Particle Technology Forum



The PTF Newsletter



This "epic" issue of our newsletter is a testament to the prolific contributions of the PTF Award winners, and their impact on science. The upcoming Summer Issue will be dedicated to sharing technical information across various subdisciplines in Particle Technology. I am soliciting contributions from **all** PTF members who are interested in sharing snippets of their research.

The deadline for <u>submission</u> is **July 1st.**

Special thanks to Mayank Kashyap for taking the pictures during the PTF dinner.

Shrikant Dhodapkar, Editor The Dow Chemical Company



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Shell Global Solutions Sponsor of the Thomas Baron Award



Sponsor of the Lectureship in Fluidization Award



Sponsor of the Young Professional Award



University of Pittsburgh Alumni Sponsor of the George Klinzing Best PhD Award

Letter from the "Chair"



With a sincere note of thanks to Reza Mostofi who led the PTF activities last two years as the chair, Bruce Hook, the next chair-elect, and I are excited to carry on the PTF tasks with help from rest of the team of volunteers. Contrary to the new "chair" picture, I am happy to be in "The Chair" having aspirations for further enhancing our efforts in focusing on the future of particle technology through involving more chemical engineering students in particle technology. Based on the input and support from all of you, I would like to work towards increased student participation at the AIChE-PTF sessions and figuring out ways to bring particle engineering in to core undergraduate US engineering curriculum.

An urgent topic for now is the PTF Awards nominations. Please note the deadline of April 30 for the initial nominations. There are many awards and I am sure many deserving candidates for these awards so please do your part and nominate someone! If you have any questions or concerns regarding the requirements, please feel free to contact Bruce and I for clarifications as well as special requests or exceptions. We are here to help. As Reza mentioned in one of the previous Newsletters, we have worked hard towards revising the rules for the Awards eligibility and this is clearly subject to further revisions based on our experience this year and input from the members. Our main objective has been to reward and encourage continued active participation by awardees in PTF activities. We expect that the award winners have made strong direct contributions to our community, least of which is being a PTF member. In case of junior members, it is expected that they are ready to follow the foot-steps of their PhD advisors in being engaged.

Coming back to enhanced participation from undergraduate and graduate students in AIChE-PTF sessions in upcoming years, I am open to your ideas and suggestions. Open questions are: How do we bring more students to the PTF sessions? What are the best ways to utilize the PTF poster session as a spring board? Can we afford to provide travel scholarships without increasing the workload of the usual small number of volunteers who help with various PTF Awards including judging of the best poster award? How about the undergraduates? Several PTF members, including but not limited to, Mayank Kashyap, Ben Freireich, Reddy Karri, Ray Cocco, George Klinzing and Shrikant Dhodapkar have been phenomenal bringing record number in of undergraduates during Saturday workshops. How do we leverage that in to regular participation and more importantly, making long-term changes to US undergraduate curricula? On that note, I participated in the IFPRI Particle Technology Education Workshop earlier this month. This was organized by Jim Litster and Jim Michaels with support from IFPRI (International Fine Particle Research Institute) and several industry members and Willie Hendrickson, president of IFPRI. This workshop included equal number of industry and academic participants drawn from several countries. While I plan to invite Jim & Jim to write more about this in a future News Letter, an obvious conclusion was that US continues to lack presence of particle technology in core engineering curriculum as compared to all other countries. I believe the PTF has a role to play and I seek active advice and suggestion from our US members, both academic and industry.

We have many interesting activities planned for this year and next, not to forget that US hosts the next World Congress in Particle Technology. Stay tuned!

Raj Dave, NJIT

Chair, PTF



PTF Award Nominations — Now Open!

As you know, thanks to our sponsors, we have a number of awards available so that we can honor those who have done distinguished work in the area of particle technology. Therefore, on behalf of PTF, I would like to ask you to nominate those outstanding colleagues, friends or students who you have always felt should be awarded and are current PTF members. These are following awards where we seek nominations this year:

- · George Klinzing Best PhD Award
- Particle Technology Forum Lifetime Achievement Award
- · Thomas Baron Award
- PSRI Lectureship Award in Fluidization
- SABIC Young Professional Award
- Dow Particle Processing Recognition Award

The Nomination process is in two steps:

(1) Short form due by **April 30, 2017**, proving the name of nominee, and up to five names of those who will provide letters of support, along with their PTF membership status, click here, <u>https://</u> <u>form.jotform.us/60587168379168</u> (*Note: If the link doesn't work with Internet Explorer, go to Google webpage and put the link in the search line*).

(2) Full package due by May 20, 2017, containing items specific to each award.

If the nominee has previously received any award from AIChE or one of its divisions/forums, an explicit statement of <u>new</u> accomplishments or work over and above those cited for the earlier award(s) must be included (max. of one double spaced page). Selected bibliography (including books, patents, and major papers published).

NOTE: It is required that the nominators are current PTF members

For the PTF Lifetime Achievement Award, at least one of the support letters must be from a former PTF Award winner. *Nominees must be PTF members.*

In a given year, the same person cannot win more than one PTF award.

Nominees must have been the member of AIChE-PTF for prior 3 calendar years (since 2014); with one exception: Best PhD must be a current member at the time of nomination and the year of award.

 One time exceptions can be made but will require the EC board approval; please send email to Bruce Hook (<u>bdhook@dow.com</u>)

Wait period for nomination after previous award: A former PTF award winner cannot be nominated for another award for at least three years (after 2014) after receiving any previous PTF award.

You will be contacted regarding the package submission process after the nomination you made is received.

Please let me know if you have any questions and please feel free to forward this information to your colleagues or other who may be interested in nominating someone.

Bruce Hook, PTF Vice Chair (<u>bdhook@dow.com</u>)

PTF Awards Lectures

Nanofluids and Colloidal Suspensions – Novel Fluid/Particle Interaction Forces and Some Relevant Applications

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The classical DLVO (Derjaguin, Landau, Verwey, and Overbeek) theory, which balances the repulsive electrostatic double layer and the attractive van der Waals forces between particles, has long been the basis for explaining the structure and stability of colloidal dispersions. However, in recent years, due to the advent of new instrumentation for measuring interaction forces in fluid-particle systems, novel forces, such as the structural force arising from the energy barrier caused by particles microstructuring, and the attractive depletion force caused by the excluded volume effect, have been characterized. This lecture highlights the role of structural forces in stabilizing nano-micro-sized particle suspensions and especially points out their importance in the variety of technological contexts such as colloidal dispersion stability, foams stabilized by fine particles, wetting, and spreading of colloidal suspensions on solid surfaces, and in cleaning of hard surfaces by using nanofluids. Theoretical results based on Monte Carlo simulations and integral equations of statistical mechanics are also reviewed. Future study is warranted to explore the role of oscillatory structural forces in materials synthesis and processing.

NOVEL FLUID-PARTICLE INTERACTION FORCES

SUSPENSIONS OF NANO-SIZED PARTICLES, SMALL POLYMER LATEXES, GLOBULAR PROTEINS AND SURFACTANT MICELLES (E.G., LIQUID DETERGENTS) IN LIQUIDS ARE CALLED NANOFLUIDS. NUMEROUS PRODUCTS SUCH AS PAINTS, INKS, COATINGS, EMULSIONS, FOAMS, GELS AND POLYMER LATEXES, AND PROCESSES SUCH AS COAGULATION, FLOCCULATION, SEDIMENTATION, LUBRICATION, AND PAPER MAKING DEPEND TO A LARGE EXTENT ON THE DISPERSION QUALITY AND STABILITY OF PARTICLE SUSPENSIONS. THE LAST DECADE HAS SEEN AN INTENSIFIED INTEREST IN UNDERSTANDING THE NATURE OF INTERACTIONS IN SUCH CONCENTRATED SUSPENSIONS OR COLLOIDAL DISPERSIONS.

The structural forces appear when the colloidal particles are confined in the gap between two surfaces, (1-3). Figure 1 shows the interaction between two macroparticles in the presence of small particles which can be solvent molecules, ions, solute molecules, polymeric macromolecules, surfactant micelles, proteins, or other nano-colloidal particles. When the separation distance between two large particles is of the order of several small particles diameters, the small particles tend to form layering structures between them. This long-range structure induces a repulsive structural barrier that contributes in preventing the large particles from flocculating or coalescing. When the separation distance between two large particles is smaller than the diameter of the small particles (so that no small particles can fit in the gap between the large particles), a net attractive force/depletion force between the large particles is expected due to the osmotic pressure difference between the bulk and confined regions. In general, the effective interaction induced by the small particles between two large particles is found to the oscillatory, including both the attractive depletion and the repulsive structural energy barrier.



Figure 2 illustrates the origin of the structural forces. Figure A represents the interaction between a solid flat wall (or macroparticle) and a colloidal dispersion of nanoparticles of diameter, *d*. Because of the entropic excluded volume effect, the particle density near the wall (n_s) is higher than that in the bulk (n). Therefore, the pressure (P_s) normal to the wall increases, and the nanoparticles tend to form layers (i.e., structure). When nanoparticles are confined between two opposing surfaces (i.e., macroparticles or flat walls) with a narrow gap (i.e., a film), the structured region near the two opposing surfaces overlaps and the density oscillation induced by both surfaces starts to interfere, giving rise to an oscillatory structural force. A simple relation between the particle density distribution and the disjoining pressure (A) (i.e., the pressure exerted by nanoparticles on the film surface) given by the contact value theorem is shown in B of Figure 2.



As a result of the volume excluded effect near the wall, the particle density is higher than that in the bulk. The pressure normal to the wall increases. Particles tend to layer (structure).

Nano-fluid confined between two walls. The disjoining pressure profile follows the particle density distribution. A direct, theoretical approach to the study of particle structuring phenomenon inside a liquid film is to use a numerical simulation, either the Monte Carlo or molecular dynamics method (3-5).

The Ornstein-Zernike (OZ) theory provides a theoretical approach to calculate the correlation function in a many body system. It states simply that the total correlation function h(r) between two particles, which is related to radial distribution function g(r) by h(r)=g(r)-1, consists of two parts (Figure 3). The first part is the direct correlation between these two particles, denoted by c(r), and the second part is contributed by all possible indirect correlations through the other particles n the system. The latter can be expressed exactly as the convolution of the direct correlation function and the total correlation function. The above explanation can be expressed by the OZ integral equation. In order to solve the OZ equation, an appropriate closure relation between the two correlation functions is needed. The Percus-Yevick equation is the most widely used closure for hard sphere systems.



We employed the grand-canonical-ensamble Monte Carlo Simulations (3) using the hard sphere particles confined in two hard walls (See Figure 4).

Typical density distributions of particles across a film of thickness 3*s* are shown in this Figure 5, for the average particle concentration in the film ranging from 15 vol % to 35 vol %. The three peaks (at -1, 0, and +1) indicate that particles inside the film form three layers parallel to the film surfaces. Also the figure shows that, at a given film thickness, as the particle concentration inside the film increases, the particle-layering becomes more pronounced.



Figure 6 shows a surface plot of in-layer RDF versus in-layer particle distance and concentration (5). At low concentration, the particles inside a layer pack randomly and form a liquid like 2-D structure. At high

concentration limit (43 vol%), two new peaks near $\sqrt{3}$ and $\sqrt{7}$ can be seen, indicating the hexagonal packing. The film thickness is two particles diameters.

Fig 6 Particle Structure Formation Inside Confined Geometry Versus Concentration



Figure 7 depicts the pressure exerted by small particles on the surfaces of the film (i.e., the structural disjoining pressure) at different bulk concentrations as a function of film thickness (3). It can be seen that the structural disjoining pressure exerted by particles in a thin film oscillates around zero and that it can be positive (i.e., structural barrier) or negative (i.e., attractive depletion) depending on the thickness of the film. The period of oscillation is nearly the effective diameter of the particle for the concentrations used here. When the film thickness is about an integer multiple of the particle diameter, the disjoining pressure is positive and when the film thickness is around 1.5, 2.5, 3.5, the effective particle diameter, the disjoining pressure is negative.



H - Film Thickness (Scaled by Particle Diameter)

Crocker et al. (6) measured the long-range entropic forces that arise between two micrometer-sized colloidal spheres in a fluid of much smaller colloidal spheres using a line-scanned optical tweezer (Figure 8). They measured the interaction potential between an isolated pair of 1100 ± 15 nm diameter PMMA (polymethylmethacrylate) spheres (Bangs Labs, Inc) induced by a background of smaller, 83 nm diameter PS (polystyrene) spheres (Seradyn, Inc).



J. C. Crocker, J. A. Matteo, A. D. Dinsmore and A.G. Yodh Phys. Rev. Lett, 82, 4352-4355, 1999

This new technique allowed them to measure the functional form of the potential with sub- k_BT energy and 15 mn spatial resolution. At the lowest small sphere concentrations, the potential was monotonically attractive, while a higher concentrations an oscillatory potential was observed, due to the liquid structure of the small spheres (see Figure 9). Surprisingly, the large spheres came together only rarely at the higher concentrations, suggesting a new means for stabilizing suspensions using entropy alone.



J. C. Crocker, J. A. Matteo, A. D. Dinsmore and A.G. Yodh Phys. Rev. Lett, 82, 4352-4355, 1999

The entropic interaction potentials measured with small sphere volume fractions ranging from $f_s = 0$ to 0.42 (the large sphere volume fraction was less than 10^{-7}). At the lowest volume fractions [curves (*b*), (*c*)] the potential is monotonically attractive, resembling the Asakure-Oosawa depletion model. As more spheres are added, a repulsive barrier forms [(*d*), (*e*)], then a secondary minimum (*f*), before becoming fully oscillatory [(*g*), (*h*)]. The spheres for curve (*h*) never reached the primary depletion minimum. Each curve had to be shifted a small amount horizontally to register their primary minima, due to the roughly 15 nm sphere polydispersity. The weak attraction seen in the $f_s = 0$ case is presumably due to van der Waals attraction.

RELEVANT APPLICATIONS

During the past two decades our research group has worked on several problems of interest to industry in which structural forces in nanofluids and colloidal dispersions appear to play an important roll and they are listed in Figure 10 (1-2).

Fig 10 Role of Oscillatory Structural Forces in Technological Systems

- A. Colloidal Particle Suspension Stability
- B. Foams Stabilized by Fine Particles
- C. Spreading and Wetting Nanofluids on Solid Surfaces
- D. Hard Surface Soil Cleansing

A. Colloidal Particle Suspension Stability

For a binary mixture of large and small particles, the potential of the mean forces between large particles is obtained from the Ornstein-Zernike equation. We incorporated the small particles in our numerical simulations by using this potential of the mean force as the interparticle effective interaction (7-11). Our numerical results reveal the phenomenon of strong particle aggregation due to the attractive depletion force exerted by small particles. In the absence of the effect of gravity, this aggregation can result in flocculation and the formation of particle clusters thereby forming "void" structures, while under the influence of gravity, the aggregation ca greatly affect the sedimentation rates.

In Figure 11 we compare the vertical density equilibrium distribution of a system containing 20V% small particles with that of a system without small particles. The sedimentation separation is more complete when there are small particles. The explanation is that due to the depletion attraction contributed by small particles, the neighboring large particles like to "stick" to each other, the distances between the neighboring particles become smaller, and thus the condensed part occupies less volume.

