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Impact, Fire, and Fluid Spread Code Coupling for Complex Transportation Accident Environment Simulation

Transportation accidents frequently involve liquids dispersing in the atmosphere. An example is that of aircraft impacts, which often result in spreading fuel and a subsequent fire. Predicting the resulting environment is of interest for design, safety, and forensic applications. This environment is challenging for many reasons, one among them being the disparate time and length scales that are necessary to resolve for an accurate physical representation of the problem. A recent computational method appropriate for this class of problems has been described for modeling the impact and subsequent liquid spread. Because the environment is difficult to instrument and costly to test, the existing validation data are of limited scope and quality. A comparatively well instrumented test involving a rocket propelled cylindrical tank of water was performed, the results of which are helpful to understand the adequacy of the modeling methods. Existing data include estimates of drop sizes at several locations, final liquid surface deposition mass integrated over surface area regions, and video evidence of liquid cloud spread distances. Comparisons are drawn between the experimental observations and the predicted results of the modeling methods to provide evidence regarding the accuracy of the methods, and to provide guidance on the application and use of these methods. [DOI: 10.1115/1.4005735]

Introduction

Transportation safety environments are important to fundamental work done at Sandia National Labs. An impact followed by fuel dispersal and fire is an example of one of the environments of interest. These environments can be tested, but are costly and difficult to fully instrument. Being able to simulate such an environment is useful for understanding details that cannot be measured and for probing many environments for a fraction of the cost of performing the tests. Many sources exist for modeling capabilities to predict impact and structural dynamics of events involving high deformation. Also, there are many models for fire and fluid flow. However, there is little information found in the open literature describing the use of a combination of these capabilities. Indeed, traditionally the most advanced methods for addressing these types of problems have been fairly decoupled, with the structural code being used primarily to describe the state of the structure following the impact if used at all. One example of this is found in the report on the response of the World Trade Center towers to aircraft impacts in the year 2001 [1]. Structural results are presented, but fluid dynamics are not coupled directly. Another recent example involves fluid simulations initiated on the basis of data from experimental testing of a small-scale impact [2].

Accurate validation quality data on such events are scarce. Many impact tests are found described in the literature, but only a small fraction of these tests involve liquids. Normally impact tests are focused on the impacts themselves, and details relevant to a fire prediction like liquid distributions and particle sizes are not found in the post-test analysis. Several years ago, a series of tests was performed at Sandia National Labs where some effort was

taken in determining the fate of the liquid following a high speed impact. Among the reports of this event is an article [3] that details the experimental methods used to evaluate the fluid dynamics. One of the tests in particular had good liquid spread data. With the development and description of a new capability to predict this combined environment [4], this dataset is valuable for evaluating the accuracy of the modeling methods.

Sandia National Labs through the Advanced Simulation and Computing program develops engineering simulation tools appropriate for modeling a wide range of physical environments. One of these tools is Presto, a three-dimensional explicit, transient dynamics code utilizing the SIERRA framework [5]. Presto is used to predict material response to structural impacts with significant deformation. Also using the SIERRA framework, Fuego is a low Mach number fluid mechanics code with chemical reactions, heat transport, and mass transport. The fact that both of these codes are implemented in the same framework facilitates combined environment predictions using both of the codes in their appropriate regimes of accuracy. Liquid dynamics in the structural code analysis are often modeled with a smoothed particle hydrodynamics (SPH) method that discretizes the liquid to Lagrangian spheres. Morphologically, the spherical elements from the structural mechanics code are acceptable to the Lagrangian/Eulerian fire code. A method was developed to execute a data transfer of the mass and momentum from the structural code, which provided the basis for the subsequent analysis. Development has since focused on defining appropriate transfer methodologies, understanding the physics required to improve the accuracy of the model assumptions, and establishing the accuracy of the mass and momentum transfer that is executed between the codes.

This work presents an interesting engineering scaling challenge that can be illustrated by examining the time scales involved in this type of event. Figure 1 shows general time scales that are needed to address the class of problems of interest. There are at least 10 orders of magnitude between the smallest time step and the largest time scale of interest. Presently, problems of this nature that involve 5–6 orders of magnitude between the fundamental steps and the ultimate goal are challenging. It is clear that for the

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Fig. 1 An illustration of typical computational time scales

immediate future that computing these types of environments will require assumptions that allow such predictions to be tractable, and that identifying and retaining the most significant physics is important to assure model accuracy.

Coupling multiphysics codes is nontrivial, and typically requires model assumptions as the predicted environment transfers between the two codes. This often involves known physical inadequacies with errors and uncertainties that are difficult to assess. Possessing a reasonable dataset for comparison, this work seeks to assess the accuracy of the methods and to build understanding of the importance of several model assumptions by comparing the simulation predictions to the experimental results. This paper presents some of the methods that are in development and presently being used to perform these calculations, and provides evidence of the accuracy that can be obtained from this type of methodology.

