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NEW METHODS FOR PREDICTING SHOCK AND IMPACT INDUCED DISPERSAL OF CONTAINED LIQUIDS

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ABSTRACT

The ability to predict the dispersal of liquids from impact or shock-induced environments is not mature. The environment might include complex physics such as multi-phase transport, solid deformation, structural dynamics, atomization, and Richtmyer-Meshkov instabilities. Simulation tools generally have heretofore been unable to capture the physics of many events of this nature due to the complexity of real physical systems and of the physics. A new method is described that couples the output from a structural dynamics simulation to initialize a computational fluid dynamics simulation. The codes used for this method were both developed under the SIERRA architecture, and are tools that were developed at Sandia National Labs (SNL) for predicting structural mechanics and fluid mechanics scenarios. The coupling occurs in one direction, in that the structural code is not informed by prediction results from the fluid code. A dimensionless parameter is used to define the chronology of the mass transfer from the structural to fluids transfer. Five scenarios have been heretofore simulated. Two of these are shock-induced dispersals, three are impact induced dispersals. Two scenarios have been simulated that have corresponding experimental data that make them amenable to validation. The comparisons that have thus far been performed suggest the capability yields results of reasonable accuracy. Results from each of the five scenarios have contributed to the understanding of the optimal use of this method for making predictions of liquid dispersals in complex environments. The need for additional validation data to build confidence in these modeling methods is apparent, and the range and type of data that would be helpful are apparent in the output that is produced from the various simulations.

INTRODUCTION

Predicting the liquid dispersal from an impact or detonation of a contained liquid is important to being able to assess many safety and consequence scenarios. Examples of scenarios of interest include transportation incidents where high-speed vehicles full of fuel impact a rigid structure. Several examples of such types of events occurred on September 11, 2001 when terrorists hijacked commercial aircraft and flew them into commercial and government buildings in New York and Washington DC, distributing fuel throughout the building and causing collapse of the structures based on the structural and thermal damage [1]. Analysis efforts related to this scenario motivated the early work in this regard. Another example of such an event occurred at the Savannah River site, where a spent nuclear fuel processing tank exploded [2]. These two scenarios are examples of the range of problems of this nature that occur. Such problems can vary in many ways including intentional to unintentional scenarios, low-speed to high-speed velocities (i.e., varying Mach regimes), ranges of fluid types (fuels, water, Newtonian, non-Newtonian), and differing geometric complexity. Motivating reasons for studying this class of problems can include design qualification, forensics analysis, hazard assessment, and test design.

The physics of liquid dispersal events of contained liquids vary significantly in relevant length- and time-scales. Early structural mechanics predictions require very small time steps, on the order of tens of nanoseconds. Ultimate event prediction time scales can vary from minutes to hours (the duration of the World Trade Center fires was months). Significant length scales can also vary greatly.

Structural mechanics predictions of these events are possible with existing computational methods, and many commercial and research software packages are capable of making qualified predictions of impact events. Such tools generally are not capable of reaching the time-scales required to predict the final liquid dispersion, nor have the resolution required to predict the break-up and spread of the liquid. Furthermore, physics such as turbulence, evaporation, atomization, and chemical reactions are generally not current components of the structural mechanics codes that predict the initial impact and dispersal. These physics are not as important at the short time-scales, while they become increasingly important at longer times.

Silde et al (2011) [3] measured the liquid dispersal from experimental impacts of liquid tanks into hard targets. Liquid drops were measured and these data were used in the fluid code for the drop transport calculations. Around the same time, work at SNL by the author and colleagues was starting that took advantage of a structural mechanics prediction to initialize the dispersal of the fluid from a similar event in a dilute spray low-Mach number reacting flow computational fluid dynamics (CFD) code [4-8]. To date, no other known efforts of this type have been found in the literature. Key to the Sandia capability is the liquid break-up model, the Taylor Analogy Break-up (TAB) model of O'rourke and Amsden (1987) [9], which is used to model the break-up of liquid drops. Also, the temporal coupling is achieved through a dimensionless criterion, the dimensionless separation distance between the drops. A dimensionless separation distance can be calculated for each drop. When the minimum separation distance exceeds a critical value, the drop is marked for insertion in the fluid mechanics code. The dimensionless separation distance is calculated as follows:

$$B_i = \min_{j=1\ to\ N} \left\{ \frac{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}}{d_i/_2 + d_j/_2} \right\}; i \neq j$$

In this equation, *x*, *y*, and *z* are the drop Cartesian coordinates, and *N* is the total number of drops (smoothed particle hydrodynamics [SPH] particles in the case of this methodology). B_i is the minimum dimensionless separation distance for particle *i*. B_i is compared to *Bcrit*, a user specified criterion normally between 1.0 and 1.7. This type of coupling will be referred to as SM/FM coupling, short-hand for solid mechanics/fluid mechanics coupling.

Table 1. SM/TM coupling scenarios

Scenario	Realizations	SPH#	Fluid Mesh	References
Water Slug Impact	7	417K	355K	Brown et al., 2012 [6]
Aluminum Tank Impact	12	1-50K	250-2,000K	Brown, 2010 [8]
Sled Track Brake	4	320-2,500K	700-2,000K	Brown and Metzinger, 2011 [7]
Detonation Outside Tank	10	50-400K	370-2,940K	Brown, 2013 [5]
Detonation Inside Tank	2	45K	530K	Brown et al., 2014 [4]

Results have been reported from five scenarios employing this SM/FM coupling methodology (summarized in Table 1). Three scenarios are impact scenarios, characterized by the sub-Mach number impact of a liquid tank or the sub-Mach number impact of a structural element on a contained liquid (the Sled Track Brake scenario). Two scenarios are impulse (detonation) scenarios. These are scenarios that are initiated by a shock wave (Mach number of 1.0). The shock wave interacts with the structural container and liquid, resulting in a dispersal of the contents. Relevant length and time-scales vary for each of the scenarios. Table 1 lists the computations that have been performed and documented. Each of these involved multiple realizations, with parameters varied in a way that the results can be meaningfully interpreted to quantify the importance of the parameters that were varied from test to test.

