



Nonlinear Dynamics of a Diffusing Interface

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NONLINEAR DYNAMICS OF A DIFFUSING INTERFACE

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Excitation of two miscible viscous liquids inside a bounded enclosure in a microgravity environment has shown the evolution of quasi-stationary waves of various modes for a range of parameters. We examine computationally the nonlinear dynamics of the system as the interface breakup and bifurcates to resonance structures typified by the Rayleigh-Taylor instability mechanism. Results show that when the mean steady field is much smaller than the amplitude of the sinusoidal excitation, the system behaves linearly, and growth of quasi-stationary waves occurs through the Kelvin-Helmholtz instability mechanism. However, as the amplitude of excitation increases, nonlinearity occurs through subharmonic bifurcation prior to broadband chaos.

Introduction

We examine computationally the nonlinear dynamics of flow fields, which destabilizes an initially stable sharp interface between two miscible liquids inside a cavity. The two fluids are subjected to oscillatory vibration in a microgravity environment, and serve as a model to understand effects of g-jitter. The instability of the interface between the two miscible liquids caused by bifurcation of the flow field serves as a model problem to study transport phenomena in a wide range of microgravity applications such as crystal growth of acousto-optic optoelectronic materials, protein and solution crystal growth. We consider a parametric space of relevance to microgravity applications.

The microgravity environment is particularly useful for transport phenomena involving nonhomogeneous bulk fluids due to minimization of buoyancy induced flows. However, vibration effects, which cause g-jitter, can serve as a source to induce convective flows. In order to quantify effects of g-jitter we designed an experiment to study effects of prescribed sinusoidal forcing on the stability of two miscible liquids¹. The experimental results show that for the frequency band of interest (0.1 – 10 Hz) and disturbance amplitude (0.2 – 20 milli-g) the interface can indeed become unstable and generate quasi-stationary waves up to four modes. The instability of the interface was shown to be caused by Kelvin-Helmholtz (K-H) instability². The flow field destabilizes to an oscillating parallel shear flow and causes the interface to evolve like a vortex sheet. The parametric space for the experiment ranged from Stokes-Reynolds number (Res) of 0.002 to 0.5. In this computational study, we extend Res to 43.

We address the dynamical state of the flow field to gain insight on the predictability of the system. Of interest is the number of modes that can be generated for a quasi-stationary wave prior to its breakup. We examine the characteristic response of the system to various amplitude and frequency of excitation. We show that for Res $O(1)$ the flow field responds isochronously to the input excitation, thus generating a limit cycle. The number of modes generated at the interface is correlated with the magnitude of Res. With increasing Res, the system becomes nonlinear and responds with harmonics of the input frequency. A subharmonic bifurcation occurs, similar to a two torus bifurcation, prior to broadband chaos. In the neighborhood of the chaotic state, there is breakup of the interface. The mechanism of the breakup is due to Rayleigh-Taylor instability.

In the following, we consider an infinite dimensional system as a dynamical model. We analyze the dynamical state of the system from its time history, pseudo and phase space trajectories, and power spectrum. The dynamical state of the system is correlated with the local bifurcation of the interface.

Formulation

The problem of interest is shown in Figure 1, two miscible liquids with distinct density meet initially at a planar interface. This realization has been shown to be possible in a microgravity environment. The two fluids are subjected to a body force parallel to its interface. The body force

$$g(t) = ng_0 + mg_0 (\cos \omega t + \theta) \quad (1)$$

consists of the steady background DC component (ng_0), the excitation AC component with amplitude (mg_0), circular frequency ω , and phase angle θ .

The dynamical model of the problem consists of the Navier-Stokes equations coupled with species continuity. For a square cavity ($H=L$) with characteristic length, time and velocity scales selected as,

$$L_c = \sqrt{\bar{v}/\omega}, T = 1/\omega, U_c = \frac{\Delta\rho}{\bar{\rho}} \frac{mg_0}{\omega} \quad (2)$$

The dimensionless incompressible Boussinesq equations in vorticity-stream function relationship can be expressed as,

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\zeta \quad (3)$$

$$\frac{\partial \xi}{\partial t} + Re_s \left[u \frac{\partial \xi}{\partial x} + v \frac{\partial \xi}{\partial y} \right] = \left[\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} \right] + \quad (4)$$

$$(AR + \cos(t + \theta)) \frac{\partial C^*}{\partial x}$$

$$\begin{aligned} \frac{\partial C^*}{\partial t} + Re_s \left[u \frac{\partial C^*}{\partial x} + v \frac{\partial C^*}{\partial y} \right] = \\ \frac{1}{Sc} \left[\frac{\partial^2 C^*}{\partial x^2} + \frac{\partial^2 C^*}{\partial y^2} \right] \end{aligned} \quad (5)$$

The velocity components and vorticity are defined as,

$$u = \frac{\partial \psi}{\partial y}, v = -\frac{\partial \psi}{\partial x}, \xi = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \quad (6)$$

The boundary conditions are no-slip along the wall boundaries (Γ)

$$\vec{V} \cdot \vec{n} = 0 \text{ on } \Gamma \quad (7)$$

and the condition of impermeability normal (\vec{n}) to the boundary,

$$\nabla C^* \cdot \vec{n} = 0 \text{ on } \Gamma \quad (8)$$

Since we are considering an initial value problem, the concentration field has prescribed values of 1 and 0 for

the left and right fluids respectively, with a value of 0.5 for the interface,

$$C^*(x, y, z, 0) = \begin{cases} 1.0 & 0 \leq x \leq L/2 \\ 0.5 & x = L/2 \\ 0 & L/2 \leq x \leq L \end{cases} \quad (9)$$

