Planar Richtmyer-Meshkov Instabilities and Transition

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Abstract. A numerical study of the evolution of the multimode planar Richtmyer-Meshkov (RM) instability in a light-heavy (Air-SF₆, Atwood number A=0.67) configuration involving a Mach number Ma=1.5 shock is carried out. Our results demonstrate that the initial material interface morphology controls the evolution RM characteristics, and provide a significant basis to develop metrics for transition to turbulence. Depending on the initial \( \text{rms} \) slope of the interface, RM evolves into linear or nonlinear regimes, with distinctly different flow features and growth rates, turbulence statistics and material mixing rates. We have called this the bipolar behavior of the RM instability. We demonstrate an important practical consequence of our results: reshock effects on mixing and transition can be emulated at first shock if the initial \( \text{rms} \) slope is high enough.

1. Introduction

In many areas of interest such as, inertial confinement fusion, understanding the collapse of the outer cores of supernovas, and supersonic combustion engines, vorticity is introduced at material interfaces by the impulsive loading of shock waves, and turbulence is generated via Richtmyer-Meshkov (RM) instabilities [1]. RM adds the complexity of shock waves and other compressible effects to the basic physics associated with mixing; compressibility further affects the basic nature of material mixing when mass density and material mixing fluctuation effects are not negligible.

Because shocks and turbulence are involved, resolving all relevant physical scales in RM simulations becomes prohibitively expensive. Classical large eddy simulation (LES) approaches [2] are particularly inadequate for RM driven flows because of the dissipative numerics needed for shock capturing. Alternatively, by combining shock and turbulence emulation capabilities based on a single (physics capturing numerics) model, implicit LES (ILES) [3] addresses the difficult issues posed by under-resolution and provides a natural effective simulation anzatz for their simulation. As we consider simulating RM instabilities we must address the effects of initial material interface deformations. The inherent difficulties with the open problem of predictability of material stirring and mixing by under-resolved multi-scale turbulent velocity fields, are now compounded with the inherent sensitivity of turbulent flows to initial conditions (ICs) [4]. Under-resolved material mixing promoted by under-resolved velocity field and ICs in shock-driven turbulent flows is thus a substantially more difficult problem.

Turbulent material mixing can be usefully characterized by the fluid physics involved: 1) large-scale entrainment, 2) stirring due to velocity gradient fluctuations, and, 3) molecular diffusion. At moderately high Reynolds number (Re) – when convective time-scales are much smaller than those associated with molecular diffusion, we are primarily concerned with the numerical simulation of the first two convectively-driven (interpenetration) mixing processes, which can be captured with...
sufficiently resolved ILES. Here, we further test ILES in this context using a simulation model that uses the Los Alamos National Laboratory (LANL) RAGE code [5]. Issues of initial material interface characterization and modeling difficulties, and effects of IC resolved spectral content on transitional and late-time turbulent mixing driven by planar RM have been previously examined [6]. The present work continues our investigation of the effects of initial interfacial morphology of the air-SF$_6$ interface in affecting planar RM [7]; our special present focus is on addressing whether reshot effects on mixing and transition to turbulence can be achieved on first shock.

2. Simulation and Analysis Approach
The planar shock-tube configuration involves low (air) and high (SF$_6$) density gases, presumed ICs at the material interface initially separating the gases, and eventual reshot off an end-wall (Figure 1). The contact discontinuity between air and SF$_6$ is modeled as a jump in density using ideal gases with $\gamma_{air}=1.4$ and $\gamma_{SF_6}=1.076$, respectively, with constant pressure across the initial interface at rest. A shocked air region is created upstream satisfying the Rankine-Hugoniot relations for a Mach 1.5 shock. The shock propagates in the ($x$) direction through the contact discontinuity (from the light to heavy side) and reflects at the end of the simulation box on the right. Periodic BCs conditions are imposed in the transverse ($y,z$) directions. The air/SF$_6$ interface is shocked at $t=0$, reshot by the primary reflected shock at $t \sim 3.5$ ms, and then by the reflected rarefaction at $t \sim 5$ms. The material mixing layers are further affected at later times by reflected compression and weaker secondary reflected shock waves, Evolution and interaction of the shock and air/SF$_6$ interface (e.g., Figure 1) is in good agreement with those of similar previously reported studies [6].