This paper reviews the results of the past calculations employing the SM/FM coupling, and focuses on the findings of the parametric variations. The scenario results suggest the importance of various parameters on the quantitative results. The importance of parameters that were varied in multiple scenarios is better understood based on the breadth of the analysis results. Then, single realizations from each scenario are analyzed using new techniques to evaluate the potential for modifications to the existing coupling methodology. Finally, some recommendations are made on the basis of the presented evaluations for methods to improve the quality of the predictions using this technique.

SCENARIOS

This section describes the scenarios that have been evaluated with SM/FM coupling listed in Table 1. Descriptions will focus on the geometry, conditions, and parameters evaluated. Two methods were used for the solid material. Both cases that used SPH for the tank involved an aluminum structure. Subsequent analyses employed finite element models for the tanks and other surrounding objects. Table 2 provides additional detail on the various scenarios. Subsequent sub-sections provide further information.

Table 2. Details on the SM/FM coupling scenarios

Scenario	Solid model	Parameters Varied	Fluid	Compared to data?	SM time
Water Slug Impact	SPH	Geometry Wind *Bcrit*	Water	Particle Sizes Liquid Deposition Liquid Spread	120 ms
Aluminum Tank Impact	SPH	SM Mesh FM Mesh *Bcrit* SM run time	Heptane	No	12-18 ms
Sled Track Brake	Finite Element	Impact Velocity Liquid Depth SM Mesh	Water	In Progress- Liquid Deposition	140 ms
Detonation Outside Tank	Finite Element	Explosive Intensity SM Mesh FM Mesh *Bcrit*	Water	No	20-300 ms
Detonation Inside Tank	Finite Element	Quantity of Explosive	Nuclear Fuel Reprocessing Fluid	No	80 ms

SIMULATION SOFTWARE

In all cases described herein, the solid mechanics code is what was formerly known as Presto, and is a module in the SIERRA/Solid Mechanics (SM) suite of codes. The fluid mechanics code is what was formerly known as Fuego, and is a module in the SIERRA/Fluid Mechanics (FM) suite of codes. Both codes are designed under the open source SIERRA framework [10, 11], and are more fully documented in internal limited distribution manuals maintained at Sandia National Labs.

WATER SLUG SCENARIO

This scenario represents the highest quality data comparison performed for this capability to date. A cylindrical aluminum tank (illustrated in Figure 1A) was filled with water and mounted on a rocket sled track. The tank was accelerated to approximately 100 m/s, and impacted into a concrete target that caused rupture of the tank and dispersal of the liquid. The best data for comparison extracted during the test included the liquid spread (cloud of water), and the final deposition pattern of the liquid. Video provided liquid spread data, and deposition data came from a series of collection pans that were positioned around the impact point. The particle size data were limited, but still helpful. The sensitive equipment was not positioned such that significant drops were observed. What small drops were observed still provided useful benchmark data.

A.

B.

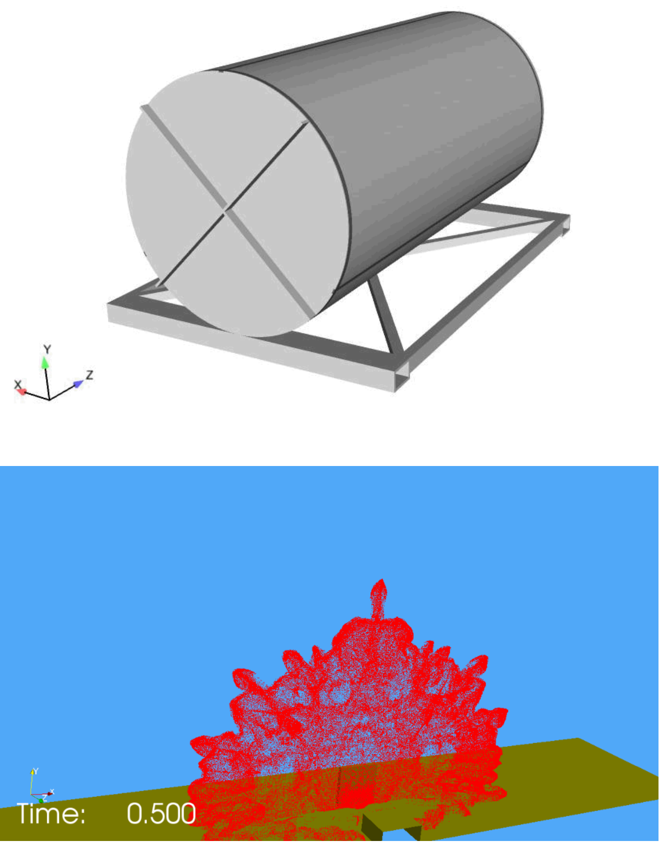

Figure 1. An illustration of the Water Slug Impact tank (A) and predicted dispersion (B) [6].

