Particle Separation Control
for Efficient Biofuel Energy Generation

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Synopsis

The project involved development of an agent-based computer model for transport of particulate matter in biofuel production systems, as well as application of this model to two different types of biofuel generation systems. The computational model examines particles of both spherical and non-spherical shape transported in a flow with complex geometry. The particles can be non-adhesive or adhesive, e.g., via van der Waals or liquid bridging adhesion. The agent-based model integrates to a finite-volume fluid dynamics code (U2RANS) to account for effects of particle transport in a flow. Applications of the computational method was made to: (1) combustion of biowaste particles, such as grain hulls or pellets, (2) separation of particles from the surrounding aqueous medium (de-watering), and (3) enhancement of algae growth rate in algae-based biofuel production systems.

In the first application area, the particle agents in the model represent pieces of biowaste products, such as wood chips or grain hulls. In this part of the project, we shared our computer code with a collaborator at the University of Iowa specializing in combustion, and worked together with the investigators at Iowa to train a graduate student in using this code. The University of Iowa graduate student then used the code to compute biowaste particle combustion in a stoker burner, with comparison to experimental results obtained at Iowa.

In the second application area, we examine methods for separation of particles from the surrounding aqueous medium. This type of de-watering problems arise in many areas of biofuel generation, e.g., in processes attempting to concentrate algae from suspension in algae production systems prior to oil extraction. We have identified a new fluid dynamic phenomenon in which a particle suspension flowing through a corrugated tube exhibits a

drift of the particles toward the tube center. The underlying mechanics of this new phenomenon have been identified and described mathematically.

In the third application area, we examine experimental data on the effect of fluid mixing on algae growth rate, which various from results showing that mixing enhanced growth rate by more than 250% to other results showing that it has little or no effect. We have coupled a model for algae growth to our particle transport model, and have integrated the combined model to spectral-based direct numerical simulation code for turbulent flows. The numerical model was then used, together with simpler heuristic models, to clearly identify the conditions under which significant enhancement of algae production occurs in a turbulent flow. The computational results are able to explain the widely divergent experimental data on algae growth rate enhancement and clearly delineate the conditions for enhancement of algae growth by mixing. Of particular interest is that finding that algae growth rate saturates at mixing rates beyond a critical value, so that for more rapid mixing no further enhancement is observed.

Introduction

Particulate flows are encountered in an extraordinarily broad array of industrial, environmental and biological problems, encompassing within it diverse subfields such as aerosol dynamics, sediment transport, colloidal dispersions, fluidized beds, and cohesive granular flows. Many of these flows are of great importance in generation of alternative energy sources, including biofuels and hydrogen. For instance, it is common to utilize biowaste products, such as wood chips, corn stalks, grass, cereal hulls, etc., to generate electricity by combustion processes. The biowaste products are processed into small pieces (particles, often of non-spherical shape), which are then fed into a combustion chamber, sometimes together with traditional combustion sources such as coal. Particle flow problems govern the fuel feeding process, the combustion process, and the ash collection process – all of the key processes for biowaste power generation. As a second example, one of the most promising technologies for generation of both biodiesel and of hydrogen comes from algae production. Two key aspects of reducing the cost of algae production are that are enhancing the algae growth rate (with minimal energy input) and efficiently extracting oil and hydrogen from the algae. Both of these concern optimization of a flow containing adhesive particles (algae cells) interacting with the surrounding turbulent fluid flow in geometrical regions (bioreactors) of complex shape.

Particle Transport Model

The primary focus of the current project is to develop, implement and test new computational methods for prediction of particulate flows typically observed in biofuel and hydrogen generation systems, as discussed above. To be useful, these computational methods need to be able to efficiently handle systems with large numbers (tens of thousands) of particles; function with particles that are adhesive, collide frequently, and are in general non-spherical; and solve for flows and particle transport in geometrically complex regions. The following advances were made during the course of the project:

1. A new highly efficient discrete element method (DEM) was developed for flows with adhesive particles (Journal Paper 6). The method uses a multiple time scale approach to achieve rapid computational speeds with large number of particles. New models are proposed for rolling, sliding and twisting resistance of particles exposed to adhesive forces.

