Non-equilibrium Thermodynamics of Rayleigh-Taylor instability

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Abstract. Rayleigh-Taylor instability (RTI) has been studied here as a non-equilibrium thermodynamics problem. Air masses with temperature difference of 70K, initially with heavier air resting on lighter air isolated by a partition, are allowed to mix by impulsively removing the partition. This results in interface instabilities, which are traced here by solving two dimensional (2D) compressible Navier-Stokes equation (NSE), without using Boussinesq approximation (BA henceforth). The non-periodic isolated system is studied by solving NSE by high accuracy, dispersion relation preserving (DRP) numerical methods described in Sengupta T.K.: High Accuracy Computing Method (Camb. Univ. Press, USA, 2013). The instability onset is due to misaligned pressure and density gradients and is evident via creation and evolution of spikes and bubbles (when lighter fluid penetrates heavier fluid and vice versa, associated with pressure waves). Assumptions inherent in compressible formulation are: (i) Stokes’ hypothesis that uses zero bulk viscosity assumption and (ii) the equation of state for perfect gas which is a consequence of equilibrium thermodynamics. Present computations for a non-equilibrium thermodynamic process do not show monotonic rise of entropy with time, as one expects from equilibrium thermodynamics. This is investigated with respect to the thought-experiment. First, we replace Stokes’ hypothesis, with another approach where non-zero bulk viscosity of air is taken from an experiment. Entropy of the isolated system is traced, with and without the use of Stokes’ hypothesis. Without Stokes’ hypothesis, one notes the rate of increase in entropy to be higher as compared to results with Stokes’ hypothesis. We show this using the total entropy production for the thermodynamically isolated system. The entropy increase from the zero datum is due to mixing in general; punctuated by fluctuating entropy due to creation of compression and rarefaction fronts originating at the interface and reflecting from the walls.

Introduction

RTI arises whenever fluids of different densities at rest are in an unstable arrangement. This results in distortion of the interface by baroclinic vorticity generation due to misaligned density and pressure gradients, aided by gravitational acceleration [2, 3, 4, 5, 6, 27, 28]. RTI plays a major role in various contexts, as in inertial confinement fusion, combustion problems, supernovae explosions and geophysics. RTI constitutes an important modeling and simulation test case for codes involving various characteristics and aspects of turbulence, transport and diffusion in flows governed by non-uniform density gradients [7]. In rapid compression and expansion processes, the system ceases to be in thermodynamic equilibrium [30]. RTI is a
non-equilibrium thermodynamic problem wherein the expansion and rarefaction of waves can be captured only by implementing the compressible flow formulation without using BA. For variations in temperature not exceeding 10 degrees, variation in density is at most 1% and this small variation can be ignored [4]. Atwood number (A) considered here is 0.1, where \( A = \frac{\rho_u - \rho_l}{\rho_u + \rho_l} \) and \( \rho_u \) is the density of the upper fluid and \( \rho_l \) that of the lower, as shown in the schematic of the problem in figure 1 with a temperature difference \( \Delta T = T_l - T_u \) of 70K between two compartments, where \( T_l \) is the temperature of the lower fluid and \( T_u \) that of the upper. Mikaelian [43] states that “...direct numerical simulations are the best way to assess the validity of BA” in his investigation of BA in RT and Richtmyer-Meshkov (RM) instabilities. Wei and Livescu [25] note that there are higher order effects which are obscured by BA for lower A values.

Experimental studies have been carried out on different aspects of RTI. Investigation of the growth of instability and turbulent mixing at the interface of two fluids, with different density ratios and experimental tank cross-sections [13], displayed increase in the width of the mixing region due to stretching of large scale motions. Similar experiment was performed, with and without tilting the 2D experimental tank, to study RTI [14]. Mixing efficiency in RTI by instantaneous removal of a plate between the fluid layers has also been investigated [15]. Measured velocity field imposed at the onset of RTI experiment was used to initialize three-dimensional (3D) simulations in [16]. RTI leading to turbulent flow was experimented with variable accelerations in [18]. Recently, an experimental investigation on the effects of forced small-wavelength, finite-bandwidth initial perturbations on miscibility of RTI leading to turbulence has been carried out [17].

