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Inflows/Outflows Driven Particle Dynamics in an Idealised Lake

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Abstract

This paper considers fluid mixing driven by inflows connected to a circular shallow lake using a numerical framework consisting of a shallow water hydrodynamic model and a passive particle-tracking model. With the flow field driven by alternate inflows predicted by a shallow water model, particle trajectories are traced out using a particle tracking model. The horizontal fluid mixing dynamics are then interpreted using dynamics system analysis approaches including finite-time Lyapunov exponent (FTLE) and Lagrangian coherent structure (LCS). From the simulation results, it is confirmed that periodic inflows are able to create a weak dynamic system in an idealised circular lake, with the particle dynamics controlled by a single dimensionless parameter associated with the inflow duration. The mixing and transport property of the lake changes from regular to chaotic as the value of the dimensionless parameter increases until global chaotic particle dynamics is achieved. By further analysing the advection of particles injected continuously to the inflows (freshwater), the fate of “freshwater” particles in a “polluted” lake is tracked and revealed. The results provide useful guidance for engineering applications, i.e. transferring freshwater from rivers to improve the water quality in polluted water bodies such as lakes. The presented approach will be able to facilitate the design of ‘optimised’ schemes for such engineering implementation.

Keywords: Shallow environmental flow, Lagrangian particle dynamics, particle tracking, inflows and outflows, finite-time Lyapunov exponent, Lagrangian coherent structure

1. Introduction

In environmental shallow water flows, horizontal mixing is a particularly important process affecting water quality. Horizontal mixing may dominate water exchange in large shallow water bodies and has important implications in interpreting the movement of waterborne micro-organisms, e.g. algae, which are linked to water quality. Therefore, understanding the mechanism of fluid mixing is crucial for planning and operating pollutant control measures and informing other environmental engineering practice. Numerical approaches have been widely developed and reported to simulate pollutant transport and impact on water quality in environment flows (e.g. [1-3]). However, it remains to be a challenge and further research is needed to better understand the mixing and transport processes in environmental shallow flows because the underlying flow hydrodynamics and mixing processes are highly complex and affected by complicated domain geometry and driving factors.

Of particular interest to environmental engineering practice is the horizontal mixing and transport in enclosed or semi-enclosed shallow flow systems, where the flow hydrodynamics is not only induced by surface stresses created by winds but also influenced by connected inflows

and outflows. Wind-induced mixing and transport properties in enclosed or semi-enclosed shallow flow systems have been previously studied by many researchers. Kranenburg [4] investigated chaotic advection in a circular idealised shallow basin induced by periodic wind stresses using analytical velocity fields. Liang et al. [5] developed a numerical approach to study wind-induced chaotic advection in several circular basins with more complicated bathymetries. The approach was extended to investigate the Lagrangian particle dynamics in a mine tailing pond with realistic bathymetry and geometry [6]. Károlyi et al. [7] showed that chaotic particle dynamics in a shallow rectangular basin could be well described using finite size Lyapunov exponents (FSLE). Lee et al. [8] simulated the wind-induced hydrodynamics in Kranenburg’s model lake using a two-layer shallow flow model and traced out the Lagrangian dynamics in the two fluid layers using a particle tracking method.

Compared to the wind-induced mixing and transport processes in enclosed shallow water bodies, the influence of inflows/outflows on fluid mixing has received less attention and requires further research. Many large freshwater lakes are connected to major river networks and their flow hydrodynamics may be influenced or dominated by inflows/outflows. Better understanding of the

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fluid mixing phenomena driven by inflows and/or outflows is therefore of crucial importance for a wider range of engineering applications including water quality control. Compared with wind stresses which usually directly act across the whole water surface area, inflows/outflows may only provide driving forces that locally influence the flow hydrodynamics; but the locally changed momentum may be spread out to the rest of the water body and affect the flow hydrodynamics in the entire domain. Therefore, the transport and mixing processes induced by inflows/outflows are expected to be different from those induced by winds and should be further investigated and understood.

Based on the theory of dynamical system (e.g. [9-10]), Lagrangian methods, which typically involve the use of passive particle tracking technique, have been well-developed and widely used in the last few decades to investigate fluid mixing dynamics in environmental shallow flows [11-15]. This paper aims to investigate the mixing and transport processes induced by inflows/ outflows using a Lagrangian particle tracking model driven by flow fields created from a 2D finite volume shallow water model. The particle dynamics will be analysed using dynamics system analysis methods including finite-time Lyapunov Exponent (FTLE) and Lagrangian coherent structures (LCS).