2. A level-set based method is developed which allows particles to be transported on a Cartesian mesh even in highly complex flow domains (Journal Paper 5). The method was implemented for a micronozzle flow field, as well as other flows fields of interest. The level-set method is much faster than the previous method, which requires searching for particle positions on a complex mesh at each particle time step.

3. A new, highly efficient model was developed for transport and collision of ellipsoidal particles (Journal Papers 5, 9 and 10), which can be used to represent elongated biofuel pellets or chips. The model introduces new methods for modeling of collision or non-spherical particles.

4. A new computational method was introduced for modeling particles transported in the presence of an electric field (Journal Paper 4). This method is a common approach to particle separation/extraction processes.

Biowaste Combustion

We have worked, together with our collaborators at the University of Iowa, to integrate the discrete-element model for particle transport with a combustion model for the particles. The particle/combustion model is then integrated with the finite-volume fluid dynamics code U2RANS. The computations use our level-set method to allow rapid particle transport simulations in combustion units of complex shape. Sample biofuel combustion calculations have been performed by our colleagues at the University of Iowa using our combined computer code (see Figure 1). These calculations also utilize a radiation module added to the code to compute radiant heat transfer between a particle and the combustion unit wall.

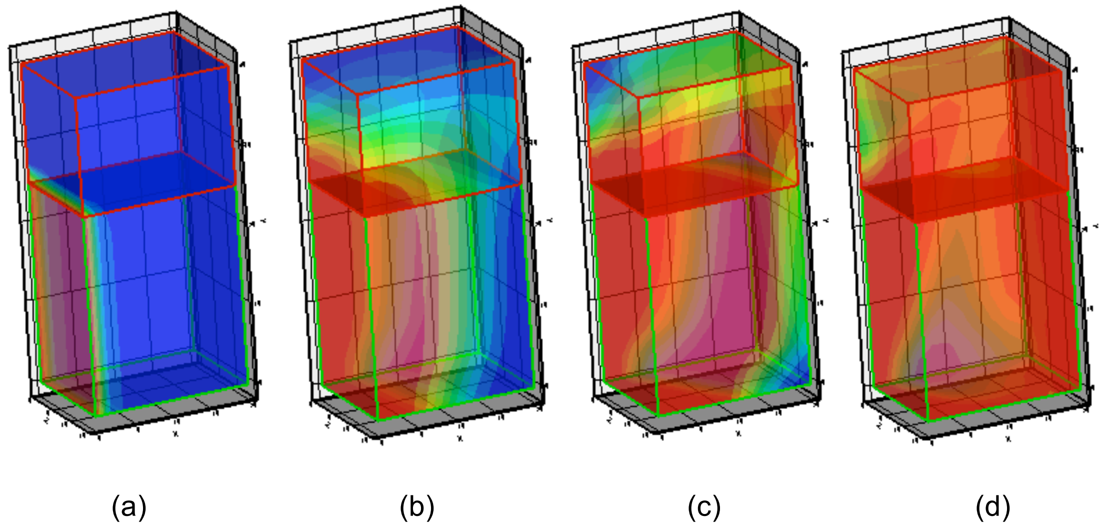

Figure 1. Time series of three-dimensional temperature profiles in a rectangular combustion unit obtained from simulation of biofuel particles injected at the left-hand wall of the combustor. (Courtesy of Albert Ratner, University of Iowa.)

Particle Separation Process

We have shown in a series of two papers (Journal Papers 3 and 8) that particles immersed in a suspension exposed to oscillating straining rate will tend to drift toward the nodal points of the straining field. The reason for this drift has been clearly explained and modeled in terms of the dynamic properties of the damped Mathieu equation (Journal Paper 8). This new fluid dynamic phenomenon is demonstrated to cause an inward drift of particles in a corrugated pipe flow toward the pipe center (Figure 2), thereby separating the particles from the surrounding fluid (Journal Paper 3). An illustration of this process is given in Figure 2, showing the particle positions from an end view at three different times during the separation process. The separation process is particularly efficient at low Reynolds numbers, and hence would work well for smaller tube sizes characteristic of microfluidic systems. The particle focusing is related to the tube corrugations, and does not occur in the absence of tube corrugations. A theory has been developed explaining why the particles exhibit the focusing phenomena, and predicting the rate at which focusing occurs for different tube geometries.

