Numerical simulations of Xe-air interfacial turbulent mixing flows

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Abstract. Richtmyer-Meshkov instability (RMI) and resulting interfacial turbulent mixing are studied. HYDRA, an AWE three dimensional Eulerian Massively Parallel Processing (MPP) code, is utilized to numerically investigate such a RMI mechanism in a convergent shock tube. Characteristics of interfacial mixing layer are quantified by mass and molecular mixing fractions. It is shown that a discrete feature significantly influences RMI and interfacial mixing process, and the perturbed transmitted shock front strongly amplifies turbulent mixing.

1. Introduction

Richtmyer-Meshkov instability (RMI) occurs when different density or compressibility fluids with interfacial perturbations are subject to an impulse acceleration, e.g. shock waves (Meshkov, 1969; Richtmyer, 1960). RMI is a fundamental fluid phenomenon, consisting of a non-stationary and nonlinear physical process. Recently, it is under an intensive investigation in such contexts as an inertial confinement fusion (ICF), supernova collapse, shock lithotripsy, sonoluminescence, detonation-driven shock (Youngs, 1994; Muglera & Gauthier, 2000; Brouillette, 2002; Dimotakis, 2005; Cook, 2009; Liu, 2010; Shankar et al, 2011).

It is therefore valuable now to better understand the dynamics of these instabilities in a three-dimensional and more complicated geometry. In this study, we are concerned with multi-material interfacial instabilities and turbulent characteristics of a three-fluid system, a heavy gas (Xenon, Xe) enclosed by a light gas (Air), initially separated by two randomly-perturbed surfaces (material interfaces).

To perform such a study, HYDRA, in addition to TURMOIL3D, applying the Monotonic Integrated Large Eddy Simulation principle for RTI and RMI problems Youngs (1994), is developed. We implement it to investigate the physics of shock-interface interaction and mixing evolution in the convergent geometry and with the feature present.

To develop and validate mixing model and understand shock induced instabilities and interfacial mixing process, at AWE a convergent shock tube (CST), which can produce a cylindrical shock, has been designed and commissioned (Holder et al, 2003; Barton & Holder, 2004; Parrish et al, 2008). In earlier experiments, mainly SF₆ was used as a dense gas. The mixing of the gases was imaged with a shadowgraph technique. Recently various diagnostics...
including laser sheets and high speed imaging were implemented, and the test cell was re-designed, too. Xenon (Xe), instead of SF$_6$, is considered for in future experiments as it is more environmentally friendly.

In following, we firstly describe the experimental work of interest and its flow characteristics in Section 2. Section 3 then briefly explain numerical implementation and the suitability of the HYDRA for investigating the physics of shock-interface interaction and mixing. Section 4 presents density, mass fraction, vorticity and simulated shadegraph images to visualize and qualitatively describe the RMI and mixing process. Subsequently, the analysis of the local and global properties of turbulent mixing is provided. We also discuss aspects some key interfacial mixing parameters in support of the mixing model development. Finally, a summary of the results and conclusions are drawn in Section 5.

2. Experimental setup

The AWE convergent shock tube (CST) was designed to investigate Richtmyer-Meshkov turbulent instability growth on a cylindrical dense gas interface. It was initially designed in 1995 and has since evolved to meet many challenges in terms of environment, diagnostics and safety. Figure 2 sketches of experimental setup, geometry dimensions and working principle.

Figure 1. AWE Convergent shock tube facility, simulation domain and working principle.

In the design, a three-fluid four-zone system is partitioned: a test cell of a heavy gas (Xenon, Xe) enclosed by light gas (Air) on either side; and a detonable gas chamber on the
The particular properties of Air, Xe (or SF$_6$) and Detonation gas used in the simulation are summarized in Table 1. Upon experiment, a cylindrical shock was produced by simultaneously detonating the oxyacetylene gas with 30 mini spark plugs. The detonation shock then propagates towards the center of the convergent geometry.

### Table 1. Gas properties of fluids and initial conditions, as used in the simulation.

| Property                          | Air         | Xe          | SF$_6$      | Detonation gas |
|-----------------------------------|-------------|-------------|-------------|----------------|
| Density ($\rho$, $\times 10^{-3}$ g/cc) | 1.184       | 5.890       | 5.970       | 1.261          |
| Molecular mass (M, g/mol)         | 29.04       | 131.29      | 146.07      | 29.25          |
| Ratio of specific heats ($\gamma$) | 1.402       | 1.667       | 1.090       | 1.166          |
| Specific heat at constant volume ($C_v$, $\times 10^8$ Mb cc/g K$^{-1}$) | 716.75      | 95.46       | 633.98      | 1,687.75       |
| Speed of sound ($a$, $\times 10^{-4}$ cm/$\mu$s) | 343.0       | 176.9       | 136.9       | 309.4          |
| Pressure ($P$, $\times 10^{11}$ Mbar) | 100.000     | 100.000     | 100.000     | 1,500,000      |
| Internal Energy ($E_0$, $\times 10^8$ Mbar cc/g) | 211,490.0   | 27,845.0    | 186,120.0   | 7,292,700.0    |

