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THE SIMULATION OF CHAOTIC MIXING AND DISPERSION FOR PERIODIC FLOWS IN BAFFLED CHANNELS

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Abstract—We report numerically generated flow visualisation simulations for the flow of an incompressible Newtonian fluid within a two-dimensional channel which can contain periodic baffles. For *unsteady* flows in this geometry a regime of chaotic advection is observed when baffles are present. The unsteadiness takes one of two forms: a "natural" unsteadiness caused by a symmetry breaking instability of the flow, or a "forced" unsteadiness generated by applying an oscillatory component to the flow. This chaotic advection is shown to provide an efficient mixing mechanism and has a number of applications in the process industry. Enhanced transverse mixing is observed which results in increased transfer properties, reduced fouling rates and, in some circumstances, a reduction in axial dispersion, as recently experimentally reported in the literature.

INTRODUCTION

The observation that simple two-dimensional unsteady flows can result in chaotic advection was clearly demonstrated by Aref (1984), and other authors (e.g., Chaiken *et al.*, 1986, Chien *et al.*, 1989). A detailed study of chaotic mixing has been published by Ottino (1989), and an excellent review of the application of chaos in dynamical systems to chemical engineering is given by Doherty and Ottino (1988). There seems obvious applications of these observations to a process engineering situation where efficient mixing is often an important requirement. By forcing the flow into an unsteady chaotic mixing regime the mixing rates can be rapidly increased and controlled. Most of the work carried out so far on chaotic advection has concentrated on simple flow regimes in simple geometries (e.g., the blinking vortex potential flow studied by Aref, 1984, or the low Reynolds number cavity flow studied by Chien *et al.*, 1986). The aim of this paper is to demonstrate the potential of chaotic advective mixing in a ducted "engineering" geometry for a non-linear flow regime.

Bellhouse *et al.* (1973) have made pioneering studies of the way in which long stroke oscillations can improve fluid mixing in furrowed channels. Typically their device operates with a peak oscillatory Reynolds number ($Re_0 = \rho 2\pi\Omega x_0 H/\mu$) in the range of 0–100, and Strouhal number [$St = (1/2\pi)(H/x_0)$] in the range 10^{-3}–5×10^{-2}, where ρ and μ are the fluid density and viscosity, respectively. Ω the frequency of oscillation, x_0 the centre to peak amplitude of oscillation and H the maximum channel width. Sobey (1980) carried out extensive two-dimensional numerical studies for this flow regime and Stepanhoff *et al.* (1981) found good agreement between simulated and observed flow patterns. Brunold *et al.* (1989) found that efficient eddy mixing could be achieved in sharp edged channels and baffled tubes, and Dickens *et al.* (1989) observed that short stroke flow pulsation in a baffled tube could also give a near plug flow residence time distribution for the regime $St = 2$, $Re_0 = 550$ and net flow Reynolds number (based on mean velocity and tube diameter) $Re_n < \sim 100$. From experimental flow pattern studies an optimum geometry for mixing was established with a baffle area constriction of order 50% and a baffle spacing of order 1.5 tube diameters (Brunold *et al.*, 1989).

Using a two-dimensional simulation, we wish to show clearly the different regimes of behaviour that can be found for laminar flow in a baffled channel. The use of colour graphics to display the results of "particle tracking" simulations enables a direct visual appreciation of aspects relating to both mixing and dispersion. For unsteady flows, such techniques are necessary in order to capture the full motion of fluid in the system. Instantaneous plots of, for example, the velocity field at various times in the flow are inadequate, as the length scale for fluid motion between plots is not conveyed.

There are a wide range of possible variables, and for this study the observations are restricted to simple geometries, namely either a reference parallel channel or a periodic baffled channel of the specification shown in Fig. 1. The numerical simulation will explore the effect of net flow Reynolds number Re_n and peak oscillatory Re_0 at a fixed St of 1.0.

THE NUMERICAL SIMULATION

The simulation used for this work is in two parts: a fluid mechanics model, which generates a velocity field, and a particle advection procedure, which calculates the locations of (in this case) *passive* marker particles as they are advected by the velocity field.