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In all the cases, the particles near the bottom are well layered. This is shown by the pronounced oscillations near the bottom in the vertical density profiles. The two photos shown in Figure 12 depict the final stage of the sedimentation process of colloidal suspension with and without nonionic micelles.



Fig 12 Gravity Sedimentation Experiment Showing Consolidated Zone



It is shown in the Figure 12 that for latex particles in 6wt% micellar solution, the separation is more complete and the particles in consolidated zone are likely to stay in contact with other particles than in the case when latex particles is dispersed in water. The colloid crystal structure was also observed with iridescent color. Figure 13 shows a photograph of a gravity sedimentation experiment. All tubes contain 2 vol.% large particles (2.85 μ m). The first tube (left) contains no fine particles, second tube (middle) contains 2 vol.% small particles (26 nm) and the third tube (right) contains 4 vol.% small particles. This photograph was taken 30 h after the experiment was started. The presence of 4V% of 26nm particles (the third tube) can stabilize the system by forming small particle layers between the larger particles (11).

Fig 13 Gravity Sedimentation Experiment Showing Consolidated Zone

Photograph for gravity sedimentation. All tubes contains 2V% large particles (2.9 µm).

- A. 2V% of large particles.
- B. 2V% of large particles with 2V% small particles (26 nm)
- C. 2V% of large particles with 4V% small particles



"Effects of Interparticle Interactions on Stability, Aggregation and Sedimentation in Colloidal Suspensions," X.L. Chu, A.D. Nikolov and D.T. Wasan, <u>Chem. Eng. Comm.</u>, <u>148-150</u>, 123-142 (1996).

Before each run, all tubes were shaken thoroughly to ensure that the particles were well dispersed, then we placed them vertically and let sedimentation occur. After some time the suspension in the tubes appears as the three distinct zones which are separated by clear "interfaces". In the top part, there is a transparent zone call "blanket" where there are no large colloidal particles. In the middle part, there is a milk-like "compression" zone, where there are some large particles-the concentration of large particles in this zone can be estimated by the degree of transparency of the liquid. The last part at the bottom is the white colored "consolidated" zone, where the large particles are most closely packed. The photograph depicted in the Figure was taken 2.5 hours after the experiment was started.

This photograph already shows the drastic difference in sedimentation caused by the presence_of fine particles. The height of the consolidated zone indicates the amount of the large particles being deposited by sedimentation at the bottom.

We plot in the Figure 14 the height of the consolidated zone for the three cases. The most striking result is that in the second tube (with 2v% 26nm plus 2V% 2.85 μ m), most large particles are deposited at the bottom of the tube in a very short time period (2-3 hrs), compared to the reference case (about 24 hrs for the first tube).

We see that in our sedimentation experiments, the sedimentation process takes about 72 hours, compared to the 24 hours for the reference case (the first tube, without fine particles) and the 3 hours for the case of a small amount of fine particles (the second tube, 2V% fine particles).

It is worth pointing out that, although the addition of fine particles can change the effective viscosity and consequently the sedimentation velocity, this is not a dominant factor in our experiment since only a small amount of fine particles (2V%) are used in our experiments. Without considering the particle interactions and the particle structure formation, the change in the sedimentation velocity due to the addition of fine particles in our experiments can be estimated from Batchelor's equation.

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In contrast to the very large change observed in our experiments. Moreover, the sedimentation velocity increases (as observed in our experiment), not decreases, as had been predicted based on the increase of viscosity concept. Therefore, such a large change in sedimentation velocity is due to the particle flocculation mechanism caused by the attractive depletion force.

Fig 14 Gravity Sedimentation Experiment: Consolidated Zone Versus Time



[&]quot;Effects of Interparticle Interactions on Stability, Aggregation and Sedimentation in Colloidal Suspensions," X.L. Chu, A.D. Nikolov and D.T. Wasan, <u>Chem. Eng. Comm.</u>, <u>148-150</u>, 123-142 (1996).

B. Foams Stabilized by Fine Particles

Particle-stabilized aqueous foams are encountered in the processing of solid waste (e.g., during boiling), food, chemical, and agricultural products, froth flotation, and radioactive waste treatment and immobilization processes (12-14). Uncontrollable foaming can severely impact the production rate and ultimately the cost-effectiveness of a chemical process. The solid particles in boiling suspensions, in the absence of any surfactants, stabilize the foam lamella and enhance the foaminess. Previously we identified at least two types of particles in such three-phase foaming systems: hydrophilic colloidal particles dispersed in the aqueous phase and biphilic particles (i.e., with some area of the particle wetted by water and the other part is not). These biphilic (or amphiphilic) particles attach to the surfaces of the foam lamella, provide a steric barrier against the coalescence of bubbles, and thereby enhance foam lamella stability and foaminess.

A foam lamella is formed during the generation and interaction of bubbles during the boiling of aqueous suspensions. Hydrophilic colloidal particles get trapped inside the lamella. Subsequently, due to the confined boundaries of the film (lamella), these particles form a layered (i.e., stratified) structure inside the foam lamella. Monte Carlo simulations of the film containing particles show that the concentration of the colloidal particles is higher in the film/lamella than that in the bulk. Furthermore, our theoretical calculations show that, at a higher particle concentration, a better particle in-layer structure develops(5) that increases the energy stabilization barrier, inhibiting particle diffusion from the film to the bulk meniscus. The repulsive structure barrier (i.e., the structural disjoining pressure) arising due to the colloid particle in-layer structure formation offers a novel stabilization mechanism for macrodispersions such as foams and emulsions. In fact, we have produced aqueous foams in surfactant-free particle suspensions using nanosized silica particles.

Figure 15 shows a photograph of the color strips in whited reflected light in stratifying foam lamella stabilized

with 20 vol%, 19nm silica particles.

Fig 15

Foaminess in the Presence of Hydrophilic Silica Nano-Particles



Photograph of the color stripes in white reflected light in stratifying foam lamella stabilized with 20 vol%, 19nm silica particles

Figure 16 shows:

A. Well-defined strips of different colors in a vertical foam film formed from 44vol.5 monodispersed latex suspension with 156-nm-dia.

B. Latex particle layering and structuring inside thinning vertical film

C., D. diffraction patterns revealing particle structural transition from layered to 2-D in-layer hexagonal packing

E. Capturing of foam lamellae with color stripes; foam generated from a solution to 20 vol.% silica particles with diameter of 19nm.



A. Photo depicts well-defined stripes of different colors in a vertical foam film formed from 44 v% monodipersed latex uspension with diameter 155 nm. B. Schematic presentation of the latex particle layering and structuring inside thinning vertical film; C and D. Offraction patterns revealing particle structure larger and to 20 n-layer hexagonal packing; E. Photo captures foam lamellae with color stripes; foam generated from a solution of 20 V% silica particles with diameter of 19 nm.

Nikolov and Wasan, Langmuir, 8(1992), 2985-2982

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Figure 17 shows:

- The Amphiphilic particles containing both the hydrophilic and the hydrophobic parts. The hydrophobic attaches to the air bubble while the hydrophilic stays outside the air bubble.
- The Hydrophobic particles are inside the air phase.

Due to the adsorption of the Amphiphilic particles, steric stabilization is formed and this stabilizes the foam lamella and increases foaminess.

Fig 17 Particle Amphiphilic at Air/Water Interface



Figure 18 shows a plot of the foaminess air forced sludge concentration. The foaminess increases as the amphiphilic particle concentration increases. The foam was generated by boiling the simulated nuclear waste (13).



Figure 19 shows a three-dimensional surface plot depicting the dependence of foaminess on the concentration of both Amphiphilic and hydrophilic particles. Curve A depicts results of the experiment when the simulated sludge contained Amphiphilic particles only, and curve B depicts the foaming results when only hydrophilic particles where present. The results of runs 1-4 are also marked on this figure. The figure shows that foaminess increases with an increase in the concentration of the two types of particles. However, hydrophilic particles produce a maximum of about 260 vol% of foaminess (i.e., the amount of gas incorporated into the system whereas Amphiphilic particles resulted in a significantly higher degree of foaminess (i.e., 900 vol%) over the same range of particle concentrations. The photographs of the attached (or biphilic) particles for different runs are also shown in the figure.



Wasan, D. T., Nikolov, A., Shah A. Ind. Eng. Chem. Res., 43, 3812-3816, 2004

Our research addresses two different but interrelated studies. The first deals with the fundamental understanding of the causes of foaming and stability of the foam as highlighted in the preceding section. The second is the practical need to find an effective antifoam or defoaming agent to minimize the production of foam during processing. Antifoam and defoaming agents have been developed to help industries such as nuclear waste, paper, pulp, coatings, ink and printing.

Antifoaming

On the basis of the mechanistic understanding of foam generation and stability, and the oscillatory structural forces, we developed an improved antifoam agent (IIT 747), since the commercial antifoam agent (Dow Corning 544) was found to be ineffective in the aggressive physical and chemical environment in the Defense Waste Processing Facility (DWPF) sludge receipt and adjustment process as indicated by the foaminess data presented in the Figure 20 (13). The addition of the IIT antifoam was found to be more effective in minimizing foam and was more effective over time than Dow Corning 544. The improved antifoam agent, IIT 747, was subsequently tested in a pilot plant at the Savannah River Site (SRS) and with real waste in their shielded cells. The antifoam developed by us is now being used in the Defense Waste Processing Facility (SRS).



C. Spreading and Wetting of Nanofluids on Solid Surfaces

The completely wetting pure liquids spread over solid surfaces, but wetting and spreading behavior changes if liquids contain nanosize spherical particles or surfactant micelles, globular proteins and macromolecules. The classical concepts of wetting and spreading of simple liquids do not apply to nano and complex fluids. The complex nature of the interacitons between the paricles in the nanofluid and with the solid substrate greatly alters the spreading dynamics under the action of the structural disjoining pressure gradient (15-20). Presented here in Figure 21, is a plot of spreading of nanofluid and viscosity on Y axis as a function of concentration. It can be seen that as concentration is increased the spreading of nanofluid increases dramatically. However with increase in concentration the viscosity also increases significantly which instead should have decreased the spreading as has been predicted by the classical theory of fluid mechanics. Thus proving that well established concepts of spreading of simple fluids do not apply to nanofluids. Let us examine the complex interactions before the nanoparticles in the fluids and the solid surface.



Nanofluid concentration (effective vol %)

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The wedge film was formed by blowing a small air bubble (diameter 200 mm) against an optically smooth glass plate in a suspension of monodisperse, charged latex spheres in deionized surfactant-free water (15). The volume fraction of spheres in the fluid was 7 vol.%, and they had a surface charge of 0.8 mCcm22, a diameter of 1.01 mm, and a density of 1.05 g cm23. The optical signal was digitized for analysis.

The latex particles tend to form a 2D colloid crystal structure at a thickness of the wedge film equal to twice the particle diameter (that is, about 2 mm). However, the particle in-layer structure changes to a disordered structure when the film thickness exceeds three particle diameters (see Figure 22). The co-existence of this ordered–disordered structure depicted here is reproducible, and was observed for several hours.

Fig 22 Schematic of Experimental Setup to Study Particle Structuring in a Wedge Film



D. T. Wasan, and A. D. Nikolov Nature, 423, pp 156-159, 2003

Figure 23 shows the particle in-layer radial distribution function, g(r), that we obtained from the image analysis of over 2,000 particles. This figure shows the co-existence of both the 2D hexagonal and cubic packing domains in the wedge film.



D. T. Wasan, and A. D. Nikolov Nature, 423, pp 156-159, 2003

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The spreading coefficient, S, was estimated as a function of the number of particle layers in the wedge film. Our calculations show that the spreading coefficient increases with a decrease in film thickness, that is, with the decrease in the number of particle layers inside the film. Also, we notice (See Figure 24) a significant change in the slope of the curve at a thickness of the wedge film equal to twice the particle diameter.

In Figure 24 we plot disjoining pressure, obtained by using an analytical expression based on statistical mechanics. The pressure is high (nearly 50,000 Pa) near the vertex, because the hard spheres are 'pushed' into the region by the spheres farther out. The pressure oscillates as 1,2,3 and 4 layers of hard spheres can be accommodated between the wedge confinement, and ultimately becomes the bulk hard-sphere pressure.



The oscillatory structural forces resulting from the ordering of particles has implications in the spreading of colloidal fluids on solids.

Nanofluid film spreading on solid surfaces has many applications. I will be presenting two such application below, one of which is hard surface soil cleaning.

D. Hard Surface Soil Cleaning

This schematic here (Figure 25) shows the ordering of nanoparticles in the wedge region resulting in spreading of nanofluid as a thin film separating the oily sill from the hard surface (15,21).

One can see, in the Figure 26 that the micellar nanofluid penetrates between the oil and the glass surface. The speckled band between the dark and light areas in figure B and C shows the formation of small water lenses (the white spots) between the oil and solid surface. In effect, two contact lines are established: the first is between the oil droplet, solid surface and aqueous film, (outer line) and the second is between the oil droplet, solid surface and aqueous film, (outer line). The thickness of the speckled band increases with the lapse of time since the inner contact line recedes more rapidly than the outer contact line, figure D. Eventually the oil droplet is separated completely from the solid surfaces by a thick water film with a dimple as shown in figure E.



D.T. Wasan and A.D. Nikolov Spreading of Nanofluids on Solids, Nature, 423, 156-159 (2003)

Fig 26 Dynamics of Oil Removal from Solid Surface in the presence of Micelles



CONCLUDING REMARKS

The oscillatory structural forces become increasingly important when colloidal particles are confined where their structural properties are strongly modified in comparison to their bulk properties. Behavior of colloidal suspensions in confined geometries is of particular interest in materials processing where the movement and deposition of nano-sized particles can be manipulated by controlling these forces.

We have merely scratched the surface when it comes to applying the concepts of particle layering or selfassembly to understanding processes like crystallization, filtration and sedimentation or to building materials of desired structural and optical properties. As we obtain a deeper understanding of the forces involved in arranging nano-sized and colloidal particles, the opportunities for chemical engineers to apply those results multiply.

ACKNOLEDGEMENTS

I wish to emphasize that the work resulting in this award lecture was due to many contributions of my former graduate students, post-doctoral associates and especially my long-time co-worker Dr. Alex Nikolov, Research Professor in the department.

