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PHYSICS-BASED SIMULATIONS TO ENABLE GAME-CHANGING NOVEL EXPLOSIVE AND PROTECTIVE TECHNOLOGIES

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14. ABSTRACT
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Existing simulation tools have become quite advanced over the past decade and they incorporate a wide variety of capabilities. Despite these advancements, their predictive capability, especially for the class of problems of present interest, has been quite poor. The fundamental difficulty is in lack of complete understanding of the complex physics of multiphase flow under conditions of extreme compressible turbulence. In order to accomplish these intellectual and technological objectives, we have studied in detail micro and mesoscale problems.

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Physics-Based Simulations to Enable Game-Changing Novel Explosive and Protective Technologies

AFOSR-FA9550-10-1-0309

Final Report for 2013

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Executive Summary

The overall goal of this research is to contribute to national defense and security by advancing the state-of-the-art in explosive dispersal of particles/droplets and replacing current empiricism with a physics-based fundamental approach. This will enable game-changing advancements in (i) lethality technologies for the development of next generation tunable-output explosives, (ii) force-protection technologies for defeating improvised explosive devices and mines, and (iii) counter-terrorism technologies for neutralizing chemical and biological weapons of mass destruction.

The core intellectual objective is to radically advance the field of *Compressible Multiphase Turbulence* (CMT) by systematically answering key outstanding questions. We will advance a rigorous physics-based formulation of CMT and thereby enable accurate high-fidelity simulations with true predictive capability. The longer-term technological objective is to facilitate the development of a Virtual Explosive Dispersal Facility (VEDF), which can be used to perform physics-based simulations of explosive dispersal of particles/droplets in applications of interest to DoD.

We have focused on the following two key questions: (1) Can the current modeling and simulation approaches accurately predict explosive dispersal particles observed in the above examples (and other related experiments)? (2) If not, what additional fundamental understanding is needed that can be translated to improved modeling and simulation capabilities?

Existing simulation tools have become quite advanced over the past decade and they incorporate a wide variety of capabilities. Despite these advancements, their predictive capability, especially for the class of problems of present interest, has been quite poor. The fundamental difficulty is in lack of complete understanding of the complex physics of multiphase flow under conditions of extreme compressible turbulence. In order to accomplish these intellectual and technological objectives, we have studied in detail the following micro and mesoscale problems:

- Investigate at the microscale the complex thermo-mechanical interaction between an isolated particle and the surrounding rapidly expanding compressible flow. Develop rigorous physics-based closures for interphase coupling between the particle and the gas.
- Extend the interphase coupling model to finite Reynolds and Mach numbers, and to account for the effects of deformation and compressive heating in case of strong-shock-particle interaction. Our initial effort was to develop and test a point-particle model to accurately predict the mass-average velocity and temperature of the particle. However, from the direct numerical simulations it was noted that the peak values of stress and temperature are far higher than the average values. Efforts are underway to extend the point-particle models to predict these peak values as well.
- Extend the interphase coupling models from an isolated particle to a cluster of particles by incorporating the effect of finite volume fraction. Here both the limits of dilute and dense volume fractions must be considered. In the former only the indirect particle-particle interaction as mediated by the surrounding gas will be important, while in the later limit additional effects of direct particle-particle collisional interaction must be modeled. This work is in collaboration with Drs. J.L. Wagner, S.J. Beresh, and S.P. Kearney at the Sandia National Laboratories.
- Existing compressible multiphase flow formulations are not universal. There are two classes of formulations in use. The first class of formulations apply to situations of dense

compressible multiphase flows, where compression of the dispersed phase plays an important role. Multiphase formulations of this type follow along the lines of the original work by Baer & Nunziato [1]. The later class of formulations are appropriate for less dense and less intense scenarios, where the compressional effect on the particles can be ignored. Here we seek to develop a unified multiphase formulation that seamlessly handless both these limits accurately. Such a formulation is of critical importance, since explosive dispersal problems of present interest start from a dense flow limit to quickly evolve into a dilute particulate flow. This work has been initiated in collaboration with Dr. T.P. McGrath at NSWC-Indian Head, MD.

- Rigorously apply the interphase momentum and energy coupling models to problems of shock-particle and detonation-particle interaction and validate the coupling model against available high-quality experimental results. In particular, validation of thermal coupling models is of great interest, as there are not adequate validation-quality experimental measurements of particle and gas temperature immediately following a strong-shock or detonation particle interaction.
- Investigate the process of explosive dispersal of particles, starting from the initial instability of a rapidly expanding layer to its subsequent dispersal process. Here the initial inviscid instability analysis was first extended to viscous instability analysis, where the effect of viscosity is to identify a most amplified spherical mode. We are in the process of extending the gas-gas contact interface instability analysis to multiphase particulate fronts. An important advancement in the stability analysis is the realization of the key role of interface thickness in dictating the wave number of the most amplified mode. The linear stability analysis has also been extended to nonlinear stages of bubble and spike growth regime and investigated through direct numerical simulations.
- Rigorously validate the micro and macroscale formulations and results against high-quality experimental data available at the Air Force Research Laboratory Munitions Directorate and at the DOE NNSA Laboratories.
- Train students and postdocs in problem of defense and security science and engineering.

2. Introduction

Lethality technologies to develop next generation tunable-output explosives, force-protection technologies to defeat improvised explosive devices (IEDs)/mines, and counter-terrorism technologies to neutralize chemical and biological weapons of mass destruction (WMD) are of great importance to our Nation's security and defense. Fundamental to these technologies are the ability to control explosive dispersal of particulates/droplets, to direct the location, time and rate of energy release, and to mitigate the effects of blast, fireball and impacting projectiles.

It is now possible, and will likely become increasingly so in the future, to produce multifunctional explosives whose microstructural details of particle size distribution and chemical composition can be controlled to great precision. Thus, there is clear opportunity for engineering next generation tunable weapons systems that can deliver a controlled amount of energy, to an exact location, at a precise moment, and at a desired rate. Tunable explosives, however, have not yet been fully realized in practical systems. The key missing link is to connect the microstructural details of the explosive to the resulting spatio-temporal details of macroscale dispersion, turbulent mixing and volumetric energy release. If this challenge can be addressed game-changing capabilities, such as quantum increase in energy release or localized release for low collateral damage, can be realized.

Compressible multiphase turbulence is at the heart of this problem. Advances in our fundamental understanding of compressible turbulent multiphase flows will positively impact many other problems of interest to DoD. For example, the devastating effects of IEDs arise from the fragments, debris and incendiaries that they explosively disperse. To effectively protect against these projectiles it is important to accurately know the momentum and energy imparted to them in an explosion. Or in the case of blast mitigation with water mist, it is the complex thermo-mechanical interaction of the water droplets with the compressible turbulent flow that mitigates the blast.

Compressible multiphase turbulence is in its infancy and poses a grand challenge as it combines three complex physics: turbulence, compressibility and multiphase flow. The urgent need for better fundamental understanding is clear from the national defense and security applications. Although substantial progress has occurred over the past several decades in the individual areas of turbulence, compressible and multiphase flows, our understanding when all three mechanisms are simultaneously active is rudimentary.

The primary objective of the ongoing work is to radically advance the field of compressible multiphase turbulence by systematically answering key outstanding questions. We will advance a rigorous physics-based formulation and thereby enable accurate high-fidelity simulations with true predictive capability. High quality experiments that have been performed (or being performed) at DoD and DOE will be used to validate the models and the simulation framework.

In particular, we will focus on the class of problems involving explosive dispersal of particles and droplets. These dispersed particles can be inert as in the case of casing fragments or liner elements or can be reactive as in the case of multiphase explosives. Using fundamental advances in modeling and simulation of compressible multiphase turbulence we perform predictive physics-based simulations of selected explosive dispersal problems. By comparing results with experimental observations and measurements the predictive capability of the new formulation is evaluated.

3. Scope and Challenge

Consider the following few examples of explosive dispersal. In Figure 1 high speed images from a thermobaric test is shown. In this case there are no particles being dispersed and therefore can be considered as single-phase baseline. The instability and turbulent nature of the expanding gas front can be clearly observed. These instabilities are thought to be associated with Rayleigh-Taylor (RT) and Richtmeyer-Meshov (RM) instabilities. But the true nature of the instability and transition to turbulence at such rapidly expanding material fronts is poorly understood.

Figure 2 shows images of an expanding cloud of aluminum particles (Particle image velocimetry of this field were also taken). In these experiments, performed at ARFL Munitions Directorate at Eglin Air Force Base, four stacked A-5 pellets (see frame e) were surrounded by a paper jacket filled with aluminum particles and the resulting pattern of explosive dispersal of particles was observed and measured. These experiments were repeated for aluminum and tungsten particles of varying particle size (see [2] for additional details).

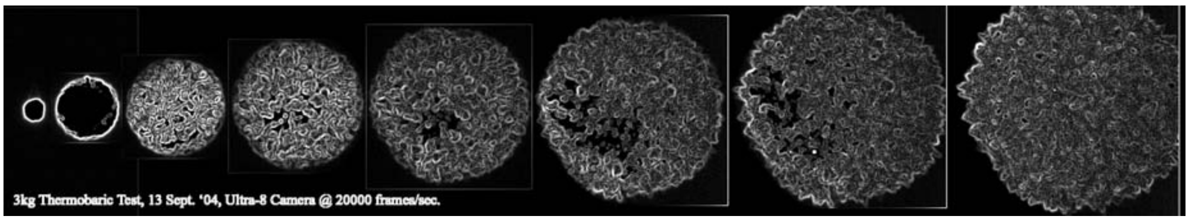


Fig 1: High speed image of a thermobaric test of 3kg TBX. The highly turbulent nature of the expanding gas contact and the associated fireball can be clearly seen (from Dr. M.R. Baer).