Methods

The complexities involved in this experiment are significant, and are not all represented in the modeling with complete accuracy. A very detailed model including all complexities would have been prohibitively difficult. For a first comparison, various simplifications were made to get a sense of the capability. Model predictions were compared with data. This initial test suggested inadequacies, and a test matrix was formulated to help understand how significant various assumptions are to the outcome of the simulated tests. Table 1 gives a list of the simulation cases that will be described in this work. This section will explain the motivation behind the categories and simulations described in Table 1, and present details on the simulations performed.

Performing a series of calculations involving various approximations gives an indication of the importance of the phenomena to the outcome of the problem. This process helps us better understand the simulation fidelity requirements, and also helps attribution of differences between models and predictions to the appropriate phenomenon. The context of this paper surrounds the study, and the results and discussion will be presented in sections corresponding to the different types of experimental data existing for comparison.

Geometry Fidelity. The original Presto geometry used for this simulation was taken from prior work where this scenario was simulated for structural analysis. Since the intent of the former work was to determine damage state, many of the minor details thought to be less relevant regarding the projectile were ignored. A cylinder with a 2:1 aspect ratio and appropriately thick alumi-

num walls was all that was employed in the model. Separate material properties were ascribed to welded joints at corresponding locations on the cylinder in the test. This is what is being called the “low” fidelity geometry in Table 1. In the actual tests, a cross shaped piece of aluminum was placed on the impact surface to help assure that the break-up on impact occurs consistently. Also, part of the support structure was added below the cylinder.

The original geometry was modified to assess the importance of these omissions. A rendering of the “high” geometry fidelity projectile is illustrated in Fig. 2. Welds beyond those in the cylinder walls were not modeled, lacking detailed information in the documentation of the tests. Further, the model is still missing certain details that were not accurately enumerated in the test report, including some additional aluminum support members in and around the undercarriage. The original cylinder was a half cylinder symmetric mesh. This was multiplied to create the full three-dimensional geometry shown in Fig. 2. The added geometry was in minor ways not fully symmetric with the rest of the object, with small variations from symmetry in the box beam support members. These variations from symmetry are probably similar in scale with those in the actual test structure.

Wind. In the post-test video, there is a slight breeze during the test as the impact liquid cloud tends to move slightly in the opposite direction that the projectile moved initially. In consultation with the test directors, we were unable to retrieve data on the speed of the wind during the test. It is unlikely that the wind was greater than a few meters per second. To better understand the effect this uncertainty has on the outcome of the test, three assumptions are made. No wind is assumed for several cases, and either 1 or 2 m/s is assumed for several others. This helps quantify the importance of the wind to the outcome of the tests, as the actual test condition likely falls reasonably close to one of the three assumptions.

Temporal Staging. Beginning this coupling work, there was no obvious parameter that was capable of prescribing the time at which particles should be moved into the fluid calculation. Because structural calculations typically rely on the decay of kinetic energy to determine their completion, such a parameter was examined. Simply transferring all the particles when the kinetic energy changes in the structural code reach a low level was the first assumption evaluated. This assured that the structural dynamics were completed, and it was therefore acceptable to transfer the mass into the code where structural dynamics were no longer calculated. This was unsatisfactory for several reasons. First, the quiescent fluid region was abruptly shocked by the introduction of a large number of liquid particles. Real events are presumed to be comparatively more gradual. Second, there is often in these types of scenarios a core of dense liquid with

Table 1 A description of the simulation cases

Case	Geometry fidelity	Wind	Temporal staging	Dimensionless staging distance (B)
1	Low	No	No	
2	Low	No	5 times	1.7
3	High	No	6 times	1.5
4	Low	2 m/s	No	
5	Low	1 m/s	No	
6	High	No	11 times	1.5
7	High	1 m/s	11 times	1.5

Fig. 2 The high fidelity aluminum geometry

particles that are together and moving slowly compared to the fast moving particles at the perimeter of the spread. This core requires more time to reach the point where its interaction with the air becomes significant. Examining spread predictions from the structural dynamics code, it was observed that the particles that were on the perimeter tended to be more separated and faster moving. Because these are probably leading edge fluid parcels, these are believed to have the earliest and most significant contact with the air. A parameter was then sought that could provide a temporal component to the transfer of mass between the codes.

In our previously described work, the coupling between the structural dynamics and fire codes was based on an evaluation of the minimum dimensionless drop separation distance [4]. This dimensionless quantity (B) is defined as the center to center particle distance (r) divided by the particle diameter (d). Because most discretized drops are of similar size for this scenario, this is a good selection for defining the temporal transfer of mass between codes. More generically, the quantity in the denominator of the dimensionless drop separation distance (B) can be a characteristic drop distance (d) like the sum of the radii of the two drops in closest proximity, which for scenarios with incipient particles varying widely in size makes more sense. The equation for the dimensionless drop separation distance used in this work is:

$$B = \frac{r}{d_{1/2} + d_{2/2}}$$

Generalized for the code, the minimum dimensionless drop separation distance for drop i is found by the following equation:

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

In this equation, x , y , and z are the drop Cartesian coordinates, and N is the total number of drops.