Of the three parameters varied in the seven cases simulated to explore sensitivity, the wind speed was the least significant to the results. This may be because the wind speed was only varied lightly between 0-2 m/s. The most significant parameter was the geometry. Whether or not the leading edge strips and under-carriage were modeled had the most significant effect on the quantitative results. The critical dimensionless transfer number was not particularly significant for most data comparison points, but use of an increased number of transfer times had a roughly 20% effect on the Sauter mean diameter. This suggests that the effect on bulk transport is not high, but can be significant if the particle sizing is significant to the accuracy of the calculation.

ALUMINUM TANK IMPACT SCENARIO

This scenario is a notional impact of an aluminum tank filled with heptane fuel. The tank is 28 cm (11 inches) square, and 2.54 cm (one inch) thick. The tank is moving at 183 m/s, and impacts an un-yielding target, as illustrated in Figure 2. It is notional, and was primarily used as a small simple demonstration of the initial capability that did not require extraordinary work to prepare the simulation or to process the data. This is the only chemically reacting fluid scenario simulated, even though one of the main objectives of this capability is to be able to simulate fuel tank impacts and the subsequent fireball. The other two impact cases were selected because they offered an opportunity to make quantitative comparisons to data. Fuel impact scenarios are complicated by the reactions. Instrumentation needs to survive not just the impact and dispersal environment, but also the fireball environment.   Existing data are limited to impact and dispersal, and are sparse.

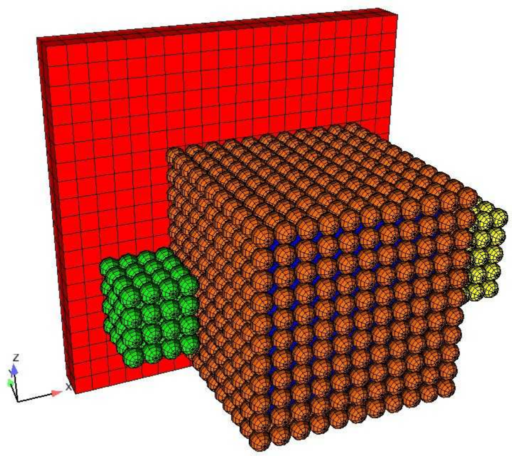

Figure 2. An illustration of the aluminum tank (orange), liquid (blue, inside the orange cube) and aluminum cubes (green and yellow) impacting an unyielding target (red).

Results from this analysis were comparative since the scenario does not have corresponding data. Since physical conditions were never varied, the results of each calculation were nominally identical. Some variation existed, although it is not obvious that the quantitative variations were significant. Visualization of results (graphical rendering of results) were more definitive, suggesting that the finer fluid mesh results conformed more to an expected resolution. The temporal coupling was evaluated, and different lengths of SM calculation time were tested. Longer SM sampling for the coupled calculation was deemed better. Despite a moderate range of spread in various quantitative results, it could not be concluded that any of the evaluated parameters had a dominant effect on the prediction.

SLED TRACK BRAKE SCENARIO

This scenario involved the brake mechanism for a rocket sled. Figure 3 illustrates the solid mechanics scenario. Rails sit atop either side of a concrete channel (gray). These are used to mount sleds that are conducted to a target area through rocket propulsion. The channel between the rails is deep, and may be filled with water to custom levels by installing dams at various locations. A pusher sled is normally used to propel the test objects. After the propulsion, it is often desirable to have the pusher sled stop before the test object. This is achieved by stopping the sled with a brake mechanism (red). In this case, the brake mechanism is a metal scoop that will rupture the dam and begin to drag through a water trench. The kinetic energy from the pusher sled is dissipated as the water is accelerated. It was observed that each test involving this type of brake mechanism produces potential validation data for this capability. The report documenting this effort [7] involved pre-test predictions that were meant to help locate instrumentation for collecting data on the liquid dispersal from one of these events. This is the only scenario in which the original SPH mass was not corrected to guarantee that the particles conserved mass from the original hex mesh through the SPH conversion and into the fluid mechanics code.

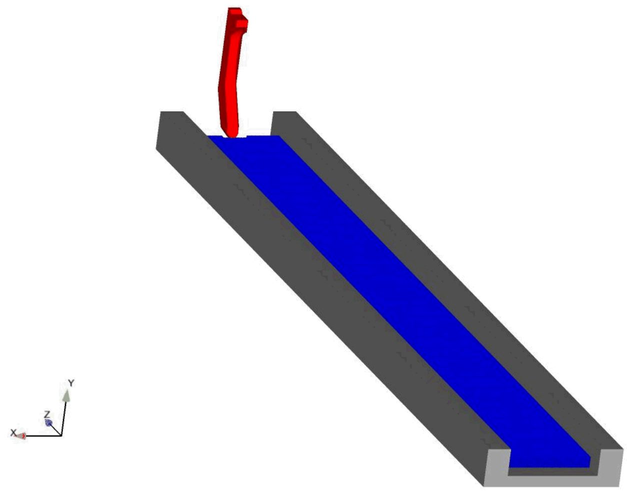

Figure 3. The Sled Track Brake scenario geometry, including the brake (red), track (gray), and water (blue).

This scenario was primarily intended to provide guidance for instrumenting a test with a rocket sled break mechanism. The scenarios calculated included variation of physical parameters, including initial velocity and water draw (depth). Two cases of higher resolution were evaluated, including one with increased SM mesh size, and another with increased FM mesh size. All scenarios were in reasonable agreement, and suggested peak mass deposition density in the range of 6-10 kg/m^3 about 1-2 meters away from the rails, and deposition around 1 kg/m^3 in the range of 5-10 meters away from the rails. A test was conducted where rain gauges and collection pans with absorptive material were placed around the point of impact to collect the water. Model comparisons are in progress. Post-test comparisons will include more geometry of the sled, and quantitative comparisons to the collected data.