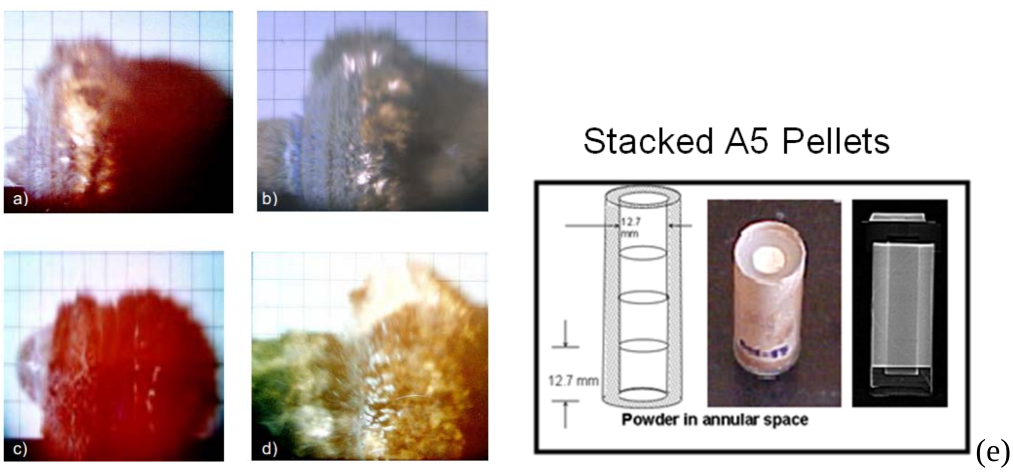


Fig 2: Early time expansion (a) An H-10 powder annulus charge at 50µs after initiation from the right side, (one inch per block) (b). 95 powder annulus charge at 50µs after initiation from the right (c) tungsten particle charge at 50µs into expansion, no combustion due to the inert metal powder (d) HSFC speed images of TSS case breakup with fragment images at 50 µs post detonation (from [2]).

Figure 3 shows an explosive spherical dispersal of glass particles. Prof. Frost and co-workers repeated these experiments under a range of conditions involving different kinds of particles and geometric configurations. In particular, we draw attention to the fact that even the qualitative behavior of instability of the material front and the pattern of particle dispersion in these three examples are quite different. Furthermore, a detailed look at these experimental results shows substantial quantitative variation, which cannot be explained with current understanding.

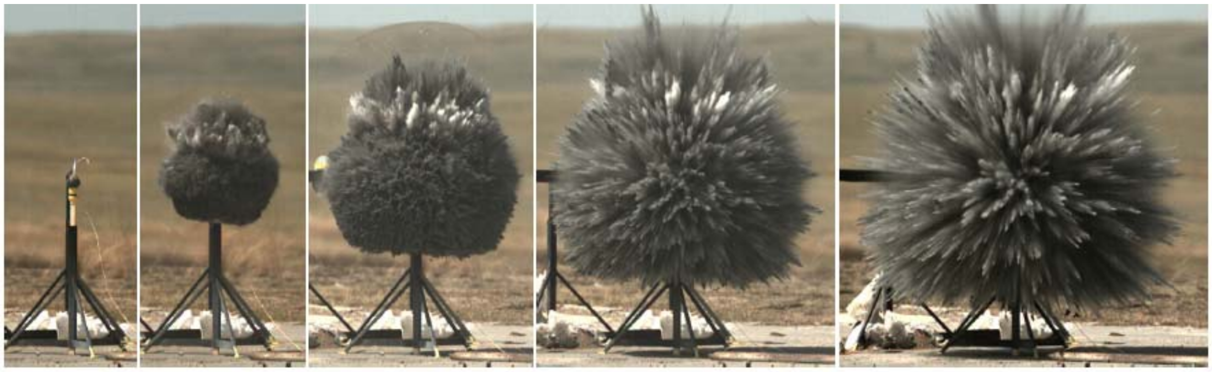


Fig 3: Spherical dispersal of glass particles with C4 explosive using 120 mm glass particles and 28g of C4. Note the needle shaped instability of the expanding particulate front. (from [3]).

We now ask the following key questions: (1) Can the current modeling and simulation approaches accurately predict explosive dispersal particles observed in the above examples (and other related experiments)? (2) If not, what additional fundamental understanding is needed that can be translated to improved modeling and simulation capabilities?

Existing simulation tools, both commercial as well as those developed and used by individual research groups, have become quite advanced over the past decade and they typically incorporate a wide variety of capabilities to handle complex geometries, particulates and droplets, ambient flow turbulence (through Reynolds-averaged Navier-Stokes and large-eddy simulation techniques). Despite these capabilities, their predictive quality, especially for the class of problems of present interest, has been quite poor. The fundamental difficulty is in lack of complete understanding of the complex physics of multiphase flow under conditions of extreme compressible turbulence. The coupling models that are in current use for mass, momentum and energy transfer between the particles/droplets and the surrounding gas are inadequate, as they are generally based on our understanding and modeling for simple steady, low-speed conditions.

The problem of explosive dispersal of particles requires us to

- Develop a universal set of governing equations for compressible turbulent multiphase flows that is applicable over the entire range of particulate concentration from the dilute limit to very dense suspension and from low-speed incompressible flows to very high-speed high density flows.
- Carefully address interphase coupling at conditions that are of relevance to DoD applications and to develop physics-based improved models of momentum and energy coupling. These coupling models will appear as closure relations in the universal set of governing equations addressed above. The interphase interaction is significantly complicated due to (a) the highly unsteady nature of the problem, (b) interaction of compressible flow features such as shocks and contacts with the particles, (c) high Reynolds number, (d) compressibility effects of high Mach number, and (e) particle-particle interaction at large volume fractions.
- Address additional complications that arise from random particle size, shape and distribution.
- Investigate the instability of rapidly expanding gas and particulate fronts and study the nature of flow transition and development of multiphase turbulence.

4. Results and Discussion

The results of the present work will be presented under five different topics. Our efforts in all these five topics have produced results that have already appeared as journal articles (or in review process or being prepared). These archival journal publications are listed as items J1 to J16 in section 6. Therefore the results and discussions to be presented here will be brief, with emphasis on only key sample results. The details can be obtained from the journal articles. In section 5 we will discuss ongoing and future research efforts that closely follow those listed here.

4.1 Theoretical Foundation - Exact Solutions For an Isolated Particle

Consider the scenarios shown in Figures 2 and 3. In each case, the dispersive pattern of millions of particles is desired. At this macroscale it will be impossible to resolve the flow around each and every particle. One needs to resort to a point-particle approach, where each particle is treated as point and its motion is computed based on aerodynamic forces that act on it. In the context of extreme compressible flows under consideration, the force on the particle will be a function of (at the least) (1) particle velocity, (2) particle acceleration, (3) local fluid velocity, (4) local fluid acceleration, (5) local particle volume fraction, and (5) other local fluid properties such as density, pressure gradient and speed of sound.

While at low-speeds (in the incompressible regime) one can correlate drag coefficient as a function of only Reynolds number based on relative velocity, this simple approach is grossly inadequate at the extreme conditions of interest here. All the other parameters, especially effects of unsteadiness, compressibility and volume fraction will play an important role. However, a naïve attempt at correlating the force on the particle in terms of the long list of parameters will be futile.

A physics-based approach to modeling this interphase momentum and energy coupling is essential for success. As a theoretical foundation, we take the limit of zero particle Reynolds and Mach numbers. In this limit the linearized compressible Navier-Stokes equations of flow around a particle can be rigorously solved. The following steps have allowed us to establish foundational results which will then be exploited in our other research:

- The problem of an isolated sphere undergoing arbitrary motion in a quiescent compressible fluid is first solved to obtain an exact expression for force. Individual mechanisms in the form of quasi-steady, inviscid-unsteady, and viscous-unsteady contributions to overall force are identified. Numerical results are in perfect agreement with the theory (see Figure 4). The resulting interphase coupling formulation offers an explicit expression for the unsteady force in the time domain and can be considered as a generalization of the classic Basset-Boussinesq-Oseen (BBO) equation to compressible flow (See journal article J1 for details).
- The above theoretical analysis was extended to the more general case of an isolated sphere undergoing arbitrary motion in a spatially-varying time-dependent compressible ambient flow. The problem was formulated in a reference frame attached to the particle and force contribution from the undisturbed ambient flow and the perturbation flow were separated. Using density weighted velocity transformation and reciprocal relation, the total force was first obtained in the Laplace domain and then transformed to the time domain. Total force was again separated into the quasi-steady, inviscid-unsteady, and viscous-unsteady contributions. The above rigorously derived particle equation of motion can be considered as the compressible extension of the classic Maxey-Riley-Gatignol (MRG) equation of motion. It

rigorously incorporates important physics that arise from the combined effects of inhomogeneity and compressibility (See journal article J5 for details).

- Finally, the above formulation for a rigid sphere was generalized to investigate the corresponding results for a droplet. Here the linearized viscous compressible Navier-Stokes equations are solved both inside and outside of the spherical drop. An expression of the transient force is first obtained in the Laplace domain and then transformed to the time domain. The total force is separated into the quasi-steady, the inviscid-unsteady, and the viscous-unsteady contributions. The new force expression reduces to known results in the limits of a drop in an incompressible flow or a rigid particle in a compressible flow (See journal article J7 for details).

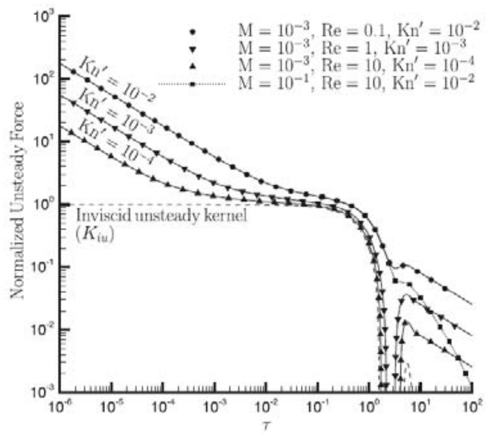


*Fig 4: Time evolution of the normalized unsteady force. Theoretical predictions are plotted as solid lines for different Mach and Reynolds numbers. Corresponding simulation results for the different cases are shown as symbols. Interestingly, excellent agreement can be observed, even at finite values of Reynolds and Mach numbers. Nonlinear effect can be shown to be important only for time larger than (1/Re*M).*

- It is well known that the computation of the history force by evaluating the convolution integral is very demanding in terms of CPU and memory requirements. In this research we seek an elegant mathematical approximation that greatly simplifies the computation of the history integrals without much loss of accuracy. This approximation will greatly benefit the computational accuracy and efficiency of Eulerian-Lagrangian approach to multiphase flows. Using rational approximation for the history kernel in the frequency-space we have developed an approximate formulation of the viscous-unsteady force which is computationally far more efficient than the traditional convolution integral. For the compressible inviscid unsteady force, the kernel in the frequency domain is a rational function. As a result the convolution integral and the differential formulation of the compressible inviscid unsteady force are identical. The viscous-unsteady kernel in the frequency-space involves fractional powers of the frequency and thus only an approximate rational form can be obtained using N-term Pade approximations. A 2-term Pade approximation has been shown to approximate the finite Reynolds number viscous-unsteady kernel to within 1% accuracy for all non-dimensional frequencies. From a simple analysis of particle motion in turbulent flows, we argue that this range of frequency is adequate for a wide range of particle properties and turbulence Reynolds numbers (see J11 for further details).