This concept is important because as a general rule, the Eulerian models without other multiphase accommodations become increasingly invalid when the Lagrangian component of the prediction of the Lagrangian/Eulerian code increases. A particle fraction greater than about 0.1 results in a 10% displacement of air in a cell, and is normally used as a peak desired threshold for a dilute spray code. A geometric analysis suggests that when the dimensionless separation distance is greater than 1.7, an infinite hexahedral system of such particles has a particle volume fraction of about 0.1. This is plotted in Fig. 3.

Fig. 3 The calculated void fraction for a given dimensionless separation distance for a regular hexahedral spaced system of uniform sphere voids

Because the instantaneous creation of the entire liquid content in the Eulerian model is not thought to best represent the behavior of the system, the use of the dimensionless drop separation distance is examined herein as a parameter used to define the temporal transfer. Temporal staging of the transfer can be achieved through analytical comparisons of the structural model predictions. At a given time, all particles are evaluated for their minimum dimensionless separation distance by comparing their position compared to all the other particles in the system. When a particle exceeds a user selected threshold for B , it can be injected. Subsequent times evaluate for injection only particles not previously injected. This temporal staging of the particles can be performed for any number of times, but is a moderately costly calculation, taking on the order of hundreds of minutes of computational time for this particular scenario on a current computer workstation processor. It further makes little sense to provide input beyond the frequency of the Eulerian time stepping of the fluid code. The number of stages (injection times) is therefore limited, with the number of time steps used for transfers varied and the dimensionless staging distance varied in these problems as suggested by Table 1. The dimensionless staging distance of 1.7 is a “safe” value to maintain the dilute spray approximation based on arguments made earlier (see Fig. 3), while 1.5 involves a bit more risk, but has not caused problems in the present scenarios. Lower values may be considered in future work. Using a value of 1 or less immediately injects all particles, so there is a finite range of sensible dimensionless separation distance thresholds for defining the transfer. At the final time step, all remaining particles are injected, regardless of their separation distances. The number of stages was also varied, taking 10 and 20 ms steps between injections. Case 2 has one fewer injection steps than case 3 because it omits the first potential injection time. Few particles were selected for injection at 20 ms, the omitted time in case 2 compared to case 1, so these cases are expected to be quite similar in terms of results. At 120 ms, all particles not previously transferred to the fluid code are injected for all cases regardless of the dimensionless separation distance.

Test Details. The test was performed for a cylinder diameter of approximately 1.2 m and a velocity of approximately 100 m/s. The full detailed test report is not openly available. The liquid spread results presented are all expressed on a dimensionless basis.

Three major experimental observations are the focus of this comparison. These are based on the data taken and prepared for during the tests.

- (1) **Drop Sizes:** Particle sizes were measured with a phase Doppler particle analyzer (PDPA) instrument well away from the impact point for one of the tests in the series. Because of the prevailing wind direction, primary spray was not sampled. Some signal was detected, likely secondary drops. The resulting test conclusion was that the drops were sized around $10 \mu\text{m}$, with the sampling location located outside the primary spray region. Some visual evidence exists above the target from this test, suggesting liquid morphology in the near impact region. Primary drops are thought to be in the millimeter to centimeter range based on photometric analysis of drops near the impact point (see for example Fig. 4).
- (2) **Cloud Spread:** Using visual photometrics, it was determined that the liquid reached approximately 40 m at peak spread distance from the center point of impact at the end of the rapid expansion phase of the impact (at about 1 s [3]). This is a useful metric, and is suggestive of the accuracy of the flow spread dampening believed to be caused primarily by the drag interaction with the air that is only modeled in the Lagrangian/Eulerian portion of the calculation.
- (3) **Liquid Deposition:** A series of $2.44 \times 3.05 \times 0.15$ m pans were located below the impact area, as illustrated in Fig. 5, and weighed before and after the test. The increase in mass

Fig. 4 The primary spray from the impact from Ref. [2] (used with permission from photographers). The water is dyed red for clarity.

was attributed to the liquid deposition. Pans were arranged regularly with respect to the target. Because the test was ostensibly symmetric, there are two data points for each location, providing grounds for experimental uncertainty estimates. The symmetry is suggested by the numbering with an apostrophe mark (') indicating the symmetrically analogous measurement pan to the base pan. Some of the pans were moved slightly in the post-test field due to impact, and in one case a pan was punctured (pan 3). The residual water was also exposed to the atmosphere where there was some unknown amount of evaporation prior to the post-test weighing (highs were $\sim 15^{\circ}\text{C}$ the day of the test, with typically low humidity found in the New Mexico high desert).