2. Methodology

The adopted Lagrangian fluid mixing modelling framework consists of a depth-average model for shallow water flow hydrodynamics and a particle tracking model for tracing out detailed passive particle trajectories. The hydrodynamic model solves the pre-balanced 2D shallow water equations (SWEs) as reported in Liang and Borthwick [16] for accurate simulation of shallow flow hydrodynamics over irregular beds involving wetting and drying. In the matrix form, the pre-balanced SWEs are written as:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} + \frac{\partial \mathbf{g}}{\partial y} = \mathbf{s} \quad (1)$$

where $\mathbf{u}$ is the vector of conservative variables; $\mathbf{f}$ and $\mathbf{g}$ are respectively the vectors of fluxes in the x and y -directions; $\mathbf{s}$ is the vector of source terms; and t is the time. The vector terms are given by [16]:

$$\mathbf{u} = \begin{bmatrix} \eta \\ uh \\ vh \end{bmatrix}, \quad (2)$$

$$\mathbf{f} = \begin{bmatrix} uh \\ u^2h + \frac{1}{2}g(\eta^2 - 2\eta z_b) \\ uvh \end{bmatrix}$$

$$\mathbf{g} = \begin{bmatrix} vh \\ uvh \\ v^2h + \frac{1}{2}g(\eta^2 - 2\eta z_b) \end{bmatrix}$$

$$\mathbf{s} = \begin{bmatrix} 0 \\ (\tau_{wx} - \tau_{bx})/\rho - g\eta \frac{\partial z_b}{\partial x} + S_{vx} \\ (\tau_{wy} - \tau_{by})/\rho - g\eta \frac{\partial z_b}{\partial y} + S_{vy} \end{bmatrix}$$

where η and z_b are the water surface level and bed elevation above datum; $h = \eta - z_b$ is the total water depth; u and v are the depth-averaged velocities in the x and y -directions; g is the acceleration due to gravity; ρ is the density of water; τ_{wx} and τ_{wy} are wind stresses in the x and y -directions, which are estimated using [17]

$$\tau_{wt} = \rho_{air} C_D U_h^2 \quad (3)$$

where τ_{wt} is the resultant vector of τ_{wx} and τ_{wy} ; ρ_{air} is the density of air; C_D is a drag coefficient; U_h is the mean velocity of wind at a particular height over the water surface which is usually chosen to be 10 m [17]. τ_{bx} and τ_{by} are the bed friction stresses which are widely estimated using the following formulas

$$\tau_{bx} = \rho C_f u \sqrt{u^2 + v^2},$$

$$\tau_{by} = \rho C_f v \sqrt{u^2 + v^2} \quad (4)$$

in which the bed roughness coefficient C_f may be evaluated using $C_f = gn^2/h^{1/3}$ with n being the Manning coefficient. Finally, S_{vx} and S_{vy} are the turbulent (viscous) terms:

$$S_{vx} = \frac{\partial}{\partial x} \left(2h\nu_{mo} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(h\nu_{mo} \left[\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right] \right)$$

$$S_{vy} = \frac{\partial}{\partial x} \left(h\nu_{mo} \left[\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right] \right) + \frac{\partial}{\partial y} \left(2h\nu_{mo} \frac{\partial v}{\partial y} \right) \quad (5)$$

where ν_{mo} represents the momentum diffusion coefficient.

The above SWEs are solved using a second-order Godunov-type finite volume method with the inviscid fluxes calculated by an HLLC approximate Riemann solver (refer to [16] and [18]) for detailed implementation). The viscous

terms are simply calculated using a central difference scheme and the friction terms are evaluated using a point-wise implicit scheme. The SWE model is then used in the Lagrangian fluid mixing modelling framework to simulate environmental shallow flows and predict the velocity fields.

With the flow velocity predicted by the aforementioned SWE model, the trajectories of the particles released in the flow can be traced out using a particle tracking model solving the following ordinary differential equations that describe a dynamics system evolving with time:

$$\frac{d\mathbf{x}}{dt} = \dot{\mathbf{x}} = \mathbf{v}(\mathbf{x}, t) \quad (6)$$

where $\mathbf{x}$ a variable representing the state of the system and may be regarded as a point at position $\mathbf{x}$ of the phase space under consideration, and $\mathbf{v}(\mathbf{x}, t)$ is the velocity of the system at position $\mathbf{x}$ and time t . For a two-dimensional spatial system as considered in this work, the particle motion equations become:

$$\frac{dx}{dt} = u(x, y, t), \quad \frac{dy}{dt} = v(x, y, t). \quad (7)$$

The trajectory of a particle released in a two-dimensional environmental flow can be then obtained by numerically integrating these equations if the flow velocities (u, v) are available. It is well-known from the dynamical system theory that the solutions to Eq. (7), i.e. Lagrangian particle dynamics, may become chaotic even when the underlying flow field is highly simple but unsteady. This is a phenomenon known as chaotic advection [11]. The procedure of solving Eq. (7) and obtaining the particle trajectories is called particle tracking. The current particle tracking model adopts the 4th-order Runge-Kutta integration method to solve Eq. (7).

Tracking a particle by solving Eq. (7) requires local velocity information at the point where the particle is located. However, the velocity information output from the SWE model is discrete (grid-based) and only available at the centres of the grid cells being used to discretise the computational domain. Herein, spatially continuous velocity information is obtained using a bilinear interpolation scheme.