The overall configuration is represented by a convergent shock tube with a dimension of 104 cm $[2, 106] \times \pi/6([-\pi/12, \pi/12]) \times 5$ cm $[0, 5]$ in cylindrical coordinates ($r$, $\theta$, $z$). The initial interfaces are placed at radius of 20 and 35 cm, respectively. A feature is superimposed at one of two randomly perturbed material interfaces to enunciate the presence of a macroscopic perturbation, as illustrated Figure 2b.

Figure 2c indicates a one-dimensional wave-diagram (X-T plane) of the convergent geometry with a pressure ratio of 15, exhibiting complex interactions between the shocks and interfaces and reflected shock and/or expansion waves. Upon detonation, an incident cylindrical shock (ICS) with a Mach number of 2.7 is generated and propagates inwards. The shock strength increases over 4.4 when it impacts on the outer interface, Air::Xe at a time of 735 $\mu$s. A reflected shock (RS.1) is generated and flows outwards, and a transmitted shock (TS.1) enters the dense fluid, Xe. At 1,005 $\mu$s, the TS.1 shock interacts with the inner interface, Xe::Air. As a consequence, a second transmitted shock (TS.2) forms with additional rarafaction waves reflected back to the Xe layer.

While hitted the apex wall at a time of 1,225 $\mu$s, the TS.2 shock is reflected back and propagates into the Air::Xe and Xe::Air interfaces, and in sequence interacts with the evolving mixing layers, in a process called reshock. The growth of the mixing layer and other mixing properties are, therefore, strongly affected by these interactions of the shock/rarefaction wave-interface, with each subsequent interaction further changing fluctuations and contributing to the formation of complex small-scale structures.

### 3. Numerical methods

In the present study, to gain a more thoroughly understanding of the mixing dynamics, we base our models on the simplified geometry of a convergent shock tube, described in Figure 2b. The shock-shock, shock-material interface interaction, resulting turbulent interfacial mixing process, the evolution of mixing properties and turbulent characteristics are complicated. The presence of a macroscopic perturbation further adds the complicity of fluid interactions and the mixing dynamics. Numerically simulating such flow phenomena is very challenging.

#### 3.1. Hydra solver

The interfacial mixing problems are generally highly dependent on small scale perturbations. To simulate such flows, it is desirable to use very fine meshes for features of interest which may only
inhabit small portions of the physical domain, but will move in space as the flow evolves. To accurately model such problems in an Eulerian, spatially fixed, frame hence requires formidably resolved meshes. Lagrangian methods, on another hand, where the mesh follows the flow, can provide the required resolution for a significantly less resolved initial mesh. However, due to the high levels of distortion inherent in mixing process, a strictly Lagrangian mesh will eventually tangle, with detrimental effects on the solution quality and numerical robustness.

For interfacial turbulent mixing flows, the Arbitrary Lagrange Eulerian method (ALE), involving a Lagrangian step followed by a remap to a non distorted mesh, seems to provide the ideal balance of the resolution a Lagrangian method provides, with all of the benefits of a Eulerian calculation.

Hydra is a three-dimensional Eulerian Massively Parallel Processing (MPP) code, developed for the solution of multi-materials hydrodynamical problems, with density, momentum and internal energy of each fluid separately solved. It uses a Lagrange and re-map methodology, such that every time cycle is divided into a Lagrangian phase, where the mesh moves with the fluid velocity, and a re-map phase where the fluid is moved back to the original fixed Eulerian frame. Recently it is extended to cylindrical and spherical polar geometrical configurations, which provides a broader capability to numerically explore interfacial mixing flows. In addition, the implementation of a semi-Lagrangian moving mesh facility, and an alternative volume fraction advection algorithm for use in highly mixed flows. Partial volume fluxes calculated using either interface reconstruction algorithm or van-Leer advection of volume fractions.

3.2. Computational domain and boundary conditions
The computational domain covers a three-dimensional CST geometry, as described in Figure 2b. A three-dimensional meshing was designated in the region of \( 2 \text{ cm} \leq r \leq 80 \text{ cm} \). To reduce the computational cost and improve the accuracy of interest regions within a limited computing power, we use one-dimensional extension to 106 cm and with a moving meshing facility. All CST surrounding walls are computationally treated as a reflective boundary.