The tank of liquid impacted a square face concrete target. The velocity was one typical of transportation, and low enough to not severely aggravate the low Mach number incompressible approximation of the fire code. Extensive evaluations of the structural results are not detailed herein, as this work is focusing on the liquid dispersal.

Model Details. The structural dynamics simulations were performed on a cluster of processors maintained at Sandia National Labs. They were run with Presto version 4.11. The water and aluminum structural materials were modeled with an SPH approximation for the dynamics [6,7]. Property values were derived from historical work and based on openly available reference data [8], with assumed Mie–Gruneisen equation of state properties for

Fig. 5 An illustration of the layout of the collection pans (not to scale) with the numbering scheme for this report

Table 2 Water properties, Mie–Gruneisen equation of state

Property	Density (kg/m^3)	C_o (m/s)	S	Gamma	Pressure cut-off (Pa)
Water	1024	1500	1.92	1.0	6890

water shown in Table 2. The target was also modeled with appropriate structural material properties, and was solved using a finite element approximation. The target was mounted at four points identical to the tests, and was allowed to deform according to the structural model predictions. Because the ground is somewhat close to the impact point, it participates in the impact. A flat strip of ground was created with an immobile boundary condition to approximate the behavior. A visual representation of this scenario at time zero is found in Fig. 6.

Since the structural impact forces are dominant in the early impact, small by comparison forces including the effect of gravity, surface tension, and drag are not computed within this framework. Water viscous forces are not explicitly modeled either, but the effects are approximated through analogy structural material properties ascribed to the liquid.

SPH predicted particle locations and velocities are saved and passed to the Lagrangian/Eulerian code. The SPH diameter is assumed proportional to the drop diameter, and used to define a drop of similar relative scale in the Fuego code. Because the thin wall aluminum structure adds complication to the liquid spread calculation, for this study the aluminum SPH particles are omitted from the Fuego portion of the simulation. An assessment of the effect of this assumption is left to subsequent work.

A plot of the Presto predicted low geometric fidelity dimensionless kinetic energy is found in Fig. 7. By 0.04 s, the kinetic energy in the original direction of travel has been almost completely eliminated. Total kinetic energy continues to decrease, as drops impact the ground surface, resulting in diverging x- and y- components of kinetic energy (note: Figs. 2 and 6 provide axes for orientation). Cases not employing staged input received the particles from predictions at 0.1 s from the Presto calculation, well after the early deformations have finished.

Fuego version 4.13.7 was used for all cases. Fuego is a low Mach number flow solver that uses a control-volume finite element to solve the Navier–Stokes equations together with reacting species transport equations; in this case, transport equations are solved for air (nitrogen and oxygen) and water vapor. In addition, Fuego can couple the Eulerian equations of fluid motion to a Lagrangian particle tracking model. The mass, momentum and energy equations of each individual particle are updated as the particle path is tracked through the fixed fluid mesh elements. Particle drag, heat transfer, and evaporation terms contribute, respectively, to distributed source terms in the fluid momentum, enthalpy, and continuity/species equations. Droplet break-up is modeled using the Taylor analogy break-up (TAB) model [9–11]. Like in previous work, we have modified the TAB model to not allow break-up on the first time step after a break-up to account

Fig. 6 A visual representation of the initial geometry for case 7. The aluminum tank is colored light gray, the target and ground are darker gray

Fig. 7 Dimensionless kinetic energy in the three coordinate directions and summed for the Presto predictions with the low geometric fidelity

for the time elapsed during the previous break-up step [4]. Although droplets interact with each other indirectly in the model through the Eulerian fluid source terms, direct droplet–droplet interactions (such as coalescence) are neglected. This may be a source of inaccuracy for regions of dense droplet distribution.

The Fuego domain was $127 \text{ m} \times 28.7 \text{ m} \times 63.5 \text{ m}$ high, with $\sim 293,000$ hex elements. Very slight biasing was used to focus mesh resolution in the target region and relax the mesh resolution at the extremities of the domain. In preliminary calculations, a finer mesh was fielded ($\sim 8\times$ more hex elements), but yielded similar spread results to within an acceptable tolerance. The refined mesh resolves a few more liquid cloud edge instabilities, but otherwise results in comparable spread distances. The mesh convergence results are omitted in this presentation except to what was just described. The target surface was declared a rebound surface for the drops, and the other surfaces deposit surfaces. This means that an impacting drop would either rebound or stick in its entirety to the surface it impacted, but not result in shattering or secondary drops. We have formulated a model appropriate for single drop impacts on dry surfaces [12], but have yet to implement it in Fuego. This omission is expected to result in an increased deposit near the primary impact regions than would otherwise be expected.