REFERENCES

- "New Vistas in Dispersion Science and Engineering", D.T. Wasan, A.D. Nikolov, D. Henderson, <u>AIChE J.</u>, <u>49</u>, No. 3, 550-556 (2003).
- "Colloidal Dispersions: Structure, Stability and Geometric Confinement," D. Wasan, A. Nikolov, B. Moudgil, <u>Powder</u> <u>Technology</u> 153, 135-141 (2005).
- 3. "Monte Carlo Simulation of In-Layer Structure Formation in Thin Liquid Films," X.L. Chu, A.D. Nikolov and D.T. Wasan, Langmuir, <u>10</u>, 4403-4408 (1994).
- 4. "A Simple Calculation of Structural and Depletion Forces for Fluids/Suspensions Confined in a Film," A. Trokhymchuk, D. Henderson, A. Nikolov and D. T. Wasan, <u>Langmuir</u>, <u>17</u>, 16, 4940-4947 (2001).
- 5. "Structural Transitions in Colloidal Suspensions in Confined Films" Wasan, D.T. and Nikolov, A.D. In *Supramolecular Structure in Confined Geometries*, S. Manne and G. Warr, Eds., ACS Symposium Series No. 736, pp 40-53 (1999).
- 6. "Entropic Attraction and Repulsion in Binary Colloids Probed with a Line Optical Tweezer", J. C. Crocker, J. A. Matteo, A. D. Dinsmore, and A. G. Yodh, Phys. Rev. Lett. 82, 4352 Published 24 May 1999
- 7. "Sedimentation of Concentrated Monodisperse Colloidal Suspensions: Role of Collective Particle Interaction Forces", Vesaratchanon, J.S., Nikolov, A.D. and Wasan, D.T., J. Coll. Interface Sci. <u>322</u>, 180-189 (2008).
- 8. "The Importance of Oscillatory Structural Forces in the Sedimentation of a Binary Hard-Sphere Colloidal Suspension," Vesaratchanon, J.S., Nikolov, A.D., Wasan, D.T., and Henderson. D. <u>I&EC Res</u>. <u>48</u>, 14, 6641-6651 (2009).
- "Role of Depletion and Surface-Induced Structural Forces in Bidisperse Suspensions," W. Xu, A.D. Nikolov and D.T. Wasan, <u>AIChE J.,43</u>,12, 3215-3222 (1997).
- 10. "The Effect of Many-Body Interactions on the Sedimentation of Monodisperse Particle Dispersions," W. Xu, A.D. Nikolov and D.T. Wasan, <u>J. Colloid Interface Sci</u>, <u>197</u>, 160-169(1998).
- 11. "Particle-Particle Interactions in Concentrated Dispersions as Probed by Capillary Force Balance with Application to Batch Sedimentation," A. D. Nikolov and D.T. Wasan, <u>Powder Technol. 88 (3)</u> 299-304 (1996)
- 12. "Foam Formation and Mitigation in a Three-Phase Gas-Liquid-Particulate System," K. Vijayaraghavan, A. Nikolov, D.T. Wasan, <u>Advances in Colloid Interface Science</u> 123-126 p 49-61 (2006).
- 13. "Foaming-Antifoaming in Boiling Suspensions", D. Wasan, A. Nikolov, A. Shah, <u>I&EC Res</u>, <u>43</u>, 3812-3816 (2004).
- 14. "Foamability of Liquid Particle Suspensions: A Modeling Study," Vijayaraghavan, K., Nikolov, A.D., Wasan, D.T. and Henderson, D. <u>I&EC Res.</u> <u>48</u> (17), 8180-8185 (2009).
- 15. "Spreading of Nanofluids on Solids" D.T. Wasan and A.D. Nikolov, <u>Nature 423</u>, 156-159 (2003).
- "Spreading of Nanofluids Driven by the Structural Disjoining Pressure Gradient," A. Chengara, A.D. Nikolov, D.T. Wasan, A. Trokhymchuk and D. Henderson, <u>J. Colloid Interface Sci.</u>, 280, 192-201 (2004).
- 17. "Wetting-Dewetting Films: The Role of Structural Forces", Nikolov, Alex; Wasan, Darsh. <u>Advances in Colloid and</u> <u>Interface Science</u>, <u>206</u>, pp 207-221 (2014).
- 18. "The wetting and spreading of nanofluids on solids: Role of the structural disjoining pressure", Wasan, Darsh; Nikolov, Alex; Kondiparty, Kirti; <u>Current Opinion in Colloid and Interface Science 16</u>, 334-349 (2011).
- 19. "The Dynamic Spreading of Nanofluids on Solid Surfaces--Role of the Nanofilm Structural Disjoining Pressure", Lim, Sandwook; Wu, Pingkeng; Zhang, Hua; Nikolov, Alex; and Wasan, Darsh; J. Coll. Interface Sci. 470, 22-30 (2016).
- 20. "Nanoparticle Self-structuring in a Nanofluid Film Spreading on a Solid Surface", Nikolov, Alex; Kondiparty, Kirti; Wasan, Darsh. Langmuir 26, 7665-7670 (2010)
- "Cleaning Dynamics of Oily Soil Using Nanofluids", Wu, Stanley; Nikolov, Alex; Wasan, Darsh. J. Coll. Interface Sci. 396, 293-306, (2013).

The Dynamics of Normal, Inverse and Sheared Fluidized Beds

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Introduction

Fluidized beds occur extensively in the chemical, petrochemical and pharmaceutical industry. Most fluidized beds are unstable to low amplitude disturbances and develop non-uniform particle distributions in the form of density waves. In fluidized beds such non-uniformities can become amplified in the bed to form fully developed bubbles (in dense fluidized beds) [1], clusters and streamers (in dilute fluidized beds) [2, 3] and slugs (in narrow fluidized beds) [1]. Since the presence of voidage or density waves are known to dramatically impact heat and mass transfer rates, and process safety and economics, it is important to understand the underlying physical mechanisms responsible for unstable flow behavior. At the same time, the dynamics of dense gas-particle suspensions are heavily influenced by granular rheology, and granular flows, by themselves can undergo instabilities. Thus, instabilities manifested by granular flows are observed in fluidized beds and an understanding of granular behavior and stresses is needed for fluidization models.

Using continuum mechanics, volume- or ensemble-averaged equations of mass and motion have been postulated to describe the flow of the fluid and particle phases in fluidized beds [4]. It is common to derive the constitutive relations for the solid phase momentum equation from the kinetic theory of dense gases [5-8]. The main difference between molecular gases and granular particles is that energy is lost due to collisions between particles, while this is not true for molecular gase collisions.

For unbounded gas-particle flows, the simplest solution to the governing equations of motion represents the steady state of uniform fluidization. In order to predict the growth of disturbances from the steady base-state, conventional methods of hydrodynamic stability analysis have been applied [9-15]. The earliest stability analysis from the work of Jackson [13] predicted that uniform fluidized beds are inherently unstable, and that such instabilities are in the form of plane waves, which propagate vertically upwards through the bed. Although linear theory can account for the existence of traveling waves in gas-fluidized beds, it can only capture phenomena occurring in close proximity to the marginal stability point. Therefore, it is not capable of predicting the ultimate fate of the instability. In order to better understand the origin of bubbles, the non-linear terms in the equations of motion have been taken into account in one-dimensional fluidized beds [16-19]. Results of non-linear analyses have shown that low amplitude disturbances can become amplified in fluidized beds to form fully-developed one-dimensional traveling waves [19].

From Bubbles to Clusters in Fluidized Beds

Bifurcation theory has been used to investigate the behavior of traveling waveforms in unbounded fluidized beds [20-24]. Using bifurcation analysis and a numerical continuation approach [20, 23] it was demonstrated that one-dimensional (1D) traveling wave solutions bifurcating from the uniform base state are unstable in the transverse direction, and that this can lead to the formation of bubble-like structures. In Figure 1, some

typical bubble-like structures are shown for a gas-fluidized bed. These represent traveling waves that move up through the fluidized bed at a constant velocity. Contour plots of solids fraction along with streamlines of the gas velocity are shown in the figure. It is important to check the robustness of the bifurcation behavior by considering different gas-particle systems. This is particularly important as bubbles are formed easily in gasfluidized beds and therefore the ability to observe them in mathematical models should not be restricted to a specific set of closures or parameters. A long series of numerical experiments were carried out by changing the model parameters and the closures and it was found that the bifurcation behavior was robust in the following sense: the traveling waves having only vertical structure emerge through a Hopf bifurcation of an unstable uniform state and the 2D traveling waves are born out of these 1D traveling waves. The high amplitude 2D traveling waves resemble bubbles in fluidized beds.

It was later established that bubbles and clusters belong to the same family of non-uniform traveling wave solutions [24]. Using a bifurcation analysis the solution structure of volume-averaged equations of motion describing unbounded fluidized beds was examined, and it was found that by varying parameters of the system, it was possible to move smoothly between the seemingly different structures observed in fluidized beds, namely bubbles and clusters. In Figure 2, contour plots of solids fraction are shown for traveling waves in gas-fluidized beds for both bubble-like and cluster-like solutions. It was observed that the traveling waves propagate in the following way: when the lower surface of a dense region becomes unstable, particles (within the solids rich region) "rain" down to fill the dilute region below. Once they pass through the dilute region, they enter the upper surface of another solids rich region. Hence, for any particle dense region, particles are lost from its lower surface and simultaneously collected on its upper surface. It is this mechanism that leads to the propagation of the density wave.

Additional work investigated instabilities in inverse fluidized beds (where the particle density is less than fluid density) and the hierarchy of bifurcations was compared to normal fluidized beds. It was shown that the Froude number and fluid to solid density ratio control the behavior of instabilities [25]. The physical mechanisms leading to density inhomogeneities in gas-fluidized beds were further investigated and it was shown that under certain simplifying assumptions, model equations of motion and continuity for the particles in a fluidized bed, can be related to those of a compressible fluid acted upon by a density dependent force. A comparison of these results with previous work on gas-fluidized beds showed that the salient features of the instability of a gas-fluidized bed are captured by the basic physics of compressible flows.

Instabilities in Bounded Fluidized Beds

Previous work had established that steady flows of gas and particles in unbounded fluidized beds lose stability to localized voidage disturbances. Work was carried out to investigate the stability of bounded gasparticle flows. The stability analysis was carried out for two sets of boundary conditions corresponding to fluidized systems having walls acting as sinks and sources of fluctuation energy [26]. The linear stability of the base state was examined by imposing a perturbation on the steady state solution in the form of a localized periodic disturbance. The governing equations and boundary conditions were then expanded in ascending powers of the perturbations through a Taylor series expansion of the nonlinear terms. Since the disturbances were assumed to be both small and smoothly varying in space and time, their derivatives were also small. Therefore, all terms of degree greater than one in the perturbations were neglected. Perturbations were assumed to take the form of a plane wave disturbance. Instabilities were characterized by computing leading eigenvalue profiles and dominant eigenfunction contour maps. The results showed two types of dominant instability patterns (symmetric and anti-symmetric) for flow in a vertical duct, both of which propagate through the bed in the form of traveling waves at speeds comparable to that of the solid phase. Moreover, model predictions showed that increasing solids fraction and decreasing particle inelasticity suppresses the disturbances. The physical mechanism of instability formation was further investigated using a term-by-term method of analysis. Results showed that the instability modes can be suppressed if solid phase inertia or inelastic particle collisions are eliminated from the momentum and pseudo-thermal energy balance equations. Moreover, it was shown that the occurrence of symmetric instability patterns is due to the inclusion of gas-phase inertia. Finally, the symmetric instabilities were shown to develop into bubble-like structures while the anti-symmetric instabilities develop into streamer-like structures. In Figure 3, a stability map is presented as a function of the average solids fraction, f, and the coefficient of restitution of the particles, ep. Within the physical parameter space, a stability analysis shows the dominant mode in the f-ep plane has three types of structures: stable patterns; symmetric unstable patterns; and anti-symmetric unstable patterns. Contour plots of solids fraction are also shown in Figure 3 to showcase a symmetric and anti-symmetric instability. These contour plots were obtained by adding a small perturbation to the steady state solution. The symmetric instability leads to cluster-like or bubble-like solutions, while the anti-symmetric instability leads to a streamer-like solution [26].

Binary mixtures of particles in fluidized beds were computationally investigated for unbounded and bounded flows. In bounded flows it was observed that segregation could occur due to competition of three diffusion forces: the thermal diffusion force, the ordinary diffusion force, and the pressure diffusion force [27]. A number of different binary mixtures were examined: 1) equal density particles with different sizes, 2) equal mass particles with different sizes and 3) equal size particles with different masses. It was observed that the species segregation in the solid phase is enhanced with a decrease in the system inelasticity, an increase in the average solids fraction or an increase in the size ratio, due to the competition of the three diffusion forces. In addition, it was found that a competition mechanism exists in the equal density case (particles with equal density but different sizes) since in the equal mass case (particles with equal mass but different sizes) small particles have a higher concentration in low granular energy regions whereas in the equal size case (particles with equal size but different masses) heavy particles have a higher concentration in low granular energy regions. By investigating equal size and equal mass systems, it was found that the breakdown of energy equipartition is mainly due to the contribution of the mass disparity, whereas the effect of the size disparity is very small if the two particle species have the same mass. For equal size particles, the flow profiles exhibit a transition with the variation of the mass ratio. For small mass ratios, the segregation between two particle species increases with an increase in the mass ratio. However, further increasing the mass ratio reverses the situation. Similar transitions were observed when the variation of the diffusion force profiles was tracked with the mass ratio. These findings are in agreement with the results for granular Couette flows. The flow of binary mixtures of particles in a fluidized bed was compared to flow of binary mixtures of particles in a channel without a gas i.e. granular channel flow. It was found that the species segregation profiles are quite similar between the bidisperse granular flows and the bidisperse gas-particle flows.

Instabilities in Sheared Fluidized Beds

A sheared fluidized bed was investigated by rotating an inner cylinder in a cylindrical fluidized bed, generating a Taylor-Couette flow. Inherent periodicity in the Taylor-Couette flow allows large length and timescales to be accessed, and so the fluidized Couette device represents a bench-top apparatus which allows for granular instabilities to form and their effect on segregation to be studied. It was observed that vortices developed and the observed instability was consistent with the Taylor-Couette instability in fluids [28]. As can be seen in Figure 4, a variety of horizontal banded structures spontaneously form in the fluidized Couette flows of binary granular materials. Shear was carried out in a well-mixed, fluidized binary mixture consisting of equal parts 138mm (white) and 462mm (rust) spheres. Particle motion (observed at the free surface) is at first azimuthal and confined to a narrow zone near the moving wall. This zone widens with rising rotation rate until it reaches the outer wall. Once particles start moving at the outer wall, a transition is seen in which particles begin to flow radially outward at the upper surface and downward along the outer wall. Particle segregation by size is observed both on the upper surface as a ring of the larger particles surrounding the inner cylinder, and as subsurface axial segregation (visible through the outer wall). These bands appear spontaneously from a well-mixed state after one to two minutes. Once formed, they are stable for all times



Figure 1: Contour plots of solids fraction (left) and streamlines of gas velocity (right) for a low amplitude traveling wave (top panels) and a high amplitude traveling wave (bottom panels). The high amplitude traveling wave has the essential features of a bubble in a gas-fluidized bed [20].



Figure 3: Instabilities in a bounded fluidized bed. Top: stability map as a function of the average solids fraction, ϕ , and the coefficient of restitution, ep, of the particles. Bottom: contour plots of solids fraction for a symmetric (left) and anti-symmetric instability (right). The contour plots were obtained by adding a small perturbation to the steady state solution [26].



Figure 2: Contour plots of solids fraction. Plots are traveling wave solutions for volume averaged equations of motion for gas-fluidized beds [24]. The results show that bubble-like and cluster-like solutions belong to the same family of non-uniform solutions.