A range of grid densities have been generated for the grid-independency study. Unless specified, simulated results from a cylindrical polar mesh of \( 780 \times 200 \times 150 \) are presented and analyzed.

3.3. Initial conditions and perturbations
The flow field is initialized in four regions distributed from the edge inwards: a high energy detonable gas, air, a high density Xe, and air. The high energy detonation gas is separated with remaining quiescent gases at thermal equilibrium and at a atmospheric pressure. As shown in Figure 2c, the incident explosive shock is initialized upon detonation and propagates towards perturbed Xe::Air material contact surfaces.

An interface representation, similar to the one employed by Liu (2010), is used here to incorporate a macro-scale feature with symmetry-breaking modes which provide more random micro-scale irregularities.

3.4. Method validation
For the purpose of the validation, firstly we numerically investigate the same configuration and flow conditions as described in Sections 3.2 and 3.3, but with a SF6 instead of Xe, as shown in Figure 2b. It was made to compare the simulations with experimental measurements, given that fact that the TURMOIL3D has been intensively validated in similar RMI and turbulent mixing studies.

Figure 2 shows a comparison of experimental and simulated results at times of 0.80, 1.0 and 1.2 ms, respectively. On the top is an experimental shadowgraph images and images showing HYDRA and TURMOIL3D respectively.
Figure 2. Comparison of experimental and simulated images at times of 0.6, 1.0, 1.27 and 1.53 ms

The 0.8 ms and 1.0 ms images show good agreement of gas position, shock position and the size and shape of the vortices forming on the lower gas interface. As time progresses to 1.27 ms the shock position is still in good agreement but the gas position in the code images has begun to lag behind that of the experiment. At a time of 1.53 ms, images are comparable in the positions of the central air void, the dense gas jets towards the apex and the air jets along the walls of the tube. The simulated images do, however, continue to lag behind the experimental images showing much less compression of the dense gas. This is probably due to the uncertainty in the SF$_6$ Equation of State, which is not well defined at a high temperature and pressure. HYDRA results are qualitatively compared with TURMOIL3D simulations confirm the capability of HYDRA in modeling complex explosively driven mix experiments.
4. Results and discussion

In this section, we firstly present temporal evolution of density and mass fraction fields, in a three-dimensional space, for the overall vortex rollup and description of internal wave structures. Figure 3 shows instantaneous density and mass fraction fields at a time of 0.8 ms, with rich small-scale structures. The creation of small disordered structures breaks symmetry and forms a complex interface topology following the passage of shock/rarefaction waves.

![Figure 3. Simulated 3D density and mass fraction contour at a time of 0.8 ms.](image)

To inspect the details of flow characteristics and interpret the simulated results, we present instantaneous and spatially averaged parameters in a two-dimensional form at representative positions. Figure 4a shows the $z-$averaged vorticity related baroclinic vorticity production field. The density contour plots show the formation of complex structures, whilst, the vorticity ($\omega, \nabla \times u$) reveals the dynamical mechanisms driving the formation of such structures. The baroclinic vorticity production plot discloses the mechanisms driving vorticity growth. Misalignment of $\rho$ and $p$ inside the vortex core has an effect given by the vortex dynamic equation.

Figure 4b displays the molecular mixing fraction profiles. The change of the volume fraction in the mixing layers increases monotonically as the shock propagates, and spreads wider with time. The peak value of the molecular mixing fraction appears near the feature and on both sides, corresponding to a high level molecular mixing of two fluids (Xe::Air). The molecular fraction approaches unity at late times, indicating a well-mixed distribution of fluids within the layers.

Figure 5 show comparisons interfacial mixing characteristics between SF6 and Xe at two different times. Note the difference in the depth of penetration of the air into the dense gas region.

5. Conclusions

In the studies, we have numerically conducted a comprehensive investigation of Richtmeyer-Meshkov instability (RMI) characteristics and resulting interfacial turbulent mixing properties, obtained from three-dimensional HYDRA simulations of a four-layer and three-fluid system, Air::Xe::Air::Detonation gas, in a convergent geometry and in the presence of a feature. The density, mass fraction, vorticity, baroclinic vorticity production and shadowgraph image are provided to qualitatively describe a typical mixing process. The perturbed transmitted shock front strongly amplifies the mixing process. It is shown that the discrete feature, in conjunction with random perturbations, significantly influences the RMI and turbulent mixing characteristics.

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Figure 4. Simulated 2D contour plots at times of 0.8, 1.0 and 1.2 ms.

Figure 5. Comparisons of Xe and SF₆ interface at times of 1.05 and 1.20 ms.

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