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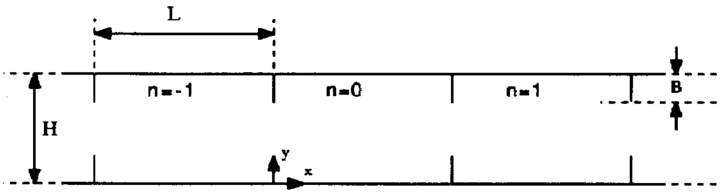

Fig. 1. The baffled channel geometry.

The fluid mechanics model is in the form of a vorticity–stream function finite difference solver for an incompressible Newtonian fluid and the scheme used is based on the work of Sobey (1980) for furrowed channels, and Howes (1988) for ducted tubes. The definition of a stream function restricts the model to *two spatial dimensions*.

The equations presented below are in a dimensionless form, with velocities scaled with peak mean oscillatory velocity ($2\pi\Omega x_0$), dimensions scaled with channel width (H), and time with the frequency of oscillation ($t = t^*\Omega$, where t^* is the dimensional time). For flows with no oscillatory component the scaling is slightly different: velocities are scaled with the mean velocity (U), and time with a combination of the mean superficial velocity and the channel width ($t = t^*U/H$). The numerical techniques used are identical for both cases.

Vorticity (ω) and stream function (ψ) are defined in the usual way;

$$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \tag{1}$$

$$u = \frac{\partial \psi}{\partial y} \tag{2}$$

$$v = -\frac{\partial \psi}{\partial x} \tag{3}$$

where u and v are the dimensionless velocities in the x- and y-directions respectively (see Fig. 1 for x and y).

These definitions lead to a Poisson relationship between ω and ψ;

$$\omega = -\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right). \tag{4}$$

From the two-dimensional Navier–Stokes equation and eq. (1), the vorticity transport equation can be derived:

$$\frac{\partial \omega}{\partial t} = -\frac{1}{St}\left(\frac{\partial(u\omega)}{\partial x} + \frac{\partial(v\omega)}{\partial y}\right) + \frac{1}{ReSt}\left(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}\right). \tag{5}$$

For the geometry of Fig. 1 the boundary conditions for these equations are as follows:

(1) No slip at the walls;

$$u = v = 0 \text{ on all walls and baffles} \tag{6}$$

(2) The total volumetric flowrate is equal to the difference in the stream function at the top and bottom walls;

For $t < 0.25$;

$$\psi = \left(\frac{\beta}{2} + \frac{1}{2}\right)\sin(2\pi t) \quad \text{at the top wall} \tag{7}$$

$$\psi = -\left(\frac{\beta}{2} + \frac{1}{2}\right)\sin(2\pi t) \quad \text{at the bottom wall} \tag{8}$$

And for $t \geqslant 0.25$;

$$\psi = \frac{\beta}{2} + \frac{1}{2}\sin(2\pi t) \quad \text{at the top wall} \tag{9}$$

$$\psi = -\left[\frac{\beta}{2} + \frac{1}{2}\sin(2\pi t)\right] \quad \text{at the bottom wall} \tag{10}$$

where

$$\beta = \frac{Re_n}{Re_0} \tag{11}$$

giving a sinusoidal volumetric oscillation.

For steady flows, the stream function is simply set to -0.5 and 0.5 at top and bottom walls respectively, with a similar 1/4 sine wave acceleration from rest. Note that the stream function boundary conditions are symmetric in order to avoid the accumulation of asymmetric numerical errors. In all cases the flow is accelerated from rest at $t = 0$ and observed to reach a fully developed state for long times ($t > \sim 10$). All results presented in this paper are for fully developed flows that are either steady or periodic.

Finite difference versions of eqs (2)–(5) form the base equations for the numerical simulation. The vorticity transport eq. (5) is used to step forward in time, the Poisson-like eq. (4) is then solved for the stream function and the velocities are obtained from the definition of stream function eqs (2) and (3). Centred differencing is used for accuracy and the explicit leap-frog method of Dufort and Frankel [see Roache, 1967] is used for the time stepping of the vorticity transport equation. The length of the time step is chosen to retain numerical stability and typically for these simulations was 0.005.