4.2 Mesoscale Mathematical Formulation

Recently, in collaboration with Dr. T.P. McGrath at the Naval Surface Warfare Center – Indian Head, MD, we have been developing a rigorous mathematical formulation for the compressible multiphase flow that is universal in its applicability. The present mathematical formulations of compressible multiphase flow fall within one of two categories. The first kind of mathematical models use ideas of rational mechanics and have been developed for dense particulate flows, where the dispersed phase undergoes strong compressional effects. But the compaction equation for particle volume fraction employed in these models is not applicable as the compression effect becomes negligible as the volume fraction decreases. The second kind of mathematical models are appropriate for dilute particulate flows, but cannot account for compressional effects and as a result fail as the volume fraction increases and start to approach packing limit. However, for the problem of present interest where a dense packed bed of particles is explosively dispersed, we require a universal mathematical formulation that spans from the dense regime to the dilute regime.

The improved universal formulation will incorporate the following important features. A revised compaction equation as shown below is being investigated

$$\frac{\partial \alpha}{\partial t} + \mathbf{u}_i \cdot \nabla \alpha + \phi \nabla \cdot \mathbf{u}_i = f(p - p_d)$$

where α is the volume fraction of the particulate phase, $\mathbf{u}_i$ is the interface velocity, ϕ is a weighting factor, whose value needs to be chosen, and $f(p - p_d)$ is the pressure equilibration contribution to particle compaction. The above formulation has the flexibility to reduce to the classic expression by Baer & Nunziato [1] in the limit $\phi \to 0$. But also has the ability to accommodate constant density particulate phase in the limit $\phi \to \alpha$. We are in the process of examining the thermodynamical consequences of the above enhanced compaction equation. Also, the mathematical structure of the resulting governing equations changes and the hyperbolicity of the system along with the appropriate definition of the speed of sound have been derived. Once the structure of the universal system has been fully established we will perform one-dimensional tests and then proceed to implement in the three-dimensional code of our group and also in the Navy hydrocode DYSMAS.

4.3 Rigorous Application to Shock-Particle Interaction

Here we build upon the solid foundation laid by the rigorous theoretical formulation outlined in section 4.1. We apply the interphase coupling formulation to the problem of shock–particle interaction. The interaction can be accurately resolved by direct numerical simulations. However, as the length scales of interest are much larger than the particle size in many applications, fully resolving the flow around millions of particles is impractical. Therefore, a point-particle approach is inevitable and in this context a rigorous model for momentum and energy exchange is very important.

Shock–particle interaction is strongly time-dependent, so unsteady mechanisms are important in momentum and energy transfer. The theoretical foundation outlined in section 4.1 provides us a rigorous physics-based function form for the different contributions to the overall force and heat transfer. Here we extend this model to account for the effects of finite Reynolds and Mach numbers. The model is used to investigate particle interactions with a planar shock wave and a spherical shock wave.

The key aspect of the present model is that it accurately accounts for the unsteady mechanisms, which are often ignored in the traditional models. During the shot duration of shock-particle interaction the fluid acceleration seen by the particle is very large and contributes to the unsteady mechanisms. The peak values and the net effects of unsteady contributions to force and heat transfer are used to measure the importance of the unsteady contributions. The results in Figure 5 show the ratio of peak values of unsteady contributions of force (frame a) and heat transfer (frame b) to their quasi-steady contributions for a wide range of particle parameters. It is clear that for a wide range of shock Mach numbers and particle Reynolds numbers the forces and heat transfer due to unsteady mechanisms are more than an order of magnitude larger and thus ignoring them can result in very large errors. Further details can be found in the journal article J2.

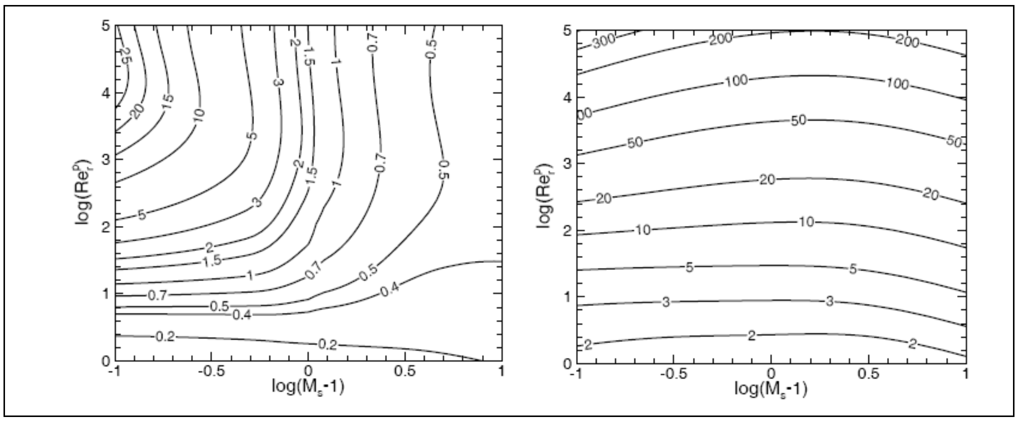


Fig 5: Here we consider the problem of force and heat transfer on a stationary spherical particle subjected to a shock. Frame (a) shows contours of the ratio of peak inviscid unsteady (pressure-gradient) force to the peak quasi-steady force (standard drag laws are limited to this quasi-steady force). Frame (b) shows the ratio of peak inviscid unsteady heating to the peak quasi-steady heat transfer. The ratios are plotted for a range of shock Mach number (x-axis) and for a range of particle size, parameterized as particle Reynolds number (y-axis). It can be seen that the ratio can be as large as 20 for the case of force and 300 for the case of heating, thus demonstrating the importance of unsteady mechanisms over a wide range of shock-particle interaction conditions.

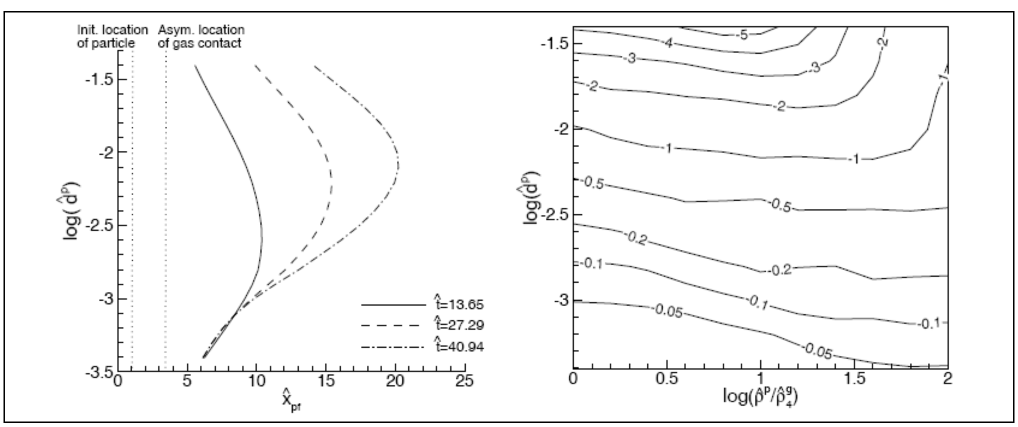


Fig 6: Here we consider the "spherical multiphase shock tube problem", where a spherical container of unit radius is initially filled with a high pressure gas-particle mixture. At t = 0 the container is removed instantaneously and the mixture is exposed to the surroundings, leading to a blast wave, gas contact, outward propagating front of particles and an expansion fan propagating inward. In the spherical geometry the gas contact reaches an asymptotic final radius, which is presented in frame (a). Also plotted

in frame (a) is the location of the particle front, as a function of particle diameter (normalized by initial charge radius), at three different times. It can be observed that (i) particles in the present example move past the gas contact into the shock-heated ambient, (ii) There is an optimal particle size that reaches the farthest at any given time, and (iii) the optimal particle size increases with increasing time. In Frame (b) we plot the error in particle front location by not including the unsteady mechanisms for varying initial particle-to-fluid density ratio (x-axis) and particle size (y-axis). It can be seen that the error in particle front location can be as large as 5 initial charge radii, and from frame (a) it can be seen that this error is a large fraction of the actual gas front and particle front location.

We extended the above investigation to consider the interesting phenomenon of particle dispersal by blast waves. A model problem, i.e., a sudden release of a compressed gas–particle mixture contained in a spherical container, is employed to investigate the fundamental physics of particle dispersal. The problem is simulated with the interphase coupling models outlined in J2. At early times, when particles are accelerated in the expansion fan, unsteady force and heating contributions are much larger than the corresponding quasi-steady contributions. Consequently, neglecting unsteady contributions leads to significant errors in particle front location (the boundary of the particle cloud - see Figure 6). The complex wave interactions in the flow have strong influence on the particle motion. As a result, the particle motion is a non-monotonic function of particle density or diameter and the evolution of particle concentration is non-uniform and unsteady. Further details can be found in the journal article J3.

4.4 Scaling Analysis

Modeling of inter-phase coupling is critical to accurate simulation of dispersed multiphase flows. In this effort, we address three important fundamental questions about inter-phase coupling: (1) Is it possible to simplify the integral representation of viscous-unsteady force? (2) Under what conditions unsteady forces are important in forward momentum coupling? (3) What parameters accurately evaluate the back effect of both the quasi-steady and unsteady forces in the fluid momentum equation? The key findings of the present study in regard to these three questions are summarized separately as follows. The details of the analysis can be found in J13-J15.

<u>Conclusions on the representation of the viscous-unsteady force:</u> In general, the viscous-unsteady force is given by a Basset-like convolution integral, whose computation is often costly. However, when both the particle and the surrounding fluid acceleration are sufficiently slow, it is possible to simplify the viscous-unsteady force and avoid evaluating the convolution integral. Here we establish the condition under which such a simplification can be made. The main conclusions are: (1) Only when the viscous-unsteady time scale (defined as the transition time for the kernel to change from the slower decay to the faster decay) is smaller than all the fluid time scales, the viscous-unsteady formulation can be simplified. The resulting simplified viscous unsteady force has a form similar to the added-mass force. (2) In turbulent multiphase flows, viscous-unsteady time scale is larger than the Kolmogorov time scale under most circumstances. Therefore, the viscous-unsteady force generally needs to be calculated using the convolution history integral. (3) For large particle-to-fluid density ratio, there exists a narrow range of particle size around the Kolmogorov length scale, where the simplified form of viscous-unsteady force can be used.

