Excerpted from an e-mail by Bucky Kashiwa (Los Alamos)

Let me take a bottom-up approach, and go about it conversationally - and from the standpoint of the physics. If you need clarification or want more detail, don't be shy about asking; I will follow up as time permits...

To me there are quite a number of unfinished items that we uncovered in our MFDRC work, and which have become more focused in some of our work since that program ended. Let us speak of three length scales of observation: the grain-scale, the integral scale, and the device scale; and let us discuss the physics that are lacking at each scale.

At the grain scale (to me) the largest looming gap in reliable knowledge is in the force between the fluid and the grains – as affected by other grains that may be nearby. (This is, in general, a multibody force.) We showed that two-body effects lead to forces that can be expressed in terms of the gradient of volume fraction (paper attached). The forces can be either attractive or repulsive, depending on the direction of relative motion between two grains. The lowest-order effect on the physics of the system is that the averaged equations for incompressible materials becomes unconditionally hyperbolic - which means that the dynamic waves can be present in the flow. The speed of these dynamic waves is very closely related to the rise velocity of bubbles in dense stationary fluidized beds, and can be used to gauge stability of the bed. In the dilute case clustering is always observed, and the size and concentration of clusters is related to the characteristic speeds of the dynamics waves.

The exact nature of the dynamic waves depends on the viscosity of the fluid, and can rarely be ignored. This is because the force needed to pull apart two grains is dominated by the viscous motion of the fluid in a very small space. When the space becomes large enough, the viscosity can be neglected - but if fluctuations are such that two grains come close together they will tend to stay close, which is why clustering occurs in the first place.

The two-body force becomes much more dicey to represent when electrostatic charges can build up on the grains (like on FCC catalyst in air). So far as I know Sundar did the order of magnitude estimate showing what charge is needed for a significant effect, but I don't think any quantitative modeling has been done for this potentially dominant force. As for the viscous part, only the zero Reynolds number limit is know (and is due to Stokes). For finite Reynolds number, no really comprehensive work is extant (I'm pretty sure).

So the two-body force is new (at least to most of the DOE crowd) and it has important implications for the dynamics y'all are trying to compute. It occurs to me that this is good news. Direct Numerical Simulation of small numbers of grains (two or three is going to be enough) in tri-periodic domains will permit determination of the model coefficients for the multibody force, in addition to the single-body force and models for homogeneous turbulence. So one can see through the grain-scale problems of getting closures for homogeneous distributions. This sets the stage for getting nonhomogeneous models by using the averaged equations with DNS closures.

The effects of nonhomogeneous distributions (including clusters) determine the integral scales, and can be made quantitative using LES (like Sundar, like Zhang, and the stuff we did during MFDRC) for which the hyperbolic equations are essential - because the statistics depend crucially on the dynamical wave speeds. The LES results generally lead to new coefficients for the forces - but not the functional form of the forces. The LES (averaged) coefficients are what one needs to go to the device scale and do something meaningful for risers, standpipes, and (nominally) packed beds - using the RANS equations closed with LES data.

There is of course a question of equilibrium that one must address when using the foregoing closure approach. In the case of LES one assumes that the evolution is a sequence of equilibrium states given by the DNS averages. In the RANS case, one assumes that the evolution is a sequence of LES states. This assumption is analogous to supposing that the molecules in a gas exhibit a local thermodynamic equilibrium, which varies from point to point. In the multifield case, one hopes that if the terms that represent 'inertia' for moving from point to point are properly included (like gradient-dependent two-body forces) then the model should work well. This point needs very careful examination, but I am bullish on a positive outcome.

Finally, I know that we never got there in MFDRC work, but we had hoped that follow-on work would systematically go after the real nut that most folks are seeking: the fully-coupled reactive flow model. I assert that the full set of physics that include heat transfer and evolution of species concentrations can be addressed in the DNS-LES-RANS approach outlined above. We are in the process of demonstrating this process in the context of nonideal detonation behavior of high explosives loaded with small inert metal grains. If we both live another few years, perhaps we can correspond once more and I can send you the paper on that demonstration. Until then, my very best regards. Bucky Kashiwa.