The difference equations are solved on a fine grid of 34×33 points, over one cycle of the geometry, using a regular spacing of grid points. The flow is assumed to be spatially periodic, with the flow in each cell identical. This is achieved numerically by substituting forwards and backwards the conditions at the exit and entry of each cell. Further details of the numerical techniques are described by Howes (1988) and Roberts (1989).

The movement of a particle X, located at (x', y') at time t is defined by the following equation:

$$u_{X,t} = \frac{1}{St} u(x', y', t) \tag{12a}$$

$$v_{X,t} = \frac{1}{St} v(x', y', t) \tag{12b}$$

where $u_{X,t}$ and $v_{X,t}$ are the velocities of particle X in the x- and y-directions at time t.

The tracking of particles is performed using a numerical integration of eq. (12) at each time step for an array of particles distributed uniformly through one cell of the geometry. Molecular diffusion may also be included in the motion of the particles by adding a random (Brownian) motion to the passive advection at each time step. The results presented in this paper, however, do not include any molecular diffusion.

SIMULATED FLOW VISUALISATION

The time evolution of horizontal coloured sectors is shown in the following set of figures. The visualisation is shown in one of two forms: either the time evolution over a number of cells, or in a more compact form, with each particle with location (x, y) in cell N [see Fig. 1] plotted at point $(x - NL, y)$, so that all particles are plotted in the same cell. As the flow conditions in each cell are identical, the latter of these two representations is equivalent to a starting condition with all cells having the same coloured horizontal layers of particles. This technique has been termed *overlay*.

Figures 2(a)–(c) show the situation for a parallel channel. In Fig. 2(a) a steady net flow of $Re_n = 100$ is applied without any oscillatory motion. From the figure, the consequences of the familiar parabolic velocity profile can be seen. In this situation the dispersion of the flow is severe because fluid elements near the wall are slower moving than elements near the centre of the channel. Mixing is also poor as reflected by the lack of radial mixing between coloured sectors. Figure 2(b) shows the effect of applying an oscillatory motion alone. The conditions of fluid oscillation are $Re_0 = 100$, $St = 1.0$. It can be readily seen that after one full oscillation the particles and coloured sectors return to their original position and no net advection or mixing has taken place. The coupled effect of net flow and oscillation is shown in Fig. 2(c). This illustrates that, under these conditions, the volumetric oscillation has no *net* effect on the fluid motion when compared to steady flow alone. Therefore, in the absence of molecular diffusion, oscillations with no baffles present will not change either the mixing or the dispersion.

In Fig. 3(a)–(d) baffles have been introduced into the channel and it is here that striking comparisons can be made with the base case flows already described. Figure 3(a) shows the flow development for a net flow of $Re_n = 100$. In this case the flow remains steady and symmetrical. The streamlines of the flow are modified by the baffles, but the overall dispersion of the flow does not appear to be significantly changed. In Fig. 3(b) the overlay technique has been used to illustrate the poor radial mixing in this flow regime. From a detailed numerical study of the fluid mechanics of flow along a periodically baffled tube, Rowley and Patankar (1984) have shown that separation occurs downstream from each baffle and symmetrical eddies form in the cavity between the wall and the baffle. As the Reynolds number increases the reattachment point moves progressively downstream until, at a Re_n of order 100, a single eddy completely occupies the wall inter-baffle region. These results have been confirmed both experimentally and numerically (Howes, 1988 and Howes and Mackley, 1987).

Figure 3(c) illustrates a potentially useful mixing mechanism that develops in the baffled channel at a Re_n between 100 and 200. At a critical Re_n the flow becomes unsteady and the symmetry of the flow pattern is broken. A periodic eddy forms successively on each opposite baffle and this results in time dependent radial velocity components developing within the channel. The consequences of this periodic eddy formation at a Re_n of 300 is seen in Fig. 3(c) and in Fig. 3(d) a clear picture of the potential ability of this system to mix fluids can be seen. The flow is periodic with a dimensionless period of 2.11, and these flow conditions could be expected to yield good mixing with some reduction in the axial dispersion when compared with laminar flow without baffles.