The concentration field equation is normalized with $C^* = (C - C_B)/(C_A - C_B)$. The parametric space (Λ) of the above set of equations

$$\Lambda = \Lambda(Re_s, AR, Sc, \theta) \quad (10)$$

consists of the Stokes-Reynolds (Re_s) number, the amplitude ratio (AR), the Schmidt number (Sc), and the phase angle θ defined as,

$$Re_s = \frac{\Delta\rho mg_0}{\bar{\rho} \bar{v}^{1/2} \omega^{3/2}}, AR = \frac{n}{m}, Sc = \frac{\bar{v}}{D_{AB}} \quad (11)$$

For the parameters of interest, the Schmidt number is kept constant as well as the phase angle. Thus the flow field as well as the dynamical evolution of the interface can be expressed as a co-dimension two problem,

$$\vec{V} = \vec{V}(x, y, t; Re_s, AR) \quad (12)$$

We used finite difference to solve the coupled set of equations (3-5). Since we are interested in the asymptotic dynamics of the system, we used an explicit scheme with a third order Adams-Bashforth technique for time discretization. The Flux Corrected Transport algorithm is used to resolve the sharp discontinuity of the interface³. A 90×90 grid size is used for spatial resolution and found to be adequate over the parametric range of interest. We mostly varied Re_s for our parametric studies, however, we found that the results are sensitive to the magnitude of AR .

Discussion and Computational Results

The parametric space considered consists of variation of the amplitude of excitation (mg_0), input frequency (ω), while keeping the background DC acceleration ($ng_0 = 10^{-6}g_0$, $g_0 = 980 \text{ cm/sec}^2$) and phase angle ($\theta = 0$) fixed. The geometric length scales ($H=L=5 \text{ cm}$) and properties of the fluid ($Sc=1079$) are fixed. The range of parameters considered is shown in Table 1.

Table 1 – Range of Parameters, $ng_0=10^{-6}g_0$

f (Hz)	Res	AR
0.5	0.1908	2.5×10^{-4}
0.5	0.2386	2.0×10^{-4}
0.5	0.2863	1.67×10^{-4}
0.5	0.3818	1.25×10^{-4}
0.5	0.4772	1.0×10^{-4}
0.5	0.7158	6.67×10^{-5}
0.5	0.95	5.0×10^{-5}
0.33	1.78	2.50×10^{-5}
0.25	2.69	2.50×10^{-5}
0.5	2.85	1.67×10^{-5}
0.5	3.80	1.25×10^{-5}
0.5	4.75	1.0×10^{-5}
0.5	5.70	8.33×10^{-5}
0.5	6.67	7.14×10^{-6}
0.5	7.60	6.25×10^{-6}
0.5	8.55	5.56×10^{-6}
0.5	9.5	5.0×10^{-6}
0.5	10.45	4.55×10^{-6}
:	:	:
0.5	42.75	1.11×10^{-6}

The metric used to quantify the response of the interface to various excitation input is its wavelength (λ) which is a function of Res and AR,

$$\lambda = \lambda(\text{Res}, \text{AR}) \quad (13)$$

Even the co-dimension two bifurcation problem is a formidable computational task because the system loses and gains stability over a dense parametric set similar to the logistic map model⁴. Even though all the fine details of the bifurcation sequence are not computed, the range of parameters in Table 1 gives a broad glimpse on typical scenarios. Over most of the parametric space, we varied mg_0 , a narrow range of ω was considered.

Effect of Flow Field on Dynamics of Interface

In order to correlate the dynamical equilibrium of the flow field in phase space with the interface response, we show in Figure 2 the local bifurcation of the quasi-stationary wave as a function of Res. The wavelength of the q-s wave decreases, or the number of modes increases, as Res increases. Breakup of the interface occurs in the neighborhood of Res=8.55 for which q-s waves no longer exist. The number of modes is dictated by the number of bends in the interface, an S shape has two modes. Transition from two to four mode q-s wave occurs for

Res>0.29. Typical interface response of four mode q-s wave is shown for Res=0.72; the four mode response extends up to Res=1.78. The mode number at the interface is sensitive to the threshold of AR, for example at Res=0.34 and AR= 5×10^{-5} a four mode structure can be suppressed by increasing AR to 1.25×10^{-4} , only two modes result. There is a transition from 4 to 8 primary modes for Res=2.85; note 3 secondary modes occur with very small wavelength at the top and bottom boundaries. This bifurcation occurs in the neighborhood of Res=1.9.

The mechanism which generates q-s waves for Res O(2.85) is basically the Kelvin-Helmholtz (K-H) instability. A row of parallel vortices is generated along the interface. These vortices serve as rotors, which stretch and fold the interface. As Res increases, Res O(4.75), there occur secondary waves riding on the primary modes on the interface. The K-H instability mechanism manifest itself perpendicular to the interface to form vortex rows. The interface no longer forms q-s waves, rather stretches and folds continuously to generate roll-up structures as typified by the Rayleigh-Taylor instability⁵. Only the initial state of the interface structure is shown, the flow field becomes quite complex with vortices occupying the entire cavity. The state of the flow field is chaotic as will later be shown.