To interpret particle dynamics, methods for analysing dynamics systems, including the finite-time Lyapunov exponent (FTLE) and Lagrangian coherent structure (LCS), are used to illustrate the organizing structures governing particle behaviours in shallow flow systems. Lyapunov exponent is an effective mathematical tool/concept for analysing the chaotic characteristics

of particle dynamics to confirm the dynamical system is sensitive to initial conditions. Lyapunov exponent σ may be defined and calculated by

$$\sigma = \lim_{t \rightarrow \infty} \lim_{\delta\mathbf{x}(0) \rightarrow 0} \frac{1}{t} \ln \frac{\delta\mathbf{x}(t)}{\delta\mathbf{x}(0)} \quad (8)$$

where $\delta\mathbf{x}(0)$ is the initial perturbation of a trajectory $\mathbf{x}(t; t_0, \mathbf{x}_0)$ and $\delta\mathbf{x}(t)$ is the grown perturbation over the time interval $[0, t]$. The Lyapunov exponents will return positive values for a chaotic system where the initially close trajectories diverge exponentially over time. The definition of Lyapunov exponent is based on the assumption that the evolution time t of the dynamical system is infinite. However, infinite evolution time is difficult to define in real-world applications and the calculation of converged Lyapunov exponents is therefore computationally expensive and challenging.

The finite-time Lyapunov exponent (FTLE) denoted by $\sigma_t^T(\mathbf{x})$ is a scalar measurement describing the level of stretching of a particle trajectory at point $\mathbf{x}_0 \in D$ from t_0 to t_0+t [19]. Herein we consider an open set $D \subset R^2$ as the spatial domain of interest is two-dimensional in this work. We define a time-dependent velocity field $\mathbf{v}(\mathbf{x}, t)$ in D and a trajectory $\mathbf{x}(t; t_0, \mathbf{x}_0)$ starting at point $\mathbf{x}_0 \in D$. The trajectory can then be traced out by

$$\frac{d\mathbf{x}(t; t_0, \mathbf{x}_0)}{dt} = \mathbf{v}(\mathbf{x}(t; t_0, \mathbf{x}_0)) \quad (9)$$

with the corresponding initial conditions given by $\mathbf{x}(t_0; t_0, \mathbf{x}_0) = \mathbf{x}_0$. The solution of the dynamic system represented by Eq. (9) may be treated as a flow map which maps the particle from initial position $\mathbf{x}_0$ to its final position $\mathbf{x}_n$ over the time interval $[t_0, t_0 + T]$. The flow map is defined as:

$$\phi_{t_0}^t: D \rightarrow D: \mathbf{x}_0 \mapsto \phi_{t_0}^t(\mathbf{x}_0) = \mathbf{x}(t; t_0, \mathbf{x}_0) \quad (10)$$

To analyse the level of perturbation to the trajectory, two points $\mathbf{x}, \mathbf{y} \in D$ are considered and point $\mathbf{y} = \mathbf{x} + \delta\mathbf{x}(0)$ is perturbed from point $\mathbf{x}$ by an infinitesimal and arbitrarily oriented distance $\delta\mathbf{x}(0)$. The growth of $\delta\mathbf{x}(0)$ in a finite time period T is then calculated from:

$$\begin{aligned} \delta\mathbf{x}(T) &= \phi_{t_0}^{t+T}(\mathbf{x} + \delta\mathbf{x}(0)) - \phi_{t_0}^{t+T}(\mathbf{x}) \\ &= \frac{d\phi_{t_0}^{t+T}(\mathbf{x})}{d\mathbf{x}} \delta\mathbf{x}(0) + \mathcal{O}(|\delta\mathbf{x}(0)|^2) \end{aligned} \quad (11)$$

where $\frac{d\phi_{t_0}^{t+T}(\mathbf{x})}{d\mathbf{x}}$ is the deformation gradient or Jacobian of the flow map; neglecting the higher order terms, the magnitude of the perturbation is finally obtained:

$$\|\delta\mathbf{x}(T)\| = \sqrt{\langle \delta\mathbf{x}(0), \frac{d\phi_{t_0}^{t+T}(\mathbf{x})^*}{d\mathbf{x}} \frac{d\phi_{t_0}^{t+T}(\mathbf{x})}{d\mathbf{x}} \delta\mathbf{x}(0) \rangle} \quad (12)$$

where A^* is defined as the transpose of matrix A and Δ is defined as the right Cauchy-Green deformation tensor:

$$\Delta = \frac{d\phi_{t_0}^{t+T}(\mathbf{x})^*}{d\mathbf{x}} \frac{d\phi_{t_0}^{t+T}(\mathbf{x})}{d\mathbf{x}}$$