<u>Conclusions on the importance of unsteady forces in forward momentum coupling:</u> The ratio between the magnitudes of unsteady and quasi-steady forces is used to evaluate the importance of the unsteady forces in forward momentum coupling. Key conclusions in regard to the importance of the unsteady forces in forward momentum coupling include: (1) Unsteady forces are important in evaluating the motion of particles of density comparable or smaller than that of

the surrounding fluid. (2) Conventionally, the unsteady forces are neglected in gas-particle flows. The present scaling analysis shows that for particles much heavier than the fluid the importance of the unsteady forces depends on the ratio between the particle size and the smallest fluid length scale and not on the particle-to-fluid density ratio. (3) In DNS of turbulent multiphase flows, the intent is to accurately compute all the turbulent length scales and their influence on particle motion. When the particle size is comparable or larger than the Kolmogorov scale (i.e., smallest fluid length scale), unsteady forces due to the smallest eddies are important in accurately evaluating the particle motion. In LES and RANS, when the particle size is larger than the smallest resolved scale, the unsteady forces due to the resolved fluid flow will be important and must be included in the computation of the deterministic component of particle motion. When the particle size is smaller than the resolved scale but larger than the Kolmogorov scale, unsteady forces due to the unresolved scales remain important and must be accounted in the closure models. (4) In shock-particle interaction, since the particle size is generally larger than the shock thickness (i.e., the smallest flow length scale), the unsteady forces dominate the quasi-steady force during shock-particle interaction. (5) For heavy particles, we observe the stress gradient and added-mass forces to be of the same order and the ratio between viscous-unsteady and quasi-steady forces to scale as the square root of the ratio between the added-mass and quasi-steady forces. Therefore, in situations where the inviscid forces dominate the quasi-steady force, they also dominate the viscous unsteady force.

<u>Conclusions on the importance of quasi-steady and unsteady forces in backward momentum coupling:</u> We define momentum coupling parameters as the ratio between the back contribution to the fluid momentum equation from the coupling force and the fluid inertial term. The momentum coupling parameter of each force contribution is estimated through scaling argument. The key conclusions are: (1) The mass fraction ratio is usually taken to evaluate the importance of the quasi-steady force in backward momentum coupling. It is shown by the scaling analysis that the momentum coupling parameter of the quasi-steady force depends on the particle mass and volume fraction ratios for heavy particles and bubbles, respectively. For heavy particles with time scale larger than the turbulence integral time scale, when Stokes number is greater than one, the back effect of quasi-steady force on the fluid motion is small and unsteady forces become dominant in backward momentum coupling. (2) The momentum coupling parameters of stress-gradient and added-mass forces are similar. The contributions of the stress-gradient and added-mass forces to backward coupling are related to the particle volume fraction. (3) The momentum coupling parameter of the viscous-unsteady force scales as the square r0oot of the products of the momentum coupling parameters of quasi-steady and added-mass forces. Therefore, for heavy particles, the back effect of the viscous-unsteady force on fluid motion depends on both particle mass and volume fractions.

4.5 Volume Fraction Effect - Application to Shock-Particle-Curtain Interaction

Here we built upon the physics-based interphase coupling model that has been rigorously validated for an isolated particle subjected to shock waves. This work has been performed in collaboration with the Sandia National Laboratories. Experiments by Wagner et al. [4], conducted in the recently constructed Multiphase Shock Tube (MST) at the Sandia National Laboratories, examined the interaction of a planar shock wave with a moderately dense particle curtain. A multiphase shock tube was used to drive a planar shock wave into a particle curtain, i.e., a dense particle field that was generated with a gravity-fed contoured seeding method, which is shown in the schematic presented in Figure 7. The initial volume fraction of particles in the mixture was about 20%. High-speed imaging and pressure measurements showed that the interaction between the incident shock and the particle curtain resulted in an upstream-propagating reflected shock and a downstream-propagating transmitted shock. After the passage of the shock wave, the particle curtain was observed to spread rapidly as it propagated downstream. The data suggested the expansion of the particle curtain to be associated with a difference in gas properties across the streamwise thickness of the particle curtain, although the exact physical mechanisms remained unexplained from the experiments.

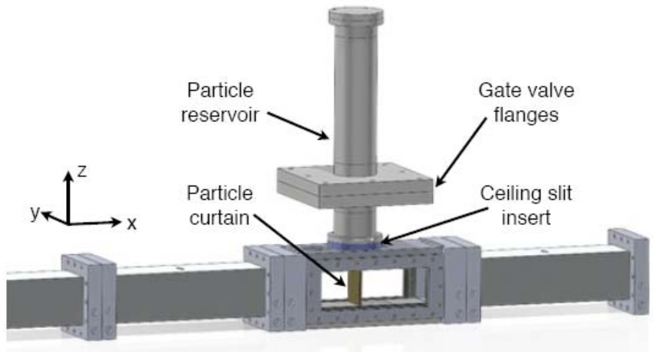
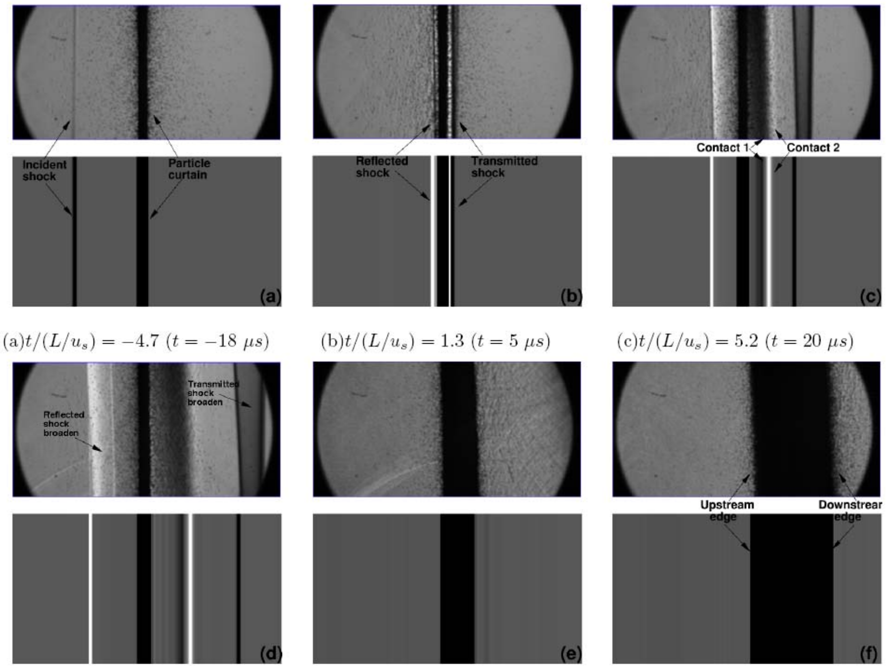


Fig 7: Schematic showing the MST test section that is used to generate the dense particle curtain. The flow direction is left to right.

The experimental conditions were simulated to investigate the underlying physics of shock-particle-curtain interaction and to validate the present compressible particle-laden flow model. The physics in the interaction between a shock wave with a dense gas-particle mixture is markedly differently from that with a dilute mixture. Following the passage of the shock wave, the dense particle curtain expands rapidly as it propagates downstream. In the simulations, the particles are viewed as point-particles and are traced in a Lagrangian framework. Compared to the standard drag law, four major improvements are made in the present interphase coupling model: (1) unsteady force contributions to particle force are included; (2) effect of compressibility on hydro- dynamic forces is included; (3) effect of particle volume fraction on hydrodynamic forces is included; (4) effect of inter-particle collision is taken into account. The complex behavior of the dense particle curtain is due to the interplay between two-way coupling, finite particle inertia, and unsteady forces. Incorporation of these effects requires significant modeling improvements and these improvements are observed to be essential for the simulation results to agree with the experimental data.

Figure 9 shows the qualitative comparison between Schlieren images obtained from the experiments and the simulations. More detailed quantitative comparison is shown in Figure 8, where on the *x-t* diagram the position of the shocks and the particle curtain are compared. The simulations show the rich details of the particle-laden flow arising from the shock-particle-curtain interaction. The physical mechanism responsible for the expansion of the particle curtain have been identified.



(a)$t/(L/u_s) = -4.7$ ($t = -18\ \mu s$) (b)$t/(L/u_s) = 1.3$ ($t = 5\ \mu s$) (c)$t/(L/u_s) = 5.2$ ($t = 20\ \mu s$)

(d)$t/(L/u_s) = 9.1$ ($t = 35\ \mu s$) (e)$t/(L/u_s) = 37.2$ ($t = 112\ \mu s$) (f)$t/(L/u_s) = 70.7$ ($t = 213\ \mu s$)

Fig 8: Numerically generated Schlieren images (contours of gas density gradient in region without particles) are compared with corresponding experimental results for the case of a shock of Mach number 1.92 interacting with a particle curtain of 2 mm thick at 21% volume fraction of 115 μm particle. Results are shown at 6 different times. Close correspondence between the experiments and simulations can be observed.

The trajectories of the edges of the particle curtain computed with the present model are shown in Figure 10 and are compared with those computed with the standard drag law of Clift and Gauvin.37 It can be observed that the upstream and downstream edges of the particle curtain calculated by these two models are substantially different. The present model yields results that match the experimental data much better than the standard drag law. If the standard drag law is used, both the upstream and downstream edges of the particle curtain move slower than the experimental results. For the downstream edge, at t = 150, the locations computed by the present model, the standard drag law, and measured in the experiment are 19.23L, 10.56L, and 20.47L, respectively. In other words, the standard drag law underestimates the downstream edge location by about 50%. As a result of the underestimate on the downstream edge, the expansion of the particle curtain is also underestimated by the standard drag law. Therefore, it can be concluded that if the above improvements in the force model are not considered, the interaction between a shock wave and a dense particle curtain and the resulting expansion of the particle curtain will not be captured accurately. These results are summarized in the journal article J6.

