

Restructuring of colloidal aggregates in turbulence

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Aggregation (Coagulation, Flocculation)



up to milimeters

Picture: Soos et al., J. Colloid Interface Sci. (2008)



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Picture: Korin et al., Science (2012)



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Ecology and Inland Fisheries

























Structure of colloidal aggregates

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Moussa et al., Langmuir (2007)



[1] Babler et al., Langmuir (2010), [2] Soos et al., J. Colloid Interface Sci. (2008), Ehrl et al., Langmuir (2008)



Aggregation kinetics in flows

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Open aggregate Dense aggregates Small d_f large d_f Consider an aggregate *i* colliding with an aggregate j i, j = number of primary particle per aggregate $K_{ij} \sim (R_i + R_j)^3 \sim (i^{1/d_f} + j^{1/d_f})^3$

 \Rightarrow d_f can be estimated from measuring the aggregation rate



Aggregation kinetcs: Population balance equations

- Homogeneous suspension
- Aggregation, breakup, and restructuring
- Evolving fractal dimension
 - At a given time, all aggregates have the same d_f

$$\frac{dN_i}{dt} = \frac{1}{2} \sum_{j=1}^{i-1} K_{A,j,i-j} N_j N_{i-j} - N_i \sum_{j=1}^{\infty} K_{A,i,j} N_j$$
$$- K_{B,i} N_i + \sum_{j=i+1}^{\infty} g_{i,j} K_{B,j} N_j$$

- *K*_{A,i,j}: Porous sphere model [1]
 - Takes into account hydrodynamic and colloidal interaction
- $K_{B,i}$: Critical stress model [3]

[1] Babler, AIChE J. (2008), Babler et al., Langmuir (2010), [2] Babler et al. J. Fluid Mech. (2008), Babler et al. PRE (2012)













- Polystyrene particles
- $d_p = 420 \text{ nm}, \phi = 2 \times 10^{-5}$
- Coagulant: Al(NO₃)₃, 0.16 w%
- Fully destabilized particles





Experimental

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- PBE to solve for $N_i(t)$
- Parameterized function for *d_f(t)* to describe the evolution of the aggregate structure



• $d_{f,\infty} = 2.34$ from regrowth experiments









Fitting $d_f(t)$ and c(t) to the evolution of $\langle R_g \rangle$ and I(0)







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Onset and duration of restructuring





Onset and duration of restructuring

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• The onset of restucturing is more sensitive to the shear rate G



Onset and duration of restructuring



- The onset of restucturing is more sensitive to the shear rate G
- The duration of restructuring scales with the shear rate G



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Conclusions

- Restructuring, in terms of the evolution of the fractal dimension, has been explored by fitting a PBE model to a set of experimental data.
- Restructuring sets in as the aggregates reach a certain size, and it is finished before they reach the steady state size.
- The aggregate size for the onset of restructuring depends stronger on the shear rate than the steady state aggregate size. This contradicts findings of Vanni and Gastaldi, *Langmuir* (2011) who studied open isostatic clusters by DEM.
- Restructuring is relatively fast and is duration scales approximately with the shear rate.
- Macromixing becomes important at high stirring speeds.





Initial fractal dimension







Final fractal dimension







Breakage parameter



Backup Slides



Evolution of df and breakage param

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• Fitting independent time evolution of d_{f} , c, and q