Figure 4: Segregation in a Taylor-Couette fluidized granular bed. Banding patterns for fluidized granular flows for white ($138 \mu m$) and rust ($462 \mu m$) particles, 50/50 vol% mixture. The fluidized granular bed is imaged through a transparent outer cylinder. The number of bands increases as the rotation rate increases [28].

we have considered (up to ten minutes). Upon increasing the rotation rate, the bands appear to sometimes split into two daughter bands, which may be alternately "thick" and "thin". A variety of initial conditions (well -mixed, vertically segregated, horizontally segregated) all yield the same segregated state.

Concluding Remarks

While we have an understanding of many aspects of instabilities in fluidized beds, a large number of research questions remain unanswered. One would like a better understanding of scale up in fluidized beds. Ideally one would like to carry out experiments and simulations for a bench scale apparatus and use the results to predict behavior at the pilot scale and manufacturing scale. One would like to be able to do this with heat transfer, mass transfer and reactions in order to predict the scale up of chemical reactors. Another important area of research is further development of closures for two phase flow equations; in particular, further work is needed for the solids phase stress for non-spherical and cohesive particles. In addition, more work on coarse graining for CFD and CFD-DEM of gas particle flows is needed in order to resolve manufacturing scale fluidized beds.

References

1. Kunii, D. and O. Levenspiel, Fluidization Engineering. 1991: Butterworth-Heinemann.

2. Juan, A.H., Instabilities induced by concentration gradients in dusty gases. J. Fluid Mech., 2001. 435: p. 247-260.

3. Agrawal, K., et al., The role of meso-scale structures in rapid gas–solid flows. J. Fluid Mech., 2001. 445: p. 151-185.

4. Jackson, R., The Dynamics of Fluidized Particles. 2000: Cambridge University Press.

5. Lun, C.K.K., et al., Kinetic theories for granular flow: inelastic particles in couette flow and slightly inelastic particles in a general flow field. J. Fluid Mech., 1984. 140(223-256).

6. Lun, C.K.K., Kinetic theory for granular flow of dense, slightly inelastic, slightly rough spheres. J. Fluid Mech., 1991. 233: p. 539-559.

7. Jenkins, J.T. and S.B. Savage, A theory for the rapid flow of identical, smooth, nearly elastic, spherical particles. J. Fluid Mech., 1983. 130: p. 187-202.

8. Jenkins, J.T. and M. Richman, Kinetic theory for plane flows of a dense gas of identical, rough, inelastic, circular disks. Phys. Fluids, 1985. 28: p. 3485-3494.

9. Anderson, T.B. and R. Jackson, A fluid mechanical description of fluidized beds. Equations of motion. Ind. Eng. Chem. Fundam., 1967. 6: p. 527-539.

10. Anderson, T.B. and R. Jackson, Fluid mechanical description of fluidized beds. Stability of the state of uniform fluidization. Ind. Eng. Chem. Fundam., 1968. 7: p. 12-21.

11. Pigford, R.L. and T. Baron, Hydrodynamic stability of a fluidized bed. Ind. Eng. Chem. Fundam., 1965. 4: p. 81-87.

12. Bachelor, G.K. and J.M. Nitsche, Instability of stationary unbounded stratified fluid. J. Fluid Mech., 1991. 227: p. 357 -391.

13. Jackson, R., the mechanics of fluidized beds. I: the stability of the state of uniform fluidization. Trans. Inst. Chem. Eng., 1963. 41: p. 13-21.

14. Bachelor, G.K., Secondary instability of a gas-fluidized bed. J. Fluid Mech., 1993. 257: p. 359-371.

15. Koch, D.L.S., A. S., Particle pressure and marginal stability limits for a homogeneous monodisperse gas fluidized bed: kinetic theory and mumerical simulation. J. Fluid Mech., 1999. 400: p. 229-263.

16. Fanucci, J.B., N. Ness, and R.H. Yen, On the formation of bubbles in gas-particle fluidized beds. J. Fluid Mech., 1979. 94: p. 353-367.

17. Hirayama, O. and R. Takaki, Analysis of nonlinear waves in a one-dimensional fluidized bed. Fluid Dyn. Res., 1997. 21: p. 233-247.

Particle Technology Forum

18. Liu, J.T.C., Nonlinear unstable wave disturbances in fluidized beds. Proc. R. Soc. Lond. A., 1983. 389: p. 331.

19. Needham, D.J. and J.H. Merkin, The propagation of voidage disturbances in a uniform fluidized bed. J. Fluid Mech., 1983. 131: p. 427-454.

20. Glasser, B.J., I.G. Kevrekidis, and S. Sundaresan, One- and two-dimensional travelling wave solutiuons in gas fluidized beds. J. Fluid Mech., 1996. 306: p. 183-221.

21. Goz, M.F., On the origin of wave patterns in fluidized beds. J. Fluid Mech., 1992. 240: p. 379-404.

22. Goz, M.F., Bifurcation of plane voidage waves in fluidized beds. Physica D, 1993. 65: p. 319-351.

23. Glasser, B.J., I.G. Kevrekidis, and S. Sundaresan, Fully developed travelling wave solutions and bubble formation in fluidized beds. J. Fluid Mech., 1997. 334: p. 157-188.

24. Glasser, B.J., S. Sundaresan, and I.G. Kevrekidism, From bubbles to clusters in fluidized beds. Phys. Rev. Lett., 1998. 81: p. 1849-1852.

25. Howley, M.A. and B.J. Glasser, A comparison of one-dimensional traveling waves in inverse and normal fluidized beds. Physica D: Nonlinear Phenomena, 2005. 201(1–2): p. 177-198.

26. Liu, X., B.J. Glasser, and M.A. Howley, Instability of bounded gas-particle fluidized beds. AIChE Journal, 2007. 53(4): p. 811-824.

27. Liu, X., M. Metzger, and B.J. Glasser, Granular and gas–particle flows in a channel with a bidisperse particle mixture. Chemical Engineering Science, 2008. 63(23): p. 5696-5713.

28. Conway, S.L., T. Shinbrot, and B.J. Glasser, A Taylor vortex analogy in granular flows. Nature, 2004. 431(7007): p. 433-437.

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Quadrature-Based Moment Methods for Fluid-Particle Flows

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1 Introduction

Given the difficulty of obtaining experimental data for multiphase flows, detailed numerical simulations are a promising tool for understanding the impact of operating conditions and physical properties on the flow dynamics. However, even the "simplest" case with monodisperse particles of known size and shape in a continuous fluid phase is challenging to simulate across the full range of scales and parameters of interest [Marchisio & Fox (2013)]. Here, a brief overview of the challenges and modeling approaches for dealing with fluid–particle flows is presented.

1.1 Polydisperse fluid-particle flows

The numerical simulation of polydisperse fluid-particle flows arising in technological and environmental applications is challenging due to their multiscale nature (figure 1). The principal characteristics of these flows are the following:

- · continuous fluid phase (Newtonian, non-Newtonian, etc.),
- · disperse particle phase (solid particle, droplet, bubbles, etc.),
- · size (chemical composition, etc.) distribution of particles,
- · finite particle inertia (as measured by Stokes number),
- · collisions (particle-particle, particle-wall),
- · variable mass loading (very dilute risers to dense fluidized beds),
- · multiphase turbulence (due to mean shear and momentum coupling between phases).

The complex physics of these flows results in many modeling challenges:

- · Strong coupling between fluid and particle phases.
- · Wide range of particle volume fractions (even in same flow).
- · Inertial particles with wide range of Stokes numbers.
- · Collision-dominated to collision-less regimes in same flow.
- · Granular temperature of disperse phase can be small and large in same flow.
- · Polydispersity (e.g. size, density, shape) is almost always present.

Hence we need a modeling framework that can handle all aspects.



Figure 1: Bidisperse gas-particle flow (PR-DNS of Subramaniam group). Large (small) particles have different mean and fluctuating velocities, and the fluid velocity varies significantly inside the computational domain due to momentum coupling.

1.2 Kinetic-based modeling approach

The kinetic theory modeling approach is summarized in figure 2. The principal feature is the formulation of a mesoscale model with physics-based closures derived from the "exact" microscale model. The mesoscale model can have a large number of phase-space variables to describe the particle size distribution, particle velocity distribution, etc. A tractable macroscale model for large-scale simulations is sought by using mathematical closures of the mesoscale model. A well-known example of this procedure is the derivation of the Navier-Stokes equation in the kinetic theory of ideal gases where the closed mesoscale model is the Boltzmann equation.

In fluid-particle flows, the mesoscale kinetic equation for the particle phase typically has one of the two following forms.

• Kinetic equation (KE) (monodisperse particles) for number density function (NDF) $n(t, \mathbf{x}, \mathbf{v})$ where **v** is particle velocity:

$$\frac{\partial n}{\partial t} + \frac{\partial v_i n}{\partial x_i} + \frac{\partial}{\partial v_i} \left[A_i(t, \mathbf{x}, \mathbf{v}) n \right] = \mathbb{C}$$

with closed acceleration A and particle-particle collision operator \mathbb{C} . In words, the NDF is the number concentration of particles with velocity \mathbf{v} at spatial location \mathbf{x} at time t. Here, the acceleration term is coupled to the continuous fluid phase due to drag.

 Generalized population balance equation (GPBE) (polydisperse particles) for the NDF n(t, x, v, ξ) where ξ is, for example, particle mass:

$$\frac{\partial n}{\partial t} + \frac{\partial v_i n}{\partial x_i} + \frac{\partial}{\partial v_i} \left[A_i(t, \mathbf{x}, \mathbf{v}, \xi) n \right] + \frac{\partial}{\partial \xi} \left[G(t, \mathbf{x}, \mathbf{v}, \xi) n \right] = \mathbb{C}$$

with closed acceleration **A**, growth **G** and collision/aggregation operator \mathbb{C} . In words, the NDF is the number concentration of particles with velocity **v** and mass ξ at spatial location **x** at time *t*. Here, the growth term is coupled to the continuous fluid phase due to mass transfer.

The KE/GPBE is coupled to Navier-Stokes equation for the continuous fluid phase. The KE and GPBE are derived from a microscale model and, hence, the functional dependencies of the acceleration, growth, collision/aggregation operators are **known**. Therefore, in principle, the mesoscale model can be solved



Figure 2: The kinetic theory modeling approach uses microscale DNS (see figure 1) to develop a closed mesoscale model that captures the relevant physics. Macroscale computational fluid dynamics (CFD) models are derived from the mesoscale model by using mathematical closures in terms of the moments.

exactly for the NDF. However, in practice, even a numerical solution is intractable due to the large number of independent variables and the complexity of the flow. For large-scale simulations, a simpler approach is needed, preferably one that can be coupled with an existing computational fluid dynamics (CFD) code.

1.3 Moment methods

One approach for developing macroscale models is referred to as *moment methods*. Starting from the mesoscale model, Eulerian moment transport equations can be derived:

• **KE:** Define (1-D) velocity moments as $M_k := \int v^k n \, dv$, and integrate KE to find their transport equation: $\partial M_k = \partial M_{k+1} = \int e^{k-1} A_k \, dv$

$$\frac{\partial M_k}{\partial t} + \frac{\partial M_{k+1}}{\partial x} = k \int v^{k-1} A n \, \mathrm{d}v + \int v^k \mathbb{C} \, \mathrm{d}v$$

where $M_0 = \rho_p \alpha_p$, $M_1 = \rho_p \alpha_p U_p$, $M_2 = \rho_p \alpha_p (U_p^2 + \Theta_p)$. Here α_p is the particle-phase volume fraction, U_p is the particle-phase velocity and Θ_p is the granular temperature. M_{k+1} is referred to as the free-transport (or kinetic) flux of M_k , and is unclosed for the largest k. The terms on the right-hand side are source terms due to acceleration and collisions.

• **GPBE:** Define joint velocity-mass moments as $M_{k,l} := \int v^k \xi^l n \, dv d\xi$, and integrate GPBE to find their transport equation

$$\frac{\partial M_{k,l}}{\partial t} + \frac{\partial M_{k+1,l}}{\partial x} = k \int v^{k-1} \xi^l An \, \mathrm{d} v \mathrm{d} \xi + l \int v^k \xi^{l-1} Gn \, \mathrm{d} v \mathrm{d} \xi + \int v^k \xi^l \mathbb{C} \, \mathrm{d} v \mathrm{d} \xi$$

where $M_{0,1} = \rho_p \alpha_p$, $M_{1,1} = \rho_p \alpha_p U_p$, $M_{2,1} = \rho_p \alpha_p (U_p^2 + \Theta_p)$. Moments $M_{0,0}$, $M_{0,1}$, $M_{0,2}$, etc. are needed for the mass distribution, while moments with k > 0 are needed to account for the correlation between the particle mass and velocity for finite Stokes number.

The terms above in red require mathematical closure because the NDF *n* is unknown. However, if we can approximate the NDF from knowledge of a finite set of its moments, then these equations will be closed. The classical example is the *hydrodynamic model* where we assume that the NDF is a functional of α_p , U_p and Θ_p , which leads to the gas dynamics equations for mass, momentum and energy. The hydrodynamic model will be valid when the NDF is mainly determined by the collision operator. In the absence of collisions (e.g. dilute flows or negligible granular temperature), a more general moment-closure method is needed. Closure with quadrature-based moment methods (QBMM) is shown schematically in figure 3.



Figure 3: Quadrature-based moment methods reconstruct the NDF from a finite sets of its moments. The reconstruction takes the form of a sum of weighted delta functions that exactly reproduces the known moments in each grid cell at each time step. Here, the 3-D solver is a classical finite-volume CFD code. The 6-D solver is a direct solver for the NDF in 3-D physical and 3-D phase space.

2 Quadrature-Based Moment Methods

The Basic Idea: Given moments, reconstruct the NDF. However, there are several important things to consider:

- · Which moments should we choose?
- What method should we use for reconstruction?
- How can we extend the method to multivariate phase space?
- How should we design the numerical solver for the moments?

In all cases, we must be able to demonstrate *a priori* that the numerical algorithm is robust and accurate. Another key point is that the method must be very fast because we will need to do the inversion in every grid cell at every time step during the CFD simulation.

One classical method for approximating 1-D integrals is Gaussian quadrature [Gautschi (2004)], which the following properties:

• The formula

$$\int g(v)n(v)\,\mathrm{d}v = \sum_{\alpha=1}^N n_\alpha g(v_\alpha) + R_N(g)$$

is a Gauss quadrature iff the N nodes v_{α} are roots of an N^{th} -order orthogonal polynomial $P_N(v)$ (\perp with respect to n(v)). This formula is exact if g(v) is a polynomial of order less than 2N.

• A robust inversion algorithm for moments $M_k = \int v^k n(v) dv$ exists to find the weights and abscissas:

$$\{M_0, M_1, \dots, M_{2N-1}\} \stackrel{\text{QMOM}}{\Longrightarrow} \{n_1, n_2, \dots, n_N\}, \{v_1, v_2, \dots, v_N\}$$

The algorithm solves a small (N) eigenvalue/eigenvector problem, which is relatively fast.