![Figure 1](image1.png)

**Figure 1.** Schematic of RTI in a box. The mixing region, boundary conditions and the initial interface position have been depicted.

![Figure 2](image2.png)

**Figure 2.** Variation of non-dimensional \( \lambda \) with \( T \) and relative humidity from [42], along with the variation obtained by regression analysis of these data.

Youngs carried out 2D and 3D numerical simulations of turbulent mixing of miscible fluids by RTI [19, 20]. Transition stages of 3D RTI between two incompressible, miscible fluids were presented using DNS in [7]. In [21], LES was used to simulate RTI and a relation between the rate of growth of the mixing layer and the net mass flux through the plane related with the initial position of the interface was obtained. Monotone implicit LES (MILES) using finite-volume technique was implemented for the numerical study of the influence of initial perturbation on turbulent RTI in [22]; Cabot and Cook [23] simulated RTI for a Reynolds number (\( Re \)) up to
32,000, which was supposed to explain type-Ia supernova. Detailed evolution of single-mode RTI was studied in [24]; the growth stages with high and low perturbation $Re$ (defined with respect to $A$, kinematic viscosity $v$, gravitational acceleration and perturbation wavelength) was studied in [25]; RTI driven by stabilizing and destabilizing accelerations in intermediate stages of simulation was investigated in [26]. Total entropy of RTI in an isolated system has been recently studied in a non-equilibrium framework [6, 27] using high-resolution DRP schemes [8] with compressible flow formulation.

### Formulation of the problem and numerical implementation

In the present study two cases are investigated. Case 1 represents a rectangular domain with dimension $0 \leq x \leq 60$ and $0 \leq y \leq 30$ and Case 2 represents a square, with dimension $0 \leq x \leq 60$ and $0 \leq y \leq 60$. In Case 1, the domain is discretized with uniformly spaced 3000 points in the $x$-direction and 1800 points in the $y$-direction and in Case 2, 3000 points in the $x$-direction and 3600 points in the $y$-direction. No-slip, adiabatic conditions are imposed on the walls (AB, BC, CD, AD) as shown in figure 1. The governing equations and the problem formulation are as given in [6, 27]. The system of equations can be expressed in terms of fluxes, given in Hoffman & Chiang [12] as follows:

$$
\frac{\partial \hat{Q}}{\partial t} + \frac{\partial \hat{E}}{\partial x} + \frac{\partial \hat{F}}{\partial y} = \frac{\partial \hat{E}_v}{\partial x} + \frac{\partial \hat{F}_v}{\partial y}
$$

(1)

where the conserved variables, inviscid and viscous fluxes are, respectively, given by, $\hat{Q} = \left[ \rho, \rho u, \rho v, \rho e_t \right]^T$; $\hat{E} = \left[ \rho u, \rho u^2 + p, \rho u v, (\rho e_t + p) u \right]^T$; $\hat{F} = \left[ \rho v, \rho u v, \rho v^2 + p, (\rho - \rho_s) g y, (\rho e_t + p) v \right]^T$; $\hat{E}_v = \left[ 0, \tau_{xx}, \tau_{xy}, u \tau_{xx} + v \tau_{xy} - q_x \right]^T$ and $\hat{F}_v = \left[ 0, \tau_{yx}, \tau_{yy}, u \tau_{yx} + v \tau_{yy} - q_y \right]^T$. In these expressions, $\rho$, $p$, $u$, $v$, $T$ and $e_t$ represent the density, the fluid pressure, Cartesian components of fluid velocity, the absolute temperature and the specific internal energy of the fluid, respectively, and $\tau_{xx}$, $\tau_{xy}$, $\tau_{yx}$, $\tau_{yy}$ are the components of the symmetric viscous stress tensor and are related to the gradients of velocity as

$$
\tau_{xx} = 2\mu \frac{\partial u}{\partial x} + \lambda \nabla \cdot \vec{V} ; \quad \tau_{yy} = \left( 2\mu \frac{\partial v}{\partial y} + \lambda \nabla \cdot \vec{V} \right) \quad \text{and} \quad \tau_{xy} = \tau_{yx} = \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)
$$

