

## **SIMULATION OF HYDRATE AGGREGATE STRUCTURE VIA THE DISCRETE ELEMENT METHOD**

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### **ABSTRACT**

As the oil industry moves from a heuristic of avoidance of hydrates to a heuristic of risk management time dependent phenomena of hydrate formation and plugging must be known. One of the key parameters to this process is the aggregation of hydrate particles, the fractal networks they form, and the effect these two parameters have on flow. Unfortunately the aggregation and fractal structure information is extremely difficult to acquire experimentally, for this reason a three-dimension discrete element method (3D-DEM) model has been implemented.

The 3D-DEM model calculates detailed solutions to Newton's equations of motion for individual particles. In addition these particles are coupled with the surrounding fluid through computational fluid dynamics (CFD). This coupled 3D-DEM can be used to investigate what the effects of shear, suspending viscosity, attractive forces, and other relevant variables have on the structure, stresses, and positions of the hydrate particles over time. In addition, the effect on viscosity has been calculated using CFD and compared back to basic hard sphere theory.

*Keywords:* clathrate hydrates, rheology, DEM, CFD

### **NOMENCLATURE**

CFD Computational Fluid Dynamics  
DEM Discrete Element Method  
LB Lattice Boltzmann

### **INTRODUCTION**

Hydrates have been of particular interest to oil and gas companies since they were shown to block pipelines by Hammerschmidt in 1934 [1]. Since

that time hydrate flow assurance heuristics have evolved from hydrate avoidance to hydrate management. Management of hydrates is a particularly difficult topic since the flow and agglomeration of the hydrate slurries must be understood. To aid in this conceptual understanding discrete element modeling (DEM) coupled with computational fluid dynamics (CFD) has been undertaken. These simulations will help

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to enhance our fundamental understanding of hydrate agglomeration by simultaneously providing access to variables like fractal dimension and rheological property parameters.

### SIMULATION METHODOLOGY

DEM is a family of simulations used in simulating bodies (i.e. particles) subject to bulk motion. DEM is typically used in situations where there are large discontinuities which cannot be described by continuum solutions (e.g. granular materials) [2]. DEM explicitly accounts for the forces and motions of all individual particles throughout time by integrating Newton's equations of motion.

The Lattice Boltzmann (LB) method is a type of computational fluid dynamics based on the Boltzmann equation. The system is discretized into a lattice of velocity vectors representing an ensemble of fluid particles at this location. As time evolves particles can move to or collide with particles at other lattice points. The rules that govern these collisions are consistent with Navier-Stokes equations of state, yielding satisfactory CFD results. In addition LB has the advantage that it greatly simplifies boundary conditions. Interactions with boundaries are treated as elastic collisions with particles [2]. This is a great simplification over other methods (i.e. finite difference method) where a solvable mesh must be found [3]. For this work, code from Prof. Tony Ladd at the University of Florida has been used and modified [4].

### RESULTS

To first verify the code for our simulations hard spheres were tested in planar shear. Shear stress for the runs were computed and the relative effective viscosity was compared against the hard sphere relationship of Krieger and Dougherty [4]. As can be seen in Figure 1 the simulations are in good agreement with the model.

To test the effect attractive forces have on flow, capillary bridge attractive forces from Rabinovich *et al.* [6] have been implemented into the simulations. The effect this has on relative viscosity is plotted in figure 2. Here relative viscosity is plotted against volume fraction and is compared against the hard sphere base line.

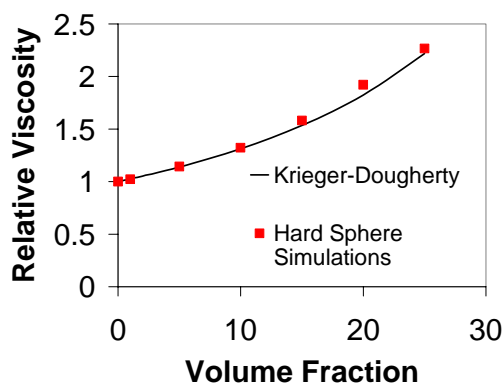


Figure 1: Hard sphere simulations show good agreement with Krieger-Dougherty relationship.

Figure 2 clearly shows how attractive forces increase the relative viscosity of the system as the volume fraction increases. At very low volume fractions (i.e. 1%) the spheres do not interact and attractive forces have no effect. However as the volume fraction increases the spheres interact more and form aggregates. In these simulations it is seen that these aggregates occlude volumes of liquid and are deformed by the shearing fluid, both of which increase the effective viscosity of the system.

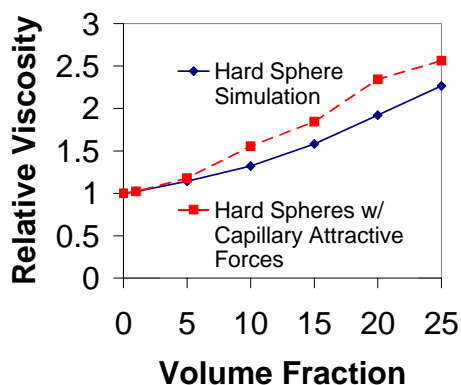


Figure 2: Attractive forces increase the relative viscosity over the hard sphere base case.