RAGE solves the multi-material compressible conservation equations for mass density, momenta, total energy, and partial mass densities, using a 2nd-order Godunov scheme, adaptive mesh refinement (AMR), a variety of numerical options for gradient limiters and interface treatments [5]. As used in the present work (with no interface treatments and a van Leer limiter), RAGE models a Schmidt number $Sc \sim 1$ miscible material interface, and high Reynolds-number ($Re$) convection-driven flow with effective viscosity $\nu_{eff}$ determined by the small-scale cutoff [6].

![Figure 1. Planar shocktube experiment.](image)

As in [5], integral measure analysis is based on transverse-plane averaged quantities,

$$\langle f \rangle(x) = \int f(x,y,z)dydz / \int dydz,$$

$$Y_{SF_6} = \rho_{SF_6} / \rho, \quad \psi(x) = \langle Y_{SF_6} \rangle, \quad M(x) = 4\psi(x)[1-\psi(x)], \quad \delta(t) = \int M(x)dx,$$

where $\rho$ is the mass density, $\rho_{SF_6}$ is the SF$_6$ partial mass-density, $Y_{SF_6}$ is the SF$_6$ mass fraction, $M(x)$, $\delta(t)$, cross-stream averaged, and integrated mixing width. The instantaneous mixing region is defined by a slab of volume $V$ about the center of the mixing layer constrained in the $x$-direction by requiring $M(x) > 0.75$. Analysis of turbulence characteristics is based on data deviations around transverse planes within the instantaneous mixing region, using,

$$\bar{u} = \langle pu \rangle / \langle \rho \rangle, \quad u = \bar{u} + u', \quad \omega = \nabla \times \bar{u}, \quad 2k = \rho \bar{u}'u', \quad \rho = \langle \rho \rangle + \rho', \quad R = \rho'^2,$$
\[ K = \int k \, dx \, dy \, dz / V, \quad \Omega = \int \rho \omega^2 \, dx \, dy \, dz / V, \]

where \( u \) is the velocity field, \( k \) is the local turbulent kinetic energy, \( R \) is the mass-density variance, \( \omega \) is the vorticity, \( K \) and \( \Omega \) are the mean turbulent kinetic energy and mass-weighted enstrophy, and summation over repeated indices is assumed.

The initial interfacial morphology is defined by the initial rms slope, \( \eta_o = \kappa_o \delta_o \sim (\nabla \chi \cdot \nabla \chi) \), where \( \chi(y,z) \) is the local deviation of the initial material interface around the mean interface location, \( \kappa_o = 2\pi / \lambda_o \), \( \lambda_o \) is a representative wavelength of the perturbation in the initial interface, and \( \delta_o = \delta(t=0) \) denotes the initial interface thickness (Figure 2). Thus, a high value of \( \kappa_o \) denotes a highly corrugated interface with high rms slope.

![Figure 2. Initial material interface characteristics.](image)

The quantity \( \kappa_o \) is used in the study of homogenous stochastic processes, where it is called the mean zero-crossing frequency [8]. In practice, the initial material interface value of \( \kappa_o \) is computed by checking for sign changes of the mass density fluctuation over lines within transverse planes and averaging their occurrences (Figure 3); for \( t > 0 \), \( \kappa(t) \) is similarly evaluated within the mixing region. Mathematically, \( \kappa \) is associated with \( \kappa^2 = \int q^2 E_R(q) dq / \int E_R(q) dq \), where \( E_R(q) \) is the instantaneous R spectra in the mixing region, \( q \) is the wavenumber magnitude, and thus, \( \kappa \) is related to the Taylor microscale; such connections are exemplified below.

