XXI ICTAM, 15–21 August 2004, Warsaw, Poland

CHAOTIC ADVECTION AND MIXING IN PULSED SOURCE–SINK SYSTEMS

Mark A. Stremler, Baratunde A. Cola
Department of Mechanical Engineering, Vanderbilt University
VU Station B 351592, Nashville, TN 37235, USA

Summary Laminar mixing in high-aspect-ratio volumes can be achieved by pulsing an arrangement of source–sinks pairs. We will present a chaotic advection analysis for pulsed source–sink systems in unbounded, circular, and rectangular domains. This analysis will be used to identify the optimal operating parameters for producing chaos.

INTRODUCTION

Achieving efficient and uniform mixing of laminar flows in high-aspect-ratio volumes is of practical interest in the design of many micro- and meso-scale fluid systems. One example of particular importance is DNA microarray analysis, a biological tool used widely in genomic research [1]. The typical microarray implementation uses DNA molecules suspended in a fluid volume that is approximately 7.5 cm by 2.5 cm by 50 μm, which we can view as a Hele–Shaw cell. The success of this tool depends in large part on having the suspended molecules uniformly sample as much of the surface as possible. Standard usage relies solely on molecular diffusion of the DNA and thus requires long sample times (at least 12 hours) and high DNA concentrations; both of these requirements limit the incredible potential of this technology. One would expect that improved results can be obtained by transporting the molecules with an imposed flow, and that significant enhancement is achieved when the flow produces chaotic advection. We refer to this process of building a system to mix by chaotic advection as 'designing for chaos' [2].

Under the Stokes flow approximation, the depth-averaged velocity in a Hele–Shaw flow can be represented by a velocity potential. Thus, assuming that the transport of molecules across the surface is determined by the depth-averaged velocity, an effective mixing system can be designed by considering chaotic advection in a two-dimensional potential flow. The flows of interest will transport molecules on a time scale much shorter than that of diffusion, so we expect the flow kinematics to provide a good representation of the overall molecule dynamics.

A potential flow that generates chaotic advection and can be implemented in a practical device [3] is produced by pulsing an arrangement of sources and sinks. Jones and Aref [4] present a comprehensive analysis of chaotic advection in a system consisting of one point source and one point sink in the unbounded plane. The source and sink each have strength q and are operated alternately, with switching between the singularities occurring periodically with frequency $1/T$. An important component of this system is the procedure whereby fluid extracted at the sink is subsequently reinjected at the source. The analysis in [4] concentrates primarily on a 'first out–first in' protocol that can be realized physically by collecting the extracted fluid in a tube beneath the sink, then turning the tube over and reinjecting the fluid at the source. It is shown in [4] that the flow is dominated by chaotic advection over a wide range of operating parameters. The details of the chaos change with the reinjection procedure, but the occurrence of chaotic advection persists.

The results for the unbounded plane provide a reasonable basis for designing a high-aspect-ratio mixing device. A variation on this system has been applied to enhancing microarray analysis [5], with preliminary results demonstrating that increased signal levels can be achieved an order of magnitude faster with pulsed source–sink mixing than with the traditional method. In contrast to the existing chaotic advection analysis [4], the real flow is bounded and the sources and sinks must operate in pairs in order to conserve volume. These are substantial changes that will impact the extent and character of the chaos, and thus an optimization of mixing in this system must be based on an analysis of chaotic advection in a bounded domain with source–sink pairs. Analytic solutions exist for source–sink pairs in unbounded and various bounded domains, making it possible to carry out a comprehensive analysis similar to that in [4]. We will present the results of this analysis for pulsed source–sink pairs in unbounded, circular, and rectangular domains.

MATHEMATICAL FORMULATION

Consider first the flow due to a source–sink pair in the unbounded plane. Superposition of a point source with strength q located at $z_{\rm p} = x_{\rm p} + {\rm i}y_{\rm p}$ in the complex plane and a sink with strength q at $z_{\rm n}$ produces a flow with complex potential

$$F(z) = (q/2\pi)\left[\log\left(z - z_{\rm p}\right) - \log\left(z - z_{\rm n}\right)\right]. \tag{1}$$

Time dependence, and hence the opportunity for chaotic advection to occur, is introduced into the system by periodically switching operation among a set of source–sink pairs. Here we will consider only two source–sink pairs, $(z_{\rm p1}, z_{\rm n1})$ and $(z_{\rm p2}, z_{\rm n2})$, but more complex arrangments are obviously possible. For a period of time T the motion of a particle in the plane is governed by (1) with $(z_{\rm p}, z_{\rm n}) = (z_{\rm p1}, z_{\rm n1})$. This flow is then stopped, and the particle is advected for time T with $(z_{\rm p}, z_{\rm n}) = (z_{\rm p2}, z_{\rm n2})$. Switching between the two pairs is continued periodically. Particles extracted from the domain through a sink are reinjected through a source during the next cycle of operation. Thus, for example, particles extracted through $z_{\rm n1}$ are reinjected through $z_{\rm p2}$.