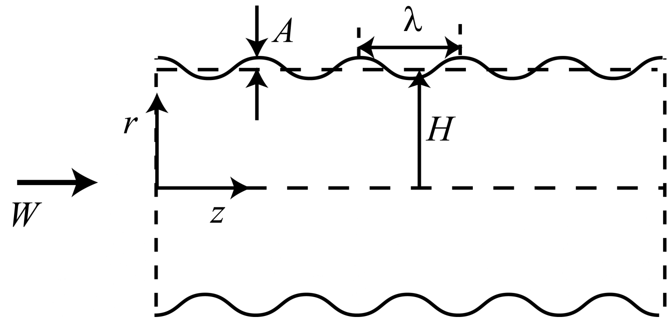

Figure 2. Schematic diagram of flow in a corrugated pipe.

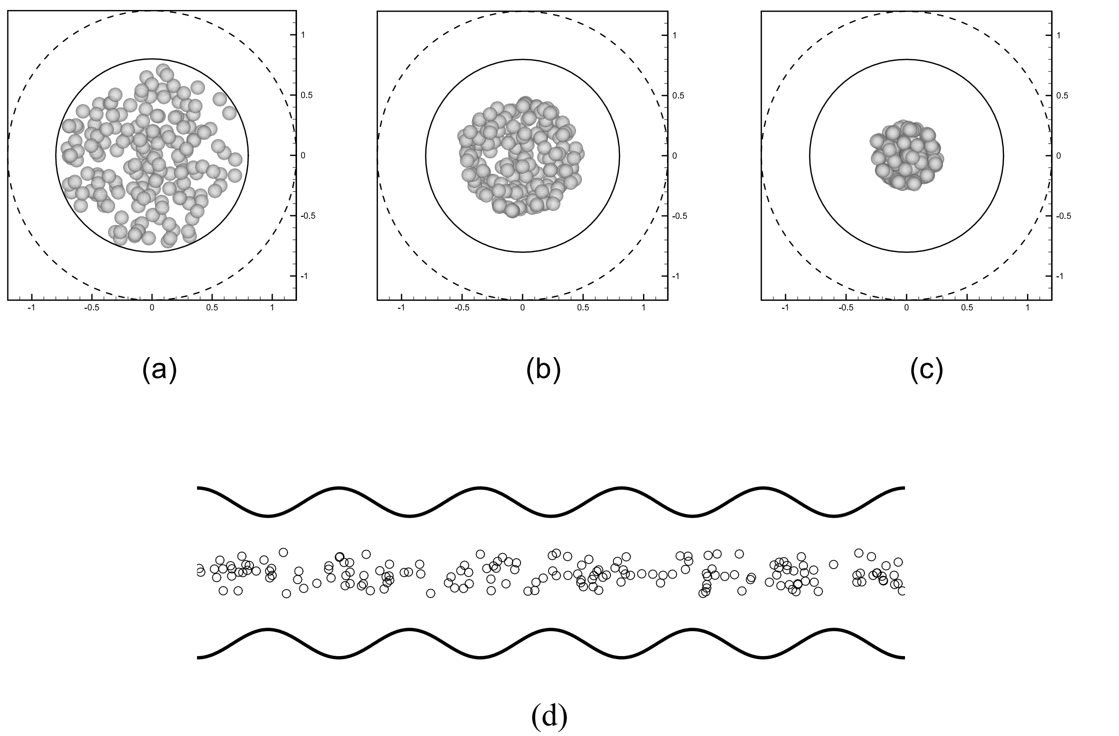

Figure 3. Time series showing particles focusing at the center of a corrugated tube for a case with Reynolds number Re = 10, from an end view. The dashed circle denotes the maximum (crest) of the tube corrugations and the solid circle represents the minimum (trough) of the corrugations. The side view in frame (c) is shown in frame (d).