![Figure 3. Zero-crossings of \( \rho' \); L denotes the transverse dimension of the computational domain.](image)

Various simulations based experiments were performed in terms of well-defined initial material interface perturbations. The local material interface deformation is given by:

\[ \chi(y,z) = \Gamma \sum a_{n,m} \sin(\kappa_n y + \phi_n) \sin(\kappa_m z + \phi_m), \]

where \( \kappa_n = 2\pi n / L, \kappa_m = 2\pi m / L, -1/2 < a_{n,m} < 1/2 \), \( \{ \phi_n, \phi_m \} \) are random phases, \( \Gamma \) is used to prescribe \( \delta_o \), and \( a_{n,m}, \phi_n, \phi_m \) are random coefficients. The participating modes are constrained by the requirement, \( \lambda_{min} \leq L/(2\pi(n^2 + m^2)^{1/2}) \leq \lambda_{max} \). A variety of IC perturbations and grid resolutions (using up to two levels of AMR) were considered. The baseline resolution involved a \( 820 \times 240 \times 240 \) grid (\( \Delta_{min}=0.1 \text{cm} \)); a much finely resolved \( 1640 \times 480 \times 480 \) grid (\( \Delta_{min}=0.05 \text{cm} \)) was used for selected representative cases. The various cases are organized into two distinct categories having significantly different (low and high) initial rms slope \( \eta_o \) (Table 1).
3. Scaling Integral Mixing Width with IC Parameterizations

As noted in our previous related work [6,7], inspection of the evolution of the mixing layer width \( \delta(t) \) (Figure 4a) for relatively small \( \eta_o \) (\( \eta_o < \pi/2 \)), shows growth rates in agreement with predictions of classical linear theory (growth proportional to \( \eta_o \)) [9]. Higher \( \eta_o \) results in larger deposition of baroclinic vorticity which leads to thicker mixing layers. The energy produced by passage of the shock is mostly in the shock direction and leads to growth of the initial modes in that same direction and increased the mixing layer widths. However, for \( \eta_o = \pi/2 \), the theory is valid only for a very short time after the material interface is shocked. Soon thereafter, the growth rate drops and this is not consistent with linear theory.

In contrast, for high \( \eta_o \) (\( \eta_o > \pi/2 \)), the growth is found to be inversely proportional to \( \eta_o \). For higher \( \eta_o \) there is a much larger deposition of baroclinic vorticity. With the higher \( \eta_o \) interface the vortex centers are closer to each other and they interact, giving rise to the production of more smaller scale modes as is only possible through non-linear processes. Here the energy of the flow, because of the nonlinear interaction, is more isotropic. Interestingly, the increase in \( \eta_o \) does not result in increase in the mixing layer width but leads to production of more small scales and thus more dissipation.

Similarly to the work in [10], we have found useful to plot the layer thickness \( \kappa (\delta - \delta_o) \) vs. time scaled with \( \kappa \delta_o \) (Figure 4b), where \( \delta_o \) is the initial mixing layer growth rate computed from the early-time simulation data (after the shock has traversed the material interface). Results for low \( \eta_o \) and high \( \eta_o \) collapse into distinctly different correlation groups – suggesting transition to non-linearity above a threshold value \( \eta_o \sim \pi/2 \). These results demonstrate what we have denoted the bipolar behavior of the RM instability [7].

For interfaces with low \( \eta_o \), the growth the mixing layer is ballistic with no mode coupling, the evolution of RM is linear (\( \sim t \)), and follows the scaling of [9]. Increasing \( \eta_o \) in the low-\( \eta_o \) group increases the deposition of baroclinic vorticity on the initial material interface and leads to higher layer growth. In contrast, increasing \( \eta_o \) in the high-\( \eta_o \) group also increases the deposition of baroclinic torque, but this leads to a reduced mixing width growth rate (\( \sim t^{0.5} \)), associated with the production of small scales by non-linear mode coupling that are additionally dissipative.