The wavelength (λ) of the interface, up to the breakup, decreases asymptotically as Res increases, shown in Figure 3. The wavelength is estimated from its average value at the center of the cavity. The dependence of λ on Res follows a power law

$$\lambda \propto C \text{Res}^{-n} \quad (14)$$

C is a constant and n is less than 1; the decrease in wavelength is similar to a turbulent cascade. In contrast the maximum magnitude of the velocity $|V|_{\max}$, shown in Figure 4, increases with Res and also follows a power law in which n is greater than 1,

$$V_{\max} \propto C \text{Res}^n \quad (15)$$

The functional relationship of λ and V_{\max} on Res illustrate the global trends. Much more details would be needed to show the bifurcation details as found for example in the logistic map.

Dynamical State of the Flow Field

We characterize the dynamical state of the system from the time history of the asymptotic dynamics of the flow field. The limit set of the time history is obtained

from both the pseudo and phase space trajectories. For a given frequency and amplitude of excitation, the response of the system is obtained from its power spectrum. The estimated power spectrum for the v component of the velocity field is calculated from,

$$\tilde{P}_v(f) = \frac{1}{R} \left| \int_0^R V(t) e^{-i2\pi f t} dt \right|^2 \quad (16)$$

in which R is the finite duration of the time interval. The smooth spectral estimate $P_v(f)$ is obtained using a Hanning window for filtering, and a convolution relation as,

$$P_v(f) = W_s(f) * \tilde{P}_v(f) \quad (17)$$

$W_s(f)$ is the spectral window for filtering. The power spectrum is estimated using the Cooley-Tukey algorithm, which employs the use of Fast Fourier Transforms^{6,7}. The dynamics of the flow field is evaluated from a representative point of the flow field. For each data set we kept 10,000 points.

We now analyze the dynamical state of the flow field, which generates the q - s waves shown in Figure 2. For low $Res=0.19$ which yields a two-mode q - s wave, the flow field oscillate isochronously, see Figure 5a, with the input frequency $f=0.5$ Hz. The power spectrum shows that the v component of the flow field responds with a frequency of 0.5 Hz, the same scenario was found for the u component. The pseudo-phase space trajectory, found by lagging the velocity with a constant k , of the v component indicates that the dynamics approach a limit cycle attractor for the selected location (0.33, 0.56) in the flow field. This indicates that for the given parametric input to the system, its future behavior will always tend to oscillate in phase with the input frequency.

When nonlinearity becomes important, Figure 5b $Res=0.48$, harmonics of the fundamental frequency appear. While the u component of the velocity field is periodic, as shown above, the v component of the velocity shows a decrease in amplitude with every oscillation. The combination of the signal is shown in the phase space trajectory, which shows a nonchaotic attractor. This attractor is a smooth surface with the attributes of stretching and folding in phase-space.

With increasing nonlinearity in the system, Figure 6 $Res=0.72$, the flow field responds with a modulated amplitude signal in the v component. Such modulation gives rise to nonchaotic attractors as evidence from the pseudo-phase space trajectory of $v(t+k)$; this attractor is

similar to the Rossler funnel⁸. The flow field responds with harmonics (1.0, 1.5 Hz) of the fundamental input frequency of 0.5 Hz; the 1.5 Hz component is very minute and is barely discernible. The gradual decrease in the amplitude of the u component of the velocity field gives rise to the dense limit cycle attractor. The combination of the signal of the u and v component is shown in the (u, v) phase-space trajectory, which shows the evolution of a nonchaotic attractor. It is known that strange nonchaotic attractors exist for quasi-periodically forced systems^{9,10,11}, however they are not smooth manifolds in phase space. Even though the attractors shown in Figure 6 are nonchaotic, they are not strange. This study gives insight into parametric regions for which an infinite-dimensional system may display these so-called strange nonchaotic attractors.

A rational subharmonic bifurcation is shown in Figure 7. When Res is increased to 1.78 for an input frequency of 0.33 Hz, both the u and v component of the velocity field show harmonic response of the fundamental frequency. A complex nonchaotic attractor illustrating stretching and folding arises in phase-space. A subharmonic bifurcation occurred in the neighborhood of $Res=2.69$, $AR = 2.5 \times 10^{-5}$. In contrast to the above cases, both the u and v components show response at one-half the input frequency of 0.25 Hz as well as higher harmonics. The response frequency of the system is phase-locked to the input frequency due to the rational relationship of the frequency ratio. Note that a subharmonic attractor is generated in phase space with a contraction of volume, since the system is dissipative; this reduces the complexity of the attractor in comparison to the lower values of Res . The amplitude ratio AR plays a significant role in the bifurcation sequence, for the same Res value of 2.69 if AR increases to 1.7×10^{-5} then the subharmonic bifurcation disappears, only harmonics of the fundamental frequency occurs.

The dynamics of the system for which it transitions from q - s waves to tendril structures and breakup is shown in Figure 8. Corresponding to the tendril structure, $Res=4.75$, is an irrational frequency component of the fundamental input frequency shown in the power spectrum. Similar to $Res=2.69$, there is a subharmonic attractor with contraction of volume in phase space. This corresponds to the two-torus bifurcation as proposed by Newhouse, Ruelle, and Takens¹². The mechanism of K-H instability which causes secondary waves on the interface gives rise to the complexity of the flow field which generates these waves. In the neighborhood of the breakup region, $Res=7.6$, there is a resulting broadband power spectrum distribution which shows that the system responds to all the frequency components within the interval of 1.0 Hz. Since the dynamics of the system

changes after breakup, we partitioned the signal of the v component into two intervals. Contraction of volume occurs in phase space for the first interval. The second interval from 160 to 400 secs shows the asymptotic dynamics of the system which yields a chaotic attractor. This attractor has the attributes of folding and stretching which typifies unpredictability. The results for Re_s in the interval of 7.6 to 42.75 show that there is a sequence of window for which the system gains stability to become periodic and loses stability to become chaotic similar to the logistic map.