Algae Growth Enhancement

We have coupled a well-known model for algae growth rate in a light-limited environment, which is typical of commercial algae production systems, to our discrete-element method code, together with the Beer-Lambert law for light attenuation by the algae. The resulting numerical method is used to examine the effect of fluid mixing on algae growth rate (Journal Paper 2). A simple model is first examined in which the algae with a single frequency in accordance to

$$y_n(t) = -\frac{H}{2} + \frac{H}{2}\cos(\omega t + \phi_n) \qquad (1)$$

where H is the depth of the algae-containing mixed layer, ω is mixing frequency, and ϕ_n is a random variable with uniform probability distribution in the interval $-\pi/2 < \phi_n < \pi/2$. The various parameters in the model are selected based on experimentally-obtained values for typical algae production systems. A plot is given in Figure 4 showing the increase in algae growth rate with time for different values of the mixing frequency, where the case with $f \equiv 2\pi\omega = 0$ corresponds to no mixing. It is found that the effect of mixing on algae growth saturates at a certain mixing frequency, which was not previously realized. Increase in mixing rate beyond this saturation point will cost energy, but not enhance algae growth.

It is also found that the extent to which algae growth rate is increased by fluid mixing is highly dependent on the fraction of the algae-containing fluid layer which is penetrated by the light. This latter length scale is associated with the inverse of the light decay rate $\phi\sigma$, where ϕ is the algae concentration and σ is a light attenuation coefficient. Figure 5 shows that at large light penetration depths (small values of $\phi\sigma$), there is little or no enhancement of algae growth rate by fluid mixing. However, at smaller light penetration depths (large values of $\phi\sigma$), while the overall growth rate decreases, the enhancement of growth rate by mixing dramatically increases. These findings are in agreement with experimental data of a number of studies, some of which show small enhancement of growth rate with mixing and some showing large enhancement. Indeed, some experimental studies have demonstrated that growth rate enhancement with mixing increases, on a percentage basis, with increase in algae concentration, but the reason for this finding was not previously understood.

Our algae growth / particle computational model was then implemented together with a pseudo-spectral method for direct numerical simulation of homogeneous turbulent flow (Figure 6), in which all scales of a turbulent flow are predicted. The results for algae growth rate enhancement in turbulent flow was in qualitative agreement with results from our simple single-frequency model, provided that the mixing time scale is set equal to the eddy-turnover time scale of the turbulent flow (defined as the turbulence integral length scale divided by the root-mean-square velocity fluctuation).

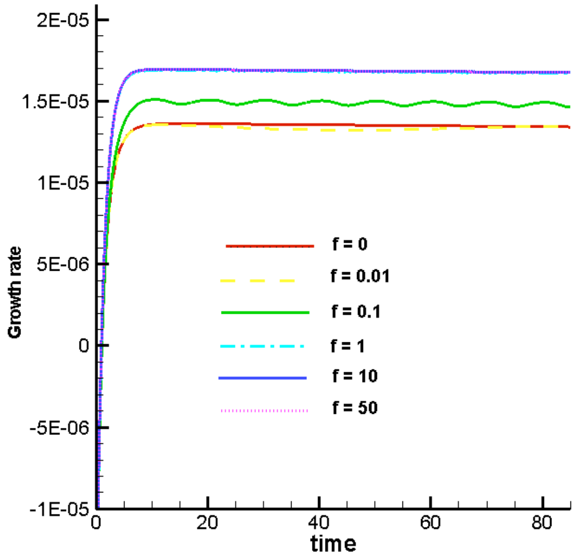

Figure 4. Enhancement of algae growth rate for different dimensionless mixing frequencies.

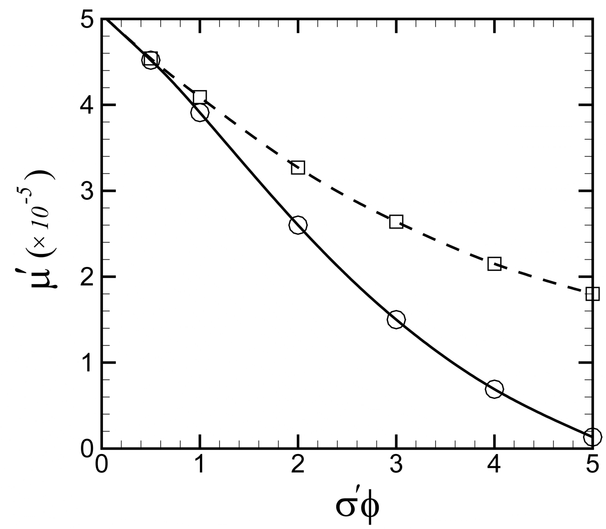

Figure 5. Variation of maximum algae growth rate μ with the inverse depth of the illuminated layer $\sigma'\phi$ for cases with no mixing (circles and solid line) and with rapid mixing ($f' = 1$; squares and dashed