![Table 1. Planar Shock-tube Simulations](image)

| \( \eta_{min} \) | \( \eta_{max} \) | \( L(\frac{1}{2}, \frac{1}{2}) \) | \( L(\frac{1}{2}, \frac{1}{3}) \) | \( L(\frac{1}{3}, \frac{1}{3}) \) | \( L(\frac{1}{6}, \frac{1}{6}) \) | \( L(\frac{1}{12}, \frac{1}{12}) \) | \( L(\frac{1}{24}, \frac{1}{24}) \) |
|---|---|---|---|---|---|---|---|
| \( \delta_o \) (cm) | 0.5 (low \( \eta_o \)) | 5 (high \( \eta_o \)) |
| \( \kappa_o \) (cm\(^{-1}\)) | \( \pi \) | \( \pi/2 \) | \( \pi/4 \) | \( \pi/6 \) | \( \pi \) | \( \pi/2 \) | \( \pi/4 \) | \( \pi/6 \) |
4. Can Transition to Turbulence Occur on First-Shock?

Our analysis above on the effects of initial interfacial morphology indicate that for high $\eta_o$, RM develops into a non linear regime and transition to turbulence is suggested. In what follows, we systematically compare reshocked low-$\eta_o$ results with first-shock high-$\eta_o$ results. The reflecting wall is located such that reshock impacts the material interface at $\sim 4000 \mu s$.

Figure 5. Mixing width evolution. (a, left): low-$\eta_o$ (reshocked); (b, right): high-$\eta_o$ (first-shocked-only).

Figure 5a shows the growth of mixing layer for the low-$\eta_o$ cases. Before reshock, the growth of mixing layer is consistent with Richtmyer’s classical theory [9], i.e. growth is proportional to $\eta_o$ of the interface. However, after reshock, the growth trends reverses and is now consistent with the nonlinear regime (Figure 5b). This shows that integral mixing-width growth trends for shocked high-$\eta_o$ are consistent with those of reshocked low-$\eta_o$. Figure 6a shows the evolution of the simulated Taylor microscale $\kappa(t)$ for the low-$\eta_o$ case. Before reshock, $\kappa(t)$ is virtually constant. When the mixing layer is reshocked, $\kappa(t)$ jumps suddenly indicating smaller-scale production. Similar effects are seen for the high-$\eta_o$ case at first shock (Figure 6b).

Figures 7 and 8 show the computed evolution of the mean turbulent kinetic energy $K$ and mean mass-weighted enstrophy $\Omega$ for the low-$\eta_o$ and high-$\eta_o$ cases. After reshock, non-linear mode coupling increases the population of small scales (higher $\kappa(t)$ in Figure 4), increasing $\Omega$ (Figure 8), which dissipates $K$ faster (i.e., following $-dK/dt \sim 2\nu_{eff}\Omega$) – thus reducing $K$ (Figure 7). For the low-$\eta_o$ group there is no mode coupling and no production of new small scales before reshock, and the evolution of $K$ follows closely that of $\Omega$. Figure 7a shows the evolution of $K$ with time for the low-$\eta_o$ case. Before reshock, $K$ increases with increasing $\eta_o$; after reshock, $K$ decreases with increasing $\eta_o$ – similarly to the shocked high-$\eta_o$ case.

Figure 6. Taylor microscale evolution. (a, left): low-$\eta_o$ (reshocked); (b, right): high-$\eta_o$ (first-shocked-only).
The concept of transition to turbulence is inherently vague; it has been traditionally viewed in terms of rapid increase in population of motions with smaller length scales, which can lead to an inertial subrange in the turbulent kinetic energy spectra (e.g., [11], and references therein). The spectral bandwidth of the turbulence has been scaled by a turbulent Reynolds number [12], usually taken as a ratio of integral-to-Kolmogorov length scales.