Summary and Conclusions

We considered the nonlinear dynamics of flow fields, which destabilizes an interface through the Kelvin-Helmholtz instability mechanism to cause quasi-stationary waves. The wavelength decreases asymptotically as Re_s increases up to the breakup region; the decrease in wavelength is similar to a turbulent cascade). We show that when the system becomes nonlinear there is a transition from two to four mode q - s waves which gives rise to a host of nonchaotic attractors due to harmonics of the fundamental frequency in the response signal of the velocity component. Bifurcation of the system from q - s waves to tendril structures introduces a rational subharmonic bifurcation. Chaos occurs through an irrational subharmonic bifurcation, which corresponds to a two-torus bifurcation; the interface breaks up and the Raleigh-Taylor type of instability is manifested. Though Re_s was not varied continuously to capture all the bifurcation details, the subset of the parametric space considered lead insight into the dynamical behavior of the system.

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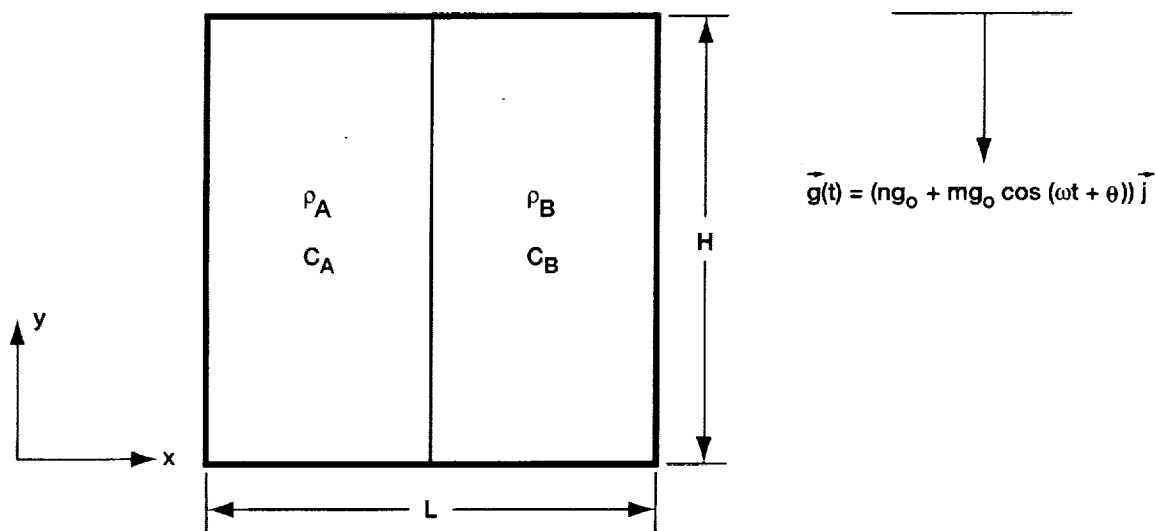


Figure 1—Physical description of two fluids in contact at an interface.