Figures 4(a)–(f) show the effect that fluid oscillations can have on the flow within a periodically baffled channel. In Figs 4(a) and (b) fluid oscillation alone is applied under the conditions $Re_0 = 100$, $St = 1.0$. The simulation shows the advection of particles over one full cycle. Starting at $t = 0$, the second simulation shows the position at the half period position ($t = 0.5$), and the third after one full cycle ($t = 1.0$). Under these circumstances the Reynolds number is sufficiently high to cause symmetrical eddies to be formed downstream of each baffle. With each oscillation, fluid near the wall of the channel is drawn into the downstream eddy that is formed as the flow accelerates, on flow reversal this eddy is ejected into the centre of the channel. In this way an efficient mixing flow is achieved within each inter-baffle region. At the conditions defined for Figs 4(a) and (b) the flow is period repeating and symmetrical about the horizontal centre line of the channel. Figure 4(b) shows that above and below this plane, efficient mixing appears to have occurred. In addition, Fig. 4(a) shows that the dispersion along the channel is small.

Figures 4(c) and (d) show the situation for a higher Re_0 of 300 and $St = 1.0$. Under these conditions the centre line symmetry of the flow is broken and the flow becomes more complex. Figure 4(d) in particular shows that excellent mixing could be expected within any one baffled cell. This mixing is not exclusively in the central part of the channel but extends well into the inter-baffle region and close to the walls. The basic mixing mechanism is similar to that previously described at a lower oscillatory Reynolds number although here the breaking of centre line symmetry leads to a greater complexity of mixing.

In Figs 4(e) and (f) the final simulation shows the coupled effect of oscillation and net flow. The oscillatory conditions are the same as described in Figs 4(c) and (d) with a net flow of $Re_n = 100$. It can be seen in Figs 4(e) and (f) that the previously observed good mixing of Figs 4(c) and (d) is retained. The crucial new aspect shown in Fig. 4(e) is that the net advection of the particles appears to be rather uniform along and across the channel. The oscillatory flow fluid mixing has dominated over any net flow radial velocity profile. It would therefore be expected that both good mixing and low dispersion could be achieved under these circumstances.

DISCUSSION AND CONCLUSIONS

The early simulations described in this paper illustrate clearly the common difficulties encountered in achieving good radial mixing and low dispersion for laminar flow in a smooth walled channel or tube. In these situations molecular dispersion is generally the only way in which species within the duct will become mixed, and the heat and mass transfer rates to and from the walls will consequently be low. Our simulations show that the introduction of periodic baffles initially has little effect with steady flow alone; however above a net flow Reynolds number $Re_n > 100$ a periodic eddy shedding flow is predicted. This *unsteady* (though periodic) flow regime results in good radial mixing. Consequently a simple method for enhancing mixing, heat and mass transfer rates can be identified for flows with $Re_n > 100$. This observation is consistent with the heat transfer findings of Mackley *et al.* (1990) who found that the introduction of periodic baffles in a circular tube significantly increased the heat transfer coefficient characteristics when compared to an unbaffled tube. This is in sharp contrast to the results of Rowley and Patankar (1984) who predicted numerically that the presence of baffles in a tube could actually decrease the heat transfer coefficient for *axisymmetric* flow conditions. The unsteadiness is likely to result in a small increase in the pressure drop. The enhancement in mixing and transfer rates, however, would undoubtedly improve the efficiency of an unbaffled device.

We believe that the instability generated by the fluid mechanics solver is of a genuine fluid mechanical origin rather than a numerical instability. A detailed study by Roberts (private communication) of the steady flow in an unbaffled channel yielded perturbation Tollmien Schlichting waves in agreement with an "exact" solution reported by Ghaddar *et al.* (1986) for a Reynolds number of $Re_n = 700$. This gave us confidence that the solver was behaving accurately in this Reynolds number regime.

The particle tracking and overlay procedure provide a powerful visual method of depicting anticipated levels of mixing and dispersion in the channel. Howes (1988) has developed a method to utilise the particle advection in order to obtain a single parameter dispersion coefficient and we are currently developing a further scheme for quantifying levels of mixing from overlay pictures of the type we have shown.