Physical properties, viz. dynamic viscosity ($\mu$), second coefficient of viscosity ($\lambda$), specific heat capacity ($C_v$), and thermal conductivity ($\kappa$) are regarded as constants in this formulation. The heat conduction terms, $q_x$ and $q_y$ are given by, $q_x = -\kappa \frac{\partial T}{\partial x}$ and $q_y = -\kappa \frac{\partial T}{\partial y}$. The closure of system of equations is provided by the ideal gas equation and is used to define energy as, $e_t = C_v T + \frac{(u^2 + v^2)}{2}$.

### Stokes hypothesis

The Lame coefficients $\lambda$ and $\mu$ appearing in the stress-strain constitutive relation (with $\mu$ as shear viscosity and $\lambda$ as second coefficient of viscosity or dilatational viscosity [32]) is related to compressibility of the flow [30]. Stokes’ hypothesis states that bulk viscosity ($\kappa = \lambda + \frac{2}{3} \mu$) is set to zero for any flow. This is irrelevant with incompressibility assumption, which in itself is an approximation, even for a very low speed flow. It implies that the thermodynamic pressure is equal to the mechanical pressure [33, 34, 35, 36]. There have been critiques [32, 33, 34, 35, 36, 41] on Stokes’ hypothesis [37]. It is weakly justified for mono-atomic rigid molecule gases [33, 36]. Compilations by Liebermann [32], Karim and Rosenhead [38] and Rosenhead [39] state that $\lambda$ is independent of $\mu$ and can be orders of magnitude higher in amplitude, while the sign is reversed. Emanuel [33] and Gad-el-Hak [34] questioned the hypothesis and its applicability for flows such as re-entry into planetary atmosphere. Cramer [40] showed that many common fluids including
are given by [42], shown in figure 2. Thus, the viscous normal stress components in the present formulation

\[ \tau_{xx} = \frac{1}{\text{Re}} \left[ \left( \frac{4}{3} + \frac{\kappa}{\mu} \right) \frac{\partial u}{\partial x} + \left( \frac{2}{3} + \frac{\kappa}{\mu} \right) \frac{\partial v}{\partial y} \right] \]

\[ \tau_{yy} = \frac{1}{\text{Re}} \left[ \left( \frac{4}{3} + \frac{\kappa}{\mu} \right) \frac{\partial v}{\partial y} + \left( \frac{2}{3} + \frac{\kappa}{\mu} \right) \frac{\partial u}{\partial x} \right] \]

The experimental \( \lambda \) variation with temperature is shown for dry and saturated air in figure 2, as discrete points and the curved line is obtained by using regression analysis of these data. We specifically focus on the role of Stokes’ hypothesis on non-equilibrium thermodynamics related to RTI and its computation in the present study. We do not require any initial perturbations here, as strong rotationality appears at the junctures of the interface with the side-walls [6, 27]. This study is similar in scope to the experiments reported in [13] and [14]. In the present computations, we have used \( \text{Re} = 10^7, \text{Pr} = 0.7, \Delta T = 70K, Ga = 0.23489, Ec = 0.01 \) and \( Fr = 12.2586 [27, 6] \) and such large values are indicative of the ability to perform calculations very accurately using the proposed formulation and numerical methods to capture the thermodynamic process which is far from equilibrium.

