MASTER

Source-sink induced chaotic advection for enhanced groundwater remediation

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Abstract

Efficient mixing of pollutant-consuming bacteria and polluted groundwater can potentially enhance natural remediation of groundwater. This could provide a faster and more cost-efficient method than currently applied remediation techniques. As turbulence in groundwater flow is absent, efficient mixing can only be achieved by producing chaos in the flow. Chaotic advection may result from time-dependent flow induced by sources and sinks.

Three different source-sink systems are investigated using numerical simulation of particle trajectories: the pulsed source-sink system, the switched dipole system and the rotated dipole system. First, a system consisting of a sequentially pulsed source and sink was investigated both in two dimensions (2D) and in three dimensions (3D). In 2D this system can be described by a single dimensionless parameter $\Gamma$, based on the strength and the separation distance of the source and sink as well as the pulse time. The efficiency of chaotic mixing was explored by determining the location and nature of the periodic points: elliptic points are the centers of non-mixing regions, while hyperbolic points are the centers of stretching and folding in the flow (essential to efficient mixing). The system showed chaotic dynamics for all parameter settings investigated. Periodic points were identified up to order six and were arranged along branch-like structures with higher-order periodic points generally located further away from the source and sink. When $\Gamma$ is decreased, the periodic points move towards the source and sink and some point are destroyed. In addition, small $\Gamma$ leads to an increase in the surface area of elliptic islands. Of all the investigated parameter settings, the system with $\Gamma = 10.4$ is likely the best mixer. In the 3D case, symmetry reduces the flow dynamics to 2D planes and the observed dynamics is similar to the 2D case.

The effects of dispersion on the pulsed source-sink system are investigated by the application of a small perturbation to the velocity field. This method has been used in previous studies to simulate the effects of inertia in chaotic systems and might also be used for dispersion. The perturbed system shows the breakup of elliptic orbits and the change of elliptic orbits into partially overlapping bands. As no comparative material is available, experimental verification of these results is needed.

In addition to the pulsed source-sink system, two systems of sequentially reoriented dipoles are studied. The switched dipole flow and the rotated dipole flow. Both these systems could be described by a single dimensionless variable $\Upsilon$ and showed confinement of material within a circle connecting the sources and sinks. As $\Upsilon$ decreases more elliptic islands appear in the switched dipole flow. The case $\Upsilon = 0.9$ showed no elliptic islands. Many more hyperbolic period-1 points were found for the rotated dipole flow compared with the switched dipole flow. This suggests that the rotated dipole flow mixes better, at the cost of taking twice the time and more surface area of elliptic islands. Of all the investigated cases, the case $\Upsilon = 1.26$ is likely the best mixer.

The possibilities of constructing a translucent laboratory model for the groundwater system are investigated for future validation of the numerical findings. Borosilicate glass spheres with a diameter of 9 mm were placed in a mixture of glycerol with water. This setup was able to make single spheres virtually invisible. When testing a setup consisting of multiple spheres, distortions were observed that significantly reduced the transparency of the setup. These distortions were attributed to optical inhomogeneities within the glass spheres, also observed with shadowgraph measurements. Temperature treatment of the spheres and better control of the lighting conditions resulted in a significant reduction of the observed distortions.
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Chapter 1

Introduction

Contamination of soil and groundwater is a large environmental problem. Sources of contamination range from leaking underground storage tanks and hazardous waste sites to agricultural sources such as fertilizers and pesticides. In general pollutants degrade naturally as a result of microorganisms that convert these contaminants to harmless materials. This process of biodegradation is very slow, often requiring several decades of time. Biodegradation of contaminants in soil is limited by a non-uniform distribution of microorganisms across the contaminated region. In some cases high concentrations of pollutants inhibit efficient biodegradation. Moreover, subsurface transport of pollutants, microorganisms and their nutrients is based on diffusion and is therefore very slow. Efficient mixing of microorganisms with pollutants and nutrients might significantly accelerate the process of biological remediation resulting in a faster and cost-efficient biological remediation technique.