We believe the oscillatory flow simulations are significant in two respects. Firstly the simulations show that oscillatory flow in baffled tubes can be a very efficient way of generating well-mixed flows and in some cases low-axial dispersion can also be achieved. The good global mixing suggests that improved heat and mass transfer can be achieved when compared with an unbaffled tube operating at a similar Reynolds number. In addition, the low dispersion will result in a device giving a near plug flow residence time distribution. Good mixing, heat transfer and low axial dispersion are generally the crucial ingredients required for efficient continuous process engineering units, used for example as a reactor or heat exchanger, and it is clear that this system offers an energy efficient alternative to existing designs. In particular the fact that the mixing is produced by oscillatory flow means that the net flow is only constrained to have a $Re_n < Re_0$. This in turn means that low net flow velocities can be chosen thereby ensuring a more compact design than say turbulent flow channel or tubular reactors. The energy requirements of an oscillatory flow device have not yet been fully investigated, but preliminary results carried out in this laboratory indicate that the energy efficiency of these oscillatory flow devices is very high.

A detailed examination of Figs 4(c)–(f) at or near the walls of the channel reveals that the type of fluid mechanics described in this simulation also offer interesting possibilities in terms of the surface purging properties of the device. During any one cycle, fluid near the wall is drawn from the wall and consumed in the vortex that forms downstream from each baffle. Particularly when the symmetry of the centre line is broken, the resulting eddies formed in the baffled region rapidly sweep the surface. If molecular diffusion is introduced, the surface removal of particles becomes even more efficient. This property suggests that the device operating in this simulated regime could give enhanced membrane filtration and also reduce fouling, for example in a pasteurisation unit. It also seems likely that nature may have exploited some of the phenomena described in this paper. The pulsed nature of blood flow may ensure that stagnant zones behind "natural baffles" are avoided, or might interact harmonically with some natural instability resulting in improved transfer properties.

The second aspect that we feel to be of importance is the way that the simulation can follow the onset of chaotic motions. This point particularly applies to the

