Forward and Reverse Modeling of the Three-Dimensional Viscous Rayleigh-Taylor Instability

Boris J.P. Kaus and Yuri Y. Podladchikov
Geologisches Institut, ETH Zentrum, Zürich, Switzerland

Abstract. A combined finite-difference/spectral method is used to model the 3D viscous Rayleigh-Taylor instability. Numerically calculated growth rate spectra are presented for an initial sinusoidal perturbation of the interface separating two fluids with amplitude $10^{-3}H$ and $0.2H$, where $H$ is the height of the system. At small initial amplitude, growth rate spectra closely follow linear theory, whereas the calculation with higher initial amplitude shows wavelength selection towards 3D perturbations. Numerical simulations and analytical theory are used to evaluate the applicability of previous 2D numerical models, which is shown to depend on (1) the wavelength and amplitude of an initially 2D sinusoidal perturbation and (2) the amplitude of background noise. It is also shown that reverse (backward) modeling is capable of restoring the initial geometry as long as overhangs are not developed. If overhangs are present, the possibility of restoring the initial conditions is largely dependent on the stage of overhang development.

Introduction

The Rayleigh-Taylor (RT) instability arising when a heavier fluid overlies a fluid with lower density has attracted attention of the Earth science community for some time. There are numerous situations, where a RT-type model is applicable to nature. Examples are batholiths [Pons et al., 1992], salt tectonics [Podladchikov et al., 1993], and convective thinning of the lithosphere [Houseman and Molnar, 1997]. The RT instability has been intensively studied by laboratory experiments [e.g. Talbot et al., 1991], analytical methods (linear and nonlinear stability analysis, e.g. Ribe, 1998; Conrad and Molnar, 1997) and numerical simulations (e.g. Schmeling, 1987; Podladchikov et al., 1993). Numerical calculations of the viscous RT instability, however, have been restricted to the 2D case, mainly because of limited computational power. Three-dimensional numerical simulations have been reported, but were done for viscous fluids with inertial forces (e.g. He et al., 1999). In this paper, forward and reverse numerical simulations of the 3D viscous RT instability in absence of inertial forces are presented.

Mathematical Model and Numerical Method

The Rayleigh-Taylor instability for the slowly creep- ing flow of viscous incompressible Newtonian fluids with constant viscosity is described by the Stokes system of equations, which are given by:

\[ \frac{\partial V}{\partial t} = 0 \]  
\[ -\frac{\partial P}{\partial x} + \mu \Delta V + \rho g = 0 \]  

where $P$ is pressure, $V=(u,v,w)$ is velocity, $x=(x,y,z)$ are coordinates, $\mu$=viscosity, $g=(0,0,-g)$ is the gravitational acceleration and $\rho$ is the density of the fluid. Non-dimensionalization was done taking $H$, $H^2g\Delta\rho/\mu$, $Hg\Delta\rho$ and $\mu/Hg\Delta\rho$ as characteristic length, velocity, pressure and time respectively, where $\Delta\rho$ is the density difference between the upper and lower fluid. The equations (1-2) are solved here for a Cartesian box with height $H$ and an aspect ratio of 5:5:1. The boundary conditions are periodic for the lateral directions and no-slip on the upper and lower boundaries. The numerical method used for solving eqns. 1-2 is a 3D extension of the method used by Schmalholz and Podladchikov [1999] to model folding instabilities. It uses a spectral method for the horizontal directions and a conservative finite difference method on a regular grid for the vertical direction. The interface-tracking algorithm is a 3D extension of the particle-line method described in [Ten et al., 1998].

Infinitesimal and Finite Growth Rate Calculations

An unstable system consisting of two superposed immisible fluid layers each of thickness 0.5 and same viscosity is considered. Infinitesimal initial perturbations on the interface separating the two fluids grow exponentially with time according to the relation $A(t) = A_0 \exp(gt)$, where $A_0$ is the initial amplitude, $q$ is the growth rate and $t$ is time, which can be calculated using a linear stability analysis (e.g. Chandrasekhar, 1961; Conrad and Molnar, 1997; Turcotte and Schubert, 1982). The initial spatial perturbations on the interface are split into a series of “normal modes”:

\[ z_{int}(x,y) = 0.5 + dh_{int}\cos(k_x x)\cos(k_y y) \]  

Copyright 2001 by the American Geophysical Union.