DETONATION OUTSIDE TANK SCENARIO

This scenario involved two geometrically different tanks of liquid. An external detonation was modeled as an expanding shock wave, and the spherical wave was modeled on external surfaces of the structure as an impulse source term. This is one of the more simple methods for predicting structural response to a shock within the SM code. A cylindrical and a hexagonal tank were employed, with the hexagonal tank being open at the top. This was a notional scenario, and does not directly correspond to existing data. The aspect ratio (height to width) of the geometry was 2. The open top hex mesh is shown in Figure 4. The aluminum tanks (gray) were modeled as welded structures, with the weld points being pre-disposed to fail under stress compared to the non-welded body parts. Liquid in the tank was modeled as water (blue). The tank was located on a rigid pedestal (red), with the detonation occurring at about a characteristic length horizontally from the base of the tank (not pictured).

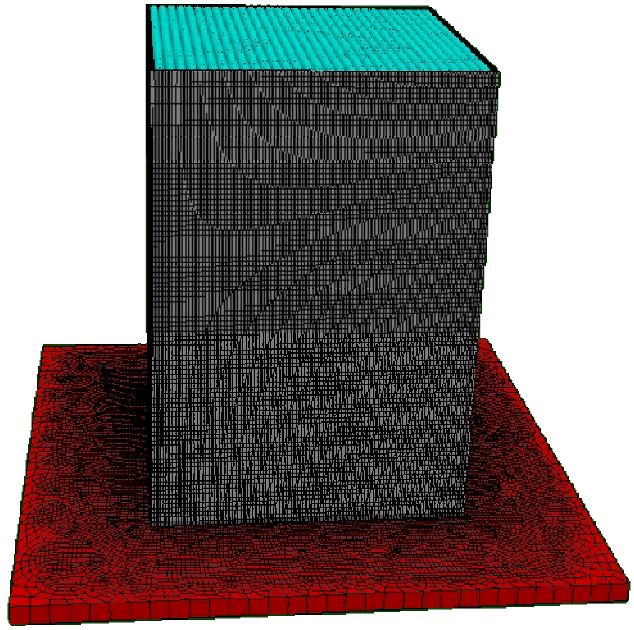

Figure 4. The coarse hex Presto mesh

This study was the first to evaluate a detonation induced spread with this couple capability. The major physical parameters varied included the shape of the tank and the intensity of the detonation. Numeric parameters varied included the critical dimensionless transfer number (*Bcrit*), the SM resolution, and the FM resolution. The focus of the analysis was on the adequacy of the models in terms of two FM approximations: the low-Mach number approximation and the dilute spray approximation. All scenarios were deemed adequate, even though standard limits of the approximations were exceeded for short times in some scenarios.

DETONATION INSIDE TANK SCENARIO

This scenario was motivated by an interest in demonstrating the SM/FM coupling capability for a tank explosion scenario, with geometry illustrated in Figure 5. A project to evaluate the nuclear safety of explosively dispersed actinides in the process of being refined for reactor fuel was conducted. As the liquid source material was a complex mixture, this scenario is the only case representing a highly complex fluid. Fuels and water are adequately represented as Newtonian single-component fluids. This fluid was modeled as closely as possible given the existing framework in the simulation codes. The scenario this effort is based upon was an explosion accident that occurred at Savannah River in the 1970s [2]. An explosion occurred in a storage tank, which resulted in the dispersal of highly hazardous materials. The most important parameter to the safety of personnel in the area is the exposure to the contaminants. Most post-event hazards can be mitigated by engineering controls. However, airborne respirable particulates represent a problem that often lacks appropriate controls because they can linger in the air and transport to different locations. This new code coupling capability was viewed as a capability to make unique predictions to assess the aerosol source term from this type of accident. While this scenario is a real event, there was no practical data for comparison. Even the intensity of the explosion source was not known.

Besides being distinguished by involving a complex liquid, this scenario necessitated new structural mechanics methods. Since an internal detonation involves significant shock reflections, it was deemed necessary to model the air medium in the tank as well as the water and explosive. The air was also modeled with SPH particles. This allowed for improved modeling of the energy transport in the tank during detonation. The SPH particles that modeled the air were not used in the coupling, although this is an interesting topic for future computational efforts.