Fluid motion in groundwater systems takes place through small pores. On a macro scale this flow behaves as a potential flow, following Darcy’s law. Generally velocities in a groundwater system are very small. Turbulent flows are often used in mixing applications and have been proven to be highly efficient mixers. Because of the small flow velocities in groundwater systems, turbulent flows cannot be created. Efficient mixing in laminar flows can be achieved using chaos. These so-called chaotic flows can arise in very simple systems and have the key property that fluid elements are stretched and folded by the flow. This property causes nearby particles in a chaotic flow to diverge exponentially fast, which is the basis of the efficient mixing capabilities of these flows. As fluid elements are stretched and folded in a chaotic flow, their surface area increases. This in turn promotes diffusion to decrease gradients in concentrations, which is called mixing. An example of the stretching and folding dynamics observed in chaotic flows is shown in figure 1.1 where snapshots of a dye trace simulation on a periodically rotated dipole flow are shown.

Before chaotic advection can be applied to enhance groundwater remediation a thorough analysis of enhanced mixing in porous media is required. Therefore chaotic advection in potential flows needs to be studied. In addition, the effect of micro-scale dynamics on the mixing in porous media should be investigated. An important micro-scale effect is dispersion of tracer particles due to large variations in velocities on the micro scale. Dispersion causes groups of tracer particles to spread, an effect that is not included in the potential flow description given by Darcy’s law.

The field of chaotic advection was pioneered by H. Aref who showed that chaotic advection can be achieved in a two-dimensional (2D) potential flow, forced by two blinking point vortices [Aref, 1984]. Later Jones et al. (1988) showed that chaotic advection is also possible in a potential flow...
without circulation using a system of an alternately pulsed source-sink system, consisting of a single source and a single sink \cite{Jones and Aref, 1988}. Inspired by this work, a more practical system consisting of several dipoles operated sequentially has been investigated by several researchers using numerical simulations. Applications range from groundwater flow \cite{Bagtzoglou and Oates, 2007} \cite{Lester et al., 2009} to flow inside microfluidic devices \cite{Hertzsch et al., 2007} \cite{Beuf et al., 2010} \cite{Stremler and Cola, 2006}. All these systems were investigated in 2D only. A typical setup of wells to achieve chaotic advection in groundwater flow is shown in figure 1.2. Experimentally the

2D simulations performed on the systems of dipoles have been verified with the use of a Hele-Shaw cell \cite{Metcalfe et al., 2010} \cite{McQuain et al., 2004}. A Hele-Shaw cell is a shallow layer of fluid enclosed between two plates. It can be shown that the flow inside such a Hele-Shaw cell behaves as a potential flow, similar to flow in porous media.
The main difficulty in experiments on actual porous media flow is that it is difficult to measure inside the medium as porous media are usually not translucent. To investigate porous media in a lab setup several experimental techniques are used. Depending on the application, MRI measurements, X-ray/CT techniques as well as gamma radiation methods or optical methods can be used [Werth et al., 2010]. In particular transport properties on the micro scale, such as dispersion of tracer particles, can be investigated using an artificial porous medium that is made translucent by matching the index of refraction of a translucent solid phase with a translucent liquid phase. This so-called refractive-index matched (RIM) porous medium can be used to measure transport properties using advanced optical techniques. From these measurements 3D time-resolved position data of tracer particles in the flow can be obtained.

In this project several systems of sources and sinks are investigated numerically. First a system of an alternatingly pulsed source and sink, referred to as the pulsed source-sink system, is investigated. This system is identical to that explored by work of Jones and Aref (1988) but here we focus on the location and nature of periodic points which are essential to chaotic advection. The analysis of this system is extended with a study on the influence of inertia. In addition, a 3D version of the pulsed source-sink system is investigated. As a next step, we consider other source-sink systems based on periodically reoriented dipoles. In contrast to previous work on these systems, (Lester et al., 2009, Hertzsch et al., 2007, Beuf et al., 2010 and Stremler and Cola, 2006) the current study involves an unbounded domain as this is a more realistic representation of the application on groundwater mixing. Again the focus is on the location and nature of periodic points and the effects of inertia and dispersion. To validate the numerical findings and to investigate micro-scale effects on the mixing properties of porous media in future experiments, the possibilities of constructing a RIM artificial porous medium are considered. The aim of these investigations is to ultimately contribute to the understanding of chaotic dynamics in porous media so as to eventually obtain an optimised system for enhanced groundwater remediation.