In our context, we use the thickness of the layer, $\delta(t)$ as a measure of the integral scale, and the mass-density Taylor micro-scale $\lambda(t)$ – related to the spatial zero crossing frequency through $\lambda(t)=2\pi\kappa(t)$ – as proxy for the small scales. Here, we use $\eta(t)=\kappa(t)\delta(t)$ as measure of the spectral bandwidth. Figure 9 shows that the rms slope of the interface $\eta(t)$ increases with time. As the flow becomes non-linear (high $\eta$), finer resolution results depict increased small-scale production as indicated by higher $\eta(t)$ and longer self-similar ranges in the spectra of $R$ (Figure 9) – which can be associated with higher effective Re [6]. As in [5], the q-shelled spectra are obtained by averaging 2D $E_{d}(q)$ evaluated at cross-stream planes within the mixing slab region defined above.

Late-time $\eta(t)$ in Figure 9 gives the initial rms slope at reshock (for $t\approx3000-4000$ µs); when $\eta(t) > \pi$, it is high enough for transition to non-linearity (and eventual turbulence) to become possible. Figure 10 (left) shows the evolution of $\eta(t)$ after the mixing layer is reshocked. The fact that $\eta(t)$ increases with time for all cases suggests that spectral bandwidth is increasing (which can also be understood as an increase in turbulent Reynolds number). The late time saturation of $\eta(t)$ for the highest $\eta_o$ in Figure 10, indicates faster disappearance by dissipation of the smallest scales of the flow. Due to mode coupling there is a much larger (and faster) increase in spectral bandwidth for the high-$\eta_o$ group. Our observations suggest that sudden increases in $\eta(t)$ and $\kappa(t)$ can be consistently used as basis for metrics to indicate flow transition.
Mixing visualizations in shocked high-\(\eta_o\) and shocked / reshocked low-\(\eta_o\) cases are shown in Figure 11 in terms of volume distributions of mass fraction of SF\(_6\) at selected times, \(t=3000\ \mu s\) after the first shock (or \(t=3000\ \mu s\) after reshock). Figure 11 exhibits qualitative similar mixing features for both cases; for shocked low-\(\eta_o\) there is distinctly less mixing as compared to the other two cases. Figure 12 shows the probability density function (PDF) of mass fraction of SF\(_6\) at the same selected times. PDFs for the shocked high-\(\eta_o\) and reshocked low-\(\eta_o\) show similar features, whereas the PDF for shocked low-\(\eta_o\) shows predominantly higher values indicating less mixing.

5. Conclusions
We have examined the effects of initial interfacial morphology of the air-SF\(_6\) interface in affecting planar RM. Vorticity production at shock time and eventual mode coupling (and transition) thereafter will depend on the initial interfacial characteristics, as well as on the particular \(A, Ma\), and (light/heavy or heavy/light) configuration considered. However, the initial \textit{rms} slope of the material interface appears to be a relevant parameter in determining whether the flow is in the linear ballistic regime, or in a non-linear mode coupling regime. We have called this the \textit{bipolar behavior of the RM instability}.

In the linear regime, the impulsive theory [9] predicts the mixing layer growth trends: as the initial \textit{rms} slope increases the growth rate increases. Less mode coupling is seen, as inferred by the smaller spectral bandwidth, and the primary production of enstrophy is baroclinic. In the nonlinear regime, the mixing layer growth rate trends are the inverse of that predicted by the theory. There is significant
mode coupling and our proxy for spectral bandwidth makes a sudden jump which we view as suggesting transition to turbulence.

Some of our findings for the nonlinear regime are not consistent with heuristic notions one might have of statistically steady turbulence, and are likely a consequence of the non-equilibrium nature of the RMI. The fact that slower growth rate of the mixing-layer width is associated with more material (interpenetration) mixing demonstrates that mixing-layer width growth-rate, bulk $Re$, and material mixing are not causally connected. Our observations have a very straightforward physical explanation: higher initial material interface slopes lead to production of more smaller scales which dissipate turbulent kinetic energy faster, reducing the growth rate. An important practical consequence of our results is that reshock effects on mixing and transition can be emulated at first shock if $\eta_0$ is high enough.

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