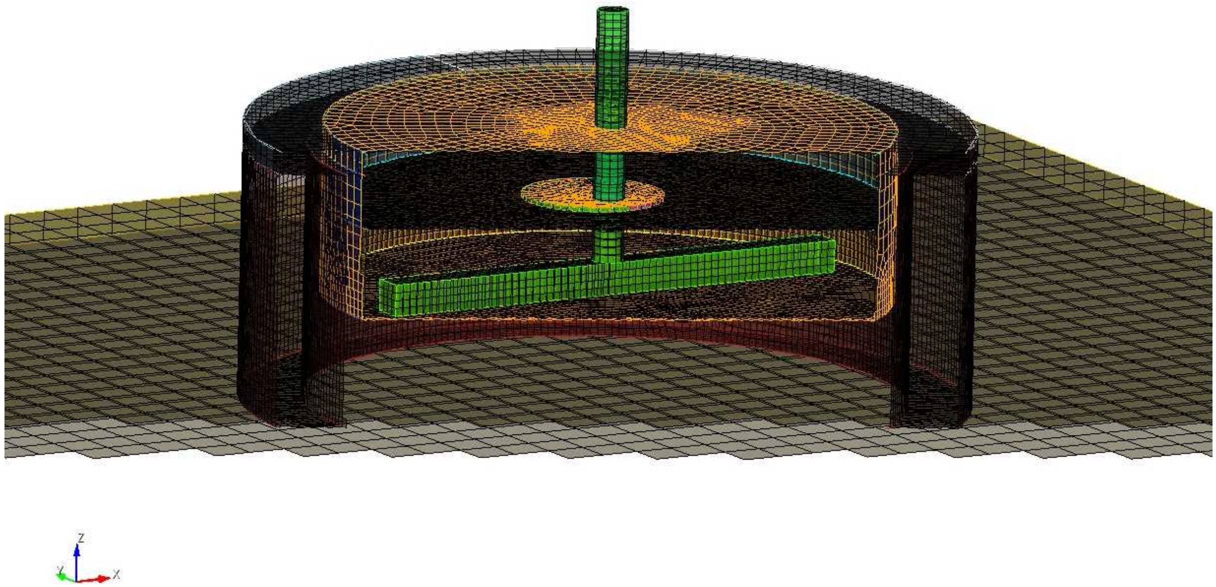

Figure 5. A semi-transparent cut-away view of the simulated geometry for the low energy scenario.

The results documented for this scenario did not involve significant parameter variations other than the detonation intensity (explosive energy), and was mostly a demonstration calculation. The scenario involved slightly more complex geometry than any previous case, as it involved the modeling of air in the SM calculation, and necessitated a dimensional modification for particle transport in the low energy detonation scenario. The dimensional modification was necessary to prevent transport of particles out of the tank that did not emerge through the linear rupture in the top of the tank. This scenario is also the first one in which a detailed analysis of particle data was made by producing a histogram of aerosol particle size distribution.

The multi-component nature of the liquid was not modeled in this particular test. The Newtonian fluid model capability was used to predict the dynamics of the detonation with surrogate properties that were estimated to be close to that of the actual material. The most serious concern in this regard is that the evaporation model was over-predicting the loss of aerosol particles.

FURTHER EVALUATIONS

In each of the above scenarios, there was a core of material that did not meet the insertion criterion (i.e., *Bmin* > *Bcrit*) by the last time step. At the last time step from the structural mechanics (SM) code, a decision was made on what to do with the remaining mass. In all cases except the Denitrator simulation (Detonation Inside a Tank), the remaining mass was injected at the last time step regardless of the insertion criterion. This conserved mass, but resulted in a large single injection at the final insertion time. This final injection has some undesirable features. First, the insertion criterion helps assure the dilute spray approximation is not severely exceeded. The final injection is not subject to this control. This may result in instability, however this has not been generally observed except in limited cases (the Detonation Inside a Tank scenario). This feature was evaluated for the Detonation Outside a Tank scenario, and shown to be an issue for some of the scenarios. Second, the insertion criterion has the effect of tapering the mass insertion in a way that is thought to be physical, in the sense that the multiphase interactions are increasingly relevant for the liquid mass transport with time. The transfer criterion functions as a model for this behavior. There is a dense spray region of the dispersal in all the cases that is not appropriately modeled from a multiphase physics perspective. Because this dense spray region has comparatively low kinetic energy, the dilute spray approximation may not be the best way to model the behavior. Third, a larger mass injection represents a discontinuous step in the introduction of kinetic energy. It is posited that the mass and energy coupling with this methodology is better modeled if the coupling does not induce large instantaneous source terms in the fluid solver.

A significant effort has not previously been made to investigate the final injection. Selecting a single case from each scenario described above, the structural mechanics simulation results are analyzed herein with a focus on the final injection. Table 3 describes the specific cases from each scenario that are evaluated herein.

Table 3. Cases evaluated in higher detail in this study

Scenario	Case	B_{crit}	SPH#	Reference
Water Slug Impact	Case 7	1.5	417,792	Brown et al., 2012 [6]
Aluminum Tank Impact	cfs1.3	1.3	19,653	Brown, 2010 [8]
Sled Track Brake	S1/F1	1.3	322,016	Brown and Metzinger, 2011 [7]
Detonation Outside Tank	Hex3 (Case 5)	1.3	49,152	Brown, 2013 [5]
Detonation Inside Tank	HighE	1.5	44,813	Brown et al., 2014 [4]

MASS AND KINETIC ENERGY ANALYSIS OF COUPLING INSERTION

The above issues are quantified for the sub-set of cases from the five scenarios. The purpose of this analysis is to begin to quantify the behavior of the coupling dynamics in such a way that they can be modified to better model the behavior of the dense spray portion of the coupled problem. Figure 6 shows the cumulative fraction of kinetic energy and mass for five scenarios versus injection (time). Kinetic energy leads mass, as the faster moving mass is generally selected for earlier insertion in the fluid code. A large fraction of the mass is remaining at the final time step in all cases. Significant kinetic energy is also found in the last insertion, albeit a smaller fraction of the total.

These plots suggest that with the possible exception of the Detonation Inside Tank scenario that the final injection represents both a significant mass and kinetic energy step function imposed on the fluid mechanics calculation. Earlier it was described in several scenarios how the transfer criterion (*Bcrit*) did not show up as one of the parameters of high significance in the evaluation of various cases. It was shown as significant, but not to the level of other parameters. This suggests that modifications might be made to the transfer criterion to advance the rate of mass transfer. This can already be done by selecting a lower critical transfer criterion (i.e., decreasing *Bcrit*). There are additional considerations, which are detailed in the next section.

