On the Simulation of Dropletization

Rainald Löhner[1], Joseph D. Baum[2], Fumiya Togashi[3] and Orlando A. Soto[4]

[1] Center for Computational Fluid Dynamics
George Mason University, Fairfax, VA 22030, USA
e-mail: rlohner@gmu.edu, web page: https://cfd.gmu.edu/

[2]Applied Simulations, Inc., McLean, VA 22101, USA

ABSTRACT

Consider the following situation: a high explosive charge is surrounded by a liquid in gas. The explosive is detonated, expanding the liquid, which then breaks up into streaks and blobs. Due to shear, these blobs then break up into droplets. The droplets also vaporize in the surrounding gas. A secondary shock impacting this mass of droplets and vapours may then lead to ignition and combustion. Some of the original liquid mass may remain as a liquid (e.g. on the ground or walls), leading to pool fires once combustion has started.

In order to attempt to model these complex multiphysics phenomena, we have **coupled several solvers**. All of the solvers are based on unstructured grids, and use standard edge-based data structures for speed. The different solvers comprise: a) For the gas part: an explicit TVD or FCT solver for chemically reacting, compressible flow; b) For the liquid part: a semi-explicit TVD solver for the advective-diffusive terms and a Poisson solver for the pressure terms of the near-incompressible flow; c) A volume of fluid approach for the free surface of the liquid; d) The Chemkin package for chemistry (11 species, 21 reactions); and e) A particle update technique that allows for droplet breakup and vaporization.

At every timestep, the solver handling the compressible flow passes the pressures to the near-incompressible flow solver. In turn, the velocities obtained from the near-incompressible flow solver are imposed for the compressible flow solver in the regions occupied by the liquid.

The transition from liquid to blobs or droplets uses an approach similar to large-eddy simulation: once the near-incompressible VOF flow solver can no longer discretize accurately the free surface, the poorly resolved regions are automatically transformed to blobs (large droplets) and transmitted to the compressible flow solver. There, they are allowed to break up further into droplets. Several options are possible for this step (we have implemented the widely used Reitz model). Figure 1 shows a typical example.

The main focus of the paper is the transition from liquid to blobs. This is perhaps the most questionable part of the coupled approach, and deserves further elucidation and discussion.

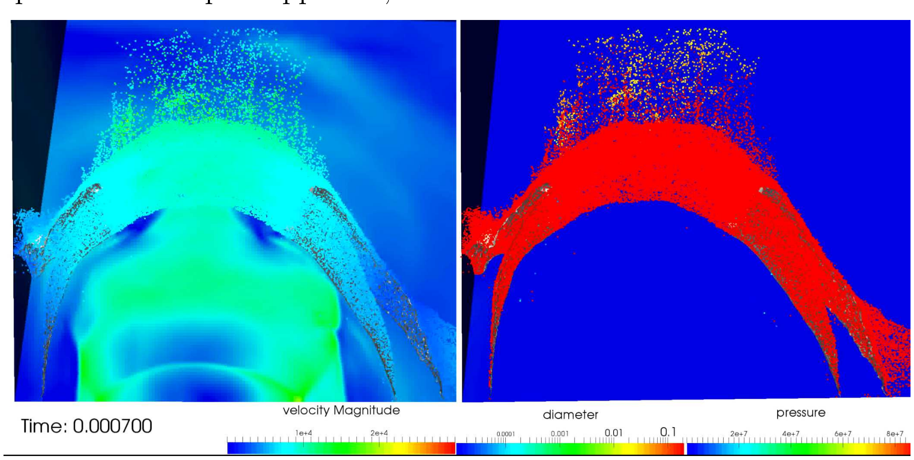

Figure 1 Velocity, Pressure, Free Surface and Particles at $T = 0.7\ ms$