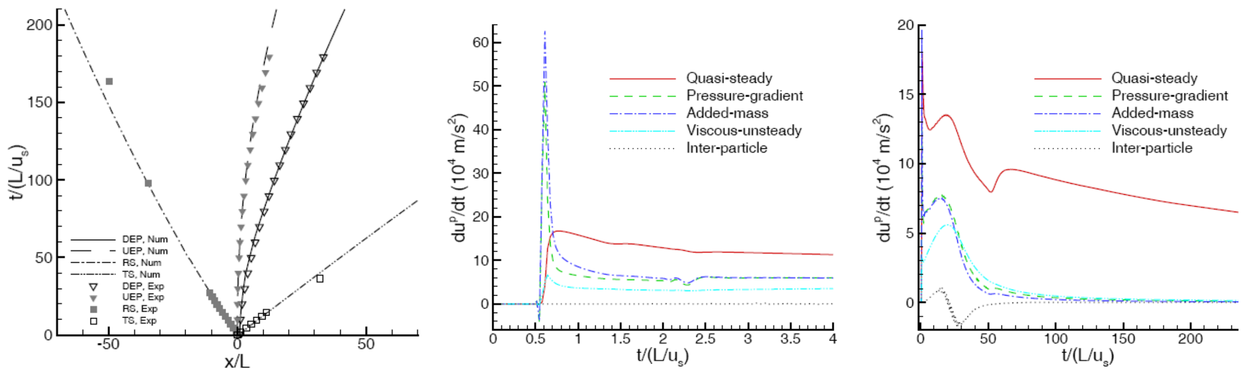


Fig 9: (a) Comparison of the Reflected shock (RS), Transmitted shock (TS), Upstream edge of particles (UEP), Downstream edge of particles (DEP) obtained from experiments and simulations. Excellent agreement is seen. The importance of including the different contributions to force is demonstrated in frames (b) and (c), where the different force contributions are plotted on short and long time scales. Over the initial short time period (see frame b), during the shock passage over the particle curtain, the unsteady forces (pressure-gradient, added-mass, viscous unsteady) are much larger than the quasi-steady force. But more interestingly, even long after the passage of the shock the net contribution of the unsteady forces remain comparable to the quasi-steady contribution. These unsteady forces are typically ignored in standard modeling approaches and therefore can result in substantial error.

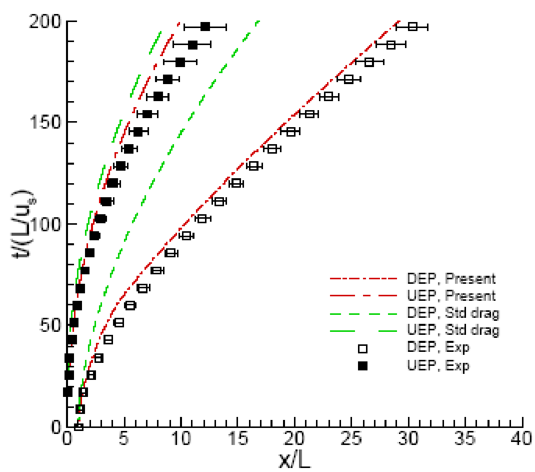


Fig 10: Trajectories of the upstream and downstream edges of particle curtain for Case 1 computed with the present model ("Present") and the standard drag law37 (\Std drag"), compared with the experimental results ("Exp").

4.6 Modeling and Simulation of Particle-Detonation Interaction

Here we are interested in the problem of a strong shock interacting with a particle, where the shock strength is of sufficient magnitude that the deformation and the compression of the particle cannot be ignored. In particular, we are interested in the problem of detonation-particle interaction in the context of condensed phase detonations, where the density of the products of detonation is substantial and the post-shock pressure can be significantly larger than the yield strength of particle. But experiments of shock interaction with a deforming particle (SIDP) in the context of metal particles subjected to an intense shock in a condensed matter ambience are rare in the literature, due to the complex nature of such experiments. Modeling and simulation is an attractive alternative that can provide time resolved details of such particle interaction with a strong shock wave. This is the approach that has been pursued here and this work is conducted in collaboration with researchers at Lawrence Livermore National Laboratory and at the University of Illinois, Urbana-Champaign.

The primary goal of this task is to extend the earlier described theoretical model presented in section 4.2 and propose a SIDP model that includes the leading order effects of particle deformation and compression heating. To reach this goal, we first carry out DNS of a deforming particle subjected to a strong shock in condensed matter. The material properties are characterized by appropriate equations of state (e.g., Mie-Gruneisen EOS). The DNS results show the interaction details, such as shock reflection, refraction and evolutions of average properties of particles. Based on the knowledge obtained from the DNS study, we improve the model by including the effects of particle deformation and compression heating. We note that shock interaction with a deforming particle (SIDP) occurs in other interesting applications as well. For example, shock interaction with a droplet or a bubble can lead to significant deformation of the droplet or the bubble. In fact a sufficiently strong shock can lead to violent breakup and fragmentation of the droplet or bubble, see e.g., [5-7]. The present simulation and modeling effort was limited to modest deformation of the particle and will not include more complex scenarios such as breakup and fragmentation.

Figure 11 shows the DNS results of an aluminum particle subjected to an intense shock in nitromethane (shock speed is 4800 m/s, the post-shock pressure and velocity are 10.7 Gpa and 2270 m/s). Details of particle deformation, and fully resolved pressure and thermal fields computed at the microscale are shown in frames a-d. The time evolution of particle velocity and average temperature obtained from the DNS are shown in Figures 9e and 9f. Such resolution is, however, impossible at the mesoscale, where millions of particles must be considered. So a point-particle approach is employed at the mesoscale, where all the microscale details must be accurately encapsulated into mass, momentum, and energy coupling models. Shown in Figure 9e and 9f are the particle velocity and temperature predicted by conventional drag and heat transfer point-particle models (these simple models are typically used in meso and system-scale simulations). It is quite clear that such standard models result in very large errors, since they have not been developed and tested for the intense pressure and temperature conditions representative of detonation particle interaction. As a consequence, it can be expected that meso and system-scale simulations performed with the standard models to result in serious error. In contrast, physics-based coupling models developed by our group can be seen to perform quite well. Thus, Figure 11 captures the serious limitations of the standard micro-to-meso coupling models and illustrates the importance of physics-based models rigorously developed from microscale simulations performed for extreme conditions.

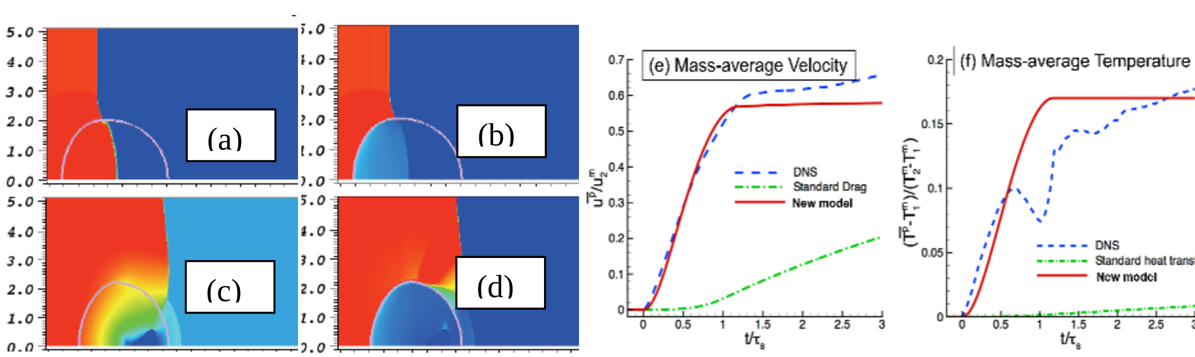


Fig 11: ALE3D simulations of intense shock propagation over an aluminum particle embedded in nitromethane (simulations performed by Dr. Najjar at LLNL). Frames (a) & (c) are pressure and (b) &

(d) are temperature contours at 0.3 and 0.8 nanoseconds, respectively. Frames (e) and (f) compare time evolution of nondimensional particle velocity and volume-averaged temperature against standard and improved physics-based models.

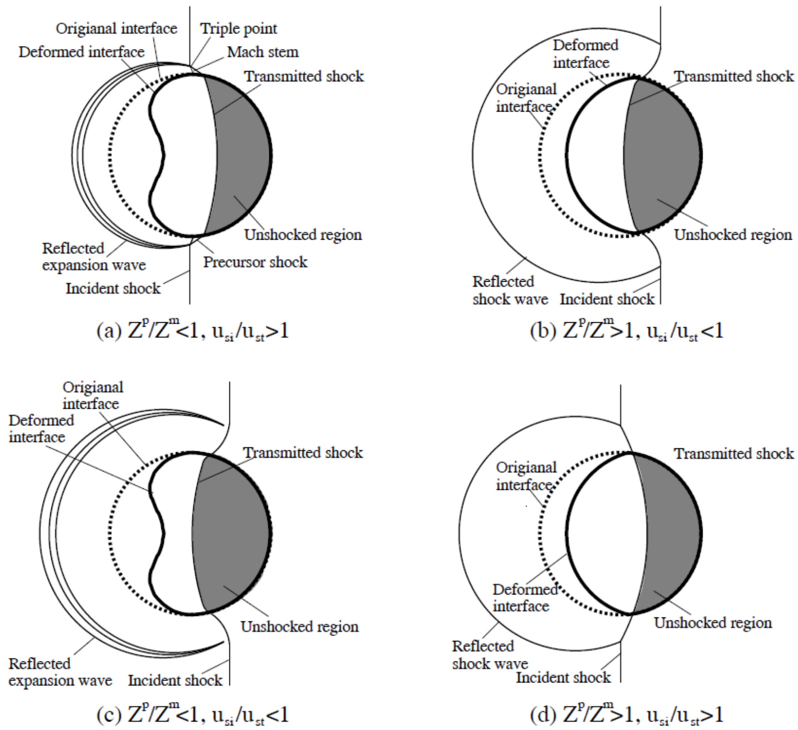


Fig 12: Representative scenarios of flow field arising from shock interaction with a deformable particle for different shock impedance and shock speed ratios.

The results of the direct numerical simulations have been generalized to broader strong-shock-particle interaction conditions. Representative scenarios of flow fields arising from SIDP are shown in Figure 12 for different combinations of the impedence ratio z_p / z_m and the shock speed ratio u_{st} / u_{si} (here z_p, z_m are the shock impedence in the particle and in the surrounding matrix and u_{st}, u_{si} are the incidence and transmission shock propagation speeds in the matrix and in the particle). The former ratio determines the reflected wave to be a expansion fan or a shock wave, while the latter ratio determines the shape of the transmitted shock (see Figure 12). In summary, there are four different scenarios: (a) a reflected expansion fan and a convex transmitted shock (z_p / z_m < 1 and u_{st} / u_{si} > 1); (b) a reflected shock and a concave transmitted shock (z_p / z_m > 1 and u_{st} / u_{si} < 1); (c) a reflected expansion fan and a concave transmitted shock (z_p / z_m < 1 and u_{st} / u_{si} < 1); and (d) a reflected shock and a convex transmitted shock (z_p / z_m > 1 and u_{st} / u_{si} > 1). The above presented are sample results. Further details can be found in the journal article J9.