It should be mentioned that Δ is a time-dependent 2×2 real symmetric matrix with real eigenvalues. The magnitude of linearized stretching is governed by this deformation tensor with the largest eigenvalue of Δ indicating the largest stretching extent in the flow and the corresponding eigenvector defining the direction of stretching. Finally, FTLE can be defined using the maximum eigenvalue of the tensor Δ :

$$\sigma_{t_0}^T(\mathbf{x}) = \frac{1}{|T|} \ln \sqrt{\lambda_{\max}(\Delta)}$$

The algorithm for calculating FTLE in the 2D environmental flows considered in this work is designed by advecting passive particles for a finite time interval. A mesh of appropriate resolution (referred to as FTLE mesh) is first created to define the initial locations of passive particles by assigning a particle to the centre of each of the FTLE cells. The particles are then advected using the proposed particle tracking model and the deformation gradient of each of the particles is subsequently used to compute FTLE. If the initial and final positions of a particle are respectively denoted as $\mathbf{x}_{ij}(t_0)$ and $\mathbf{x}_{ij}(t_1)$ (with $t_1 = t + T$), the deformation gradient of a particle can be then approximated using a central difference scheme on the FLTE grid:

$$\left. \frac{d\phi_{t_0}^{t+T}(\mathbf{x})}{d\mathbf{x}} \right|_{\mathbf{x}_{ij}} \approx \begin{bmatrix} \frac{x_{(i+1)j}(t_1) - x_{(i-1)j}(t_1)}{x_{(i+1)j}(t_0) - x_{(i-1)j}(t_0)} & \frac{x_{i(j+1)}(t_1) - x_{i(j-1)}(t_1)}{y_{i(j+1)}(t_0) - y_{i(j-1)}(t_0)} \\ \frac{y_{(i+1)j}(t_1) - y_{(i-1)j}(t_1)}{x_{(i+1)j}(t_0) - x_{(i-1)j}(t_0)} & \frac{y_{i(j+1)}(t_1) - y_{i(j-1)}(t_1)}{y_{i(j+1)}(t_0) - y_{i(j-1)}(t_0)} \end{bmatrix} \quad (15)$$

For each particle, the deformation gradients at all four directions are calculated and the largest gradient is considered to be the FTLE

at $\mathbf{x}_{ij}(t_0)$. Based on this algorithm, the FTLE distribution (measuring the average or integrated separation between trajectories) over the entire 2D flow domain can be obtained to indicate the dynamics of particles.

The concept of Lagrangian coherent structure (LCS) is derived from a dynamic system perspective [20]. Considering a dynamic system as defined in Eq. (9) with inherently chaotic particle trajectories, the hyperbolic points and their associated stable and unstable manifolds are considered as the organizing structures that determine the dynamics of the system [21-23]. Particles close to the hyperbolic points trace out the stable and unstable manifolds by working forward and backward against time, respectively. The stable and unstable manifolds separate the regions of different dynamics and play a role as the skeletons of the particle dynamics in the dynamic system.

In practical applications, the system dynamics is usually complicated, and it is difficult to identify these hyperbolic points and trace out the invariant manifolds. However, special structures traced out by particle patches may have the ability to attracting or repelling particles as invariant manifolds do, and these special structures are referred to as Lagrangian coherent structures (LCSs) [24]. In other words, LCSs are often locally the most strongly attracting or repelling material surfaces in the flow system. In two-dimensional flow systems, LCSs are defined by the material lines depicting the hyperbolic regions, which effectively act as the barriers of particle transport.

Along with the application of the FTLE scalar field $\sigma_{t_0}^T(\mathbf{x})$, a more quantitative and mathematical definition of LCS is given by Shadden et al. [19] as the locally maximum ridge of $\sigma_{t_0}^T(\mathbf{x})$. In this context, the curvature of the field $\sigma_{t_0}^T(\mathbf{x})$ is introduced using the Hessian matrix Σ :

$$\Sigma = \nabla^2 \sigma_{t_0}^T(\mathbf{x}) \quad (16)$$

Herein Σ is a symmetric matrix with real eigenvalues and orthogonal eigenvectors. Let λ_n be the smallest eigenvalue and $\mathbf{n}$ be the corresponding eigenvector; the associated LCS is the set of (all) points in the field satisfying the following conditions:

$$\mathbf{C1.} \lambda_n < 0; \quad \mathbf{C2.} \nabla \sigma_{t_0}^T(\mathbf{x}) \cdot \mathbf{n} = 0 \quad (17)$$

It is clear that LCSs as defined can effectively reveal the underlying fluid structures in a two-dimensional time-dependent flow

system that is not typically evident from the Eulerian fluid description perspective.

3. The model lake and hydrodynamics

The Kranenburg's idealised circular lake [4] is adopted in this work to investigate the fluid mixing characteristics in an enclosed or semi-enclosed shallow environmental flow system. The wind-induced flow hydrodynamics and particle dynamics in Kranenburg's lake have been intensively simulated and analysed by Liang et al. in [5] and [25]. This work will focus on the fluid mixing induced by inflows/outflows.

Figure 1. Initial water depth and the inflow/outflow channels of the idealised lake.