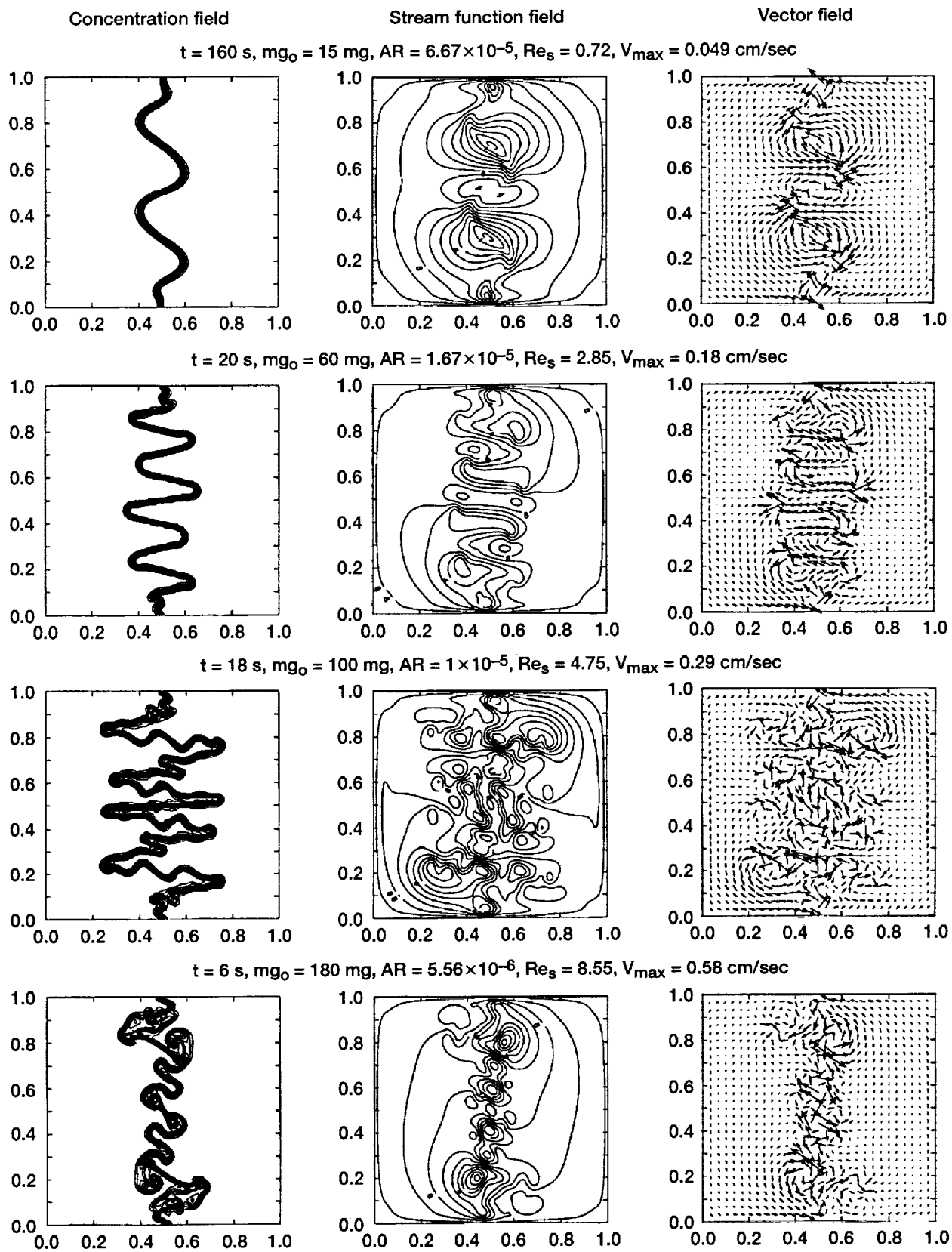


Figure 2.—Bifurcation of quasi-stationary waves showing increasing density of modes up to breakup ($Re_s = 8.55$), $f = 0.5 \text{ Hz}$, $ng_0 = 10^{-6}g_0$.

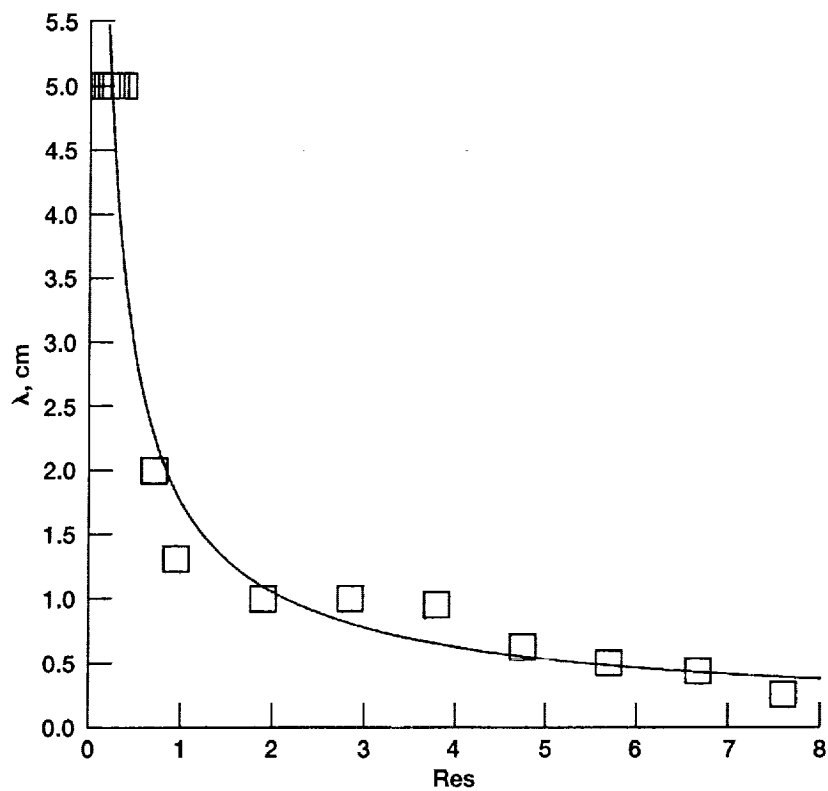


Figure 3.—Wavelength (λ) as a function of Stokes-Reynolds number.

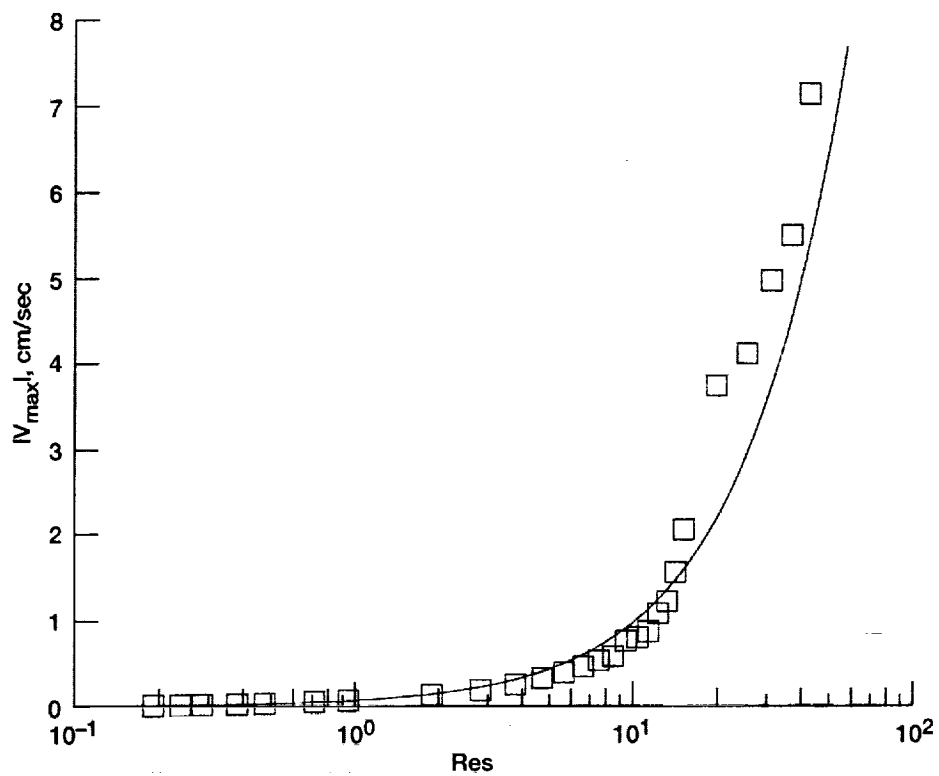


Figure 4.—Maximum velocity as a function of Stokes-Reynolds (Res) number.