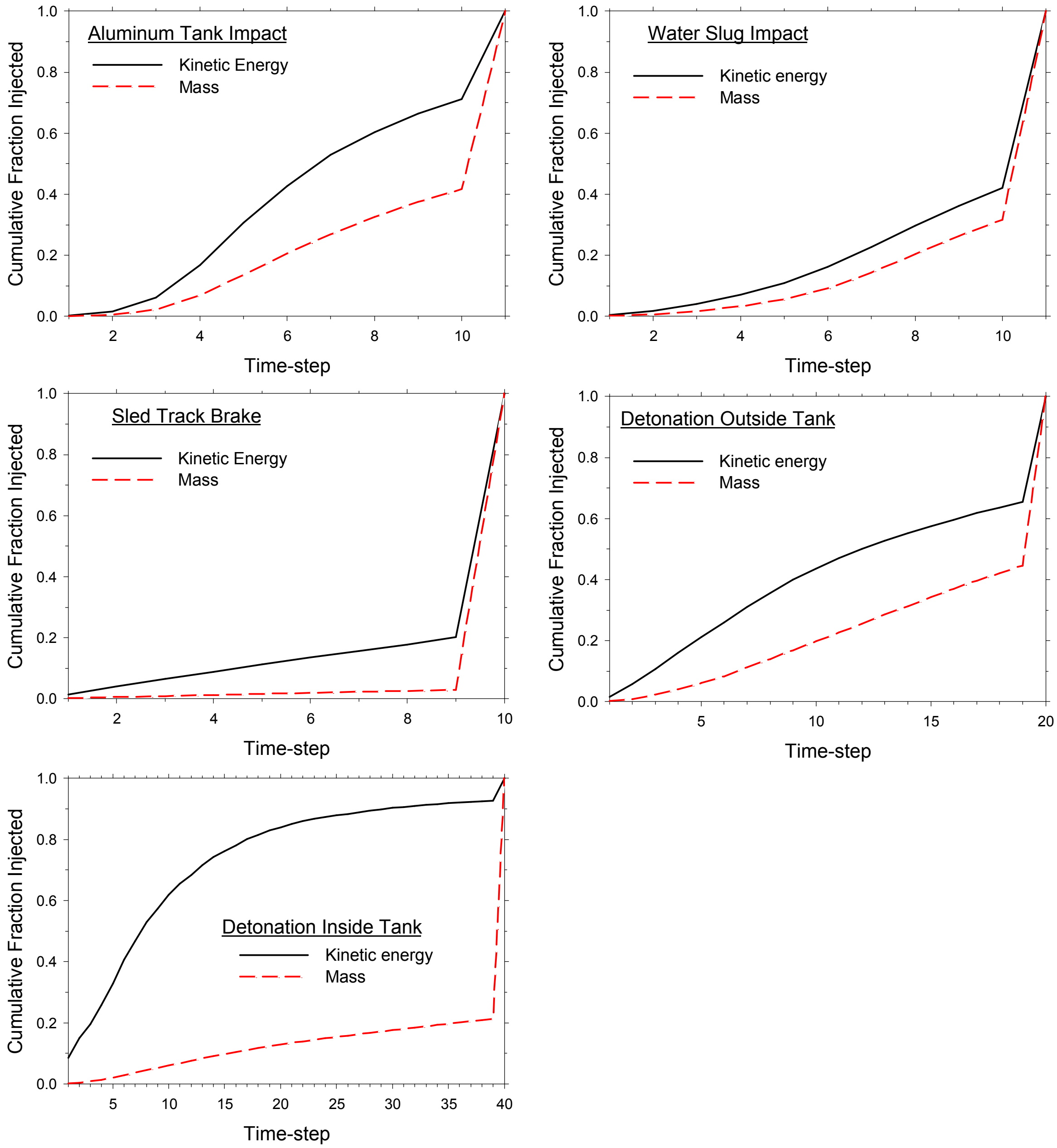

Figure 6. Cumulative kinetic energy and mass fraction injected as a function of time step for five cases, one for each scenario.

FINAL INSERTION ANALYSIS

To help better understand the nature of the last input file, some new analysis methods have been employed. It was observed that there are occasionally clumps of particles that would never meet the transfer criterion (B_i > *Bcrit*) because the particles are either not moving, or moving together. Even with extended times, many of these particles will not tend to separate and be selected for insertion. Figure 7 shows a visualization of two such findings. The first (A) is from the Detonation Inside a Tank scenario. Liquid is plotted in color, and the outline of the mesh showing the location of the tank is shown in light gray. Notice that well outside the major