The bathymetry of the lake is defined using the following equation for still water depth h_k , which is a function of the radial distance from the centre of the lake:

$$h_k = H(1/2 + \sqrt{(1/2 - 1/2 * (r/R))}) \quad (18)$$

where $H = 0.5\text{m}$ is a weighted mean water depth; $R = 120\text{m}$ is the radius of the model lake; r is the distance from the centre of the lake. Two 8m wide inflow channels are connected to the main water body at the northwest and northeast directions to facilitate inflow boundary conditions. A 12m wide outlet is attached to the south, where a fixed water level of 0.251m is imposed as boundary conditions. The bathymetry (initial water depth) and the configuration of the inflow and outflow channels are illustrated in Figure 1.

To predict the flow hydrodynamics, the computational domain is discretised using a uniform grid of 210×210 square cells at a resolution of 1.2m. The gravitational acceleration g equals 9.81m/s^2 . The Manning coefficient n is set to 0.025. The p_{vt} for calculating turbulent fluxes is chosen to be 3.4 for a circular basin [26]. The initial water depth in the inflow/outflow channels is set to be 0.251m, to

give the same water level as the ambient flow in the main water body. The inflow discharge is maintained at $20\text{m}^3/\text{s}$ during the whole simulation. Simulations are run for 12 hours until the flow field becomes steady.

Figure 2. Steady-state streamlines driven by: (a) inflow from northeast; (b) inflow from northwest.

Figure 3. Time histories of velocity component u at the four gauges.

Figure 2 presents the steady flow fields driven respectively by the inflows from the northeast and northwest inlet channels. Taking the flow field driven by the northeast inflow as shown in Figure 2(a) as an example, most of the circular domain is occupied by two big gyres that

are separated by a streamline traced out by the main flow across the lake from inflow channel to outlet. The two-gyre system is similar to the flow pattern induced by wind stresses as presented in Kranenburg [4] and Liang et al. [5] but the rotation directions of the gyres are opposite. In the wind-induced flow field, water velocities are directed against the wind direction in deeper part of the lake, and with the wind in the shallower areas, which clearly different from the inflow-driven flow field as shown in Figure 2. The time histories of the x -direction velocity component at the four gauge points located inside the basin at (70, 0), (0, 70), (-70, 0) and (0, -70) are recorded during the simulation and presented in Figure 3, confirming the flow field become steady after about 6 hours.

4. Particle dynamics results and discussion

To study the inflow/outflow driven Lagrangian particle dynamics and fluid mixing properties in the circular model lake, a simple dynamic system is created and considered. Each of the two inflow channels is assumed to be controlled by gates, which are open or closed alternately to create a simple periodic flow field. In the first half of a period (T), the northeast inflow channel is open whilst the northwest channel is closed; the opposite operation is implemented in the second half of the period. To simplify the simulations and better reveal the inherent fluid mixing dynamics, it is further assumed that the flow adapts instantaneously to follow the change of inflow conditions. Following Kranenburg's wind-induced flow system [4], a dimensionless parameter is derived to control the level of fluid mixing in this simple dynamic system, given as

$$\mu_i = \frac{\ln(H/z_0)}{8\kappa} \frac{Q_{in}t_f}{R_0hw} \quad (19)$$

where $z_0 = 2.8$ mm is the roughness height of the bed; $\kappa = 0.4$ is the von Kármán constant; Q_{in} is the constant inflow discharge; h and w are the water depth in and width of the inflow channels; t_f is the duration of the inflow, i.e. half of the period T ; and R_0 is the characteristics length of the lake which is conveniently chosen to be the radius of the lake. The parameter μ_i as defined in Eq. (19) may be regarded as a dimensionless inflow duration parameter related to the inflow duration t_f (half of the period). In fact, μ_i may be interpreted as a dimensionless time and is essentially the ratio between the travel distance during the inflow duration $Q_{in}t/hw$ and the characteristics length R_0 . Therefore, the particle dynamics in this idealised model lake is actually controlled by the length of

the inflow duration, when other related flow parameters are fixed, e.g. inflow rate, channel width, etc.

4.1 FTLEs, LCSs and particle dynamics

To properly visualize the distribution of FTLEs and reveal LCSs, a grid of 420×420 cells (twice the resolution of hydrodynamic grid) is used to define the initial locations of passive particles. FTLEs, with their values normally falling between 0 and 0.2 in the current case, are plotted as contour maps in the 2D domain in an order of minutes^{-1} . On the contour plots, the LCSs are automatically filtered out as red lines (the highest values) based on the adopted colour scheme. The forward-tracking LCSs, generated by tracking the particles forwards in time, are locally the most strongly repelling material surfaces in the flow, pushing the particle to leave these LCSs. So in time-forward simulations, these LCSs may not be easily visualized by tracing particles. On the other hand, the backward-tracking LCSs are generated by tracking the particles backwards in time and are locally the most strongly attracting material surfaces in the flow. Particles near to these backward-tracking LCSs will be attracted to trace out their specific structures during a simulation.