Before analysing the three source-sink systems the theoretical fundamentals regarding groundwater flow and chaos are discussed in chapter 2. This section is followed by a discussion of the pulsed source-sink system in section 3. The source-sink systems based on periodically reoriented dipoles are discussed in section 4. The RIM artificial porous medium is discussed in section 5. This report ends with a presentation of the conclusions and a discussion in chapter 6.
Chapter 2

Theory

This chapter describes the basic theory needed for the investigation of chaotic advection in groundwater systems. First the fundamentals of groundwater flow are discussed briefly. In this part the transport mechanisms and the governing equations for groundwater flow are discussed. The second part of this chapter is devoted to the basic theory regarding chaos.

2.1 Groundwater flow

In this section some theory regarding flow in groundwater systems is discussed. A more extensive discussion of this subject can be found in Bear (2010) and Stauffer (2005). Groundwater flow takes place through small pores between grains of sand or within rocks. The microscopic details of the flow velocity and pressure are very complex. To obtain macroscopic information on the flow in porous media the microscopic details of the flow through individual pores is not of interest. Therefore, quantities such as flow velocities and pressure are averaged over a small volume containing several pores. This is shown in figure 2.1 where the black square represents the so-called representative elementary volume (REV). At the scale of the REV the microscopic details of the problem are lost and the flow can be modeled as a continuum.

Figure 2.1: Schematic representation of a representative elementary volume in a porous medium. Figure from [Stauffer, 2005].
The macroscopic flow through porous media obeys an empirical relation known as Darcy’s law which describes the relationship between velocity $\vec{v}$ and pressure $p$ inside the porous medium. That is,

$$\vec{v} = \frac{k}{n\rho\nu}(\nabla p - \rho\vec{g}), \quad (2.1)$$

where $\rho$ and $\nu$ are the density and the kinematic viscosity of the fluid, respectively. These quantities are averages over the REV. The vector $\vec{g}$ describes the gravitational acceleration. The porosity $n$ describes the relative volume occupied by the pores in the porous medium and the permeability $k$ is a measure of the ease with which flow can pass through the porous medium. The velocity from equation (2.1) is irrotational and the flow can be described as a potential flow. Darcy’s law is valid when inertia and dispersion can be neglected. The relative importance of inertial forces with respect to frictional forces is given by the Reynolds number:

$$Re = \frac{vd}{\nu}, \quad (2.2)$$

where $d$ is a characteristic length in the system. For porous media this characteristic length can be represented by a characteristic pore scale length. Groundwater systems generally have low flow velocities resulting in low Reynolds numbers. This justifies neglecting the effects of inertia.

In addition to Darcy’s law, conservation of mass states that

$$\nabla \cdot \vec{v} = 0, \quad (2.3)$$

where the density of the fluid and the porosity are assumed constant.

Transport of tracer materials such as pollutants in groundwater flow is dependent on three different processes. These processes are advection, diffusion and dispersion. Firstly, tracers are transported with fluid particles by the flow; this effect is referred to as advection. Diffusion causes transport of tracers from regions of high concentration to regions of lower concentration of these pollutants. This microscopic effect causes a small collection of tracer particles to spread out, equalizing concentrations. At the microscopic level the fluid velocities vary strongly. This variation causes small collections of tracers to spread. This spreading effect is called mechanical dispersion and is not included in the macroscopic description given by Darcy’s law.

### 2.2 Chaos

Chaotic systems are systems that behave irregularly and unpredictably. In contrast to noisy dynamics caused by for example thermal fluctuations in electric circuits, the irregularity and unpredictability in chaotic systems is the result of the system itself and is caused by extreme sensitivity to initial conditions. Chaos can arise in very simple systems, provided that the system has a nonlinear component.

Chaotic dynamics can be observed in a wide variety of situations and on different scales, ranging from the dynamics of the earth’s magnetic field, the weather and the solar system to dynamics of the economy and chemical reactions. The study of chaotic systems is also important from an engineering perspective as machines can exhibit chaotic behavior [Tél and Gruiz, 2006]. The theory presented in this section outlines the basic principles of chaos relevant to this work ([Speetjens, 2001], [Tél and Gruiz, 2006] and [Water, 2010]).
2.2.1 Maps and Poincaré sections

The irregularity of chaotic systems makes them more difficult to study as one would with regular motion. Instead of studying the dynamics of a system as a function of time, chaotic systems are generally studied in their phase space where interesting structures can often be observed. In phase space, each state of the system is represented as a point. For example, the motion of a pendulum in time can be studied in a traditional way by looking at the position versus time. Alternatively the dynamics of the pendulum can be studied by looking at the velocity versus position, which we call phase space. Phase spaces are often higher dimensional spaces, which complicates visualisation. In the general case of 2D motion the phase space would be four dimensional: one dimension for each velocity component of the velocity vector $\vec{v} = (v_x, v_y)$ and one dimension for each component of the position vector $\vec{x} = (x, y)$.