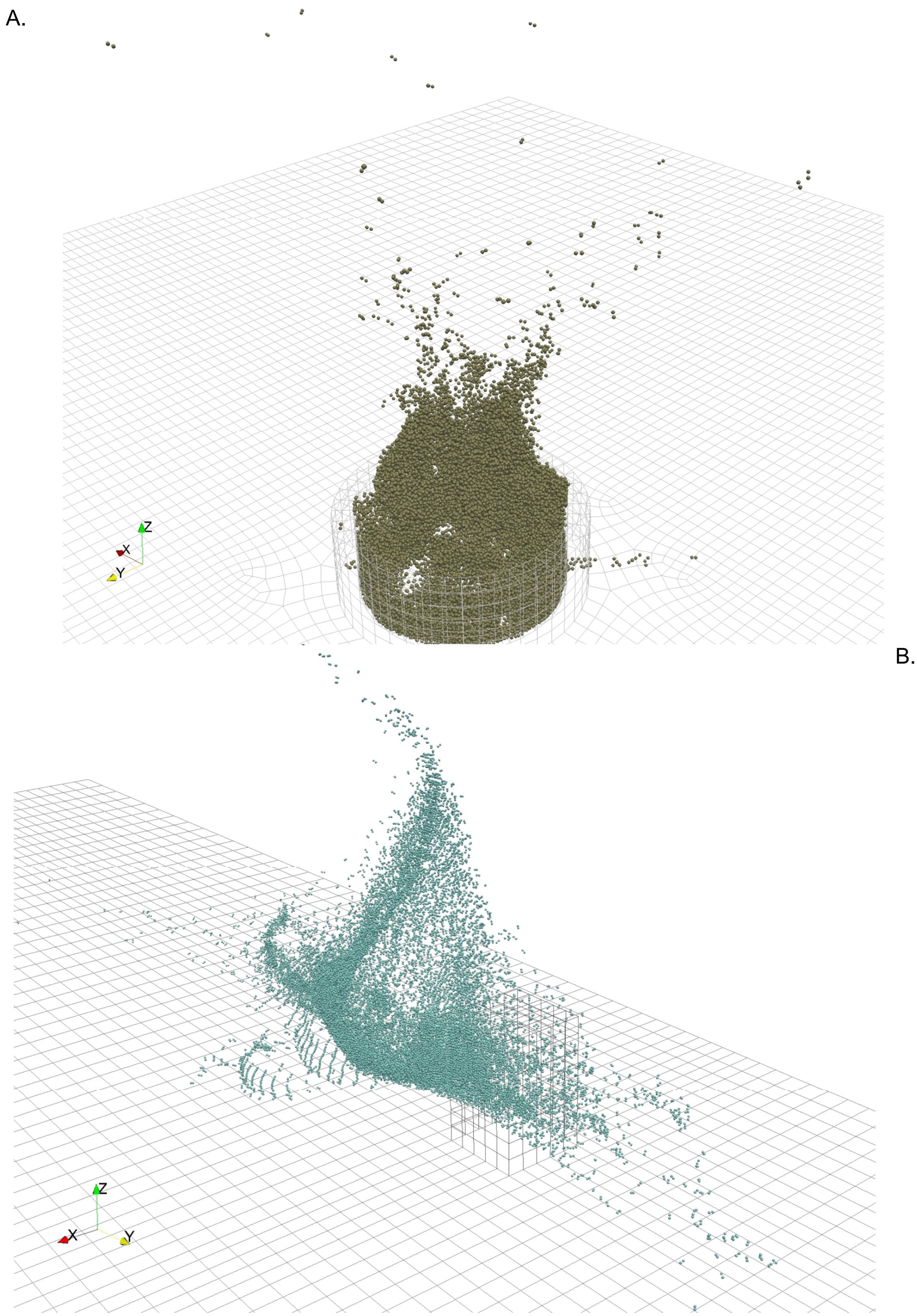

Figure 7. Two images illustrating the last injection for A. The Detonation Inside a Tank scenario and B. The Detonation Outside a Tank Scenario.

grouping of particles there are binary particle pairs. Many particles are high above the cylindrical tank, suggesting that particles have high velocity, having traveled the furthest from the tank. The *Bcrit* condition never selects these for insertion. These may be understood to be physically representative of larger particles than were modeled with the SPH resolution. Thus, assuming that these particle pairs are of near uniform velocity, it might be appropriate to combine the particles and rely on the break-up model in the fluid mechanics solver to manage the subsequent transport. These particles were not modeled (by omission) from the original calculations. It would be sensible to retain more of the mass of this final injection step, while removing the liquid that clearly cannot escape the tank and is in bulk configuration. Further model development will be required to improve on this condition. Figure 7 B shows a similar plot from the Detonation Outside a Tank scenario. The tank was initially on a pedestal, which is illustrated with a darker gray mesh in the figure. Like the Detonation Inside a Tank scenario, this one exhibits binary pairs at the fringes of the distribution. Another feature this scenario illustrates well is that of linear chains of particles. Further along the positive-x direction, there are strings of particles. These are not selected for injection earlier on because they are clumped in a line. The curved shape of the line suggests that they may separate at longer times, as they were likely completely linear at the initial time.

Were it possible to capture and model the binary pairs appropriately, they could be inserted earlier, shifting the mass and kinetic energy distributions presented previouly upward. The current insertion criterion based on a dimensionless insertion parameter, B_i, cannot currently capture this. An appropriate quantitative model for this would need to be formulated. The same may be true for the linear chains. It also would seem to be sensible to develop a way to assess the final injection and couple to classical bulk multi-phase modeling methods like level-set or volume of fluid when appropriate. This would allow for an improved representation of a wider range of scenarios.