Figure 4 presents the FTLE distribution maps of $\mu_i = 2.7$ computed through forward-tracking (Figure 4(a)) and backward-tracking of particles (Figure 4(b)) for a duration $t = 50T$. Both of the forward and backward-tracked FTLE maps show nearly symmetrical patterns about the vertical diameter of the model lake owing to the alternating inflow forcing from the north-western and north-eastern directions. The main flow channels are covered by red colour indicating high FTLE and high separation rate. The areas covered by the dark blue colour have zero FTLEs, indicating zero separation rate. Theoretically, FTLEs should commonly have non-zero values. Actually, the sizable zero-FTLE zones in Figure 4(a) and Figure 4(b) are mostly created manually for those rapidly escaping particles. Particles initially located in these areas are washed out of computational domain before the simulation is completed, which prevents FTLEs from being quantified, and the FTLEs for these particles are simply set to zero. Since the particles in these areas rapidly move out of the domain without interacting with the surrounding particles, the dark blue zones are featured with low/zero fluid mixing. For the dynamic system with low μ_i , the FTLE distribution map is predominately covered by blue or dark blue colours, indicating small or zero FTLEs. Therefore, the overall fluid mixing for this case is therefore poor.

Figure 4 FTLE distribution for $\mu_i = 2.7$: (a) forward-tracked FTLE; (b) backward-tracked FTLE.

An effective means to interpret the mixing property of the dynamics system is to look at the LCSs in the FTLE distribution maps. LCSs occupy the high FTLE zones. Between these LCSs, there exist the so-called ‘valleys’ that are marked by blue or dark blue colours for low or zero values of FTLEs. While the existence of LCSs indicates the zones with high mixing rate, the valleys define the zones with low/poor mixing property (where the FTLE has a value between 0~0.05). As shown in Figure 4(a), the dynamic system for $\mu_i = 2.7$ is clearly featured with three low-mixing zones separated by LCSs, in addition to the dark blue ‘rush-out’ zone in the lower middle part of the domain where particles escape quickly. Particles initially released to these low-mixing zones will stay inside for a long time and can hardly be transported to and mixed with particles in other regions. On the other hand, particles initially located outside of these low-mixing zones (i.e. on or close to the LCSs) may travel rapidly along the representative unstable manifolds and mix with particles far away from its original locations. But they can never travel into the low-mixing zones

without further disturbances. As a result, particles that are originally near to each other may belong to different mixing zones (i.e. LCSs or valleys) and thus have entirely different behaviours. This essentially implies that the behaviour of a particle is highly sensitive to its initial conditions, which is a signature of chaos.

To demonstrate the fact that the LCSs essentially trace out invariant manifolds (or at least semi-invariant) and the lake is featured with zones of different mixing properties, three square particle patches, each with 10000 particles, are released into different mixing zones inside the lake at $t = 0$, as illustrated in Figure 5(a). The green patch is initially located in the rush-out zone, the red patch in a poor mixing zone and the blue patch on LCSs. The fates of the particles in these three patches are entirely different during the 50T of particle tracking process as shown in Figure 5(b-d). The green particles are quickly washed out from the domain by the powerful north-south cross-domain flow driven by the inflow, as shown in Figure 5(b). Located in one of the low-mixing zones, the red particle moves slowly and its shape has barely changed during the whole simulation, indicating poor mixing. The blue patch first travels to the south while it is simultaneously stretched into a filament. When it reaches the domain boundary, the filament reverses its direction of movement and travels back to north along the unstable manifolds as indicated in Figure 4. Overall, chaotic particle behaviour or rapid fluid mixing only exists in the small areas filled by unstable manifolds or LCSs for this dynamic system with $\mu_i = 2.7$.

Figure 5 Advection of three particle patches for $\mu_i = 2.7$: (a) $t = 0$; (b) $t = 10T$; (c) $t = 30T$; (d) $t = 50T$.

Figure 6 presents the FTLE distribution maps for $\mu_i = 10.8$. Obvious changes to the FTLE distribution have been detected, compared with $\mu_i = 2.7$. The LCSs that were previously only surrounding the low-mixing zones have begun to penetrate these zones and affect the particle dynamics inside. The LCSs close to the centre of lake have only changed slightly compared to those for $\mu_i = 2.7$. But substantial changes have been detected in the areas close to the physical boundary of the lake. Clearly, well-mixing zones indicated by the existence of LCSs have increased their size by penetrating into the original low-mixing zones for lower μ_i , making

the FTLE distribution to become more complicated and leading to more complicated particle dynamics.

Figure 6 FTLE distribution for $\mu_i = 10.8$: (a) forward-tracked FTLE; (b) backward-tracked FTLE.

Figure 7 shows the advection of the three particle patches for $\mu_i = 10.8$, with their original location shown in Figure 5(a). The green particle patch is readily washed out from the computational domain as it is still located in the wash-out zone. The red patch is still located in one of the well-defined low-mixing zones and particles move slowly without much mixing occurred. However, the movement of the blue particle patch has become much more complicated and traced out the structure of backward-tracked LCSs at the right-hand side of the lake. Since the forward-tracked LCSs and backward-tracked LCSs now interact with each other at the boundary of the low-mixing zones, chaotic mixing has been evidently created in these regions. As shown in Figure 7(b-c), the blue patch is repeatedly stretched and folded when they travel along the unstable manifolds from south to north. The stretching and folding actions have led to a complicated self-similar structure that fills the regions close to the eastern boundary of the right-hand side low-mixing zone, indicating chaotic particle-dynamics.