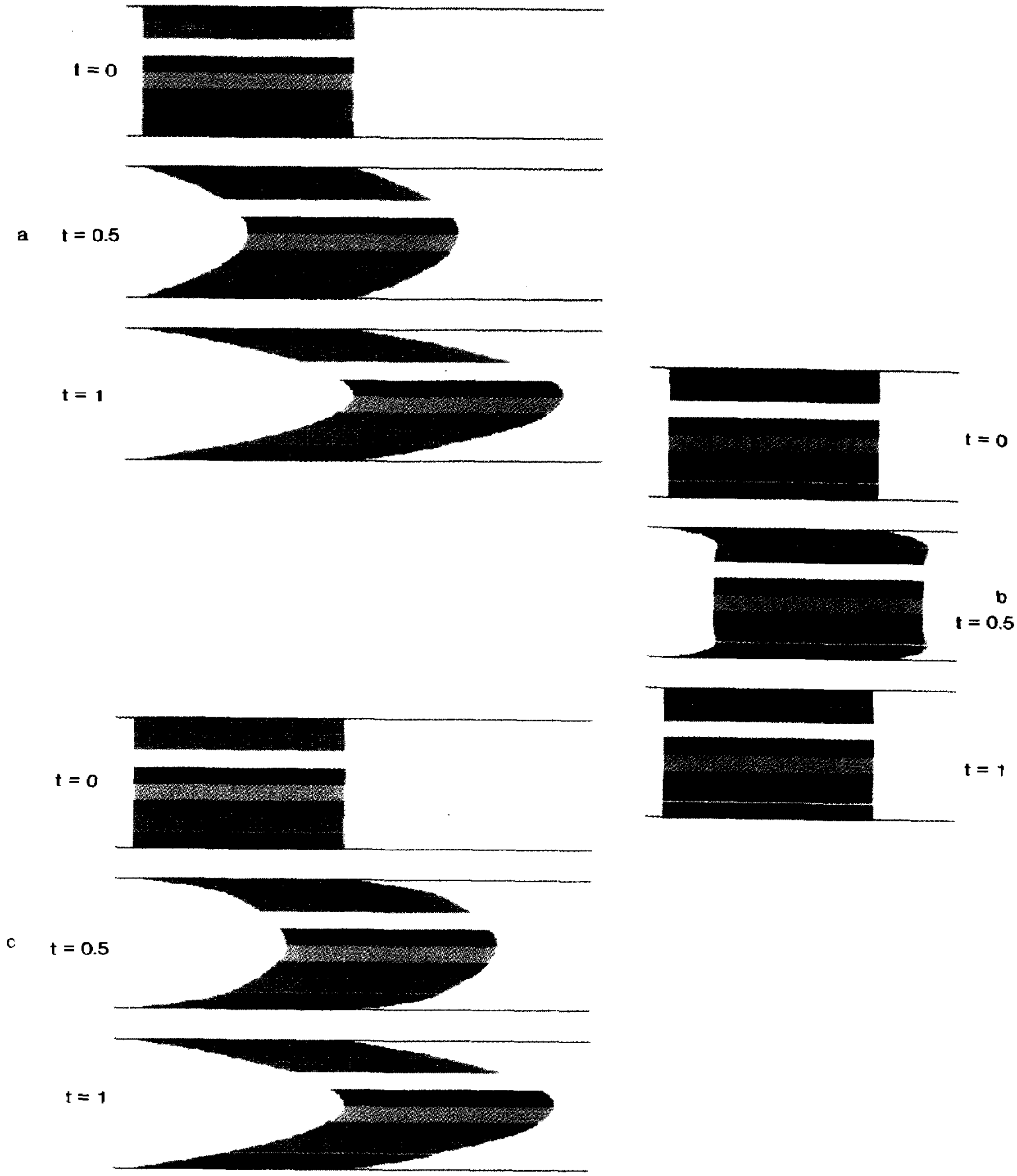

Fig. 2. Results for an unbaffled channel: (a) net flow at $Re_n = 100$, (b) oscillatory flow at $Re_0 = 100$, $St = 1.0$, (c) coupled net flow and oscillatory flow at $Re_n = 100$, $Re_0 = 100$, $St = 1.0$.