4.7 Instability of the Expanding Spherical Gas-Gas Interface

Here we begin to address the question of how an expanding material front becomes unstable and evolves into spatial patters seen in Figures 1, 2 and 3. This instability and transition problem is in its infancy. Rigorous instability analysis of such complex time-dependent highly-compressible multiphase flows has not been performed in the past. As the first step we address the instability of a rapidly expanding gas-gas interface, before proceeding to the instability of an expanding particulate front.

A high-order WENO scheme is employed to investigate the stability of a rapidly expanding material interface produced by a spherical shock tube. The flow structure is characterized by a forward moving primary shock, a backward moving secondary shock, and a spherical contact interface in-between. We consider herein the linear inviscid regime and focus on the development of the three dimensional perturbations around the contact interface by solving a one-dimensional system of partial differential equations. Numerical simulations are performed to illustrate the effects of the contact interface's density discontinuity on the growth of the disturbances for various spherical wave numbers. In a spherical shock tube the instability is influenced by various mechanisms which include classical Rayleigh-Taylor (RT) effect, Bell-Plesset (BP) or geometry/curvature effect, the effect of impulsively accelerating the interface, and compressibility effects. For an extended intermediate time period, it can be shown that the small disturbances grow exponentially as in the classical RT instability. During this stage, the exponential growth rate increases with the spherical wave number, until it saturates for very large wave numbers due to the finite thickness limitation of the numerical representation of the contact interface. The results compare favorably with previous theoretical models; but indicate that in addition to compressibility, the space-time evolution of the contact interface's thickness plays a significant role. A parametric study is performed that varies the pressure and density ratios of the initial spherical container. The characteristics of the contact interface and the applicability of various instability theories is investigated for these regimes. Furthermore, varying the pressure and density ratios aids in understanding significance of compressibility effects on the instability at different operating conditions.

A comparison of the computed growth rate with the various theoretical models [8-12] is presented in Figure 13. The predictions of planar (Taylor [8]) and spherical (Plesset [9], Espsten [12]) RT instability theories are generally close to each other indicating the relatively modest effects of compressibility and sphericity. The dominant feature of all these theories is the increase in growth rate as square root of the spherical wave number. The computed growth rate follows this scaling up to a wave numbers of about 40, beyond which the growth rate slows down and eventually saturates to a constant growth rate that is independent of the wave number. In the regime where growth rate is $\propto \sqrt{n}$ the solution to the compressible ODE by Epstein [12] compare the best with the computed growth rate. This can be expected since Epstein's theory accounts for both compressibility and radial effects.

The asymptotic constant growth rate computed for large wave numbers compares well with the local convective growth rate given by Bandiera [10]. At such large wave numbers the finite thickness of the contact interface computed in the base flow solution begins to have a strong influence. The interface does not appear as a discontinuity and the density gradient in conjunction with the local pressure gradient within the contact interface dictates the growth rate. Unlike classical RT instability, the convective instability is independent of the spherical wave number. Figure 9 corresponds to a grid resolution of N = 16000 for both the base flow and perturbation solutions. The theory by Lindl [11] follows both the low and large wave number behaviors. However, Lindl's prediction is based on incompressible analysis of a planar interface and is somewhat lower than the computed growth rate.

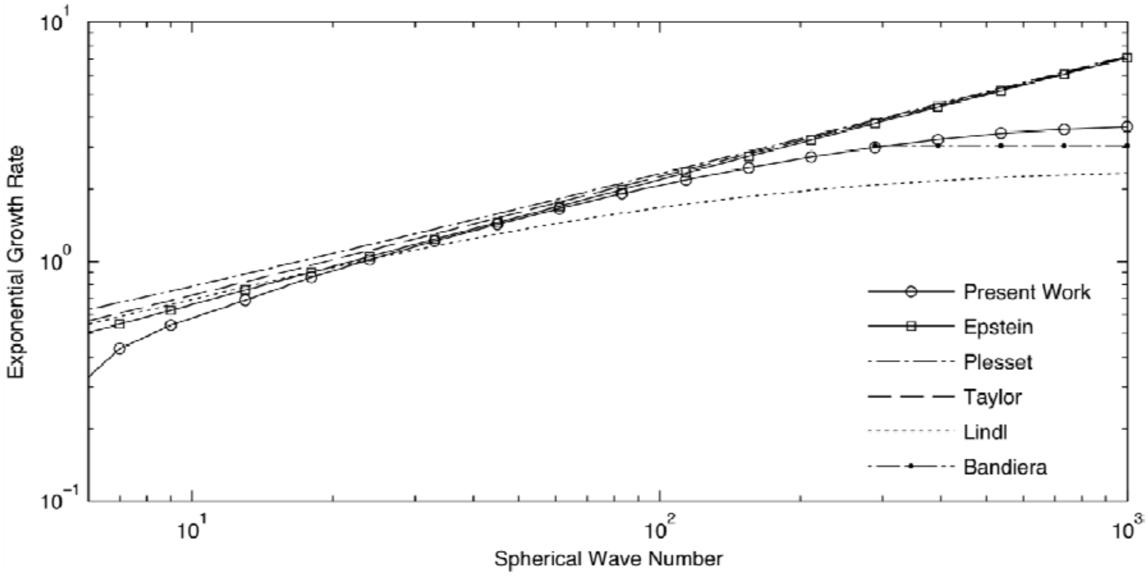


Fig 13: The effect of the wave number on the growth rate.

The above inviscid analysis has been extended to the viscous regime, where the effect of finite Reynolds number and thermal and mass diffusivities on the instability results have been examined. Figure 14 demonstrates the effect of the Reynolds number on the growth rate for a given Atwood number. For low wave numbers the Reynolds number has no effect on the growth rate. Consequently, the growth rate predicted for wave numbers less than 45 did not change as the Reynolds number went from 6.2 x 10^5 to 10^4. However, for high have numbers, as the Reynolds number decreases the peak growth rate and its corresponding wave number also decrease. As the Reynolds number is reduced from 6.2 x 10^5 to 10^4, the peak growth rate is reduced from 1.15 to 1.07 and its corresponding wave number also reduced from 400 to 100. For the limiting case of very large Reynolds number $(\mathrm{Re} \to \infty)$, the inviscid solution is recovered where the growth rate saturates and does not decline for very large wave numbers. The low-Reynolds number cases may be taken as an approximation to the turbulent flow case, in which the presence of turbulence can be modeled by an eddy viscosity that increases the effective Reynolds number. Further details can be found in the articles J4 and J8.

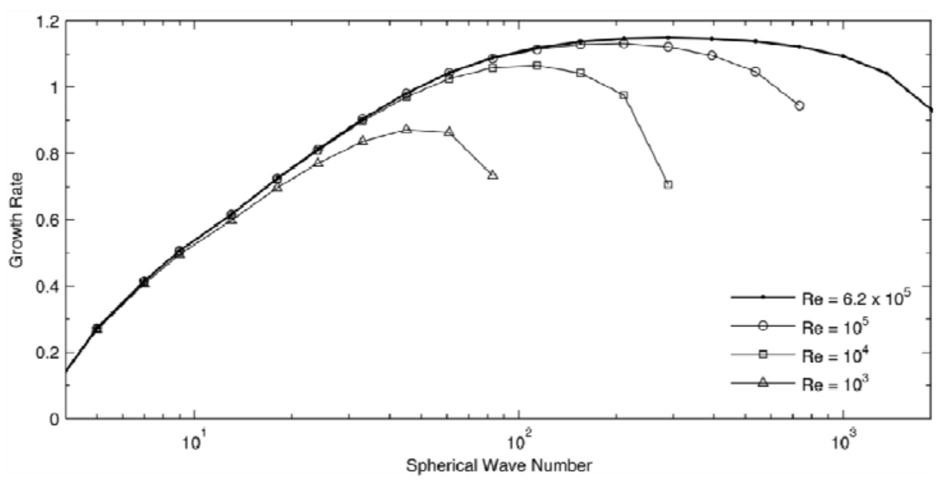


Fig 14: The effect of the Reynolds number on the growth rate for an Atwood number of 0.3575.

4.8 Instability of a Rapidly Expanding Spherical Particulate Interface

The problem under study is that of a mixture of gas and metal particles (e.g. aluminum) initially contained in a spherical diaphragm of a small radius under high pressure. The gas-particle mixture is then suddenly released as in a spherical shock-tube. The problem represents several real-life applications, such as, particle-laden detonative combustion, dispersal of metalized explosives, volcanic eruption, and ignition of solid-propellant rockets, to mention only a few. In the single-phase case, when the high- pressure gas is suddenly released from a spherical container, a forward-moving shock wave is formed along with a backward-moving rarefaction wave, whose trailing edge becomes a secondary shock due to the convergent geometry. Between the two shocks a contact interface (CI) is formed, which acts as a material interface that separates the hot driver gas from the cold driven pure gas. Due to the inherent density jump across this contact interface, Rayleigh-Taylor-Instability (RTI) emerges where inter-penetrating dimples form, around which there is considerable vorticity. In the case of a gas-particle mixture in a spherical shock-tube, a second interface is formed that separates the gas-particle mixture from the pure-gas phase. The presence of the solid particles influences the instability of the gas-gas CI, which is the subject of the present study.

In the multiphase context, the effect of the presence of metal particles on the gas-gas CI needs to be studied. The gas-particle interactions are quite complicated because there are several additional mechanisms involved, such as the quasi-steady viscous forces, the heat transfer between the particles and the gas, and the added-mass forces. The instability of the gas-gas CI is affected by the presence of the particles at two levels. In the first, the presence of the particles modifies the gas base flow, which drives the CI instability. At the second level, the gas-particle interaction produces additional perturbation source-terms in the stability equations of the perturbed gas flow. Although an Eulerian- Lagrangian approach, if utilized properly, can capture the effect of particles on the contact interface, it is harder to capture the instability of the particle interface itself if needed. Hence, a two-fluid Eulerian approach is implemented herein. The methodology employed in Mankbadi & Balachandar (2012) for the single-phase problem is extended here to investigate the complex multiphase problem.