• In all cases, the weights $\{n_1, n_2, \ldots, n_N\}$ are positive and the abscissas $\{v_1, v_2, \ldots, v_N\}$ are well defined (i.e., are in the support of the NDF).

2.1 Quadrature method of moments

The favorable properties of Gaussian quadrature led to the quadrature method of moments (QMOM) for size moments. Using QMOM [McGraw (1997)], the unclosed terms in the moment equations are approximated as

$$\frac{\mathrm{d}\mathbf{M}}{\mathrm{d}t} = \int_0^\infty \mathbf{S}(\xi) n(\xi) \mathrm{d}\xi \approx \sum_{\alpha=0}^N n_\alpha \mathbf{S}(\xi_\alpha)$$

where $\mathbf{M} = \{M_0, M_1, \dots, M_{2N}\}$ and \mathbf{S} is a "source term". Experience has shown that QMOM has the following properties:

- Exact if S is polynomial of order $\leq 2N$, otherwise a very good approximation.
- Provides good approximations with small N ≈ 4.
- When solving the moment equations numerically, the moments M must remain realizable for moment inversion, which is almost always the case.

Note that QMOM is equivalent to reconstructing the NDF [Dette & Studden (1997)] as

$$n^*(\xi) = \sum_{\alpha=0}^N n_\alpha \delta(\xi - \xi_\alpha),$$

which is **realizable** because $n_{\alpha} \ge 0$ for all α . The abscissas ξ_{α} can be interpreted as weighted samples (or "parcels") that adapt dynamically with the evolution of the moments.

2.2 Hyperbolic QMOM

For closure of the spatial flux M_{k+1} , hyperbolic QMOM for the velocity moments is preferable, for example, to CQMOM [Yuan & Fox (2011)]. As an example, consider the KE in 2-D with velocity moments $M_{i,j} = \int u^i v^j n(u, v) \, du dv$.

· Conditional HyQMOM reconstructs the velocity NDF as

$$n^{*}(u,v) = M_{0,0} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} p_{\alpha} p_{\alpha\beta} \delta(u - \bar{u} - u_{\alpha}) \delta(v - \bar{v} - \bar{v}_{\alpha} - v_{\alpha\beta})$$

where $\bar{u} = M_{1,0}/M_{0,0}$, $\bar{v} = M_{0,1}/M_{0,0}$ are the mean velocities, and the abscissas u_{α} , $v_{\alpha\beta}$ and the conditional moment \bar{v}_{α} are found from central moments:

$$C_{i,j} = \frac{1}{M_{0,0}} \int_{\mathbb{R}^2} (u - \bar{u})^i (v - \bar{v})^j n(u, v) \, \mathrm{d}u \mathrm{d}v.$$

• In 2-D velocity phase space, the nine quadrature nodes are found from 10 moments:

$$\begin{array}{ccccccc} M_{0,0} & M_{0,1} & M_{0,2} & M_{0,3} & M_{0,4} \\ M_{1,0} & M_{1,1} & & \\ M_{2,0} & & \\ M_{3,0} & & \\ M_{4,0} & & \end{array}$$

Like CQMOM, the CHyQMOM reconstruction can reproduce particle trajectory crossings, but has hyperbolic (i.e., real eigenvalues) for the spatial fluxes.

2.3 Kinetic-based finite-volume methods

Kinetic-based finite-volume (KBFV) methods were developed to ensure that the numerical solution for the moments are realizable in CFD codes [Marchisio & Fox (2013)]. The basic problem is as follows. Given the **transported moments**, solve the 2-D KE in moment form:

$$\frac{\partial M_{i,j}}{\partial t} + \frac{\partial M_{i+1,j}}{\partial x} + \frac{\partial M_{i,j+1}}{\partial y} = i \int u^{i-1} v^j A_x \, n \, \mathrm{d} u \mathrm{d} v + j \int u^i v^{j-1} A_y \, n \, \mathrm{d} u \mathrm{d} v + \int u^i v^j \mathbb{C} \, \mathrm{d} u \mathrm{d} v$$

where the right-hand side is closed using QBMM:

$$\frac{\partial M_{i,j}}{\partial t} + \frac{\partial M_{i+1,j}}{\partial x} + \frac{\partial M_{i,j+1}}{\partial y} = \sum_{\alpha=1}^{N} n_{\alpha} \left\{ i u_{\alpha}^{i-1} v_{\alpha}^{j} A_{x,\alpha} + j u_{\alpha}^{i} v_{\alpha}^{j-1} A_{y,\alpha} + u_{\alpha}^{i} v_{\alpha}^{j} \mathbb{C}_{\alpha} \right\}.$$

When developing a numerical algorithm, there are several things to consider:

- · How do we discretize the spatial fluxes?
- · How do we update the moments in time?
- How can we ensure that the moments are always realizable?

In the literature [Vikas *et al.* (2011)], it is well known that only first-order numerical schemes yield realizable moments. However, high-order schemes are needed to reduce numerical diffusion. Getting a high-order scheme to work requires additional effort as we briefly describe next.

2.4 Kinetic-based spatial fluxes

Kinetic-based spatial fluxes make use of the reconstructed NDF. In KBFV methods, the spatial fluxes use a kinetic formulation [Perthame (2003)]. For example, with the 1-D moment advection equation defined by $\partial_t M_{0,0} + \partial_x M_{1,0} = 0$, we write the flux as the sum of two contributions:

$$M_{1,0} = Q_{1,0}^- + Q_{1,0}^+ = \int_{-\infty}^0 v\left(\int n^*(v,\xi) \mathrm{d}\xi\right) \mathrm{d}u + \int_0^\infty v\left(\int n^*(v,\xi) \mathrm{d}\xi\right) \mathrm{d}v.$$

Using reconstructed NDF n^* , the downwind and upwind flux components are

$$Q_{1,0}^{-} = \sum_{\alpha=1}^{N} \rho_{\alpha} v_{\alpha} I_{(-\infty,0)}(v_{\alpha}) \quad Q_{1,0}^{+} = \sum_{\alpha=1}^{N} \rho_{\alpha} v_{\alpha} I_{(0,\infty)}(v_{\alpha})$$

where $I_{\mathbb{S}}(x)$ is the indicator function for the interval \mathbb{S} . The velocity abscissas thus define the fluxes locally in physical space and time. In the context of finite-volume methods, the flux components are used to define the flux functions at the cell interfaces, $\mathbf{G}(\mathbf{M}_l, \mathbf{M}_r)$, given moments on the left \mathbf{M}_l and right \mathbf{M}_r sides of the interface. As mentioned above, first-order flux functions lead to generally unacceptable levels of numerical diffusion. Second-order flux functions are preferred for CFD simulations.

2.5 Realizable time-stepping schemes

Given KBFV flux functions between neighboring cells, we can compute the updated moments as follows:

• First-order explicit Euler:

$$\mathbf{M}_{i}^{n+1} = \mathbf{M}_{i}^{n} - \lambda \left[\mathbf{G} \left(\mathbf{M}_{i+\frac{1}{2},l}^{n}, \mathbf{M}_{i+\frac{1}{2},r}^{n} \right) - \mathbf{G} \left(\mathbf{M}_{i-\frac{1}{2},l}^{n}, \mathbf{M}_{i-\frac{1}{2},r}^{n} \right) \right]$$

• Second-order explicit RK2SSP:

$$\begin{split} \mathbf{M}_{i}^{*} &= \mathbf{M}_{i}^{n} - \lambda \left[\mathbf{G} \left(\mathbf{M}_{i+\frac{1}{2},l}^{n}, \mathbf{M}_{i+\frac{1}{2},r}^{n} \right) - \mathbf{G} \left(\mathbf{M}_{i-\frac{1}{2},l}^{n}, \mathbf{M}_{i-\frac{1}{2},r}^{n} \right) \right] \\ \mathbf{M}_{i}^{**} &= \mathbf{M}_{i}^{*} - \lambda \left[\mathbf{G} \left(\mathbf{M}_{i+\frac{1}{2},l}^{*}, \mathbf{M}_{i+\frac{1}{2},r}^{*} \right) - \mathbf{G} \left(\mathbf{M}_{i-\frac{1}{2},l}^{*}, \mathbf{M}_{i-\frac{1}{2},r}^{*} \right) \right] \\ \mathbf{M}_{i}^{n+1} &= \frac{1}{2} \left(\mathbf{M}_{i}^{n} + \mathbf{M}_{i}^{**} \right) \end{split}$$



Figure 4: 2-D cuts through the six Lagrangian simulations of cluster-induced turbulence (CIT). The domains are shown to scale relative to the largest domain. The location of the particles is shown, which is roughly equal to the particle-phase volume fraction when scaled properly. On the largest domain (Case 6), the clusters are smaller than the box size, while on the smaller domains some clusters span the entire width of the box.

where $\lambda = \Delta t / \Delta x$ is fixed using a realizability constraint, which is more restrictive than the CFL condition [Vikas *et al.* (2011)]. RK2SSP is realizable because \mathbf{M}_i^{n+1} is a convex sum of two realizable moment sets. The flux functions are defined using velocity abscissas with second-order spatial reconstruction of the weights. In this way, the CFD code is second order in space and time.

3 Validation for Clustered-Induced Turbulence

Instead of moment methods, the KE can be simulated using Lagrangian methods where individual particles are tracked, including particle–particle collisions [Capecelatro & Desjardins (2013)]. While quite accurate, these methods are very expensive for moderately dense flows where the number of particles in the system can be many millions, or even billions. The question then arises: Do Eulerian moment methods and Lagrangian models give equivalent results?

Here, we use cluster-induced turbulence (CIT) [Capecelatro *et al.* (2015b)] to investigate this question for gas-particle flows. The simulation cases considered are as follows:

- Cases 1-6 in [Capecelatro et al. (2015a)] (see figure 4).
- Average volume fraction: α_p = 0.01.
- Density ratio: $\rho_p / \rho_g = 1000$.
- Particle Reynolds number: Rep = 0.5.
- Terminal (Stokes) velocity: $\mathcal{V} = 0.1$ m/s.
- Characteristic cluster length: $\mathcal{L} = 2.5$ mm.
- Box size for Case 6: L_x/L = 129 (2048 × 512 × 512).

The Lagrangian and Eulerian simulations are performed on same grid for the fluid phase, but not with same numerical schemes. In general, the Lagrangian simulations use high-order schemes and thus differences at the smallest resolved scales are expected. The grids are cubic with length approximately equal to the particle diameter.



Figure 5: Particle volume fraction fields for (left) Lagrangian and (right) Eulerian simulations from Case 6.

The governing equation for the Eulerian 10-moment model is

$$rac{\partial \mathbf{M}}{\partial t} +
abla \cdot \mathbf{F} = \mathbf{A} + \mathbf{C} \quad ext{where} \quad M_{ijk} = \int u^i v^j w^k \, f(\boldsymbol{v}) \mathrm{d} \boldsymbol{v}.$$

The ten moments are related to the particle-phase variables as follows:

$$M_{000}^{0} = \alpha_{p}, \quad \begin{bmatrix} M_{100}^{1} \\ M_{010}^{1} \\ M_{001}^{1} \end{bmatrix} = \alpha_{p} \boldsymbol{U}_{p}, \quad \begin{bmatrix} M_{200}^{2} & M_{110}^{2} & M_{101}^{2} \\ M_{110}^{2} & M_{020}^{2} & M_{011}^{2} \\ M_{101}^{2} & M_{011}^{2} & M_{002}^{2} \end{bmatrix} = \alpha_{p} (\boldsymbol{U}_{p} \otimes \boldsymbol{U}_{p} + \mathbf{P}_{p})$$

where \mathbf{P}_p is the (symmetric) particle-phase pressure tensor. The trace of \mathbf{P}_p is proportional to the granular temperature. In the KBFV code, a Gauss-Hermite quadrature is used to solve for the free-transport flux \mathbf{F} . The collision term \mathbf{C} is approximated by the inelastic BGK model [Passalacqua *et al.* (2011)]. As in the Lagrangian simulation, Stokes drag and gravity are used to define \mathbf{A} .

A qualitative comparison of clustering is shown in figure 5 for Case 6. While the cluster shapes are very similar, the Eulerian simulation has slightly longer/wider clusters. A quantitative comparison of selected one-point statistics is shown in figures 6 and 7. The moment method (EE-AG) has slightly fewer high α_p values than the Lagrangian (EL) simulations. This difference is likely due to numerical resolution of the smallest scales. EE-AG has slightly higher falling velocity for the particles, which is likely due to the larger clusters. In figure 7, EE-AG has lower granular temperature than EL, which is partially due to how it is extracted from the EL data in post-processing. On the other hand, EE-AG has higher turbulent kinetic energy for both phases, which is likely due to the larger clusters. In general, the domain-size dependence found with EL and EE-AG is very similar, thus either method can be used to investigate the effect of domain size. Quantitative comparisons between two-point statistics such as energy spectra confirm the qualitative observations about cluster size discussed above.

4 Extension to Dense Flows

The CIT results above are for dilute flows where only the free-transport flux is important in the Eulerian model. For dense flows, such as fluidized beds, the collisional and frictional fluxes are also very important. The numerical treatment of such fluxes is not particularly efficient using kinetic-based methods. Thus, we can combine KBFV methods for the free-transport flux with classical hydrodynamic models for the dense phase in order to treat all flow regimes in gas-particle flows.



Figure 6: Particle volume fraction PDF (left) and falling velocity (right) for all cases.



Figure 7: Kinetic energy statistics for Θ_p (left), k_p (middle), k_f (right) for all cases.

4.1 Kinetic model for all flow regimes

The gas-particle flow model for dilute-to-dense particles couples two models: the (monodisperse) particle-phase KE

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{A}n = \mathbb{C}$$

where

- $n(t, \mathbf{x}, \mathbf{v})$ is the number density function (NDF),
- v is the particle velocity,
- A is the particle acceleration,
- \mathbb{C} it the rate of change of n due to Boltzmann–Enskog collisions and frictional stresses;

and the fluid-phase equations

$$\begin{split} \frac{\partial}{\partial t} \alpha_{\rm g} \rho_{\rm g} + \nabla \cdot \alpha_{\rm g} \rho_{\rm g} \mathbf{U}_{\rm g} &= 0 \\ \frac{\partial}{\partial t} \alpha_{\rm g} \rho_{\rm g} \mathbf{U}_{\rm g} + \nabla \cdot \alpha_{\rm g} \rho_{\rm g} \mathbf{U}_{\rm g} \mathbf{U}_{\rm g} &= \nabla \cdot \alpha_{\rm g} \boldsymbol{\tau}_{\rm g} + \beta_{\rm g} + \alpha_{\rm g} \rho_{\rm g} \mathbf{g} \end{split}$$

where

- $\alpha_{\rm g} = 1 \alpha_{\rm p}$ is the gas-phase volume fraction,
- β_{g} is the mean particle drag.

In dense flows, the frictional stresses make the KE very stiff so that only the low-order velocity moments used in the hydrodynamic model are needed to describe the particle phase.