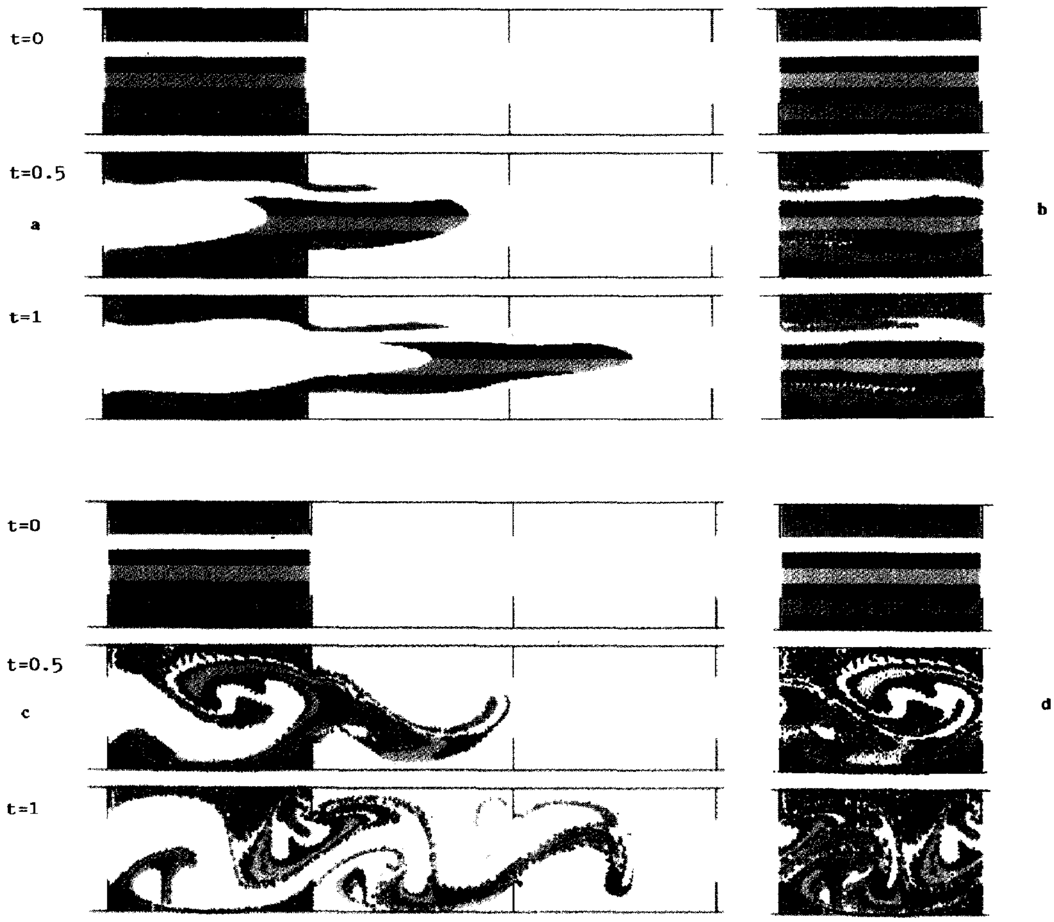

Fig. 3. Results for a baffled channel with no oscillatory component in the flow: (a) and (b) net flow at $Re_n = 100$, and (c) and (d) net flow at $Re_n = 300$.