The base flow’s discontinuous surfaces are tracked in the presence of solid aluminum particles. The density of aluminum particles relative to that of the initial compressed gas yields a ratio of 43.66. In Figure 15, the locations of the interfaces for three different combinations of particle diameter and volume fraction are depicted. Figure 2 (A) (d_p = 10 micron, initial particle volume fraction = 1.5%) illustrates the locus of the primary shock (PS), the secondary shock (SS), the contact interface (CI) separating the driver gas from the driven gas, and the particles interface (PI). In the near field, the secondary shock initially moves out but soon turns and travels inward. For very early time the secondary shock is in close proximity to both the contact interface and the particle interface. The particle interface impacts the behavior near the contact interface, especially when it collides with the contact interface and overtakes it at about t=2.5. The particles then pierce through the contact interface and are no longer in the initially compressed gas but rather are now in the shock-heated fluid. Now, consider two other extreme cases for the base flow. In Figure 15 (b) (d_p = 500 micron, initial particle volume fraction = 5%), the particle response time has become too large, and as such the particles are not responding quickly to the gas flow. In this case, the PI stays away from the CI as shown in the diagram. In the other extreme (d_p = 1 micron, initial particle volume fraction = 5%), the particle response time has become very small such that particles respond quickly to the gas, and consequently the PI and CI are close to each other, as illustrated in Figure 15 (c).

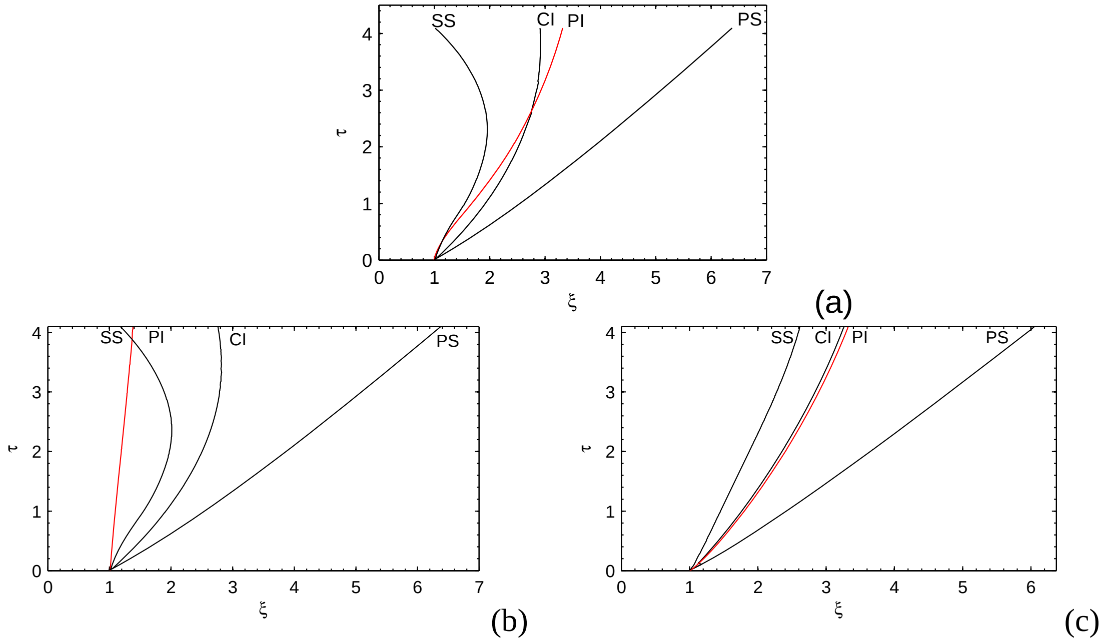


Fig 15: The $\boldsymbol{\xi}$*-* $\boldsymbol{\tau}$ *diagram depicting the radial location of the primary shock, particle interface, contact interface, and secondary shock. A) For* $d_p = 10\mu m$, $\rho_p/\rho_g = 43.66$, and ϕ_{p_0} *= 0.015. B) For* $d_p = 500\mu m$, $\rho_p/\rho_g = 43.66$, and ϕ_{p_0} *= 0.05. C) For* $d_p = 1\mu m$, $\rho_p/\rho_g = 43.66$, *and* ϕ_{p_0} *= 0.05.*

4.9 Non-linear Instability of the Expanding Cylindrical Gas-Gas Interface

When the amplitude of the perturbation grows to 10-20% of the wavelength, non-linear effect becomes important. The symmetry between the light and heavy fluids breaks down and a bubble-spike structure appears. Conventionally, bubble refers to the light fluid that rises into the heavy fluid, while spike denotes the heavy fluid that penetrates into the light fluid. The non-linear growth is characterized by the heights of the bubble and spike. In the non-linear regime, it has been shown previously using simulations, theoretical analysis and experiments that the heights of the bubbles/spikes increase at a constant velocity when a single mode perturbation is introduced at the interface. In other words, the perturbation amplitude grows linearly in time. Recently, investigations show that the growth velocities of the heights of the bubbles/spikes increase again after being at a constant value for a finite period of time.

Modeling of the non-linear growth of RTI has been intensively studied in the past. The goals of the present study are to improve the understanding of RTI in explosion flows through rigorous numerical simulations of the present problem and to examine the capabilities of the existing RTI models on predicting RTI in explosion flows. A simple extension to Miles' model is proposed, in which the effects of the transition from linear to non-linear growth is captured. In addition, the background flow density variations are included. As can be seen from Figure 16(a) the RTI can still be studied as bubbles and spikes even at late times. The mushroom-type structures are still intact. So we can conclude that, for a given wavenumber, the non-linear growth in the azimuthal and longitudinal directions are quite different. While in the azimuthal case, the structures are well behaved for large wavenumbers even for late times, severe mixing ensues for the corresponding longitudinal case (see, Figure 16(b)). This shows that for a given wavenumber, the non-linear growth does depend on the direction in which the mode is imposed.

Fig 16: (a) Bubble and spike mushroom-type structures for azimuthal wavenumber (m = 48) at time = 6:9 and (b) No clear bubble-spike pattern for longitudinal wavenumber (n = 48) at t = 6:9

5. Recommendations and Future Work

We are continuing the research along all the fronts outlined in section 4. In particular, we plan to accomplish further fundamental advances in interphase coupling modeling, experimental validation, and prediction of interfacial instability of explosive multiphase material fronts. These ongoing activities are discussed below:

Modeling: Despite the good performance of the present interphase coupling model described above, there are still several complex scenarios of practical importance, for which the coupling model requires further investigation and improvement.

1) In the limit of moderate particle clustering, the effect of local particle volume fraction can be expected to play a key role in the quasi-steady, and the unsteady force contributions. Currently we rely upon incompressible flow results to provide up guidance for modeling the volume fraction effect in the compressible flow regime. We will pursue direct numerical simulations at the microscale of steady and unsteady flows around periodic array of particles to develop fundamental understanding of volume fraction effect on quasi-steady and unsteady forces in the compressible flow regime.

2) When particle volume fraction is large, then particle-particle interaction in the form of inter-particle collisions will begin to play an important role. In [J6] we used a simple particle-pressure-based model to account for the inter-particle collision force. This simple representation was sufficient for the modest volume fraction considered in that investigation. In order to extend the formulation to higher volume fraction, more rigorous understanding of inter-particle collision is required, especially in the context of a shock wave propagating over a dense curtain of particles. On one hand we are coordinating with researchers at Sandia National Laboratories to extend their experiments [4] to denser particle curtains, where inter-particle collision will be the dominant force on the particles. A rigorous universal compressible multiphase formulation is currently under development. We have started to first explore its mathematical structure and limiting analytical and numerical behaviors. As we complete this theoretical framework, we are continuing to test the formulation by comparing its predictions against high quality experimental results, including those from the multiphase shock tube facility at Sandia National Laboratories. We are begining to perform Discrete Element Method (DEM) simulations along with our point-

particle coupling model of the hydrodynamic forces. The DEM results can be used to develop improved inter-particle collision force models and to validate them against experimental measurements. However, in the DEM approach an empirical model is required in accounting for the momentum and energy exchange during particle-particle contact.

3) Note that once the detonation wave completely sweeps across the entire explosive, the detonation wave will be transmitted as a shock wave (blast wave) through the surrounding air. At the initial stages the intensity of this shock wave is very high and the corresponding shock Mach number can be order ten. The compressible coupling models that have been developed and tested have generally been limited to subsonic and transonic conditions. Thus, there is a strong need to evaluate the appropriateness of the interphase coupling models at even extreme flow conditions, and develop new models (or modifications) as necessary.

4) We are continuing our investigation of detonation-particle interaction, where the particle undergoes significant deformation (see discussion in section 4.6). We are performing ALE3D simulations of detonation-particle interaction under varying conditions of incident shock/ detonation wave intensity, particle-to-fluid density and impedance ratios. These simulation results are being used to develop a more robust model that fully account for particle deformation into consideration. Efforts are underway to extend the point-particle models to predict not just the mass-averaged velocity and heating but to predict the peak values of stress and temperature as well.

Experimental Validation: Rigorous validation is essential at every stage of model development and integrated simulation. We have taken care to find appropriate validation data for each component of the coupling model, as well as their overall integrated contribution. As we incorporate more features into the model additional experimental results are being identified for rigorous validation.

1) The present very-strong-shock or detonation-particle interaction model has been motivated by detailed numerical simulations performed at the microscale. However, the model must be validated against high quality experimental results. Measurements of deformation and motion of an isolated particle resulting from its interaction with a detonation wave is a challenging task. We are currently collaborating with researchers at the Air Force Research laboratory - Munitions Directorate to perform this kind of experiments along with detailed time-resolved x-ray and other high-speed measurements.

2) Prof. D. Frost at McGill University and his collaborators have performed outstanding collection of experiments on explosive dispersal of particle under varying conditions. Prof. Frost is current on his sabbatical visit at our group at the University of Florida. We are closely collaborating with him and applying our modeling and simulation approach to his experimental configurations.

3) Interphase energy coupling models of shock-particle and detonation-particle interaction have hardly been validated due to paucity of high-quality experimental results. Thus, validation of thermal coupling models is of great interest. In particular, we desire validation-quality experimental measurements of particle and gas temperature immediately following a strong-shock or detonation particle interaction.

Instability: Our investigation of instability of a rapidly expanding material interface presented in section 4.5 was limited to only gas-gas interface. Thus we only considered the case of a high-density highly compressed sphere of gas (for example products of a spherical detonation) expanding into the ambient. Due to the near-constant deceleration of the gas-gas interface it initially undergoing Rayleigh-Taylor (RT) instability, which was investigated both in the inviscid and viscous limits (see section 4.5). Our analysis has established a firm mathematical methodology for investigating instability of such rapidly expanding material fronts. Over the next two years we plan to exploit this methodology and investigate the following extensions.

1) We are extending the investigation of the instability of a rapidly expanding particulate front, presented in section 4.8. We will also consider cases similar to that in Figure 2e, where the particles were placed around an explosive. The introduction of the particulate phase in the instability analysis introduces additional complexities, and the role of interphase momentum and energy coupling will be of importance.