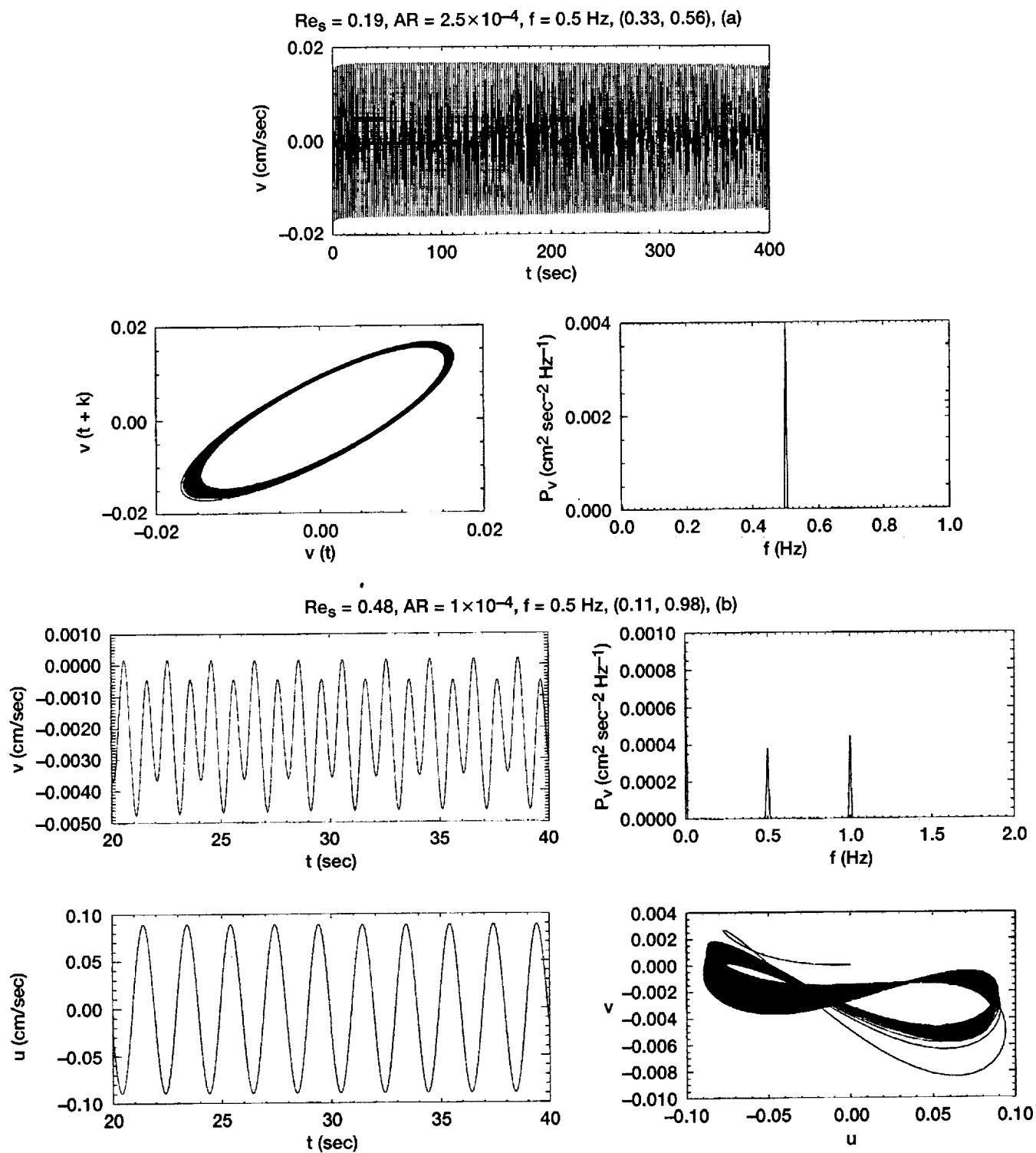


Figure 5.—Limit cycle ($Re_s = 0.19$) and nonchaotic attractor ($Re_s = 0.48$) due to aperiodic component of velocity field.

