect of break-up events, the no break-up case predicts the highest global agglomeration rate while the d_f =2.0 case has the lowest agglomerate rate, an indication that an increase in the hydrodynamic stress decreases agglomerate size, with summaries at dimensionless time t^+ = 5000 given in

Table 2. This is also evident in Figure 7, where the agglomerates with two, three, four, five and six primary particle sizes are shown with time, with the no break-up case showing the highest number of agglomerates for the five agglomerate sizes, while those with the smallest fractal dimension of d_f = 2.5 (equivalent to the highest hydrodynamic stress) show the least number of agglomerates. This phenomena was observed in previous work (Njobuenwu and Fairweather, 2015) where it was noted that agglomerate sizes reduce with increasing levels of turbulence.

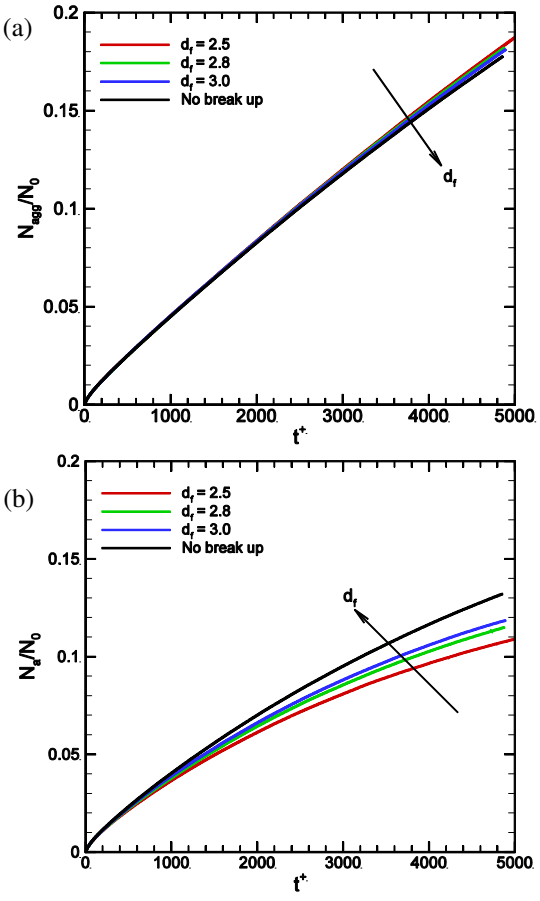

Figure 5: Influence of fractal dimension of the agglomerate structure on the time history of (a) the total number of the particle–particle collisions leading to agglomeration, N_{agg}, and (b) the total number of agglomerates, N_a, both normalised by the initial number of primary particles, N_0.

Table 2: Frequencies of the break-up (N_{bk}/N_0), particle-particle collisions (N_{col}/N_0), agglomeration events (N_{agg}/N_0), number of agglomerates (N_a/N_0) and agglomeration rate (N_{agg}/N_{col}) obtained using different fractal dimensions after a dimensionless time t^+ = 5000.

d_f	N_b/N_0	N_{col}/N_0	N_{agg}/N_0	N_a/N_0	N_{agg}/N_{col}
2.0	6.46×10^{-2}	2.81	0.172	0.065	6.14×10^{-2}
2.5	4.27×10^{-2}	2.62	0.187	0.109	7.16×10^{-2}
2.8	2.69×10^{-2}	2.52	0.182	0.115	7.23×10^{-2}
3.0	2.10×10^{-2}	2.50	0.181	0.119	7.26×10^{-2}
∞	0.00×10^{-0}	2.38	0.178	0.132	7.46×10^{-2}

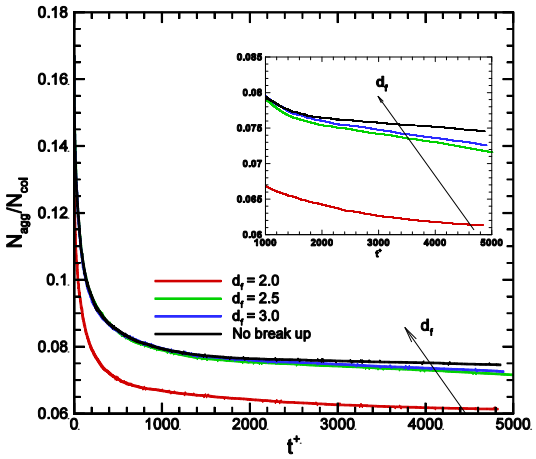

Figure 6: Influence of fractal dimension of the agglomerate structure on the time history of the agglomeration rate, N_{agg}/N_{col}.

4 Conclusions

LES and LPT have been used to simulate particle agglomeration and break-up events, together with a deterministic treatment of inter-particle collisions and particle feedback effects on the fluid phase. Agglomeration is based on the pre-collision energy momentum balance, restitution coefficient and van der Waals' interactions, while agglomerate break-up occurs instantaneously subject to a hydrodynamic stress exceeding a critical value dictated by the properties of the agglomerates modelled using their fractal dimension. Break-up events increase with simulation time and as the fractal dimension decreases. A greater number of collisions that lead to agglomeration was observed at higher levels of break-up since this increase the number of agglomerates of smaller size. Break-up events therefore reduce the number of agglomerates in the system, especially when a doublet particle is broken into two singlets. Although there is a larger number of collisions, and collisions leading to agglomeration, their ratio N_{agg}/N_{col} decreases with time due to the high number in the denominator.

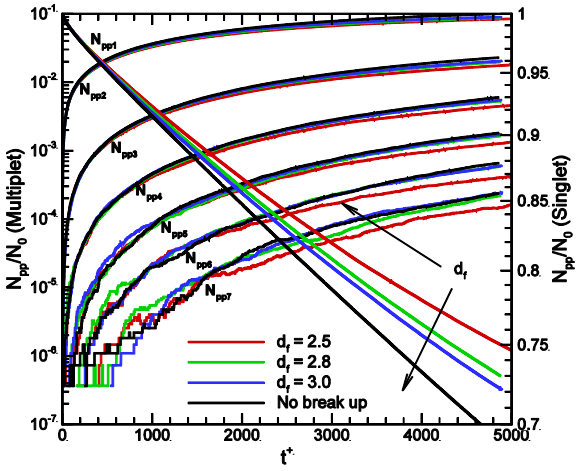

Figure 7: Influence of fractal dimension of the agglomerate structure on the time history of the population of single and multiple particles.

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