2) One of the interesting features of the spherical instability is that the growth rate only depends on the spherical model number n and does not distinguish between the combination of circumferential and azimuthal components. We plan to continue performing the non-linear analysis of the instability through direct numerical simulations, under cylindrical configuration (similar those presented in section 4.9).

6. Students, Publications & Presentations

Students:

1) Manoj Parmar (PhD 2010) - Currently employed at Innovative Scheduling Inc.
2) Yue Ling (PhD 2010) - Currently Research Scientist at Université Pierre et Marie Curie
3) Mina Mankbadi (PhD 2013) – Currently employed at NASA Glenn Research Center
4) Subramaniam Annamalai (PhD Student)
5) George Akiki (PhD Student)
6) Christopher Neal (PhD Student)
7) Angela Diggs (PhD Student – leveraged with DoD SMART fellowship at AFRL-RW)

Journal Publications:

J1) Parmar, M., Haselbacher, A. and Balachandar, S. Generalized Basset-Boussinesq-Oseen equation for unsteady forces on a sphere in a compressible flow. *Physical Review Letters* **106**, 084501 (2011).

J2) Ling, Y., Haselbacher, A. and Balachandar, S. Importance of unsteady contributions to force and heating for particles in compressible flows Part 1: Modeling and analysis for shock-particle interaction. *International Journal of Multiphase Flow* **37**, 1026-1044 (2011).

J3) Ling, Y., Haselbacher, A. and Balachandar, S. Importance of unsteady contributions to force and heating for particles in compressible flows Part 2: Application to particle dispersal by blast waves. *International Journal of Multiphase Flow* **37**, 1013-1025 (2011).

J4) Mankbadi, M. and Balachandar, S. Compressible inviscid instability of rapidly expanding spherical material interfaces, *Physics of Fluids*, **24**, 034106 (2012).

J5) Parmar, M., Haselbacher, A. and Balachandar, S. Equation of motion for a sphere in non-uniform compressible flows, *Journal of Fluid Mechanics*, **699**, 352-375 (2012).

J6) Ling, Y., Wagner, J.L., Beresh, S.J., Kearney, S.P. and Balachandar, S. Interaction of a planar shock wave with a dense particle curtain: Modeling and experiments, *Physics of Fluids* **24**, 113301 (2012).

J7) Parmar, M., Balachandar, S. and Haselbacher, A. Equation of motion for a drop or bubble in viscous compressible flows. *Physics of Fluids*, **24**, 056103 (2012).

J8) Mankbadi, M. and Balachandar, S. Viscous effects on the Rayleigh-Taylor instability of rapidly expanding spherical material interfaces. Submitted *Shock Waves*, (2013).

J9) Ling, Y., Haselbacher, A., Balachandar, S., Najjar, F.M. and Stewart, D.S. Shock interaction with a deformable particle: Direct numerical simulation and point-particle modeling. *Journal of Applied Physics*, **113**, 013504 (2013).

J10) Aarons, L.R., Balachandar, S. and Horie, Y. The mixing of cohesive granular materials featuring a large size range in the absence of gravity. *Powder Technology* **235**, 18-26 (2013).

J11) Parmar, M., Balachandar, S. and Prosperetti, A. Efficient computation of history forces using Pade approximation and its energy implications. To be submitted to *Journal of Fluid Mechanics* (2013)

J12) Mankbadi, M. and Balachandar, S. Effect of suspended particles on the Rayleigh-Taylor Instability of Spherical Material Interfaces. Under review *Physics of Fluids* (2013).

J13) Ling, Y., Haselbacher, A. and Balachandar, S. Scaling analysis of particle dispersal in multiphase explosions. To be submitted (2013)

J14) Ling, Y., Parmar, M. and Balachandar, S. A scaling analysis of added-mass and history forces and their coupling in dispersed multiphase flows. *International Journal of Multiphase Flows*, **22**, 102-114 (2013)

J15) Parmar, M., Ling, S. and Balachandar S. Multiphase energy coupling: Its form and scaling analysis, in preparation (2013)

J16) Annamalai, S., Parmar, M., Ling, S. and Balachandar S. Nonlinear Rayleigh-Taylor instability of a cylindrical interface in explosion, under review *ASME Journal of Fluids Engineering* (2013)

<u>*Conference Papers and Abstracts*</u>

C1) Ling, Y., Haselbacher, A. and Balachandar, S. Particle dispersal in rapidly expanding gas flow: Importance of unsteady force and heat transfer. *Bulletin of the American Physical Society*, **55**, EV 00007, Long Beach, California, (November 2010).

C2) Parmar, M., Haselbacher, A. and Balachandar, S. Extension of Basset-Boussinesq-Oseen and Maxey-Riley equations to compressible flows. *Bulletin of the American Physical Society*, **55**, EV 00008, Long Beach, California, (November 2010).

C3) Lieberthal, B., Stewart, D.S., Bdzil, J.B., Najjar, F.M., Balachandar, S. and Ling, Y. Simulation of deformation, momentum and energy coupling particles deformed by intense shocks. *Bulletin of the American Physical Society*, **56**, H2 00009, Baltimore, Maryland, (November 2011).

C4) Mankbadi, M. and Balachandar S. Instability of rapidly expanding spherical material interfaces. *IMECE* **2011-62400,** Proceedings of ASME International Mechanical Engineering Congress and Exposition, November 11-17, Denver, CO, USA (2011).

C5) Mankbadi, M. and Balachandar S. Viscous effects on the Rayleigh-Taylor instability of rapidly expanding spherical material interfaces. 50th AIAA Aerospace Sciences Meeting, Nashville, TN. January (2012)

C6) Balachandar, S., Ling, Y., Parmar, M. and Mankbadi, M. Compressible Multiphase Turbulence – Explosive dispersal of particles, International Conference on Numerical Methods in Multiphase Flows, State College, PA, June (2012).

C7) Parmar, M., Balachandar, S. and Haselbacher, A. Equation of motion for a drop or bubble in viscous compressible flows. *Bulletin of the American Physical Society*, **57**, P. 449, San Diego, CA, (November 2012).

C8) Ling, Y., Parmar, M., Annamalai, S., Balachandar, S. and Frost, D.L. Toward rigorous modeling of extreme compressible multiphase flows. *Bulletin of the American Physical Society*, **57**, P. 54, San Diego, CA, (November 2012).

Invited Presentations (Only relevant to AFOSR funding)

P1) CCMT and Modeling and Simulation of Obscurant Clouds, Edgewood Chemical Biological Center, US Army Aberdeen Proving Grounds, MD. July (2013)

P2) Disperse Multiphase Turbulence – Environmental & Extreme Flows, Keynote Lecture, International Conference on Multiphase Flows, Jeju, S. Korea. May (2013)

P3) Disperse Multiphase Turbulence – Environmental & Extreme Flows, Invited Lecture, Workshop on Multiphase Flows, Huazhong University of Science & Technology, (e-presentation), Wuhan, China. June (2013)

P4) Turbulence and Particles – Friends or Foes, Ecole Centrale Paris, Paris, France . September (2013)

P5) Turbulence and Particles – Friends or Foes, Keynote Speaker, Euromech Colloquium 555, Bordeaux, France. September (2013)

P6) Multiphase Flow Physics, Modeling and Simulation, Edgewood Chemical Biological Center, US Army Aberdeen Proving Grounds, MD. July (2013)

P7) Full System Integrated Simulations of Rocket Motors, Naval Surface Warfare Center, Indian Head, MD. July (2012).

P8) Modeling and Simulation of Turbulent Multiphase Flows for Explosive Particle Dispersal, Naval Surface Warfare Center, Indian Head, MD. July (2012).

P9) Compressible Multiphase Turbulence – Explosive dispersal of particles, Gordon Research Conference on Energetic Materials, Mount Snow, VT. June (2012).

P10) Compressible Multiphase Turbulence – Explosive dispersal of particles, Department of Aerospace Engineering, Texas A&M University, College Station, TX. April (2012).

P11) Compressible Multiphase Turbulence – Explosive dispersal of particles, High Explosive Research and Development Facility, AFRL-RW, Eglin, FL, March (2012).

P12) Compressible Multiphase Turbulence – Explosive dispersal of particles, Lawrence Livermore National Laboratory, Livermore, CA. January (2012).

P13) Viscous effects on the Rayleigh-Taylor instability of rapidly expanding spherical material interfaces. 50th AIAA Aerospace Sciences Meeting, Nashville, TN. January (2012)

P14) Compressible Multiphase Turbulence – Explosive dispersal of particles, Sandia National Laboratories, Livermore, CA. January (2012).

P15) Compressible Multiphase Turbulence – Explosive dispersal of particles, Center for Mixing at Extreme Conditions, Los Alamos National Laboratory, Los Alamos, NM. January (2012).

P16) Fundamental advances in compressible multiphase flows: application to explosive dispersal of particles. 48th Annual Technical Conference of Society of Engineering Sciences, Chicago, IL. October (2011).

P17) Compressible multiphase flows - Explosive dispersal of particles. 41st AIAA Fluid Dynamics Conference and Exhibit, Honolulu, HI. June (2011).

P18) Drag and lift forces on particle motion and resuspension. Department of Mechanical Engineering, University of Newcastle, Unite Kingdom, September (2010).

P19) Compressible multiphase flows: Explosive dispersal of particles. Cavendish Laboratory, Cambridge University, United Kingdom, September (2010).

P20) Microscale simulations of shock interaction with heterogeneous inclusions. Air Force Research Laboratory, Eglin Air Force Base, Ft. Walton Beach, FL. December (2011).

P21) Hierarchical approach to simulations of multiphase explosives. DTRA Meeting, Applied Physics Laboratories, Pennsylvania State University, State College, PA. December (2011).
P22) Microscale simulations of shock interaction with heterogeneous inclusions. Air Force Research Laboratory, AFOSR/AFRL Workshop, Washington, DC. July (2011).
P23) Explosive dispersal of particles - why do we need to understand compressible multiphase flows? Air Force Research Laboratory, Eglin Air Force Base, Ft. Walton Beach, FL, February (2011).
P24) Compressible multiphase flows: explosive dispersal of particles. SHAMRC Workshop, Santa Fe, NM. (2010).
P25) Particulate and agent dynamics in multiphase turbulent reacting flow. Applied Physics Laboratories, Pennsylvania State University, State College, PA. (2010).
P26) Compressible multiphase flows: Explosive dispersal of particle. US Air Force Research Laboratory, Munitions Directorate, Eglin Air Force Base, Ft. Walton Beach, FL. (2010)
P27) Compressible multiphase flows: Explosive dispersal of particle. Department of mechanical Engineering, Florida State University, Tallahassee, FL, (2010).

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