In the special case of fluid advection using a forced velocity field, every position corresponds to a specific velocity and hence the system can be completely described by the position vector only. To reduce the complexity of the system the dynamics can often be described in discrete time steps $T$. The evolution of the position over time can be described by

$$\vec{x}_{t+T} = \Phi_T(\vec{x}_t), \quad (2.4)$$

where $\Phi_T$ is the function that maps the position $\vec{x}_t$ at time $t$ to the position $\vec{x}_{t+T}$ at time $t+T$. The mapping function $\Phi_T$ can in principle be determined by integrating the equations of motion over time and hence, the mapping function contains all the details of the motion. Repeated application of the mapping function on the position results in a discrete time evolution of the position. When these discrete points are plotted in phase space a so-called Poincaré section is obtained.

2.2.2 Periodic points

There may exist special points $\vec{x}_p$ in the map, called periodic points, for which application of the map yields the same point. That is

$$\Phi_k T(\vec{x}_p) = \vec{x}_p, \quad (2.5)$$

where the superscript denotes $k$ subsequent applications of the mapping function, with $k \in \mathbb{N}^+$. A point satisfying equation (2.5) is referred to as a period-$k$ point. When $k > 1$, periodic points come in sets of $k$ points, where each member of the set satisfies equation (2.5) and the set member relate to each other via

$$\vec{x}^{(i+1)} = \Phi_T \vec{x}^{(i)}, \quad (2.6)$$

where the superscript $(i)$ labels the set members.

Different kinds of periodic points can be distinguished. The different cases in 2D as well as 3D are discussed below. A full analysis on this subject can be found in Speetjens (2001) and Tel (2006).

Two-dimensional periodic points

Consider a period-$k$ point $\vec{x}_p$ of the map $\Phi_T$ from equation (2.4). The dynamics near a periodic point can be determined by looking at the response of the map on perturbations $\Delta \vec{x}$ on $\vec{x}_p$. For small perturbations it is sufficient to approximate the response by considering only linear terms.
of the map around the periodic point. Upon $k$-fold application of the mapping function, covering a time of $kT$, the perturbed point is close to its original location. The location of the perturbed point after $t = kT$ can be approximated by

$$\vec{x}(kT) = \vec{x}_p + \Delta \vec{x}(kT) = \Phi^k_T(\vec{x}_p + \Delta \vec{x}(0)) = \vec{x}_p + \tilde{J}\Delta \vec{x}(0),$$

(2.7)

where $\tilde{J}$ is the Jacobian matrix of $\Phi^k_T$ at $\vec{x}_p$.

In 2D the general trajectory in this linearised region near the periodic point is described in discrete steps of $kT$ by

$$\Delta \vec{x}(nkT) = a_1\vec{\eta}_1 e^{\lambda'_1 nT} + a_2\vec{\eta}_2 e^{\lambda'_2 nT},$$

(2.8)

where $n$ is a positive integer counting the steps, $\vec{\eta}_1$ and $\vec{\eta}_2$ are the eigenvectors of $\tilde{J}$. Here, $\lambda'_1$ and $\lambda'_2$ are related to the eigenvalues $\lambda_1$ and $\lambda_2$ of $J$ via

$$\lambda'_i = \frac{\ln \lambda_i}{T}.$$  

(2.9)

The constants $a_1$ and $a_2$ can be determined from initial conditions. The eigenvalues $\lambda_1$ and $\lambda_2$ are related to phase space volume changes. Application of the concepts described in this chapter on incompressible fluid motion leads to incompressibility of the corresponding phase space, which results in the following constraint on the eigenvalues: $\lambda_1 \lambda_2 = 1$. Two different kinds of periodic points can be distinguished:

- **Hyperbolic points**: In this case the eigenvalues are both real. Material is attracted in one direction and repelled in another direction. The attracting and repelling directions coincide with the eigenvector directions of the matrix $\tilde{J}$. Hyperbolic points are crucial in chaotic advection as they facilitate stretching and folding in the fluid, as will be discussed in section 2.2.3. The general evolution of a tracer particle near a hyperbolic point under subsequent applications of the mapping function is shown in figure 2.2a.