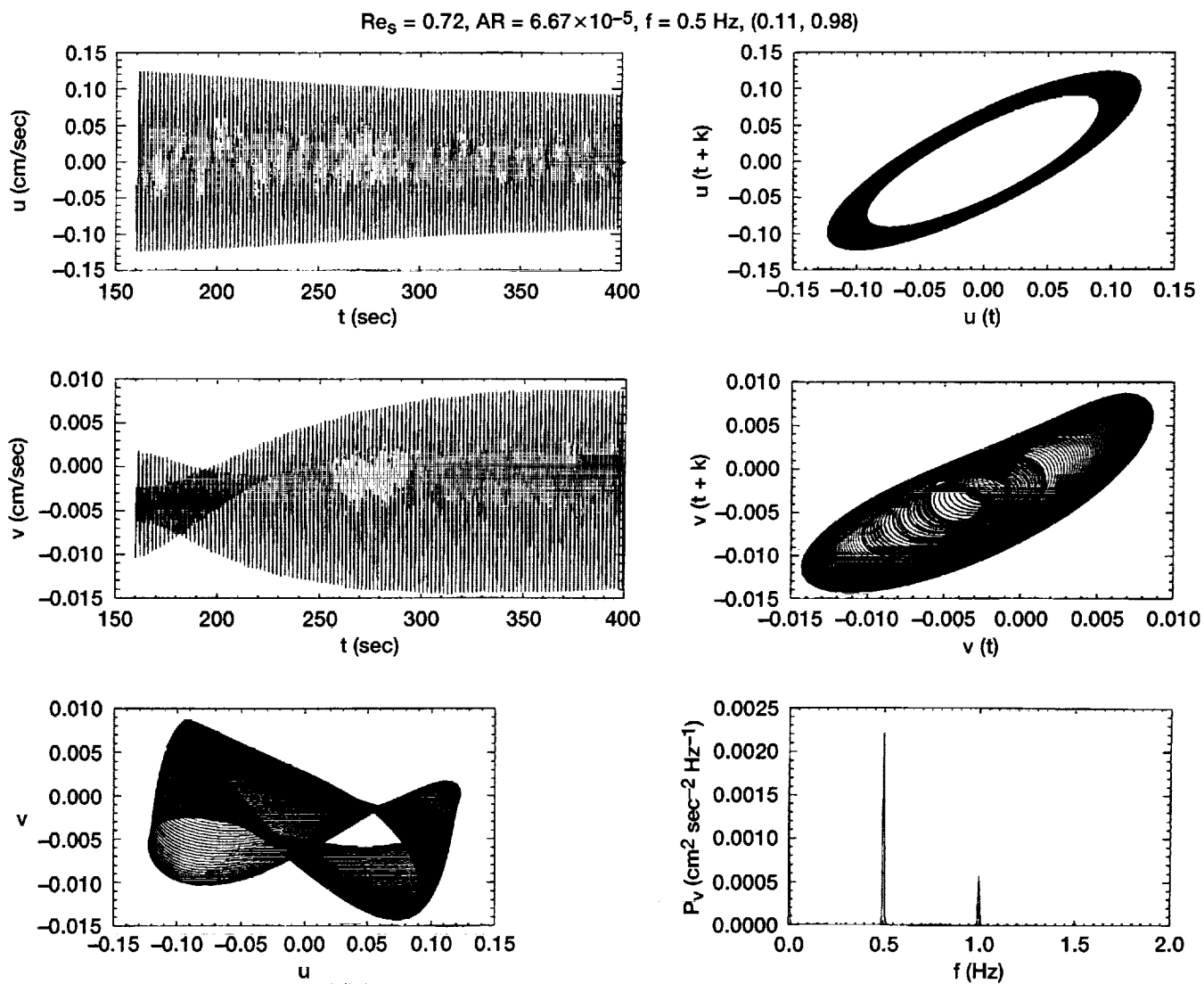


Figure 6.—Nonchaotic attractor due to periodic and amplitude modulated components of velocity field.