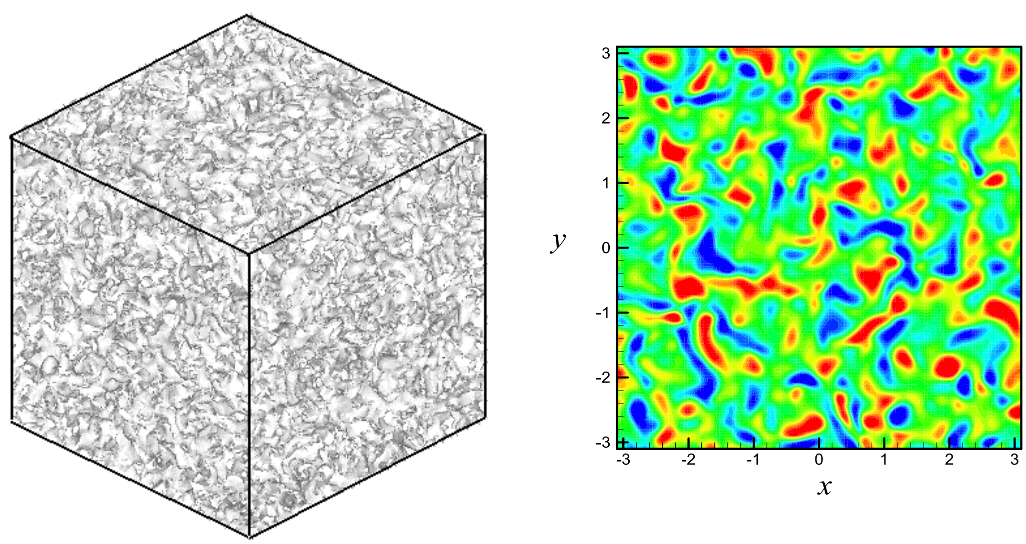

Figure 6. Plots illustrating the homogeneous turbulence flow field used for computing effect of turbulence on algae growth rate: (a) $\lambda_2 = 0$ iso-surface in a three-dimensional perspective view, illustrating the vortex structures in the turbulent flow field, (b) contours of ω_z in the $z = 0$ cross-sectional plane

In order to provide a rapid, but accurate, method for prediction of the effect of turbulence on algae growth rate, we have developed an integrated algae-hydrodynamics computational method that includes the following parts:

(1) Reynolds-Averaged Navier-Stokes (RANS) model of turbulent fluid flow in reactor,
(2) stochastic Largangian model for turbulent fluid fluctuations,
(3) simulation of light intensity in reactor, and
(4) simulation of algae growth rate within reactor.

The RANS model provides prediction for the mean velocity field and averaged turbulence quantities, such as turbulent kinetic energy and dissipation rate. The stochastic Lagrangian model solves a stochastic differential equation of the Langevin form

$$du_i' = -\frac{u_i'}{T_\ell}dt + \left(\frac{4q_i}{T_\ell}\right)^{\frac{1}{2}} d\xi\,, \qquad (1)$$

where $q_i = \overline{u_i'u_i'}/2$ is the turbulence kinetic energy associated with the i^{th} component of the fluctuating velocity field and T_ℓ is the eddy turn-over time, which is related to the turbulence dissipation rate ε and the total turbulent kinetic energy $q = q_1 + q_2 + q_3$ by $T_\ell = q/3\varepsilon$. The differential $d\xi$ is a Gaussian distributed random variable with zero mean and variance equal to the time step dt. The solution for light intensity within the reactor solves the Beer-Lambert equation with light refraction effects, and the algae growth rate model solves the Eilers-Peeters model for three-phase algae growth. The key new feature in this computational approach is the use of a stochastic Lagrangian model to connect RANS based turbulence simulations with algae growth simulations, which had not been done previously.