- **Elliptic points**: When the eigenvalues are purely imaginary, material close to the periodic point performs a rotation about this periodic point in the Poincaré section. Because of the pure rotational motion, there will be a non-chaotic region around the elliptic point where particles are observed to stay in an orbit near the periodic point, under subsequent applications of the mapping function. These orbits of particles rotating about an elliptic points are referred to as elliptic orbits or invariant surfaces. The non-chaotic region around the elliptic points is called elliptic island. The general evolution of a tracer particle in a Poincaré section near a elliptic point is shown in figure 2.2b.

The special case when $\lambda_1 = \lambda_2 = 1$ is called marginally stable and can be found at the transition from elliptic to hyperbolic.
Three-dimensional periodic points

In the 3D case some important differences can be observed with respect to the 2D case. The Jacobian $\tilde{J}$ from equation (2.7) now has three eigenvalues $\lambda_1, \lambda_2$ and $\lambda_3$ with their respective eigenvector directions $\tilde{\eta}_1, \tilde{\eta}_2$ and $\tilde{\eta}_3$. The general solution of equation (2.7) becomes

$$\Delta \tilde{x}(nkT) = a_1 \tilde{\eta}_1 e^{\lambda'_{1} nT} + a_2 \tilde{\eta}_2 e^{\lambda'_{2} nT} + a_3 \tilde{\eta}_3 e^{\lambda'_{3} nT},$$  

(2.10)

where $n$ counts the discrete time steps, $\lambda'_1$, $\lambda'_2$ and $\lambda'_3$ relate to the eigenvalues of $\tilde{J}$ via equation (2.9) and $a_1$, $a_2$ and $a_3$ are constants that can be determined from the initial conditions.

Again incompressibility requires the eigenvalues of the Jacobian matrix to satisfy $\lambda_1\lambda_2\lambda_3 = 1$. This invariably results in one real eigenvalue, say $\lambda_1$, which leaves two possibilities for the remaining eigenvalues: $\lambda_1, \lambda_2, \lambda_3$ are all real, or $\lambda_2$ and $\lambda_3$ are complex conjugates. Two basic types of periodic points can be distinguished:

- **Node**: When all the eigenvalues are real the point is referred to as a node. Two types of nodes can be distinguished: stretching nodes and compressing nodes. When $\lambda_1 > 1$ and both $\lambda_2$ and $\lambda_3$ are positive and smaller than 1, the node is of the stretching type. This structure compresses fluid in the $(\tilde{\eta}_2, \tilde{\eta}_3)$-plane, and stretches fluid along the $\tilde{\eta}_1$-direction. When $\lambda_1 < 1$ and $\lambda_2$ and $\lambda_3$ are positive and larger than 1, the node is of the compressing type. This type of node compresses fluid in the $\tilde{\eta}_1$-direction and stretches fluid in the $(\tilde{\eta}_2, \tilde{\eta}_3)$-plane. The dynamics around hyperbolic nodes are depicted in figure 2.3a. In the special case that one of the eigenvalues is equal to 1 the dynamics near the periodic point is essentially 2D and the 2D hyperbolic point, described in section 2.2.2, is obtained.

- **Focus**: When $\lambda_2$ and $\lambda_3$ are complex conjugates the periodic point is referred to as a focus. Depending on the value of $\lambda_1$ again stretching and compressing types can be distinguished. In the stretching case, $\lambda_1 > 1$ and fluid rotates about the $\tilde{\eta}_1$-direction while simultaneously being stretched in that direction. Fluid is compressed in the $(\tilde{\eta}_2, \tilde{\eta}_3)$-plane. The compressing focus is observed when $\lambda_1 < 1$. In this case the fluid is compressed in the $\tilde{\eta}_1$-direction while rotating about the $\tilde{\eta}_1$-direction as well. Fluid is stretched in the $(\tilde{\eta}_2, \tilde{\eta}_3)$-plane. The dynamics corresponding to the focus type periodic points are depicted in figure 2.3b. In the special case that $\lambda_1 = 1$ the dynamics is again reduced to 2D and similar to the 2D elliptic point as described in section 2.2.2
In some cases the dynamics is confined to 2D planes and consequently the 2D types of periodic points are obtained. These periodic points can join in the direction normal to the plane into a smooth line in 3D. This line is referred to as a periodic line. The eigenvalues normal to the line can change at different points on the line, allowing the type of dynamics (elliptic, hyperbolic or marginally stable) in the planes to change.