4.2 Moment model for all flow regimes

The moment transport equations with collisional and frictional fluxes can be written for 10 velocity moments. In the dilute regime, we have as before

$$\begin{aligned} \frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot \mathbf{F} &= \mathbf{S} \\ M_{000}^{0} &= \rho_{p} \alpha_{p}, \quad \begin{bmatrix} M_{100}^{1} \\ M_{010}^{1} \\ M_{001}^{1} \end{bmatrix} &= \rho_{p} \alpha_{p} \boldsymbol{U}_{p}, \quad \begin{bmatrix} M_{200}^{2} & M_{110}^{2} & M_{101}^{2} \\ M_{110}^{2} & M_{020}^{2} & M_{011}^{2} \\ M_{101}^{2} & M_{011}^{2} & M_{002}^{2} \end{bmatrix} &= \rho_{p} \alpha_{p} (\boldsymbol{U}_{p} \otimes \boldsymbol{U}_{p} + \mathbf{P}_{p}) \end{aligned}$$

where \mathbf{F} is the free-transport flux and \mathbf{S} is the source term due to acceleration and collisions [Fox & Vedula (2010)]. In the dense regime, we have

$$\frac{\partial \rho_p \alpha_p \mathbf{U}_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \mathbf{U}_p = 0$$

$$\frac{\partial \rho_p \alpha_p \mathbf{U}_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \left(\mathbf{U}_p \otimes \mathbf{U}_p + \mathbf{P}_p + \mathbf{G}_p + \mathbf{Z}_p \right) = \rho_p \alpha_p \mathbf{g} + \rho_p \alpha_p \mathbf{M}_{pg}$$

$$\frac{\partial \rho_p \alpha_p \mathbf{P}_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \left(\mathbf{U}_p \otimes \mathbf{P}_p + \mathbf{Q}_p + \mathbf{H}_p \right) + \rho_p \alpha_p \left[(\mathbf{P}_p + \mathbf{G}_p) \cdot \nabla \mathbf{U}_p + (\nabla \mathbf{U}_p)^T \cdot (\mathbf{P}_p + \mathbf{G}_p) \right]$$

$$= \rho_p \alpha_p \mathbf{E}_{pg} + \rho_p \alpha_p \mathbf{C}_p$$

where $3\Theta_p = trace(\mathbf{P}_p)$ and the free-transport fluxes are shown in blue.

In the dense regime, the free-transport flux can be approximated by the hydrodynamic model shown here in red:

$$\mathbf{P}_p = \Theta_p \mathbf{I} - \boldsymbol{\sigma}_p = \Theta_p \mathbf{I} - 2\nu_{p,k} \boldsymbol{S}_p$$

where the rate of deformation tensor is

$$oldsymbol{S}_{p}=rac{1}{2}\left[
abla oldsymbol{U}_{p}+\left(
abla oldsymbol{U}_{p}
ight)^{T}-rac{2}{3}\left(
abla \cdotoldsymbol{U}_{p}
ight)\mathbf{I}
ight]$$

and $\nu_{p,k}$ is an effective viscosity for the particle phase. The collisional flux (where the corresponding pressure is infinite for finite $\alpha_p \approx 0.63$) is modeled as

$$\mathbf{G}_p = \frac{p_{p,c}}{\rho_p \alpha_p} \mathbf{I} - 2\nu_{p,c} \mathbf{S}_p.$$

The frictional flux (where the corresponding pressure is infinite for finite $\alpha_p \approx 0.63$, null when $\alpha_p < 0.55$) is modeled as

$$\mathbf{Z}_p = \frac{p_{p,f}}{\rho_p \alpha_p} \mathbf{I} - 2\nu_{p,f} \mathbf{S}_p.$$

In the hydrodynamic model, the energy fluxes are modeled by $U_p \otimes \mathbf{P}_p + \mathbf{Q}_p + \mathbf{H}_p = U_p \otimes \mathbf{P}_p - \frac{2}{3}k_{\Theta}\nabla \otimes \mathbf{P}_p$ where k_{Θ} is an effective conductivity. In the dense regime, the transport equation for Θ_p is solved as the traceless, anisotropic part of \mathbf{P}_p (i.e., $\boldsymbol{\sigma}_p$) is modeled in terms of S_p .

4.3 Solution algorithm for all flow regimes

In the kinetic flux-splitting scheme for all flow regimes, the free-transport flux is treated with moment methods in dilute regions and the hydrodynamic model in dense regions. This is accomplished as follows. First, we split \mathbf{F} in the moment transport equation:

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot h_1 \mathbf{F} + \nabla \cdot (h_2 \mathbf{F} + \mathbf{G} + \mathbf{Z}) = \mathbf{S}$$

where $h_1 + h_2 = 1$ and the flux-splitting function is defined by using the kinetic, collisional and frictional contributions to the particle-phase pressure:

$$h_2 := \left(\frac{p_{p,c} + p_{p,f}}{p_{p,k} + p_{p,c} + p_{p,f} + \varepsilon}\right)^p.$$



Figure 8: Dependency of flux-splitting functions on α_p found from a fluidized-bed simulation.

The blue flux above is treated using KBFV methods, while the red flux uses the hydrodynamic model. In dilute regions, h_2 is nearly zero, while in dense regions it is nearly one (see figure 8). Thus, the exponent p determines the fraction of the free-transport flux that is treated using KBFV methods. Experience suggests the p = 4 is a reasonable choice. In a CFD simulation, h_2 will be different in every cell at every time step so that the code dynamically adjusts to the local flow regime.

The operator-splitting algorithm proceeds in two steps:

Step 1: KBFV method $\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot h_1 \mathbf{F} = \mathbf{0}$ Step 2: Hydrodynamic solver $\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot (h_2 \mathbf{F} + \mathbf{G} + \mathbf{Z}) = \mathbf{S}$

with all of the source terms S evaluated in the second step. Here, G and Z are the collisional and frictional fluxes, respectively, for the velocity moments M. The solution procedure is as follows:

- 1. Initialize all variables \mathbf{M} , $\{\alpha_p, U_p, \Theta_p, \boldsymbol{\sigma}_p\}$, and $\{\alpha_g, U_g, p_g\}$.
- 2. Calculate h_1 and h_2 .
- 3. Explicit free-transport solver:

Compute kinetic-based moment fluxes to transport the moments.

Update $\{\alpha_p, U_p, \Theta_p, \sigma_p\}$ using moments M.

4. Iterative hydrodynamic solver:

Solve for $\{\alpha_p, U_p, \Theta_p\}$ using hydrodynamic transport equations.

Solve gas-phase velocity and pressure $\{U_g, p_g\}$ equations.

- 5. Solve σ_p transport equation (not shown).
- 6. Update moment set **M** using $\{\alpha_p, U_p, \Theta_p, \sigma_p\}$.
- 7. Advance in time by repeating from Step 2 until simulation is complete.

In practice, the computational cost is dominated by the hydrodynamic solver when the flow is dense (e.g., a fluidized bed). The algorithm can be implemented with any hydrodynamic solver (e.g. MFIX, OpenFOAM) developed for gas-particle flows. The only substantial change needed in the hydrodynamic code is to insert h_2 in the definition of the free-transport flux term.



Figure 9: Particle volume fraction (left) and granular temperature (right) fields found from free-transport flux splitting code. Two left panels: $\overline{\alpha}_p = 0.01$. Two center panels: $\overline{\alpha}_p = 0.1$. Two right panels: $\overline{\alpha}_p = 0.4$.

4.4 Application to particle-laden vertical channel flow

Results for a 3-D wall-bounded vertical channel, simulated with the algorithm described above, are shown in figure 9. Three channel-average particle volume fractions were employed: $\overline{\alpha}_p = 0.01$, 0.1, and 0.4, corresponding to dilute, moderately dilute and moderately dense flows. Simulations were also run with $h_2 = 1$ for all cases (i.e., the hydrodynamic model). For the values of $\overline{\alpha}_p$, the level of granular temperature was significantly larger when the free-transport flux was treated with KBFV methods. Analysis of the results revealed the source term in the hydrodynamic model for granular temperature was too small by a factor of approximately two. In general, the flow dynamics of gas-particle flows are significantly different when the granular temperature is lower. For example, the particle volume fraction distribution across the channel width changes significantly. In dense flows, the observed bubble size is larger when the freetransport flux is treated using a moment method.

5 Concluding Remarks

- Mesoscale models have a direct link with the underlying physics and result in a kinetic equation for the velocity number distribution function (NDF).
- Quadrature-based moment methods (QBMM) solve the kinetic equation by reconstructing the NDF from its moments.
- For dilute flows, it is best to use the velocity NDF reconstruction and kinetic-based finite-volume (KBFV) methods.
- For dense flows, it is best to use a KBFV method for the free-transport flux and a "two-fluid" hydrodynamic solver for the collisional and frictional fluxes.
- The joint mass-velocity NDF allows for polydisperse particles needed in applications involving particle "size" changes.
- The QBMM algorithms described in this article are part of the OpenQBMM project (figure 10) (www.openqbmm.org).



Figure 10: Gas-particle flow simulation tools implemented in OpenFOAM as part of the OpenQBMM project.

References

- [Capecelatro & Desjardins (2013)] CAPECELATRO, J. & DESJARDINS, O. 2013 An Euler-Lagrange strategy for simulating particle-laden flows. *Journal of Computational Physics* 238, 1–31.
- [Capecelatro et al. (2015a)] CAPECELATRO, J., DESJARDINS, O. & FOX, R. O. 2015 Effect of domain size on fluid–particle dynamics in homogeneous, gravity-driven, cluster-induced turbulence. *Journal* of Fluids Engineering 138(4), 041301.
- [Capecelatro et al. (2015b)] CAPECELATRO, J., DESJARDINS, O. & FOX, R. O. 2015 On fluid-particle dynamics in fully developed cluster-induced turbulence. *Journal of Fluid Mechanics* 780, 578–635.
- [Dette & Studden (1997)] DETTE, H. & STUDDEN, W. J. 1997 The Theory of Canonical Moments with Applications in Statistics, Probability, and Analysis, John Wiley and Sons (NY).
- [Fox & Vedula (2010)] FOX, R. O. & VEDULA, P. 2010 Quadrature-based moment model for moderately dense polydisperse gas-particle flows. Industrial & Engineering Chemistry Research 49, 5174–5187.
- [Gautschi (2004)] GAUTSCHI, W. 2004 Orthogonal Polynomials: Computational and Approximation, Oxford University Press (UK).
- [Marchisio & Fox (2013)] MARCHISIO, D. L. & FOX, R. O. 2013 Computational Models for Polydisperse Particulate and Multiphase Systems, Cambridge University Press (UK).
- [McGraw (1997)] MCGRAW, R. 1997 Description of aerosol dynamics by the quadrature method of moments. Aerosol Science and Technology 27, 255–265.
- [Passalacqua et al. (2011)] PASSALACQUA, A., GALVIN, J. E., VEDULA, P., HRENYA, C. M. & FOX, R. O. 2011 A quadrature-based kinetic model for dilute non-isothermal granular flows. *Communica*tions in Computational Physics 10, 216–252.
- [Perthame (2003)] PERTHAME, B. 2003 Kinetic Formulation of Conservation Laws, Oxford University Press (UK).
- [Vikas et al. (2011)] VIKAS, V., WANG, Z. J., PASSALACQUA, A. & FOX, R. O. 2011 Realizable high-order finite-volume schemes for quadrature-based moment methods. *Journal of Computational Physics* 230, 5328–5352.
- [Yuan & Fox (2011)] YUAN, C. & FOX, R. O. 2011 Conditional quadrature method of moments for kinetic equations. *Journal of Computational Physics* 230, 8216–8246.

Interactions, Integrations and Innovations - Memories from my fluidization research and hope for the future

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By some coincidence the day of the session 270 of AIChE 2016 Annual Meeting was just the 42nd anniversary of my first step on North America to join Professor C.Y. Wen's group of West Virginia University back in 1974. Moreover, San Francisco was the very place of my first step. I thank very much the Particle Technology Forum, AIChE and SCEJ, Professors T. Tsuji (Osaka U) and H. Kamiya (TUAT), the organizer, Profs. N. Ellis (UBC), L.S. Fan (OSU), F. Johnsson (Chalmers UT), Dr. T. Knowlton (PSRI), Profs. J.R. van Ommen (Delft UT), P.G. Trinanes (U Greenwich), A. Tsutsumi (U Tokyo) and A. Yu (Monash U), the speakers, and all the attendants for realizing the honorable session for me.



Photo 1. After the session (Nov. 15, 2016)

(From left: T. Tsuji, H. Kamiya, N. Ellis, F. Johnsson, M. Horio, P.G. Trinanes, L-S. Fan, T. Knowlton, J.R. van Ommen, C. Chen, and A. Yu; Photo taken by Dr. A.S. Issangaya.)

In this article I would present an extended summary of my talk in the session by focusing on my background, on how I rediscovered the three stage law of Taketani (cf. Horio (2013)¹⁾) and applied it for my research over the subsequent two decades and on the interaction between industry and academia (or practice and theory) that have been supporting progresses of scientific knowledge in our field.

1. From the borderland

Occasionally looking down at the Monongahela River, the riverside bushes of deciduous broadleaf trees typical of West Virginia and the ups and downs of coal barge carriers from my office window on the 5th floor of WVU Engineering Building at Morgantown WVa, I started my career of fluidization research in the group of Professor C.-Y. (Jimmy) Wen. I was a late starter in the field because I spent already ten years on various fixed bed and moving bed applications for my doctor thesis under Professor Iwao Muchi. Moreover, since my degree was given from the department of metallurgy and iron-steel engineering, Nagoya University, I was just a dark horse in chemical engineering community.

In general a scientist/researcher wanders around searching for unknown things and/or paradoxes. In engineering sciences, which support technical endeavor to reach a goal, the nature of a researcher is not at all different. An engineering scientist is a pioneer in a certain borderland cultivating it focusing on the relationship between what he/she is watching there and the established system of scientific/technological knowledge. On the other hand, an engineer is a person who tries to apply all the established knowledge to realize his/her development ideas or to solve problems. After all such efforts, he/she may face some unknown things, recognize that he/she is now in a borderland and try to know and control them to pursue his/her objectives. Usually, an engineer would not appreciate just being in borderlands.

From the beginning of my career I happened to wander such borderlands. I was a chemical engineering student at Nagoya Institute of Technology but in the department of applied chemistry where chemical engineers were a minority. There in School Year 1965 I did my BS thesis work on the process analysis of fixed bed leaching process under the one-year supervision of Professor Ikuho Yamada, who was famous for his theory on multi-component distillation. Prof. Yamada persuaded us students to think over phenomena from several viewpoints of much different scales, say from molecular to plant scales, and over a wide subject areas. He provided us a special atmosphere to concentrate ourselves on mathematics and numerical simulation. In the spring of 1966 I moved to Nagoya University for my MS and PhD following Professor Iwao Muchi who was Professor Yamada's boss there in Nagoya Institute until two years before. Professor Muchi was a brave person. Receiving an offer from the new Department of Iron and Steel Engineering, he jumped into the discipline much different from chemical engineering (it was very much so particularly that time). I too was already a venturous chemical engineering student heading the borderland and just believing that molten iron only differs from water in density, several other transport properties and nothing more! Years later, Muchi models on blast furnaces, LD converters and so on became famous and pulled out complete modernization of iron/steel metallurgy. I finished my PhD on the dynamics of iron making processes, blast furnaces, hot blast stoves and sintering machines, mainly tackling with transient behaviors of fixed and moving bed.