Although the ground beneath the impact point around the sled track was flat, the surrounding terrain was moderately variable. The terrain variations are not accurately reflected in the fluid model, representing a source of uncertainty. The near region was accurately modeled, and the extent to which terrain features differ between the model and the test are not thought to be significant uncertainties because they are well away from the dense fluid region where most of the dynamics are occurring in the prediction and from the areas where data are being compared to model predictions. We conjecture that the cases involving a modeled wind may be more affected by the missing terrain because the terrain may contribute to the development of the wind flows.

Cases were run for at least 15 s of physical time. As much as 20% of the mass of the original liquid was potentially still suspended in the air at the time of termination (see Fig. 13). However the deposition between 2.5 s and 15 s was negligible (peaks changes around 2%), and not accelerating. Much of the residual mass was very small drops, which are not as significantly affected by gravitational forces compared to convection/advection. Most deposition at the measurement locations occurred within the first second.

Results and Discussion

Drop Sizes. Figure 8 shows predicted Sauter mean diameters (SMD) in the domain for each test case. The Sauter mean

Fig. 8 Predicted Sauter mean diameters for all test cases

diameter is the drop diameter best representative of the surface area to volume ratio in the system, and a good indicator of bulk spray characteristics. Cases 3, 6, and 7 all had the lowest SMD, 1–200 μm below the other cases. The commonality among these cases is that they had the higher fidelity geometry, and they were all staged input scenarios. Cases 3 and 6 are nearly identical, suggesting a finite number of staging times may be acceptable. The staged input scenario with low geometry resolution was case 2, which has SMD values typically between the rest of the cases and the ones with staged input. This suggests that both the staging and the geometric fidelity contribute to the size of the drops found in the predicted environment.

Figure 9 shows the minimum, maximum, and arithmetic number mean values of diameter for case 1, which is representative of the other cases with similar SMD as found in Fig. 8. Figure 10 shows a corresponding plot for case 7, also meant to be representative of case 3 and 6 results. Both show initial diameters in the mm–cm range (10^3 – $10^4 \mu\text{m}$), consistent with the data. This agreement mostly is a function of the SPH particle sizes and the original geometry. The close comparison to the data at early times (0–2 s) should not be attributed to any predictive accuracy. Besides significantly lower arithmetic mean diameters in case 7 compared to case 1, a very notable difference exists in the minimum drop diameter predictions. Case 7 has significantly lower minimum drop diameters. This is presumably due to the staging of the particles on transfer. The PDPA data suggest fringe diameters around $10 \mu\text{m}$, which are well below the minimum diameters predicted by the case 1 simulation, but well within the prediction

Fig. 9 Case 1 drop diameter prediction details

Fig. 10 Case 7 drop diameter prediction details

range for case 7. Break-up in these simulations is mostly a function of the droplet air interaction as modeled with the TAB model.

Drop diameters evolve from the break-up, and are mostly a function of the particle TAB break-up model employed in these simulations. The TAB model describes an analogy between a damped oscillator and the drop interaction with the surrounding gas field, with break-up being the result of large forcing functions. The improved accuracy for case 7 can be ascribed to the fact that the early drops are subjected to a more significant velocity difference compared to the gas and tend to contribute more significantly to the momentum transfer between the liquid and gas than particles injected later into a more mature gas field. This seems physically accurate, and is evidence to the importance of the staging. Another factor may be that the added aluminum geometry in the Presto calculation deflects more particles in the structural portion of the calculation and creates a wider spread of water particles. Particles grouped less with the bulk material are more prone to break-up because the velocity differential between the liquid and gas that is the primary break-up mechanism is increasingly present. This too helps physically explain the prediction results.

Cloud Size. As mentioned above, peak cloud spread distances were approximately 40 m. How to represent this in the model is not fully intuitive, as trace amounts of mass may not be resolved in the photography. We have selected a parcel density method to evaluate the peak spread distance. A postprocessing algorithm was developed to measure parcel distance from the impact point. A parcel concept is employed to facilitate calculations, taking advantage of the parcel concept employed in the code. SPH particles are initially single particles as they are introduced in the fluid domain. As these break aerodynamically, they don't form new independent particles, rather multiple particles are tracked together in the parcel that behaves as an individual group of particles might behave. The parcels are typically of comparable mass because they originate from similarly sized initial particles. The parcels normally vary slightly in mass, as initial SPH sizes were similar but not exactly the same, evaporation causes mass loss, and there is the potential parcel splitting when a critical number of drops per parcel is exceeded (5.1×10^7 was selected and used for this problem). Parcel splitting was evaluated and found to be infrequent, and not believed to be a significant problem with this methodology. Parcel density is therefore thought to be a good approximation for mass density. Mass density isn't necessarily proportional to visibility, but for dispersed drops in a similar size range it represents a good approximation. The post processing algorithm was used to generate summary data from which the results plots are extracted. The distance algorithm used was a point to point distance. Mass density in this case is probably quite

closely related to visibility. An estimate of mass density is obtained by evaluating particle parcels per unit area or volume, under the assumption that all parcels contain approximately the same mass. Parcels are summed in certain distance ranges from the impact point, and these are spherical integrals. This is the method employed for this analysis. In retrospect, it might have made more sense to use a radial distance from the axis of flight of the impacting object. Because the impact clouds are mostly shaped like a disk (especially early on, see also Fig. 18), the difference between the two methods may not be significant except at smaller distances and after the plume has matured.