Figure 7 Advection of the three particle patches for $\mu_i = 10.8$: (a) $t = 10T$; (b) $t = 30T$; (c) $t = 50T$.

As μ_i is further increased to $\mu_i = 21.6$, the mixing and transport properties of the lake have been largely enhanced as illustrated by the resulting FTLE distribution maps in Figure 8. The two large low-mixing zones located at the left and right-hand sides of the lake have been substantially shrunken and replaced by two vortex-shape islands. LCSs have extended to almost all over the lake except for several much smaller low-mixing zones. The main flow path inside the lake has also been influenced. In the previous cases with lower μ_i , the main flow path features two upper branches connected to the

inlets and one almost straight channel to the south connected to the outlet. Now the lower part of main channel is highly twisted, as shown in Figure 8(b), indicating that particles initially located in the twisted main flow channel may have different mixing dynamics rather than simply being flushed out of the domain.

Figure 8 FTLE distribution for $\mu_i = 21.6$: (a) forward-tracked FTLE; (b) backward-tracked FTLE.

Figure 9 Advection of the three particle patches for $\mu_i = 21.6$: (a) $t = 10T$; (b) $t = 30T$; (c) $t = 50T$.

Figure 9 illustrates the evolution of the three particle patches at $\mu_i = 21.6$. Some particles from the green patch have been stretched into a filamentary structure within $10T$. As time elapses, the green patch rapidly traces out a complicated skeleton of unstable manifolds. This has not been observed at the left-hand side of the lake for lower μ_i , confirming that part of the original wash-out zone has been invaded and become a well-mixing zone. Located at the centre of the low-mixing zone, the red patch still follows slow and regular movement and has not mixed with fluid particles from outside the zone. Meanwhile, the blue patch has traced out the unstable manifolds at the right-hand side of the lake, as expected. Finally, as shown in Figure 9(c) for $t = 50T$, a large area of the lake has been occupied by green or blue particles. This indicates that more comprehensive chaotic mixing has occurred in a large area of the lake although the particles in chaotic zones can never transpose into the low-mixing zones, e.g. where the red patch is located. Furthermore, although green and blue particles undergo chaotic mixing they can only mix with the particles in the same zones. That is to say, different mixing zones still exist and are separated, and global mixing has not been achieved.

The particle dynamics has substantially changed when μ_i is further increased to $\mu_i = 86.4$, and the corresponding FTLE distribution maps are shown in Figure 10. The forward-tracked FTLE distribution is no longer meaningful since almost all of the particles have left the domain after $50T$ and therefore the FTLE values cannot be calculated using the FTLE computation technique as described previously. The backward-tracked FTLE distribution (**Error! Reference source not found.**(b)) shows that the LCSs have begun to fill most of the space in the whole lake.

Figure 10 FTLE distribution for $\mu_i = 86.4$: (a) forward-tracked FTLE distribution; (b) backward-tracked FTLE distribution.

Since there are no major low-mixing areas under the current condition, the whole lake is considered to be well mixed. As shown in Figure 11, particles from the three different patches quickly develop into complicated fractals and finally the unstable manifolds are perfectly traced out by these particles, as demonstrated in Figure 11(a). When the simulation time is increased to $t = 30T$ (Figure 11(b)), the number of particles remaining in the lake quickly decreases. At $t = 50T$, there are only few particles remaining inside the domain, which indicates that the lifetime of particles is finite in an open or semi-open chaotic system.

Figure 11 Advection of the three particle patches for $\mu_i = 86.4$: (a) $t = 10T$; (b) $t = 30T$; (c) $t = 50T$.

4.2 Continuous particle dynamics, occupying rate

In the previous section, we discussed how particle patches initially located in different mixing zones are advected to develop into patterns of different levels of complexity under the influence of LCSs. In engineering applications, it is also important to know how the particles carried by the inflows are transported in and occupy the different areas in the lake. Analysis of Lagrangian dynamics of particles

injected from outside may provide guidance for effective engineering solutions to improve the quality of water by utilising the inflow/outflow-induced shallow water flows. In reality, the duration of inflows may be regulated using gates in the inflow channels and the particle dynamics will be dependent on duration and magnitude of the inflows. On the contrary, it is almost impossible to directly control the wind forces (neither the magnitude nor the duration and direction) in a natural flow system. Controlling inflows/outflows therefore may provide an effective way to alter the flow dynamics and hence improve water quality of (semi-)enclosed water bodies.

Herein passive “freshwater” particles will be introduced into the lake directly through inflows. When the respective inflow is on, 25 particles arranged in a rectangular patch are created at each time step of particle-tracking calculation in the centre of inlet area and flushed into the lake together with the inflow. The scenarios with four different μ_i are simulated for $50T$ and the corresponding occupy rates are calculated. The occupy rate is defined as the ratio between the area ever visited by freshwater particles and the total areas of the lake. It may be used as an indicator of water quality improvement.