The motion of a particle at z in the upper half plane due to a point source with strength q at $z_{\rm p}$ and a point source with

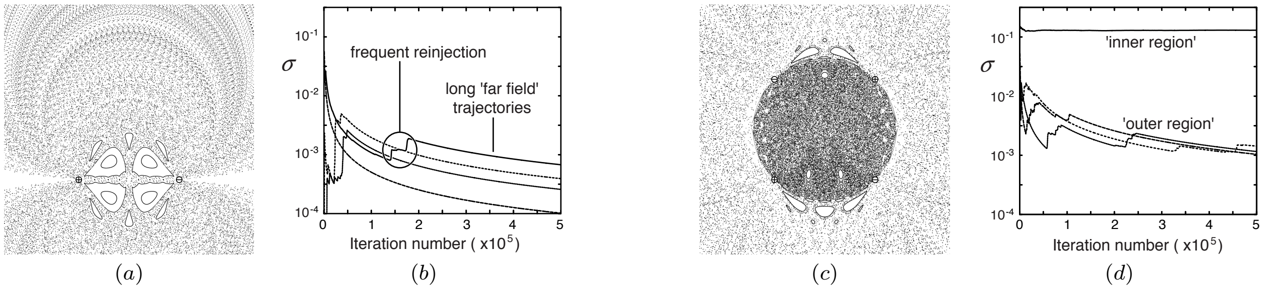

Figure 1. Chaos diagnostics for two pulsed source-sink systems in the unbounded plane. Sources are indicated by $\oplus$ and sinks by $\ominus$. Panels (a) and (c) show Poincaré maps, and (b) and (d) show convergence of the positive Lyapunov exponent for different initial positions. The system in (a)–(b) consists of one source and one sink operated alternately as in [4]. In (c)–(d) the right source and sink are operated as a pair, and then the left source and sink are operated as a pair. The dark circular area in (c) is the 'inner region'.

strength q at z_{n} is governed by the complex potential

$$F(z) = (q/2\pi)\,\big[\log(z - z_{\mathrm{p}}) + \log(z - \overline{z_{\mathrm{p}}}) - \log(z - z_{\mathrm{n}}) - \log(z - \overline{z_{\mathrm{n}}})\big], \tag{2}$$

where the overbar denotes complex conjugation. A variety of bounded domains can be obtained from (2) by conformal mapping of the z-plane to the w-plane. Circular and rectangular domains are given by the mappings

$$w = (\mathrm{i} - z)/(\mathrm{i} + z) \qquad \text{and} \qquad w = \big[1 + \mathrm{sn}^{-1}\big(K(k)\,z, k\big)\big]/2, \tag{3 a, b}$$

respectively, where $\mathrm{sn}(z, k)$ is the Jacobian elliptic sine, $K(k)$ is the complete elliptic integral of the first kind, and the parameter k is determined by the aspect ratio α of the domain through

$$\alpha = \big[K\big(\sqrt{1-k^2}\big)\big]/[2\,K(k)].$$

Operation of these systems is the same as described for the unbounded plane.

RESULTS AND OUTLOOK

Chaos diagnostics such as Poincaré maps and Lyapunov exponents are computed by numerically integrating a given particle forward in time under the constraint that during a cycle of operation the particle remain on its streamline, given by $\psi(x, y) = \mathrm{Im}[F(z)] =$ constant. Some illustrative results are shown in Figure 1 for the unbounded plane.

Panel (a) shows a Poincaré map for a case with only one source and one sink, as analyzed in [4]. There are several elliptic islands close to the source and sink, but much of the domain is occupied by the chaotic sea. The motion of a particle in the chaotic sea is characterized by periods of frequent extraction and reinjection interspersed with long forays away from the singularities along essentially curved paths. The convergence of the Lyapunov exponents in Panel (b) clearly indicates that the rapid stretching associated with chaos is caused by frequent reinjection, while the long far-field trajectories are essentially regular.

Panel (c) shows a Poincaré map for a case with two source-sink pairs arranged on the vertices of a square. The scale of the system and the operation time T are the same as in Panel (a). Particles in the far field experience long, essentially regular trajectories similar to those above. The influence of the source–sink pairs is seen in the 'inner region'. For the choice of parameters used in Panel (c), a particle in the inner region is trapped there for all time and avoids being carried into the far field. Thus this inner region experiences a sustained level of rapid stretching, as shown in Panel (d).

Bounding the domain on a scale similar to the source–sink separations forces all of the particles to remain near the sinks, eliminating the far-field trajectories and causing almost all particles to experience frequent reinjection and high levels of chaos. Pulsed source–sink pairs in a bounded domain are thus expected to mix even better than the original unbounded analysis suggests.

The details of the chaotic advection in bounded domains depend upon the domain shape and size, the source–sink configuration, the reinjection procedure, and the operation time T. We will present the results of an analysis that identifies the optimal operating parameters for producing chaos in pulsed source–sink systems.

References

[1] DeRisi J.L., Iyer V.R.: Genomics and array technology. *Curr. Opin. Oncol.* **11**:76–79, 1999.

[2] Stremler M.A., Haselton F.R., Aref H.: Designing for chaos: Applications of chaotic advection at the microscale. *Phil. Trans. Roy. Soc. London* A, in press.

[3] Evans J., Liepmann D., Pisano A.P.: Planar laminar mixer. In *Proc. IEEE Int. Workshop Micro Electro Mech. Sys., Nagoya, Japan, Jan. 26–30*, pp. 96–101, 1997.

[4] Jones S.W., Aref H.: Chaotic advection in pulsed source-sink systems. *Phys. Fluids* **31**:469–485, 1988.

[5] McQuain M.K., Seale K., Peek J., Fisher T., Levy S., Stremler M.A., Haselton F.R.: Chaotic mixer improves microarray hybridization. *Anal. Biochem.*, in press.