Paper number 2000GL011789.
0094-8276/01/2000GL011789$05.00
where \( k_x = 2\pi/\lambda_x \) and \( k_y = 2\pi/\lambda_y \) are wavenumbers in the \( x \)- and \( y \)-direction respectively, \( \lambda_x \) and \( \lambda_y \) are wavelengths in \( x \)- and \( y \)-direction, and \( dh_{int} \) is an infinitesimally small amplitude (\( dh_{int} \ll \lambda_x, \lambda_y \)). Each of these normal modes can be analyzed separately and has a non-dimensional growth rate \( q \):

\[
q = \frac{(k^2 + 2)e^{-k} - e^{-2k} - 1}{4k[-2ke^{-k} + e^{-2k} - 1]}
\]

where \( k = \sqrt{k_x^2 + k_y^2} \). The growth rate has a maximum of \( q = 0.03835 \) if \( k = 4.895 \). Note that eqn. (4) includes the 2D solution (e.g. [Turcotte and Schubert, 1982]) as a special case, i.e. \( k_y = 0 \). According to the linear stability analysis, which is only valid for very small perturbations of the interface, purely 2D waveforms have the same growth rate as an infinite number of 3D waveforms (composed by linear superposition of normal modes having wave number vectors of same length but different orientation). Thus a weakly nonlinear analysis is needed to constrain the pattern selection ([Ribe, 1998]), a situation similar to the Rayleigh-Bénard instability (see e.g. [Godrèche and Manneville, 1998] for discussion). The growth rate \( q \) can also be calculated numerically by assuming a similar initial sinusoidal perturbation but of finite amplitude \( dh \). The result of such a calculation is shown in Fig. 1. For initial amplitude of \( dh = 10^{-3} \), the numerically calculated growth rate approaches the analytical growth rate (eqn. 4) with an accuracy of 1% (Fig. 1a). However, calculations using larger initial amplitude (e.g. \( dh = 0.2 \), Fig. 1b) show a clear selection towards more 3D \( (\lambda_x = \lambda_y) \) normal mode perturbations. This result is in general agreement with the analytical calculations of Ribe [1998].

**Forward Modeling Results**

To study the competition between 2D and 3D initial perturbations, and thus to test the validity of previous 2D numerical simulations, we performed a forward simulation of an initial (non-dominant) 2D sinusoidal perturbation of the form \( z_{int}(x, y) = 0.5 - 10^{-2} \cos(2\pi x/5) \) with normally distributed (white) noise with a variance of \( 5 \times 10^{-4} \). Two-dimensional numerical simulations by Schmeling [1987] showed already that such a configuration is unstable and leads to the breakup of the initial perturbation. This was also observed in our three-dimensional simulation, with the difference that the initial 2D perturbation decomposes into irregular 3D structures (Fig. 2). A two-dimensional Fourier transform of the interface revealed that the simultaneous growth and superposition of several dominant 3D normal modes is responsible for the development of irregular 3D structures. A rough estimate of the survival of initial sinusoidal 2D perturbations vs. dominant normal modes growing out of the background noise can be made by using linear stability growth rates. The growth in amplitude of an initial 2D perturbation can be expressed \( A^{2D}(t) = A_0^{2D} e^{qt} \), whereas that of a dominant mode, growing out of noise, is \( A^{dom}(t) = A_0^{dom} e^{qt_{dom}} \). We define the characteristic time \( t^* \) as the time needed for an initial perturbation to reach an amplitude of 0.5. The initial perturbation survives if
KAUS AND PODLADCHIKOV: 3D VISCOUS RAYLEIGH-TAYLOR INSTABILITY

Figure 3. Phase diagram predicting the survival of an initial sinusoidal 2D perturbation over background noise depending on its initial amplitude \( A_0 \), initial wavelength \( \lambda_{2D} \) and the initial amplitude of the largest dominant normal mode present in the noise \( A_{dom}^0 \). Crosses show results of numerical simulations, where the initial perturbation survived, whereas open circles, x-marks and squares show results where the initial perturbation broke up into 2D, intermediate or 3D structures. Insets show the interface at the end of numerical simulations that resulted in 3D, intermediate and 2D structures respectively.