Figure 12 presents the simulation results at $t = 50T$ for different μ_i . When $\mu_i = 2.7$, particles are first transported to the central area of the lake by the inflow currents and then move straight to the south and leave the lake from the outflow channel. The occupy area is limited, and the “freshwater” particles just pass through the main flow channel and have little chance to mix with fluid particles in other parts of the lake. As μ_i increases to 10.8, particles are able to fill the entire north-south main flow channel and large areas close to the circular lake boundary. For $\mu_i = 21.6$, most parts of the lake have been occupied by the “freshwater” particles except the two low-mixing zones and a small area close to the north shoreline. It is clear that the LCSs effectively act as separatrix, preventing the “freshwater” particles from entering the low-mixing zones to dilute the possible pollutants or to wash the pollutants out of the lake. When μ_i is finally increased to 86.4, i.e. the global chaotic state as identified previously has achieved, the particle dynamics has clearly become dramatic and almost the whole lake is visited by “freshwater” particles, potentially leading to improved water quality.

Figure 12 Particle released continually into the lake: (a) $\mu_i = 2.7$; (b) $\mu_i = 10.8$; (c) $\mu_i = 21.6$; (d) $\mu_i = 86.4$.

In order to quantify the effectiveness of using “freshwater” particles to improve water quality of the model lake, the occupy rates of the four simulations with different μ_i are calculated and presented. For this purpose, the model lake is cover by 31428 uniform cells. If a cell is ever visited by at least one “freshwater” particle during the particle-tracking simulation, it is marked as being occupied. Figure 13 illustrates the changes of occupy rate during the 50T simulations with four different μ_i . After an exponential growth at the beginning, the changes of occupy rate of different μ_i quickly slow down and become quasi-steady (herein the occupy rate at the turning point is named quasi-steady occupy rate). For larger μ_i , fewer periods are required to reach quasi-steady state. This means that, when the dynamic system becomes chaotic (with sufficiently large μ_i), freshwater particles will visit more areas in the lake in fewer periods, demonstrating that the use of flesh water to flush the lake and improve water quality may be more effective when μ_i is sufficiently large.

Figure 13 Time histories of occupy rate for different μ_i .

Table 1 lists the relevant simulation results for the four scenarios, in terms of quasi-steady occupy rate, highest occupy rate and the time required to achieve them for all for simulations. For $\mu_i = 86.4$ when the dynamic system has become globally chaotic, the highly occupy rate reaches 98.94% during the 50T of simulation, effectively meaning that the whole lake has been reached by “fresh water”. The quasi-steady stage with an occupy rate of 91.29% is reached only after 3T, equivalent to 3840s or slightly more than 1 hour. For smaller μ_i when the dynamic system has not reach global chaotic stage, much lower quasi-steady and highest occupy rates are achieved. Furthermore, the time required to reach the quasi-steady occupy rate is actually longer for $\mu_i = 10.8$ and 21.6. Therefore, a chaotic dynamic system is essential when inflow/outflow-induced shallow water flows are used to improve water quality in a semi-enclosed water body.

Table 1. The convergent rates and highest occupy rates for different μ_i .

μ_i	2.7	10.8	21.6	86.4
Time to quasi-steady state (s)	940	6000	5440	3840
Number of periods (T)	23.5	37.5	17	3
Quasi-steady occupy rate (%)	19.13	49.96	79.17	91.29
Highest occupy rate (%)	20.76	54.1	86.88	98.94

5. Conclusions

A numerical modelling approach consisting of a shallow water hydrodynamic model and a passive particle-tracking model is developed and implemented to investigate the mixing and transport process induced by inflows/outflows in an idealised semi-enclosed shallow flow system. The horizontal mixing dynamics are interpreted using FTLEs, LCSs and advection of particle patches.

From the simulation results, it is confirmed that periodic inflows are able to create a weak dynamic system in a semi-enclosed shallow water body, i.e. the idealised circular model lake as considered in this work. The particle dynamics is controlled by a single dimensionless parameter associated with inflow duration, i.e. the dimensionless flow duration. The results in terms of FTLE distribution maps and the associated LCSs confirm that the mixing and transport property of the lake changes from regular to chaotic as μ_i increases. Higher mixing efficiency is achieved with higher μ_i and global chaotic particle dynamics is achieved at $\mu_i = 86.4$ in the current case study. In conclusion, chaotic mixing may be developed by using period inflow/outflow conditions, comparable to those produced by periodic wind stresses.

By analysing the advection of particles injected continuously into the system at the inflow locations, it is able to trace out the fate of “freshwater” particles in a “polluted” lake. When μ_i is low, effective mixing cannot be achieved and the “freshwater” particles are not well mixed with the “polluted” water particles in large areas of the lake, leading to low occupying rate. When μ_i is increased, more effective mixing and higher occupying rate can be achieved at a shorter time. The results provide useful guidance for engineering applications, i.e. transferring freshwater from rivers to improve major polluted water bodies, and the presented approach will be able to help design ‘optimised’ solutions for engineering implementation.

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