In Nagoya University I was also affected by Professor Genji Jimbo with his powder technology as well as his unique philosophy of engineering. My encounter with the writing of a physicist and thinker Mitsuo Taketani (1911-2000) was probably through him.

In Muchi group there was a fluidization subgroup led by my close friend Dr. Shigekatsu Mori, from whom I was always informed what's going on in fluidization research. Dr. Mori joined a year early Professor Wen's group and encouraged me to do so. It was right at the time of the oil crisis and I thought it was a chance to much widen my field.

So, from November 1974 I started my two year post doc study at WVU as noted above. My main task there was to review the state of the art of fluidization and to develop a numerical simulation model on fluidized bed combustors taking into account the pressure elevation effects (cf. Horio and Wen (1978) and Horio, Rengarajan, Krishnan and Wen (1977)). After the oil crisis the movement for coal fired FBC boiler developments was quickening. In December 1975 the Fourth International Conference on Fluidized Bed Combustion was held at McLane, Va. Attending the meeting with Professor Wen I could meet almost all players for bubbling fluidized bed combustion boiler development that time.

Enjoyable was the discussion with Professor Wen who was interested in almost everything. As far as I know he was working on coal pyrolysis, gasification and combustion, gas-solid reaction kinetics, reactor design and fluidization fundamentals that time. For fundamental issues we discussed over and over on elutriation, on which previous correlations were scattering, on a paradox for fines' low elutriation rate and on unclear conceptualization of TDH; we also discussed on phenomena around the gas distributor, lateral bubble distribution and its effect on solid mixing. Such an extremely wide interest on fundamental phenomena was due to his strong intention in chemical reaction/reactor engineering, and to the strong ties with industries. Professor Wen gave me a chance to teach graduate students for one semester with a title of *The Special Topics of Fluidization*, through which I became able to review almost all the previous discussions and achievements of fluidization.

However, it was also because of the special situation of fluidization research of that time, which I gradually recognized, and then clearly by 1980. The special feature of that time lied in the fact that the efforts to explain comprehensively almost all phenomena in fluidized beds based on the bubble dynamics had been yielded successful results by around 1970. It was an end of a long journey initiated by Lewis and Gilliland in the 1940s to uncover the secrets of fluidization. So, contrary to the enthusiasm of bubble based researches during the 1960s, the interests of researchers shifted to particle issues, distributor issues, freeboard issues, scale-up issues and high velocity, high pressure issues, all of which were out of the coverage of the simple bubbling bed theory. It was thus quite timely that the first International Fluidization Conference was held in 1975 in Asilomar, Ca.

2. Backcasting with the Taketani three stage law

Coming back to Japan I started to systematically study on freeboard phenomena including elutriation, splashing and TDH issues, distributor phenomena including jetting and dead zone issues, lateral bubble distribution and solid segregation. From the early 1980s I started writing a 305 page book entitled as "Fluidization Reaction Engineering" in Japanese with Drs. Mori and Muchi. The book was published in 1984, two years after I joined Tokyo University of Agriculture and Technology. During the book writing I had an inspiration on the history of fluidization research, which actually was a reconfirmation of Taketani's three stage law of scientific progress (1942) almost forgotten by people by that time.

The Taketani three stage law claims that the progress of knowledge of a science always go through the three stages, i.e., the phenomenology stage (or the stage of phenomenologist), then the structuralism stage (or the stage of structuralist) and finally essentialism stage (or the stage of essentialist). By using the analogies between the essence (first principle) and a differential equation, between structures and boundary conditions and between phenomena and solutions he explains that the reason is because of the constitution of things themselves. His point is that we cannot immediately jump from phenomenology to essential theory or first principle. We need structuralist approach in between. With such an understanding, we may able to backcast and define where we are and design the research project aiming at the target period with a product image. It may be worth to note here first that the Khun (1962)'s paradigm theory does not provide such strategic approach to unveil the secret of things and second that such a three stage process is essential for the cognitive process. This applies for almost all research projects from a short term project to the long term development of a new scientific theory. For further details please see Horio (2013).

Indeed, it is interesting to review from the view point of the three stage law the early elaboration, i.e., the 327 page book, 'Fluidization' by Max Leva (1959), an inventor, scientist and consultant in Pittsburgh. It contains much information on the characteristics of fluidized bed in terms of observed data and narrations, parameters evaluated, but based on concepts for homogeneous systems, correlations with dimensional

analysis and nomographs for design calculations. The bed voidage fluctuation data observed by a capacitance probe by Morse and Ballou (1951) was already included but such aggregative fluidization is explained by the aggregation of solids instead of 'aggregation' of gas into bubbles (cf. p.95 Fig. 4-10). There was no discussion on bubbles although the term 'bubbling fluidization' appears only once in Nomenclature (table 1-1). In the book we can find those famous names such as N. Epstein, LT Fan, E.R. Gilliland, of course, H.F. Johnstone, M. Kwauk, O. Levenspiel, W.K. Lewis, L. Massimilla, T. Shirai, R.D. Toomey, C.Y. Wen and/or F. Zenz but not J.F. Davidson, D. Kunii nor J.F. Grace. It was a summary of the phenomenological knowledge and some structural arguments in the period of the mid-1940s to the early-50s

But the stage/period of structuralist study had been already kicked off in 1955 by Shen-Johnstone's two phase model as a reactor model where bubble phase and emulsion phase were separately treated to explain the low conversion typical in fluidized bed reactors. Bubbling had already become one of an important issues in the book 'Fluidization and Fluid-Particle Systems' by F.A. Zenz and D.F. Othmer (1960). They shed lights on almost all aspect of particle behavior and handling in fluidized bed systems including gas and solid feed, jetting, bubbling, entrainment, freeboard, and transport lines from real process development experiences and the content is quite informative even now. However, it was published right before the revolution of Davidson's bubble model.

Davidson and Harrison (1963) demonstrated that the fluid mechanic formulation is the essence of bubbling bed although not many fluidization engineers and academia were familiar with such an approach. Since the publicaion of Shen-Johnstone (1955) it took eight years to reach the Davidson model. Then, for about a decade after the Davidson-Harrison book, almost all fluidized bed phenomena were formulated in terms of bubble hydrodynamics and bubbling bed assumptions. Such new bubbling bed approaches were summarized by the timely publications of both Kuni-Levenspiel's book '*Fluidization Engineering*' (1969) from design oriented viewpoint and '*Fluidization*' (1971) edited by Davidson-Harrison from academic viewpoint. The historical development process reviewed above clearly shows that the ten years of structuralist stage of two-phase model was the cradle of the Davidson model and the next ten years of essentialist stage.

I have described the above process several times elsewhere and many readers would have agreed my point already. One question may arise why each stage took almost ten years. On this 'velocity of paradigm progress' I have no idea yet. It is just an empirical fact. It may be different for issues of different scales and complexities and in communities of different researcher populations. Also the progress in information technology, computer capacity and artificial intelligence may change the velocity in the future. In any case we can apply the three stage law in designing our research strategy for the future by assuming the current velocity of knowledge progress.

Now, it is important to note that the second and third stages do not completely solve the all paradoxes or questions raised in the first phenomenological stage. Many questions remain unsolved except for the issues beautifully solved and became one of the pillars of the theory or the relevant academic realm. The remained issues serve for the exploration of the next round again with the three stages.

In my case, with the rediscovery of the three stage law in my research field, I defined my ten years from around 1973 as the new phenomenology stage of the second 30 years and thought that a new paradigm of structural approach should be appearing at around 1983. In the case of the first 30years the structural issue was the division of the bed into bubble and emulsion phase. However, the second 30 years' paradigms of the phenomenological stage were relevant to: 1) regions in the fluidized bed which are not simply treated by the bubble model, 2) the global behavior of bubbles (Werther and Molerus (1973)), 3) fluid and particle property dependence of bubble behavior (Geldart (1973)), 4) high velocity fluidization beyond the bubbling regime and below the dilute pneumatic transport (Yerushalmi et al. (1975)).

With the Prof. Muchi group at Nagoya university and then with my group at Tokyo University of Agriculture and Technology I intentionally tried to sweep out as many issues listed above but keeping the structural

viewpoint firm. We successfully clarified 1) the bubble eruption and fines' transport mechanism in the freeboard (Horio, Taki, Hshieh and Muchi (1980)), as well as the structure in the distributor zones concerning vertical and horizontal jetting (Horio, Nishiyama, Liu and Muchi (1983)) and dead zone formation (Horio, Kiyota and Muchi (1980)), 2) similitude of bubble distribution in different scale models (Horio, Nonaka, Sawa and Muchi (1986)), its applicability to bubble induced solid mixing (Horio, Takada, ishida and Tanaka (1986)), 3) generalized bubble diameter correlation including the effect of bubble splitting (Horio and Nonaka (1987)), and 4) flow regime (Horio and Morishita (1988)) and structure, particularly the core and annulus structure of circulating fluidization (Ishii, Nakajima and Horio (1989)) with its scaling law (Horio, ishii, Kobukai and Yamanishi (1989)).

While working on the subjects at hand one can think about the next paradigm. During the structuralist stage somebody may reach a new paradigm for the essentialist stage. Heeding such a point, I defined the period around 1993 to around 2002 the essentialist stage and focused our effort on a) the measurement of mesoscale structure of dilute suspensions, i.e., clustering nature, by laser sheet technique (e.g., Horio and Kuroki (1994)), b) complete phase diagram development from bubbling, turbulent, fast and dilute transport (Horio and Ito (1997)), c) powder compression effect of a bubble (Horio, Iwadate and Sugaya (1998)) and agglomerating fluidization (e.g., Nishii, Ito, Kawakami and Horio (1993)), Iwadate and Horio (1998)), and d) numerical simulation by DEM (e.g., Mikami, Kamiya and Horio (1996), Kaneko, Shiojima and Horio (1999), Rong, Mikami and Horio (2001), Kuwagi and Horio (2002), and Kuwagi, Takeda and Horio (2004), etc.).

The fundamental equation for the fluid-particle systems have already been developed by Anderson and Jackson (1967). However, the computer capacity in the 1960s was not sufficient to handle realistic issues. Also the locally averaged formulation of their equations were not easy to apply realistic issues such as cohesive interaction of particles and particle property distribution. I was sure that the DEM-CFD approach initiated by Tsuji, Kawaguchi and Tanaka (1993) could become one of the essentialist stage paradigms to deal with a wide variety of particle scale phenomena from the first principle. Since the computer capacity that time was still insufficient, we restricted our work within the demonstration type.

3. Industry-Academia and Practice-Theory Interactions

The above arguments are on the aspect of knowledge and academia. However, we cannot separate knowledge and practice. Knowledge is basically for practice. The R&D efforts for innovations always provide new demands for knowledge. In this respect Industry-academia interactions as well as practice-theory interactions are the very basis of innovations in knowledge. In my group, I have been always working together with industries, from energy, material, environment, food and pharmacy. Also I asked my PhD students publish both theoretical/analytical and experimental work. Except for some rare geniuses, we ordinary people have more inspiration by knowing both sides having different thinking styles and languages. This applies to most of sciences including social sciences. But it has been particularly so in the realm of fluidization. It is because particulate solids and discrete beings are so well widespread and because fluidized beds have a fascinating variety as liquid has in the molecular system. So, fluidization can be applied to almost all industries, natural phenomena and probably even to social phenomena.



Photo 2. With my former student Mr Koike (left) Inside a plant (2001)

This nature of the realm of fluidization provides pitfalls for a researcher in application. Researchers tend to be completely captured by the application field where they can keep themselves busy on many practical issues. Of course if things can be done without any problem, then fluidization should not need any more excavation and you can just reproduce fluidization engineers, teachers and consultants with no R&Ds. The reality is that even after the two 30 year periods of fluidization research, our knowledge has not been well developed to serve further technology innovations. For instance, first, since the mesoscale structure issue directly related to macroscopic estimation of gas solid slip velocity and drag force, further investigation is necessary to account for the mechanisms that generates cluster sizes and their distributions; second, complete phase diagrams have to be developed for different particle systems; third, theory for agglomerate size determining mechanisms in agglomerating fluidized beds is still half way through; and fourth, reliable, flexible and cost effective numerical simulation tool has to be developed.

Recently, I had a chance to review fluidization in natural phenomena and found that their scales are much larger than what we have been dealing with in industries. Since we can control conditions in experimental fluidized bed facilities and can reproduce phenomena as demanded, we have been able to develop a rather comprehensive knowledge on particle-fluid systems. However, if such knowledge is supposed to be applied to natural phenomena, we have no sufficient data for it.



Photo 3. Let's Scale-up our Dreams.

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Without the need from practices the academic activities on fluidization shall be weakened. From the 1940s until the 70s, the petroleum and petrochemical industries have been continuously creating R&D needs for the fluidization science. After the 1970s the oil crisis and the global warming have changed and still changing the situation. In such a changing world, technologies to deal with particulate solids will find more places. When the second 30 year period was over at around 2002, I was not sure if the third period was starting. But recently, I started to think that it has been probably so, though it could be in a much larger scales and more comprehensive manners. The transition to sustainable world is a huge task, to which our particle technology and fluidization engineering have to be responsible. So, our password should be 'Let's scale up our dreams!' Photo 3 is one of my hand drawn fans given to the speakers and chairmen in appreciation. I hope a new wind is blown from those fans.