To test how flow affects the structure of aggregates a diffuse aggregate was created, shown in Figure 3, (Figure 3a is the side view of the aggregate and Figure 3b is the top view of the same aggregate). This structure of ninety-nine particles was created using diffusion limited growth by randomly adding particles onto the

surface of the aggregate. The diffusion limited growth yielded a fractal dimension of 1.99. This aggregate was then placed in a shear flow field (going from left to right in Figure 3 a) and its structure was monitored over time. In Figure 4 (where Figure 4a is the side view of the aggregate and Figure 4b is the top view of the same aggregates), the effects of shear on this structure can be seen. The initially diffuse aggregate has broken into two smaller aggregates. Both aggregates appear to be denser in packing and more planar in shape than the initial structure.

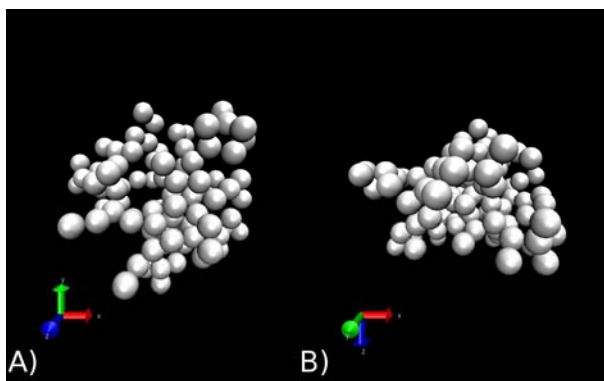


Figure 3: Initial diffusion limited aggregate structure. (A side view, B top view)

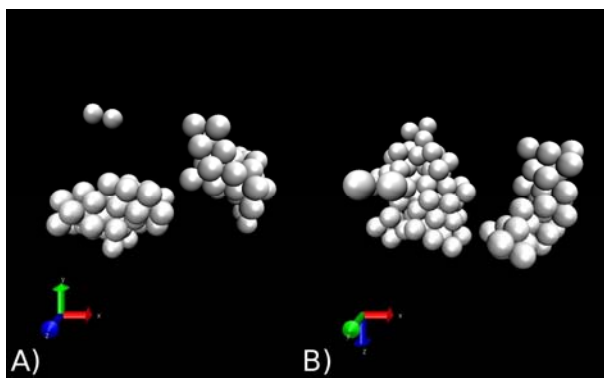


Figure 4: Fractal dimension increases due to shear over time. (A side view, B top view)

The fractal dimension for the larger aggregate (seen on the left in Figure 4a and 4b) was calculated to be 1.82. The smaller aggregate (seen on the right in Figure 4a and 4b) was calculated to be 1.97. This seems to suggest that the new aggregates are more diffuse than the original

aggregate; however one can clearly see this is not the case. The initially structure was roughly spherical and diffuse. The aggregates formed from shear flow are more planar but densely packed. Both structures give a fractal dimension of  $\sim 2$ , yet the initial diffuse structure has a much larger occluded volume. This shows that fractal dimension does give some information about the structure of the aggregates but misses out on some key properties (*e.g.* aspect ratio) as well. This shows that parameters in addition to fractal dimension will need to be considered. These simulations have shown to be a useful way in determining what these parameters may be and provide a possible tool to predict expected values.

## CONCLUSIONS

DEM coupled w/ CFD has proven to be an intriguing novel method to investigate hydrate agglomeration and the effect hydrates have on suspensions. These simulations also provide a useful way to probe the effect attractive forces have on relative viscosity. In addition they are useful in probing experimentally difficult variables such as fractal dimension while the system is undergoing shear. Finally one of the most useful pieces is that simulations allow us to visualize aggregation and the effect of flow on the aggregates, helping to enhance our conceptual understanding. This visualization can show us that even though the fractal dimension of aggregates may not be changing, the structure of the aggregates may still be changing.

## ACKNOWLEDGEMENTS

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## REFERENCES

- [1] Sloan E.D. and Koh C.A. *Clathrate Hydrates of Natural Gasses*, 3<sup>rd</sup> Edition., CRC Press, Boca Raton, FL, 2008.
- [2] Sukop M.C. and Thorne D.T. *Lattice Boltzmann Modeling*. Springer, New York, NY, 2006.
- [3] Ladd A.J.C. *Numerical Simulations of Particulate Suspensions via a Discretized Boltzmann Equation Part I. Theoretical Foundation*. J. Fluid Mech. 1994;271:285-309.

- [4] Macosko C.W. *Rheology Principles, Measurements, and Applications*. Wiley-VCH, New York, NY, 1994.
- [5] Ladd, A.J.C. and Verberg, R. *Lattice-Boltzmann simulations of particle-fluid suspensions*. J. Stat. Phys., 104:1191-1251, 2001.
- [6] Rabinovich Y.I., Esayanur M.S, and Moudgil, B.M.. *Capillary Forces between Two Spheres with a Fixed Volume Liquid Bridge: Theory and Experiment*. Langmuir. 2005;21:10992-10997.