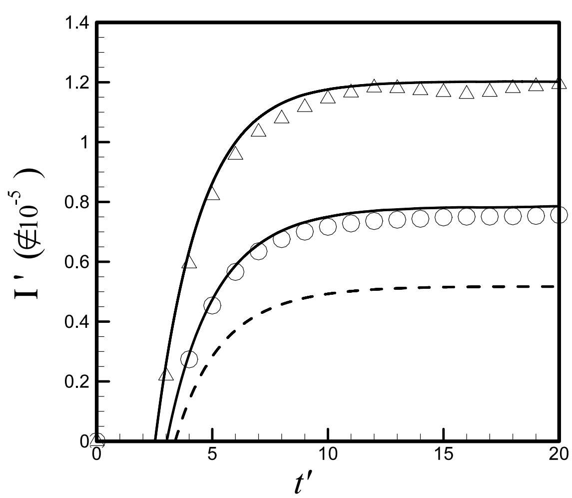

Figure 7. Predicted dimensionless growth rate as a function of dimensionless time for cases with no flow (dashed line), predictions from the direct numerical simulation of Marshall and Haung (2010) for mixing with $f_T = 0.36$ (circles) and $f_T = 1.8$ (triangles), and the corresponding predictions from the stochastic Lagrangian model with the same turbulent kinetic energy and dissipation rate (solid lines).

In Figure 7, predictions for the dimensionless algae growth rate with no flow (dashed lines) are compared with those for forced homogeneous turbulence with dimensionless mixing frequency $f_T \equiv T_S / T_\ell$ of 0.36 and 1.8, where T_S is the photosynthesis time scale. The results with turbulent flow are shown both for the direct numerical simulation (DNS) (symbols) and for the stochastic Lagrangian approach (lines). The stochastic Lagangian approach is found to match nearly exactly with the DNS results.

Final Results

This project has improved the state-of-the-art for modeling of fluid and particulate flows critical to biofuel and hydrogen generation in a number of ways. (1) We have developed a computational method for discrete-element modeling which exceeds in capabilities, speed and accuracy any other such model in the world. The model allows for adhesive particles, two-way coupling with the fluid, particle combustion, non-spherical particles, particle interaction with an electric field, and particle transport in complex domains. (2) We have utilized our computational model to discover a new fluid dynamical phenomenon allowing continuous-flow separation of particles from the surrounding liquid in a continuous manner with low energy dissipation. A mathematical theory explaining this new phenomenon has been developed and demonstrated. (3) We have integrated a stochastic Lagrangian model for algae particle motion with a RANS turbulent prediction method and a model for algae growth, and used the combined model to examine the effect of turbulent fluid mixing on algae production. A simplified model for effect of mixing on algae growth was developed and validated by comparison to simulations using direct simulation of turbulent flow. It is found that a saturation state exists beyond which more rapid mixing does not cause on increase in algae growth rate. Previous experimental results for algae growth rate, which appear to contradict each other, have been explained by our model. A stochastic Lagrangian model for turbulent fluid fluctuations was developed and used to move algae particles. The predicted values with this stochastic approach are nearly identical to those predicted with a direct numerical simulation of the full turbulent flow field. Using the computational methods developed in this study, it is for the first time possible to accurately simulate clustering and growth rate enhancement of algae particles during algae biofuel production processes.

PROJECT DATA

Students:

Gregory Hewitt, "A computational investigation of particle focusing and dispersion in corrugated tubes," M.S. Thesis, University of Vermont, December, 2009.

Kyle Sala, "A stochastic Lagrangian model of turbulent mixing for algae growth prediction in photobioreactors," accelerated M.S., University of Vermont (in progress), expected graduation Dec. 2012.

***Journal Papers*:**

Paper #1 is an invited review article covering computational methods for adhesive particle flows relevant to energy and environmental engineering. This paper is written jointly with two collaborators from Tsinghua University in Beijing, who work extensively on biofuel combustion problems. Papers #2 and #3 examine the effect on algae production rate of fluid mixing with different intensities. Papers #4 and #9 describe new particle separation methods developed during the project and demonstrated using an agent-based computational method. Paper #8 describes a new type of discrete-element model for efficient computation of flows with adhesive particles. Paper #7 illustrates use of the level-set method for particle transport in a complex domain, which was developed during the course of the present project. Paper #5 presents an extension of the discrete-element method for particles exposed to an electric field. Papers #6, 10 and 11 describe a new highly efficient computational method for non-spherical colliding and adhesive particles, and then apply the method to analysis of aggregate structures observed in blood flow. The same computational methods as described in these papers can be used for simulation of non-spherical biofuel particles in complex domains.