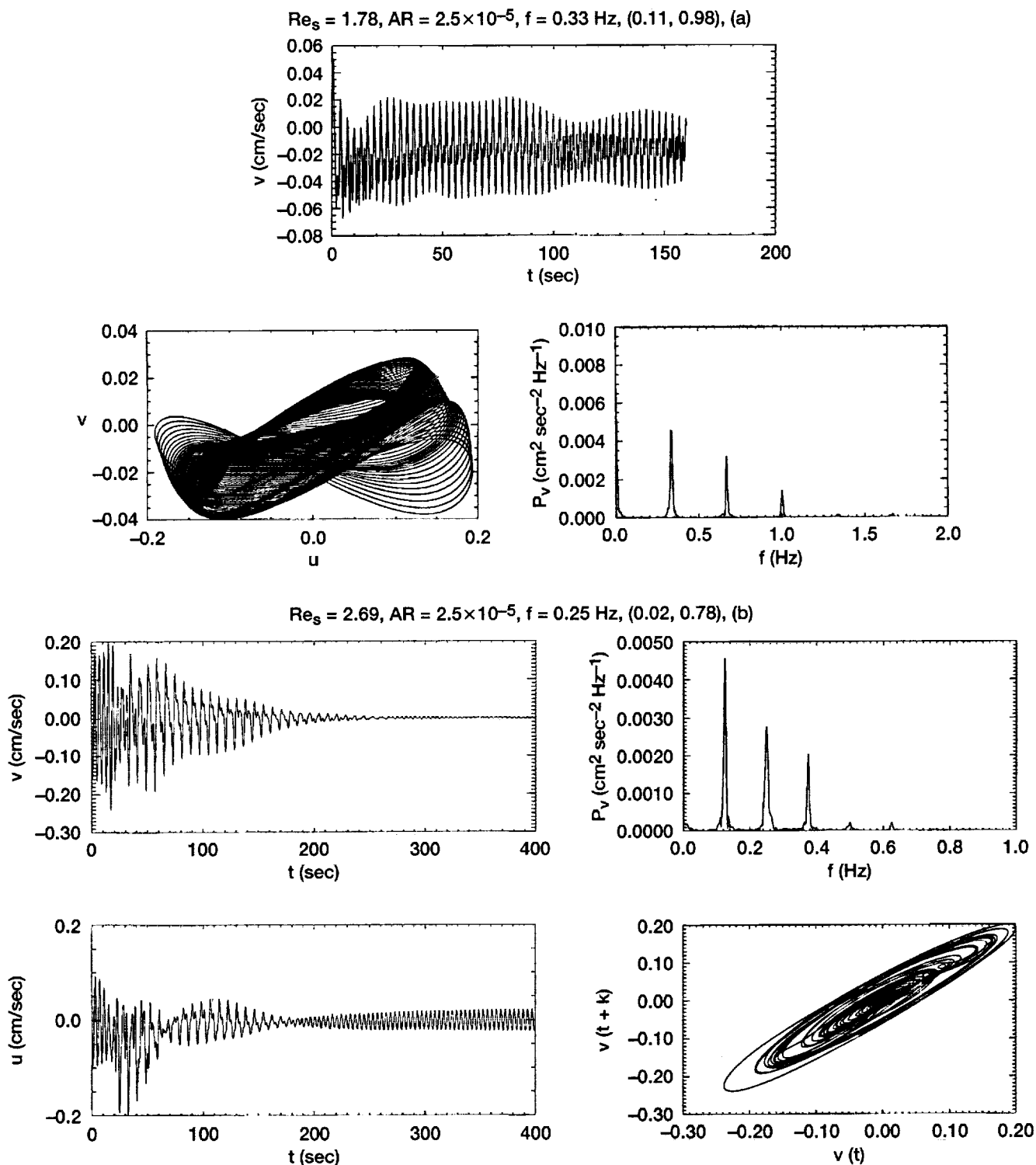


Figure 7.—Rational subharmonic bifurcation of velocity field.

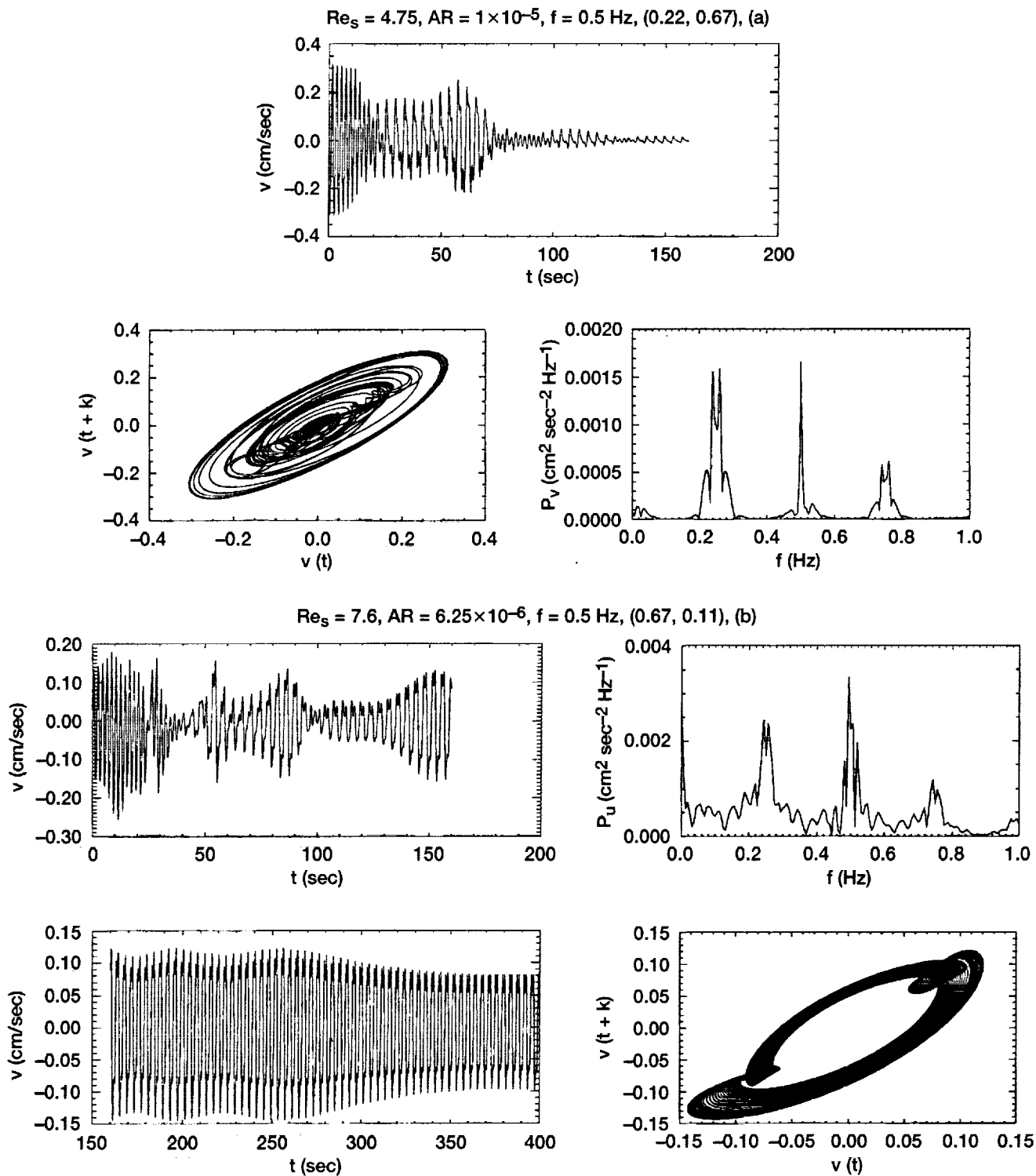


Figure 8.—Transition to chaos via irrational subharmonic bifurcation.

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