Figure 11 shows drop parcel density (count divided by distance) for 0.5 m radial bins at 2.5 s for all the cases in this study. Any parcels beyond 50 m are included in the 50 m bin. The parcel density will be roughly proportional to a mass per area, and can therefore be considered a crude estimate of the mean optical density for a ring at the given radial distance from the impact point. At 2.5 s, most of the parcels are found between 20 and 40 m away from the target, with the peak densities in most cases occurring in this region. This is not consistent with visual observations from the tests that suggest a more uniform distribution. The particularly sparse 0–15 m region for many cases as extracted here is confirmed by plotting in a graphical package the parcels. Single major peaks for cases 3, 6, and 7 are found at about 5 m distance, suggesting that the lack of geometry fidelity may be part of the reason for the unexpectedly low drop density for the other cases in the under 20 m distance range. The tendency to form a toroidal shape may not be only caused by the geometric fidelity as suggested in Fig. 11, but by other minor geometric omissions as well that have not been targeted for testing in this study.

Results in Fig. 11 suggest that the spread distances are slightly overpredicted. Beyond 40 m there are still a significant number of parcels in the predictions. Peak spread according to Fig. 11 would best be considered approaching 50 m for all of the cases, about 25% higher than the data estimate suggests. The reported peak of 40 m from the data is at 1 s, and suggests that there is some minor spread occurring beyond that time [3]. Taking into account the uncertainties in the data, these simulations appear to be a reasonably good approximation of what was found experimentally.

There could be a relationship between the moderately excessive spread and the presumed lack of particles near the impact point. A model feature that could cause this not evaluated in this study is the incorrect treatment of viscosity and surface tension in the core liquid. The SPH predictions do not treat these phenomena correctly, and when the transfer occurs, morphological information in this regard that may be important to correctly predict it may not be present in the transfer. There is a dense zone of slower moving particles near the impact point at the final transfer time. These may not be adequately modeled as individual particles. If the

Fig. 11 Predicted parcel density at 2.5 s

Fig. 12 Case 7 spread predictions

liquid is not well dispersed in that region, the surface tension and viscosity in the tests may be more significant to the liquid flow than would be predicted by modeling the particles as spheres in the fluid code. Curiously, while geometric fidelity appears to affect particle spread at distances below 20 m, it does not appear that the ultimate spread distance (35–50 m) is significantly affected by it.

Figure 12 shows the evolution of the parcel density for case 7, and is somewhat representative of trends in the remaining cases. This is reproduced to illustrate that the 2.5 s results are acceptable for evaluating particle spread distances. Drop parcel density at later times is at least as low as at 2.5 s at distances beyond 40 m. Figure 13 shows dimensionless particle mass plotted versus time, which shows that for the first 2 s that the mass in the system is relatively similar for all cases. At later times, the wind becomes a significant factor, with wind enhancing the removal of particle mass from the system as might be expected. There are basically two loss mechanisms present in these calculations. Particles can interact with the boundaries or evaporate. The wind is not thought to significantly affect the evaporation loss, and loss enhancement is therefore believed to be related to the boundary loss. Figure 14 shows a photograph and a simulation still from comparable times illustrating the similarities in predicted shape of the liquid cloud. The general edge shape is reasonably well predicted, including the edge variations that presumably originate from instability mechanisms present in the early impact. In Figure 14(a) there are noticeable decreases in spread distance at approximately $\pm 45^\circ$ from vertical. While these gaps correspond to the structural

Fig. 13 Particle mass as a function of time

Fig. 14 Experimental (a) and case 7 predicted (b) liquid spread at similar times

cross-member on the impact face (see Fig. 2), there is reason to believe that this fluid spread feature may not be due solely to these members (which are included in the fine geometry model). There were also comparatively small bolts used to secure the target at the same angular orientation. These bolts were not present in the simulations, and are believed to be the primary source of the discrepancy. Examination of the simulation predictions suggests that most of the liquid in the region of the bolts is flush with the face of the target, lending credence to this belief. This is further evidence that minor geometry configurations can have a significant effect in the outcome of these events.