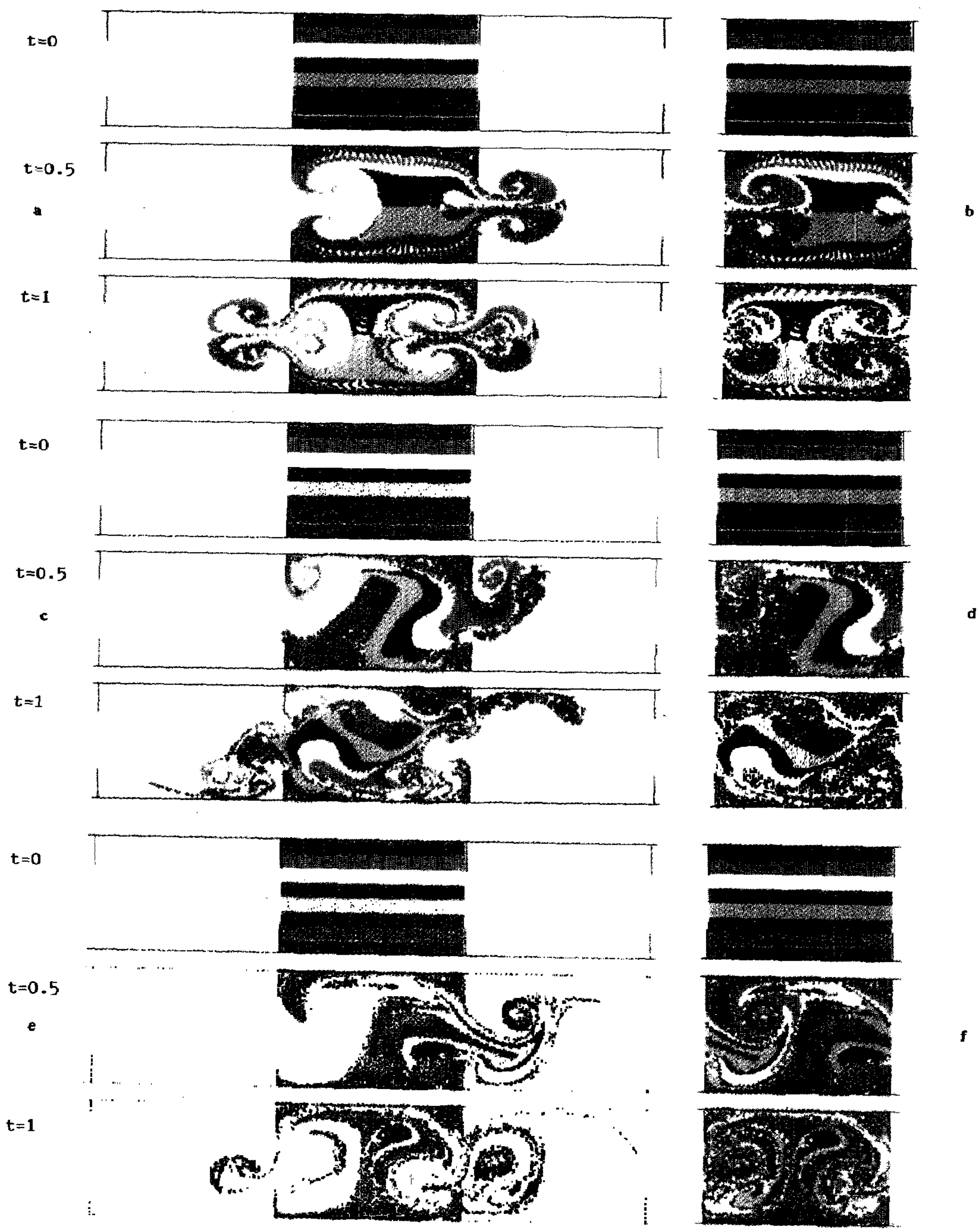

Fig. 4. Results for oscillatory flows in a baffled channel: (a) and (b) oscillatory flow at $Re_0 = 100$, $St = 1.0$, (c) and (d) oscillatory flow at $Re_0 = 300$, $St = 1.0$ and (e) and (f) coupled net flow and oscillatory flow at $Re_n = 100$, $Re_0 = 300$, $St = 1.0$. Figures 2–4 show a series of particle advection plots. The pictures show the position of an array of particles with each particle represented by a coloured spot. Each figure consists of three pictures taken at successive times during the advection process. The first picture shows the starting position of the particles corresponding to $t = 0$, the second picture shows the position of the particles at $t = 0.5$ and the third at $t = 1.0$.

oscillatory flow work. In unbaffled ducted flow the transition from laminar to turbulent flow occurs usually at a Reynolds number in the region of 2000–3000 and for any given tube over a narrow window of Reynolds number. In the case of the baffled channel, the transition from ordered flow to chaotic flow occurs at a much lower Reynolds number and also develops in complexity over an appreciably wide range of Reynolds number. It is therefore possible to explore the detailed way in which the fluid motion moves from the ordered flow shown in Fig. 4(a) to the chaotic advected flow of Fig. 4(c). The variables of stroke amplitude and frequency provide two easily changed parameters and the system seems excellent for both experimental and numerical studies. Typically the effects we have described can be seen in a 25 mm channel for a fluid oscillation 1–5 mm centre to peak amplitude at a frequency of 1–5 Hz.

A restriction on the numerical scheme we have utilised requires that the flow is two dimensional. From preliminary experiments we have carried out we believe this to be the case for the simulation conditions described in this paper. Obviously the third dimension presents more general complexity; however, we believe there is a useful range in which two-dimensional experiments and simulations can be carried out with baffled channels.

Finally in this paper the sharp edges necessary to generate eddy separation have been introduced as periodic baffles placed at the walls as this was seen as a simple geometry giving the minimum additional surface area within the channel to achieve the required effect. There are of course a number of other baffle and geometric variants possible that will give similar effects to that described here and clearly there is still significant scope for further optimisation of the geometric design. In addition, at present there is certainly an upper limit, of order $Re_0 = 700$ to which the numerical solver may be taken with any degree of confidence, there is no such limit experimentally however and the higher oscillatory Reynolds number regime ($Re_0 > 500$) offers exciting possibilities for an intense eddy mixing device that could be used for example for fast reactions, and the manufacture of fine dispersions.

NOTATION

B	baffle height
H	channel width
L	cell length
n	cell number
Re_0	oscillatory Reynolds number ($\rho 2\pi\Omega x_0 H/\mu$)
Re_n	net flow Reynolds number ($\rho U H/\mu$)
St	Strouhal number ($H/2\pi x_0$)
t	dimensionless time
t^*	dimensional time
U	mean velocity
u	local velocity in x-direction
v	local velocity in y-direction
$u_{X,t}$	velocity of particle X in direction x at time t
$v_{X,t}$	velocity of particle X in direction y at time t
x	streamwise distance
x_0	centre to peak amplitude of oscillation
y	transverse distance from bottom wall

Greek letters

β	ratio of mean and oscillatory flow (Re_n/Re_0)
μ	fluid viscosity
ρ	fluid density
ψ	stream function
ω	vorticity
Ω	frequency of oscillation

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