\[ A^{2D}(t^*) > A^{dom}(t^*) \]

This condition can be written as:

\[ \ln(A^{2D}_0/0.5) / \ln(A^{dom}_0/0.5) < q_{dom} \]  \( (5) \)

where \( q_{dom} \approx 0.03835 \) and \( q \) is calculated from linear stability analysis (eqn. 4). Full numerical simulations are in good agreement with the prediction of equation (5) and show that breaking up of the initial 2D perturbation leads in most cases to a 3D geometry (see Fig. 3). Equation (5) can thus be used to predict if an initial 2D perturbation will survive or breaks up into 3D structures.

Reverse Modeling Results

Inverse modeling is of major practical importance [Bennett, 1992; Marchuk, 1982] and reverse modeling of 3D diapiric structures is of special interest for earth scientists (e.g. 3D restoration of salt domes). Reverse modeling was done, using the same numerical code as for forward simulations, but with negative timesteps. Four reverse simulations, started at different stages, recovered the 2D initial perturbation (Fig. 4). Similar simulations showed that 1) reversing with a lower resolution (64x64x257) than that of the forward model gives approximately the same results, 2) the adding of lines to the interface, done in forward simulations, produces interpolation errors, which cumulate during reverse modeling and 3) these errors are even larger if overhangs are present. We thus speculate that restoration errors are partly due to cumulative growth of numerical errors and partly of physical origin. The physical origin of the noise effects can be explained by noting that the growth rate of the numerical errors during forward simulations is given by eqn. (4). The amplitudes of the errors grow exponentially \( (q > 0 \) for all wavelengths), but slower than the true physical (dominant) modes. Conversely, during forward modeling of stably stratified fluids or reverse modeling of initial stages of the RT instability (when overhangs are not developed yet), the numerical errors decay exponentially with a rate governed by eqn. 4, but \( q < 0 \). Therefore, it is to be expected that the reverse modeling of the RT instability is numerically more stable than the forward modeling. However, development of overhangs drastically changes the situation. The overturned layers are stably stratified and their modeling is better posed for the forward simulations then for the reverse ones. Small perturbations at the lower side of an overhang, which are due to the remeshing of the interface, start amplifying during reverse simulations. Reversing of the RT instability is thus difficult if overhangs are developed and the success of recovering the initial conditions depends on the stage of overturn development. The most extreme case would be a fully developed overturn (complete stable stratification), from which reversing will no longer recover the initial perturbation.

Figure 4. Reverse simulation of the 3D RT instability shown in Figure 2. (A) Contour plot of the interface height in the forward simulation at times \( t = 0, 85 \) and 170 respectively. (B) Reverse simulation starting from \( t = 255 \) in the forward simulation. (C) Reverse simulation starting from \( t = 170 \) in the forward simulation. (D) Reverse simulation which started from \( t = 170 \), but with added noise of maximum amplitude \( 5 \times 10^{-3} \).
Conclusions

We present fully dynamical numerical simulations of the 3D viscous RT instability. Forward simulations show that an initial 2D perturbation may decompose into 3D structures if the amplitude of background noise is high compared to the amplitude of the 2D perturbation. We quantified the 2D-3D transition, using linear stability theory (eqn. 5). Numerical simulations show good agreement with this prediction (Fig. 3). Reverse (backward) modeling of the RT instability is capable of restoring the initial 2D conditions from intensively deformed 3D structures. However, the accuracy of the reverse model deteriorates if overhangs are prominent in the 3D structures because the overhangs result in a stable configuration with little memory of the initial conditions.

Acknowledgments. We thank D. Schmid and S. Schmalholz for helpful discussions, G. Houseman, H. Schmeling and D. Yuen for reviews and J. Connolly for improving English of the paper.

References


B. Kaus and Y. Podladchikov, Geology Institute, Swiss Federal Institute of Technology, Sonnegstrasse 5, CH-8092 Zürich, Switzerland (e-mail: kaus@erdw.ethz.ch; yura@erdw.ethz.ch)

(Received May 11, 2000; revised July 19, 2000; accepted September 13, 2000.)