Liquid Deposition. As a final comparison between model results and data, liquid deposition is evaluated. Figure 15 shows a summary plot of the predicted pan mass fraction compared to that from the test. In this section, data uncertainties are shown, and the error bars are representative of the simple aleatory uncertainty from the data. They are two standard deviations in magnitude. Because this plot may be difficult to parse, the results have been summarized in Fig. 16 in a way that is easier to visualize.

Fig. 15 A detailed comparison of the pan deposition data and predictions

Fig. 16 A summary of the liquid deposition comparison

Predictions for pan 3, just below the impact point, are significantly higher than the data by approximately a factor of two. This is not unexpected, because the Fuego fluid mechanics model presently does not accurately simulate the secondary impact dynamics of multiple sprays impacting in rapid sequence and close proximity. Impacting drops all stick according to the model. In reality, one would expect a significant amount of satellite or secondary drop formation on impact, further contributing to the spread. Predictions for pans 4, 5, and 7 are all low. Cases with particle staging and high resolution tend slightly more towards the data. These may be low for the same reason pan 3 results were high. Splashing expected to occur at pan 3 would distribute mass outward, with the pans with low mass prediction being among the expected recipients of the splashed mass. Pans 2 and 8 had some predictions within the data, and some outside. Pans 6 and 9, both located directly opposite the incoming trajectory had mixed results, with some predictions within the data range and others falling outside above and below the data.

Despite the local inaccuracy, the combined accuracy of these results may be acceptable. Assuming liquid impacts on a surface where it may spread, the precise location of the liquid may not be as important as a general proximity. If one integrates the mass in pans 1 through 9, a total recovered mass can be illustrated, as in Fig. 17. Except for case 2, all overpredict the mass as measured, and most fall within the two standard deviation range of data uncertainty. There are three significant considerations when examining and interpreting these results. First is the fact that the current model suite is missing a satellite splashing model of drops formed

Fig. 17 Total predicted and measured deposited mass

on impact, and is probably a reason to expect predictions to be higher than the data near the point of impact. Secondary drop formation is likely to preferentially distribute mass outward. Second, the data are probably slightly lower than they would be if the mass were measured real-time due to evaporation. Third, the predictions as extracted and presented here are probably slightly low, as there was still mass entrained in the air at the simulation extraction time of 15 s (see Fig. 13). This uncertainty is probably best understood quantitatively, as peak deposition mass changes are around 2% of the total liquid mass for deposits extracted at 2.5 s and 15 s for all cases. This demonstrates that there is very little addition of deposit mass on the ground between 2.5 s and 15 s, with deposition expected to continue to slow. Especially considering the slight wind present in the test, lingering mass would be expected to be pushed downwind before finally depositing on a surface, avoiding final deposition in the pans. After 15 s, even with $1/2$ m/s wind velocity, one would expect the bulk of the cloud to pass over the collection pans. Despite what appears to be significant discrepancies in the local deposition predictions, the integral data comparison and the specifics of the data and model inadequacies allow us to conclude that the model is performing reasonably well. Addition of an improved liquid surface interaction model or drop impact model is left to future work, and has potential application for this class of problems.

Figure 18 shows an illustration of the full-field deposition from the predictions arranged in descending case order taken from results at 15 s time. The target is a small black rectangle, and the initial direction of the liquid tank is downwards in the plot, consistent with Fig. 16. There is moderate asymmetry in the results, which is difficult to accurately attribute, but not unexpected. Contributing factors may include initial mesh asymmetries, randomness in the droplet break-up model, turbulence model sensitivities, numeric precision, and solver accuracy as sources for asymmetry inherent in this type of simulation. All things considered, the

Fig. 18 Predicted deposition density at 15 s for case 1 (top) through case 7 (bottom) plotted on a logarithmic scale with black contours separating regions of fixed order of magnitude

symmetry is good. The influence of the wind can be seen in the deposition patterns, and is most pronounced for the 2 m/s case (case 4). For the 1 m/s cases (5 and 7), the wind effects are more subtle. At first glance, this is the most significant factor in the deposition patterns. But, the effect of geometric fidelity is well distinguishable in the densest (red) contour region as it transitions to the next lighter color. Cases 3, 6, and 7 exhibit noticeably different trends at the center-plane of impact symmetry, with increased deposition further away from the target in the direction of travel of the tank. Because the red-to-green transitional colors represent higher deposition, differences in these regions are thought to be more significant. The wind effects are most evident in the low density regions and at further distances from the target. The similarity in spread distances is also evident, as most cases have outer contours with approximately the same width.