1. Li, S.-Q., Marshall, J.S. and Yao, Q., "Adhesive particulate flow: the discrete element method and its application in energy and environmental engineering," *Progress in Energy and Combustion Science* (invited review article, in preparation).

2. Marshall, J.S. and Sala, K., "A stochastic Lagrangian approach for simulating the effect of turbulent mixing on algae growth rate in photobioreactors," *Chemical Engineering Science* (in preparation, 2010).

3. Marshall, J.S. and Huang, Y., "Effect of fluid mixing on light-limited algae growth in homogeneous turbulence," *Chemical Engineering Science*, Vol. 65, No. 12, pp. 3865-3875 (2010).

4. Hewitt, G.F. and Marshall, J.S., "Particle focusing in suspension flow through a corrugated tube," *Journal of Fluid Mechanics*, doi:10.1017/S0022112010002697 (in press, 2010).

5. Liu, G.Q., Marshall, J.S., Li, S.-Q., and Yao, Q. "Discrete-element method for particle capture by a body in an electrostatic field," *International Journal for Numerical Methods in Engineering* (in press, 2009).

6. Chesnutt, J.K.W. and Marshall, J.S., "Structural analysis of red blood cell aggregates under shear flow," *Annals of Biomedical Engineering*, Vol. 38, No. 3, pp. 714-728 (2010).

7. Mousel, J. and Marshall, J.S., "Aggregate growth and breakup in particulate suspension flow through a micro-nozzle," *Microfluidics and Nanofluidics*, Vol. 8, No. 2, pp. 171-186 (2010).

8. Marshall, J.S., “Discrete-element modeling of particulate aerosol flows,” *Journal of Computational Physics*, Vol. 228, pp. 1541-1561 (2009).

9. Marshall, J.S., “Particle clustering in periodically-forced straining flows,” *Journal of Fluid Mechanics*, Vol. 624, pp. 69-100 (2009).

10. Chesnutt, J.K.W. and Marshall, J.S., “Effect of particle collisions and aggregation on red blood cell passage through a bifurcation,” *Microvascular Research*, Vol. 78, pp. 301-313 (2009).

11. Chesnutt, J.K.W. and Marshall, J.S., “Blood cell transport and aggregation using discrete ellipsoidal particles,” *Computers & Fluids*, Vol. 38, pp. 1782-1794 (2009).

***Conference Presentations*:**

1. Marshall, J.S., “Particle segregation in the presence of oscillating straining flows,” 61st Annual Meeting of the Fluid Dynamics Division of the American Physical Society, San Antonio, Texas, Nov. 23-25, 2008.

2. Marshall, J.S., “Particle segregation in oscillating straining flows,” IMA Conference on Dense Granular Flows, Isaac Newton Institute, University of Cambridge, Cambridge, UK, Jan 5-9, 2009.

3. Marshall, J.S., “Discrete-element modeling of adhesive particle flows,” IBM-BECAT Workshop on High Performance Computing, University of Connecticut, Storrs, Dec. 17, 2008.

4. Hewitt, G. and Marshall, J.S., “Particle focusing and dispersion in suspension flow through a corrugated tube,” 62nd Annual Meeting of the Fluid Dynamics Division of the American Physical Society, Minneapolis, MN, Nov. 22-24, 2009.

5. Hewitt, G.F. and Marshall, J.S., “Particle focusing in a corrugated tube,” International Conference on Multiphase Flow, University of Florida, Gainesville, FL, May 30-June 4, 2010.

6. Marshall, J.S. and Huang, Y., “Simulation of light-limited algae growth in homogeneous turbulence,” Algae and Energy in the Northeast, Burlington, Vermont, March 17-18, 2010. (poster)

7. Marshall, J.S. and Huang, Y., “Simulation of light-limited algae growth in homogeneous turbulence,” Vermont EPSCoR Annual Conference, Burlington, Vermont, March 11, 2010. (poster)