References

- Anderson, T.B., and Jackson, R., Fluid Mechanical Description of Fluidized Beds. Equations of Motion, Ind. Eng. Chem. Fundam., 6 (4), pp 527–539 (1967).
- Davidson, J.F., and Harrison, D., 'Fluidised particles,' Cambridge University Press, NY (1963).
- Davidson, J.F., and Harrison, D., (eds.), 'Fluidisation', Academic Press, 1971.
- Geldart. Types of Gas Fluidization, Powder Technol., 7, pp. 285-292 (1973).
- Horio, M., 1. Overview of Fluidization Science and Fluidized Bed Technologies, 'Fluidized-bed Technologies for Near-zero Emission Combustion and Gasification,' ed. by F. Scala, Woodhead Publishing, 3-41, (2013).
- Horio, M., Ch. 2 Hydrodynamics, 'Circulating Fluidized Beds,' ed. by J.R. Grace, A.A. Avidan and T.M. Knowlton, Chapman & Hall, London, pp. 21-86, 1997.
- Horio, M., Ishii, H., Kobukai, Y., and Yamanishi, N., A Scaling Law for Circulating Fluidized Beds, J. Chem. Eng. Japan., 22, pp. 587-592 (1989).
- Horio, M., Ishii, H., and Nishimuro, M., On The Nature of Turbulent and Fast Fluidized Beds, Powder Technology, 70, pp.229-236 (1992).
- Horio, M., and Ito, M., Prediction of Cluster Size in Circulating Fluidized Beds, J. Chem. Eng. Japan, 30, pp. 691-697 (1997).
- Horio, M., Iwadate, Y., and Sugaya, T., Particle Normal Stress Distribution Around a Rising Bubble in a Fluidized Bed, Powder Technology, 96, pp.148-157 (1998).
- Horio, M., Kiyota, H., and Muchi, I., Particle Movement on a Perforated Plate Distributor of Fluidized Bed, J. Chem. Eng., Jp., 13, pp.137-142 (1980).
- Horio, M., and Kuroki, H., Three-dimensional Flow Visualization of Dilutely Dispersed Solids In Bubbling and Circulating Fluidized Beds, Chem. Eng. Sci., 49, pp.2413-2421 (1994).
- Horio, M., and Morishita, K., Flow Regimes of High Velocity Fluidization, Japan J. Multiphase Flow, 2, pp.117-136 (1988).
- Horio, M., Nishiyama, A., Liu, J., and Muchi, I., Horizontal Jet Penetration into Powder Beds under Different Aeration Conditions, Kagaku-Kogaku-Ronbunshu, 9, pp.609-616 (1983) (in Japanese).
- Horio, M., Nonaka, A., Sawa, Y. and Muchi, I., A New Similarity Rule for Fluidized Bed Scale Up, AIChE J., 32, pp. 1466-1482 (1986).
- Horio, M., and Nonaka, A., A Generalized Bubble Diameter Correlation for Gas Solid Fluidized Beds, AIChE J., 33, pp.1865-1872 (1987).
- Horio, M., Rengarajan, P., Krishnan, R., and Wen, C.Y., Fluidized Bed Combustor Modeling, Final Report Prepared for NASA under Contract No. NAS3-19725, Jan. 1977.
- Horio, M., Taki, A., Hsieh, Y., and Muchi, I., Elutriation and Particle Transport through the Freeboard of a Gas-solid Fluidized Bed, Fluidization, J.R. Grace, J.M. Matsen, ed., Plenum Publishing, pp.509-518 (1980).
- Horio, M., Takada, M., Ishida, M., and Tanaka, N., The Similarity Rule of Fluidization and its Application to Solid Mixing and Circulation Control, Fluidization V, Engineering Foundation, pp.151-158 (1986).
- Horio, M., and Wen, C.Y., Simulation of Fluidized Bed Combustors: Part I. Combustion Efficiency and Temperature Profile, AIChE Symp. Ser., No. 176, vol.74, pp.101-110 (1978).
- Ishii, H., Nakajima, T., and Horio, M., The Clustering Annular Flow Model of Circulating Fluidized Beds, J. Chem. Eng. Jp., 22, pp.484-490 (1989).
- Iwadate, Y., and Horio, M., Prediction of Agglomerate Sizes in Bubbling Fluidized Beds of Group C Powders, Powder Technology, 100, pp.223-236 (1998).
- Kaneko, Y., and Shiojima, T., and Horio, M., DEM Simulation of Fluidized Beds for Gas-phase Olefin Polymerization, Chem. Eng. Sci., 54, pp. 5809-5821 (1999).

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Kuhn, T., 'The Structure of Scientific Revolutions', University of Chicago Press, Chicago, 1962.

Kunii, D., and Levenspiel, O., 'Fluidization Engineering', Wiley, NY, 1969.

- Kuroki, H., and Horio, M., The Flow Structure of a Three-dimensional Circulating Fluidized Bed Observed by the Laser Sheet Technique, 'Circulating Fluidized Bed Technology IV,' AIChE, pp.77-84 (1994).
- Kuwaki, K., and Horio, M., A Numerical Study on Agglomerate Formation in a Fluidized Bed of Fine Cohesive Particles, Chem. Eng. Sci., 57, pp.4737-4744 (2002).
- Kuwagi, K., Takeda, H., and Horio, M., The Similar Particle Assembly (SPA) Model, An Approach To Large-Scale Discrete Element (DEM) Simulation, 'Fluidization XI- Present and Future for Fluidization Engineering', U. Arena, R. C. Hirone, M. Miccio, P. Saratino, eds., pp. 243-250, 2004.

Leva, M., 'Fluidization', McGraw-Hill, 1959.

Mikami, T., Kamiya, H., and Horio, M., The Mechanism of Defluidization of Iron Particles in a Fluidized Bed, Powder Technology, 89, pp. 231-238 (1996).

Morse, R.D., and Ballou, C.O., The Uniformity of Fluidization, Its measurement and use, Chem. Eng. Progr., 47, 199-204 (1951).

Nishii, K., Itoh, Y., Kawakami, N., Horio, M., Pressure Swing Granulation, a Novel Binderless Granulation by Cyclic Fluidization and Gas Flow Compaction, Powder Technology, 74, pp.1-6 (1993).

- Rong, D., Mikami, T., and Horio, M., Particle and Bubble Movements Around Tubes Immersed in Fluidized Beds A Numerical Study, Chem. Eng. Sci., 54, pp.5737-5754 (1999).
- Shen, C.Y., and Johnstone, H.F., Gas-Solid Contact in Fluidized Beds, AIChE J, 1, pp. 349–354 (1955).
- Taketani, M., On the Formation of Newtonian Mechanics, Kagaku (Science), 12, pp. 307-311 (1942) (in Japanese).
- Tsuji, Y., Kawaguchi, T., and Tanaka, T., Discrete Particle Simulation of Two-dimensional Fluidized Bed, Powder Technology, 77 (1) pp. 79–87 (1993).

Werther, J., and Morelus, O., The Local Structure of Gas Fluidized Beds, Int. J. Multiphase Flow, 1, p. 103 (1973)).

- Yerushalmi, J., Gluckman, M. J., Graff, R. A., Dobner, S., and Squires, A. M., Production of Gaseous Fuels from Coal in the Fast Fluidized Bed, 'Fluidization Technology,' ed. by D. L. Keairns, Hemisphere Publ. Co., Washington, Vol. II, pp. 437-469, 1975, (see also J. Yerushalmi, J. Turner and A.M. Squires, The fast fluidized bed, Ind. Eng. Chem., Process Design and Development, 15, pp. 47-53 (1976)).
- Zenz, F.A., and Othmer, D.F., 'Fluidization and Fluid-Particle Systems', Reinhold, 1960.

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History of Particle Technology

Historical Perspective on Electrostatics

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When was the first electrostatic spark observed is impossible to say. This occasion occurred no doubt long before the written-word was recorded on paper. The first time I (George Klinzing) was exposed to the history was at a Nishin Flour Mill Company Symposium on Electrostatics held in Mt. Hiei near Kyoto, Japan. Wolfgang Kleber gave the conference banquet speech on electrostatics showing many slides of sketches of electrostatics being demonstrated mostly for amusement. They probably can be classified as parlor games. Serious study seemed to begin in the mid 1700 with experiments done in England by Joseph Priestley the discovery of oxygen and in France by Abbe Nollet. Benjamin Franklin also began to carry out experiments on electrostatics in America. It is curious to note that all three researchers knew of the others work mainly through the Royal Society Proceedings. To attest to this interaction or interchange Priestley wrote a two volume book called "The History and Present State of Electricity" published in London in 1755. Thanks to the interest of the scientific community the Johnson Reprint Corporation in 1966 reprinted these volumes and many libraries in the world have this holding. This book has a rich bibliography of experiments and observation in electrostatics that date to the 1600's. Abbe Nollet in France produced a book entitled "Recherches sur les causes partculieres des phenomenes electriques" published in Paris in 1745. The Hathi Trust scanned this book and it is available through the University of Michigan in the scanned format. At the University of Pittsburgh has an original copy of this book in its special collection holdings. I, George Klinzing, was privileged to look through this book carefully since the paper seems quite fragile. The special collection bibliographer, Benjamin Rubin, scanned the drawings in the book and we will share these drawing of experiments later in this paper. One thing of note reading Priestley work was the high esteem that he had for Nollet and Franklin citing their works often and praising their findings. Communication occurred in these times by letters.

One interesting account of electrostatics is cited by Priestley in his book as involving the Leyden Phial as related to Dr. Franklin –

"The end of the year 1745, and the beginning of 1746 were famous for the most surprising discovery that has yet been made in the whole business of electricity, which was the wonderful accumulation of its power in glass, called at first the Leyden Phial; because made by Mr. Cuneus a native of Leyden as he was repeating some experiments which had seen with Messrs. Muschenbroeck, and Allamand, professors in the university of that city. But the person who first made this great discovery, was Mr. von Kleist, dean of the cathedral in Koenigsberg now in Russia; who, on the 4th of November 1745, sent an account of it to Dr. Lieberkuhn at Berlin. This account, as taken by Mr. Gralath out of the resister of the academy at Berlin, to which he had been communicated, is as follow. "When a nail or piece of think brass wire, &c. is put into a small apothecary's phi-

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al and electrified, remarkable effects follow; but the phial must be very dry, or warm. I commonly rub it over before-hand with a finger, on which I put some pounded chalk. If a little mercury or a few drops of spirit of win, be put into it, the experiment succeeds the better As soon as this phial and nail are removed from the electrifying glass, or the prime conductor, to which it hath been expose, is taken away, it throw out a pencil of fame so long, that with this burning machine in my hand I have taken above sixty steps, in walking around the room. When it is electrified strongly, I can take it into another room, and there fire spirits of wine with it...."

It is interesting to see the detail at which the experimenter explained their procedure and details of their findings.

Kleber presented a number of transparencies of historical experiments in electrostatics at the Mt. Heio meeting. We will comment on these at this time. Figure 1 portrays an experiment done by Ottonis De Guericke in Magdeburg in 1672 with one rotating sulfur sphere which was used as the source of electrostatic generation. This sphere was rubbed with dry hands and the second one produced a spark at the same time. Figure 2 is what can be termed as a parlor game where one lady is pumping a device to rotate a glass sphere with the gentleman having his bare feet touch the sphere and the being suspended touches the second lady's hand attracted light weight particles such as a colored feather to her hand and arms. This experiment performed in 1749 was the forerunner of electrostatic flocking, painting and powder spraying.

The classic Lichtenberg figure, Figure 3, is shown next. This figure is on record in the museum in Goerlitz, Germany. The Lichtenberg figures are branching that occurs in electric discharges on the surface or interior of insulating materials. They were names after Georg Christoph Lichtenberg who did his work on static electricity in 1777. This illustration shows the lightning patterns caused by electrostatic discharge. Figure 4, which is a copy of the introduction page, shows the American experiments were conducted by Benjamin Franklin which are contained in a book with a copy of the introduction page. The book is entitled 'Experiences et Observations sur L'Electricite published in Paris in 1752. The book also has an illustration Franklin's kite experiment with lightning in a wooden shelter, June 1752, Figure 5. Curious application of electrostatic ground are seen in the next illustration, Figure 6, showing the grounding devices used on umbrellas and lady's hats. I guess one could feel safe when walking in a thunder storm. A laboratory was able to bring lightning into its space by the illustration, Figure 7, that shows a lightning rod on a house connected by a metal chain to the receptacle in the internal of the laboratory. The next sketch, Figure 8, shows the dramatic lightning effect from a metal wire and two experimenters. It should be noted that Prof. G.W. Richmann in St. Petersburg died during the thunderstorm, June 8, 1753. His assistant survived this discharge experience. The application of electrostatics was thought to be a remedy for some human aliments. The next figure, Figure 9 shows the application of electrostatics in the field of medicine. There is rich discussion by Priestley and Nollet on the effect of electrostatics on various human maladies. The application of electrostatics to a variety of different human health problems is shown in the next illustration. In looking towards the fountain of youth electrostatics was applied. The next illustration, Figure 10, shows the application of health improvement by using the magic of electrostatics. The next two illustrations show the passage of electrostatic charge through various people, Figures 11 and 12.

The next illustration, Figure 13, comes from the book by Nollet where electrostatic charges are passed through plants and animals. The tests were conducted over long periods of time, 5 hours or more, noting the weight change of the animal. Nollet also experimented with passing electrostatic charges through a vacuum chamber shown in the next illustration, Figure 14. Heated objects were also shown in reference to electrostatic application showing the conductivity of the a flame.

The next illustration, Figure 15, also comes for Nollet indicating various arrangements with metal plates and metal bars and rods. In agriculture the application of seeding dispersion was also employed as shown in the next figure, Figure 16. Figure 17 is again a parlor game with a suspended child followed the transfer of charge through a kiss.





You can find these "Original Lichtenberg Figures" in a large numbers in the museum of Görlitz.



Figure 3



Franklin's Versuch mit dem Drachen (Juni 1752) Holzstich aus späterer Zeit.

Figure 5



Figure 2



Figure 4



Figure 6





Figure 9







Figure 8



Figure 10







Nollet untersucht den Einfluß der Elektrizität auf das Wachstum von Pflanzen und Tieren.

Figure 13



Figure 15





Figure 14



Figure 16



Figure 17

Figure 18



Figure 22



There are eight illustrations in the Nollet book which will be commented on. As noted before, these are reproduction obtained by scanning the original book illustrations by the staff of the special collections at the University of Pittsburgh.

The Figures follow in sequence from 18 to 23 in the illustrations.

Figure 18 - This illustration shows through the use of windows the effects of electrostatics beginning to the generation by the use of a rotating glass sphere having a metal chain the conduct the charging with discharging from one hand to another showing the spark.

Figure 19 - This illustration again show the effect of electrostatics from the rotating sphere source to a man through a conducting metal chain to discharge to a metal plate through his hand. Note the man is standing

on an insulator. The other parts of the illustration note the movement of a suspended rod which electrostatics in transmitted.

Figure 20 - From the spherical moving source charge is transferred to a glass container through a metal rod. Place one's hand or hands on the surface of the glass container shows how one change move the direction of the discharge.

Figure 21 - This experiment attempts to transfer charge to plants and fruits to see if there is any effect on the condition of the objects and the peak discharge.

Figure 22 - This is another experiments showing the various kinds of discharges are possible especially the atomization of liquids.

Kleber on a visit to a museum south of Moscow in 1974 found a painting of the use of electrostatics to entertain people. The Polish painter is Daniel Chodowiecky (1726-1801). Note the woman transferring the charge is standing on an insulator. See Figure 23.

One of the most curious application of electrostatics comes from Priestley's book entitled Beatification. In this experiment Bose used electrostatics to be passed through a person who was standing on a block of pitch (see Figure 18). The experimenter (Bose) who also attested that others have observed this test, noted a tingling of the skin as the current was passed through him and finally erupting from his head to produce a halo. Other experimenters attempted the same experiment without success only noting the tingling sensation but no halo. It is interesting to note that Bose wrote the first scientific book in verse.

For those interested in this early accounting of electrostatics and their various applications we highly recommend reading section of both Priestley and Nollet's books.



Figure 23

References

- 1. Bose, G.M. "Oratio inauguralis de electricitate, 2 parts", (1738), Wittemburg, Gralath's biobliotek
- 2. Nollet, Abbe, "Recherches sur les causes partculieres des phenomenes electriques" Paris (1745)
- 3. Priestley, J., "The History and Present State of Electricity 2 volumes" London (1755). Reprinted by the Johnson Reprint Corporation (1966).

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