General Discussion

The previously discussed results are very helpful in understanding the predictability of the modeling methods employed for impact to liquid spread scenarios. Overall, the capability appears to be reasonably accurate. The drop size modeling suggests that the temporally staged input and details of the impact geometry help improve the distributions such that predicted drop sizes are more consistent with the PDPA measurements at the fringes of the impact cloud. Cloud spread may be overestimated by about 25% from the nominal value. None of the model variations seemed to affect this much, suggesting that other model features not assessed here probably play a more significant role in this final spread magnitude. We presently theorize that morphological inadequacies in the treatment of the fluid and in its subsequent development are contributing to an error in the core region, and may also influence final spread distances. Liquid deposition on the ground is mostly locally inaccurate (see Fig. 16), but when looked at over larger integral areas may be acceptable (Fig. 17). The local inadequacies are clearly at least partly related to the methods used to model the surface impact of drops. We have an improved model awaiting implementation that is believed to be quite good for single drop impacts. But since the scenario clearly involves a more dynamic impact environment, with multiple adjacent impacts, the single drop model is not expected to result in much more than an incremental improvement in the prediction accuracy. It is unlikely to move 50% of the mass, as would be required to make model and experiment for pan 3 to agree. In the end, the current accuracy may be sufficient. If the liquids deposit on flat or slanted surfaces, their flow will probably smooth out the local inadequacies. Combining a surface liquid flow model with the current codes may be important to simulate some cases accurately.

These simulations have also been helpful in understanding the fidelity necessary to correctly model impact scenarios. The wind assumption seems to have a minor effect on the outcome for this exercise, and it is never clear that any of the wind approximations are better than any other. Within the range tested, the wind doesn't seem to be very important to any of the comparisons with data. The geometric fidelity and the temporal input staging were both found to be important for resolving drop sizes and possibly for predicting the spread of particles. Based on what we have learned here, it would probably be best to focus on the liquid spread distance and the tendency for the drop cloud to form the torus shape in follow-up work. An alternative treatment method for the impact core may be possible to develop within the present framework that would better approximate the behavior of a real system.

Since this work is aimed at validating an impact scenario for a fuel laden transportation vehicle, it is helpful to comment on the relevancy of this work to this problem of interest. The test involving the rocket propelled tank of water is perhaps the best existing validation dataset for model evaluation at this scale. However it does not include significant reactions other than evaporation of the liquid. A fireball will form for a more complex impact involving a fuel. Not only the size and intensity of the predicted environment are relevant, but also the rate at which ignition occurs. And the fact that the

thermal field is strongly coupled between the gas and liquid phase makes the reacting impact an extremely challenging problem. For the evaporation of the water in this case, accurate concentration data do not exist to quantify the accuracy of the predictions. Because the evaporation is an essential element to the impact of transportation fuels and because it is directly related to the details of the impact, measuring the evaporation products for this type of a test could be an excellent way to further validate the modeling method.

It was found in this study that geometry fidelity was the most important parameter evaluated. This finding raises an issue with respect to practical scenarios of this nature. Transportation vehicles tend to be geometrically complex, with a large number of complex parts. When these types of scenarios are analyzed, it is not expected that fine features will be all fully resolved. The level of geometric simplification found in this study between the low and high resolution cases are probably similar to those one would expect to find present in practical simulations of this nature. It is probably safe to conclude that increasing fidelity calculations will trend similar to what was found in this study in that the drop break-up is enhanced with the presence more geometric detail. What will be difficult to ascertain is what of level refinement is needed to resolve what level of accuracy. Until improved guidance in this regard can be obtained, it is probably advisable to evaluate multiple levels of geometric refinement to help estimate simulation accuracy for a given scenario.

Conclusions

A new method to couple a transient dynamics code with a fire Computational Fluid Dynamics (CFD) code is presented. The use of a dimensionless spacing parameter provides what is thought to be as sensible way to define transfer times. Drop size, particle cloud, and liquid spread data from a unique dataset involving the impact of a tank of liquid into a solid target provide helpful context to understand the accuracy of present models and the best methods for simulating this type of a scenario.

- Generally speaking, the model is capable of a reasonable representation of the quantified results of the tests.
- Some discrepancies exist, with most significant discrepancies being related to the final spread location of the liquid mass.
- These discrepancies are moderate in scale (~25% in spread distance, within two standard deviations for integrated deposit), and may be acceptably low depending on the application of interest.
- Of the parameters tested for sensitivity in this study, the geometry fidelity had the most significant effect on the outcome of the predictions. Data mostly suggest improved accuracy with higher fidelity geometry.
- The time staging of the mass transfer between the structural and fire codes may also be viewed as a significant feature to the model. In this case it was not as significant to the liquid spread results as the geometry fidelity, but it affected the predicted drop sizing appreciably.
- These predictions did not appear to be significantly influenced by the wind within a practical range of assumptions. However, the wind speed was very low for these tests.
- These results point to productive subsequent work. Testing should focus on measuring accurate evaporation in a practical environment, and model development should consider methods for improving the prediction of the morphology of the liquid around the code transfer times. Additional validation work is advisable to help build confidence in the accuracy of these methods.

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