Computations of the model thought-experiment are performed using compressible NSE described in [6, 11, 12]. Non-periodic boundary conditions have been implemented in both vertical \((y)\) and horizontal \((x)\) directions. High-resolution DRP schemes [8] are implemented to carry out the simulations. The numerical and physical dispersion relations are almost the same over a large range of space and time scales. Spatial discretization of convective fluxes are performed using high resolution OUCS3 scheme [1, 9]. RTI results have been validated with Read’s experiment [13] as shown in [6, 27] where the general features and primary stages of RTI have also been described.

**Results and Discussion**

**Entropy of the non-equilibrium thermodynamic system without Stokes hypothesis:**

The present study is for a non-equilibrium thermodynamic process involving air as the working substance driven by large thermal gradient, even though the flow speeds are negligibly small. Here, the entropy of the system at any point \((x_m, y_n)\) in the system is given by

\[ \Delta s_{mn}(t + \Delta t) = c_p \ln \frac{T(x_m, y_n, t + \Delta t)}{T(x_m, y_n, t)} - R \ln \frac{p(x_m, y_n, t + \Delta t)}{p(x_m, y_n, t)} \]  

(4)

We will refer to the condition at the onset as the zero-level datum for the entropy. One can compute the entropy of the entire system by using equation (4) for each computational cell and then summing over the entire domain. The resultant entropy of the system as a function of time is shown in figure 3 for the rectangular domain (Case 1), with and without Stokes’ hypothesis. Here, the entropy change with bulk viscosity is shown for three sub-cases, confirming higher rise when Stokes’ hypothesis is not used. Identical grid and time step has been used for computing the three sub-cases, varying \( \kappa \) in figure 3. It can be noted that consistently the entropy is higher without Stokes’ hypothesis and with an additional 10% increase in \( \kappa \) in Case 1, as one would expect due to the presence of higher viscous normal stress. The figure reveals that the time-variation of entropy is identical for the computations using with and without Stokes’ hypothesis for up to \( t \approx 4 \), when the convection in the box is negligibly small. Beyond this time, one
Figure 3. Total entropy for rectangular domain (Case 1) plotted as function of time; \( \Delta \) represents results without Stokes’ hypothesis and \( \heartsuit \) represents results with Stokes’ hypothesis and symbol \( \nabla \) represents results with an increased value (1.1\( \kappa \)).

Figure 4. Total entropy for rectangular and square domain plotted as function of time. Symbol \( \Delta \) represents results without Stokes’ hypothesis for Case 1; \( \square \) represents Case 2 without Stokes’ hypothesis and \( \heartsuit \) for Case 2 with the hypothesis.

notices that the computed entropy is higher without the restriction of Stokes’ hypothesis. This is due to the additional dissipative term \( \nabla (\kappa \nabla u) \) appearing in the momentum equation and \( \kappa (\nabla u)^2 \) in the energy equation. The dissipative structures arise in the systems (control volume or computational cells) which are able to exchange energy or mass with their neighbours or corresponding cells to establish a macroscopic internal order. The dissipation arising due to these structures or fronts correspond to a low entropy value visible in figures 3 and 4 and may indeed be a source of order [31]. In figure 4, entropy change is compared between rectangular and square domains. Also in this figure, the variation of entropy for Case 2 is compared with and without Stokes’ hypothesis. The relation between entropy and vorticity is given by Crocco’s theorem [29], as discussed in [27]. The rate of mean increase of total entropy is also greater and approximately double in Case 2 compared to Case 1, which is due to the fact that mixing occurs early and at smaller scales in the square box compared to the rectangular box as will be explained later with respect to figure 8. Interface instability causes spikes and bubble formation in the presence of mixing. The increase in the atypical \( M \) structures in the total entropy plot is due to pressure waves being created at the interface, which propagate in the \( y \)-direction and reflect from the top and bottom walls while the background mixing due to diffusion shows up of continuously increasing entropy. For the square box, pressure pulses take a longer time to reach the top of the box and reflect from the wall as rarefaction waves.