All five scenarios have also been re-analyzed by examining every particle, and counting the number of neighboring particles within the *Bcrit* threshold. Some particles have zero near neighbors, which would normally mark them for insertion. Any above this would not normally be inserted at the time-step of analysis. A particle with one near neighbor might be a binary pair, or the end of a linear chain. A system with two near-neighbor particles might be a component of a system that includes linearly arranged particles. A system with 4-8 particles in the near neighborhood might be arranged in a planar configuration. More near-neighbor particles assures a degree of packing in the third dimension. Any count beyond 27 suggests particles are heavily packed around the point of comparison. With these guidelines in mind, the final insertion file for the above listed cases has been analyzed, with results found in Figure 8. It was not unexpected to find the Detonation Inside Tank scenario had many densly packed particles. Nor was it surprising to find the Water Slug Impact case with a significant number of particles at higher proximity. The Sled Track Brake scenario trended at first with the Detonation Inside Tank scenario, but broke off and exhibited few particles with more than 10 others in proximity. This suggests that much of the mass may be planar, or that the system may be more sparse. This particular scenario was unique because it did not involve the volume correction mentioned earlier, which may also be a contributing factor. The Aluminum Tank Impact and Detonation Outside the Tank scenarios exhibited the most distribution from the initial impact, evidenced by the generally low number of particles in proximity. Even with a model that transitions all such particles ($n<=2$), there will still be a significant fraction of particles for many of the cases that cannot meet an adequate transfer criterion because they are in a bulk configuration (fraction represented by the intersection of the gray dashed reference line with the scenario curve). For the Sled Track Brake and Detonation Inside a Tank scenarios, this fraction is approximately 85-90%. It is much less for the other scenarios (25-50%).

Using the number of particles in proximity as a quantitative measure, it is possible to identify candidate binary pairs and linear chains of particles. Subsequent work will identify additional criteria to improve the temporal coupling between the SM/FM codes using quantitative methods discussed herein. The objective will be to identify more particles than can appropriately be transferred sooner, thus reducing the jump in kinetic energy and mass insertion at the final SM time-step.

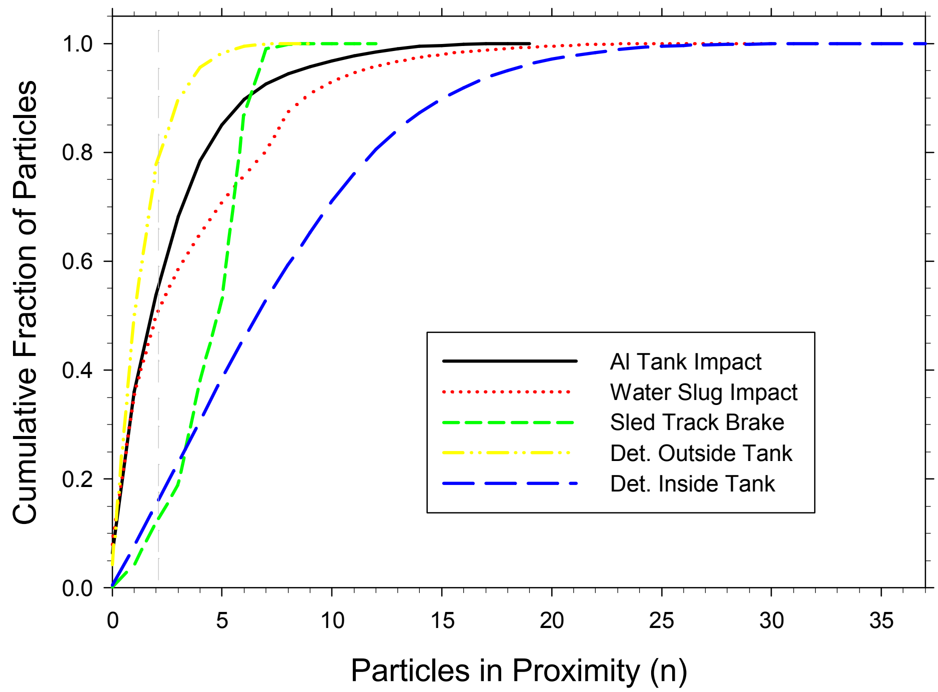

Figure 8. A cumulative distribution plot of the number of particles in proximity (based on the B number) to a source particle for the last injection for the five selected cases.

SUMMARY AND CONCLUSIONS

Analysis is presented on a code coupling methodology to solve the transport of contained liquids dispersed by an impact or impulse. The five scenarios that have thus far been simulated with the SM/FM coupling are reviewed, and this report summarizes the results of the SM/FM coupling. The scenarios represent a range of conditions, suggesting that the SM/FM coupling capability may be broadly applicable to many problems of interest. The time coupling is determined by a critical dimensionless parameter. This method of coupling results in a final mass injection with some undesirable features at the last SM timestep. The kinetic energy and mass coupling is evaluated for five selected cases, one from each scenario. The final insertion is shown to include an undesirable step discontinuity in the kinetic energy and mass for most cases. Some details of this final insertion are further analyzed. A modification to the transfer algorithms may be warranted to capture binary and linear groups of particles that cannot be captured with the current transfer criterion. Methods for identifying candidate binary particles are presented.

FUTURE WORK

A method for consolidating binary pairs has been formulated, and will be the topic of a paper to a different conference within the next year. Other analysis methods have been employed to further evaluate the last insertion step, which will also be described in subsequent reports. A method for modeling the dense region of the spray is also being considered to better model the dynamics of the core regions of spray from these types of problems. The most important follow-on effort should involve validation. This capability has not yet been compared with a wide range of data, or high-quality detailed data. This is an important next step because it will help quantify the accuracy of the method, the reduction of uncertainty being ultimately the primary goal for scientific predictive tools. Lack of existing validation comparisons relates directly to the lack of adequate data to quantify uncertainties in the model predictions. This type of data is scarce because it is difficult to instrument and capture the needed measurements to appropriately validate this type of scenario. Multi-component models will be needed to correctly model complex fluids in future efforts.

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