Pressure Waves:
Apart from the mean entropy increasing for computed NSE (with and without Stokes’ hypothesis), there is also atypical sharp variation of entropy, as shown in figures 3 and 4. This is due to the creation of multiple pressure pulses, as the working medium (air) allows formation of pressure waves starting from the interface. This is shown in figures 5 and 6 for Case 1, with and without Stokes’ hypothesis by solid and dashed lines respectively. Figures 5 and 6 show the pressure across \( y \) at \( x = 30 \) with the former dominated by pressure pulses for Case 1 at the onset of RTI, while figure 6 shows events at a later time when mixing is predominant. Effects
of bulk viscosity are visible at the interface \((y = 2.4 - 3)\) shown in figure 6, during \(t = 10.35\) to 11.25. The formation of pressure pulses from the interface towards the top and bottom of the box is associated with the fluid dynamic transient response. These pulses upon reflection from solid wall changes from compression to rarefaction pulses and vice versa and move back towards the original interface. These compression and rarefaction of the medium give rise to entropy changes, as given by equation (4), and has one to one correspondence for the variation of entropy, with compression giving rise to increase in entropy, while rarefaction reduces entropy of the system.

Reckinger et al [10] in their compressible N-S, energy and species mass fraction formulation, used periodicity in \(x\)- and \(y\)-directions, using non-reflecting boundary condition along with an additional buffer layer of increased viscosity to assist damping of the pressure wave. This is to ensure that they simulate “an infinite domain such that any pressure wave approaching the numerical boundaries is not reflected and thus does not interact with and disturb the growth of the instability”. In the present simulations, we instead capture the pressure waves by implementing non-periodic boundary conditions in \(x\)- and \(y\)-directions to report the significance of atypical entropy variation for the thermodynamic system for both rectangular and square domain in figures 5 and 6.

Evolution of density for Cases 1 and 2 are shown in figure 7 for the complete domain. Here, the
flow is not periodic in $x$-direction and the points of interface meeting the side-walls are the major sources of initial perturbations, as observed in frames 2a) and 2b) at $t = 5$. These disturbances originating at the side-walls dictate the flow evolution during RTI evident in frames 3a) and 3b) at $t = 10$. Although there are no visible differences in figure 7, indeed there are significant differences right from the onset (in terms of vortical structures), as seen in the zoomed pictures of the interface in figure 8. For example, in frame 2a), one can notice distinct vortical structure at $t = 5$, while for the square box, flow evolves more due to delayed pressure reflections from top and bottom wall, which is responsible for delayed vortex structure formations. Quite contrary to classical fluid flow description, here the flow evolves from small scales, which propagate rapidly along the interface from both the ends (the triple points at the junction of the side-walls and the interface).
Figure 8. Zoomed density contours for the present simulations for rectangular (left) and square boxes (right) shown at: (1a, 1b) $t = 3.0$, and (2a, 2b) $t = 5.0$. Twisting and stretching at the interface can be visualized in frame 2b) which is absent in frames 1a) and 2a).

Summary
In the present analysis, Ash et al. [42]'s experimental data for air is used for a new model of second coefficient of viscosity, so that the bulk viscosity ($\kappa$) is not zero. In classical approach using Stokes’ hypothesis, one uses $\kappa = 0$ for compressible NSE. These results are compared in figures 3 to 6, from the onset of RTI till the time when mixing is complete ($t = 14$). It is clearly evident that the Stokes’ hypothesis promotes dissipation, while the calculations without the same hypothesis show sharper entropy variation. Initial growth is determined by formation of pressure waves, which is dependent on the value of bulk viscosity and this is evident in figures 3 and 4. The present research helps one obtain an alternative to using traditional Stokes’ hypothesis, which results in a more accurate representation of entropy variation that exhibits the non-equilibrium thermodynamics during RTI in an inhomogeneous system. In the near future, we will extend the present study of RTI to a 3D finite non-periodic box.

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