(a) Hyperbolic node

(b) Hyperbolic focus

Figure 2.3: Phase space portraits of different types of periodic points. Particles close to the periodic point will follow paths in Poincaré sections. These paths are formed by joining the stroboscopic points for each iteration. The direction (stretching or compressing) is dependent on the eigenvalues and is not shown here. Figures from [Speetjens, 2001].

2.2.3 Manifolds

The phase space behaviour near periodic points was described in the previous section. In the present section the influence of these periodic points on the rest of the phase space is discussed.

Fluid near hyperbolic points is pushed away in one direction while fluid is attracted from another direction. These principle directions of stretching and compression can be identified by the eigenvectors of the Jacobian at this point, as discussed in the previous section. Trajectories emanating from the eigenvector corresponding to the stretching direction trace out the so-called unstable manifold. This manifold $W$ essentially is an invariant line under the mapping $\Phi^k$ such that

$$\Phi^k(W) = W \quad (2.11)$$

stating that every point on this manifold stays on the manifold after application of the mapping function.

Material points on the unstable manifold originate from the hyperbolic periodic point. Similarly the stable manifold can be defined as the invariant curve consisting of all points that approach the
hyperbolic periodic point. Stable and unstable manifolds can be traced out for arbitrary long times
and hence they are of infinite length. Note that in 3D systems these manifolds can be 2D surfaces,
but for simplicity only the 2D case will be considered here.

Because of their infinite length unstable and stable manifolds will intersect each other. Such
an intersection point is called a homoclinic point when both of the manifolds belong to the same
hyperbolic point and a heteroclinic point when the manifolds belong to different hyperbolic points.

Consider the hyperbolic point $P$ shown in figure 2.4 with its stable and unstable manifolds $W_s$
and $W_u$, respectively. Following the unstable manifold from $P$ inevitably the stable manifold will
be crossed. Because this homoclinic point $\vec{x}_h$ is on an unstable manifold so is the mapping $\Phi_T(\vec{x}_h)$
of the homoclinic point. At the same time, the mapping $\Phi_T(\vec{x}_h)$ of the homoclinic point is on the
stable manifold. This implies the existence of a second homoclinic point. Further iterations of
the mapping produce more and more homoclinic points, each lying closer to the hyperbolic point
than the previous one as shown in figure 2.4 All the points on the unstable manifold between two
successive homoclinic points are mapped between the next pair of homoclinic points. This results
in the loops shown in figure 2.4 Due to incompressibility the area between the unstable and stable
manifolds (shown in grey) between two successive homoclinic points remains the same. Because
the homoclinic points are closer together near the hyperbolic point the loops become stretched.
Similar dynamics occurs on the side of the stable manifold where successive homoclinic points are
produced by longer and longer loops of stable manifold (dashed line in figure 2.4).

![Figure 2.4: Manifold dynamics: the formation of homoclinic points. Figure from Water, 2010.](image)

The behaviour of stable and unstable manifolds discussed above shows an important property of
chaotic systems. Material located near a hyperbolic point is stretched along the unstable manifold.
This unstable manifold intersects the stable manifold and forms loops that converge towards a
hyperbolic point. The material line that was originally stretched near an hyperbolic point is now
folded onto itself. This stretching and folding dynamics is the essence of chaotic advection.
2.2.4 The KAM theorem

The KAM theorem, or Kolmogorov-Arnold-Moser theorem, describes the breakup of elliptic orbits around periodic points under small perturbations [Tél and Gruiz, 2006]. As discussed in section 2.2.2, non-chaotic regions can be found around periodic points of the elliptic type. Particles in these elliptic islands describe periodic motion around the corresponding periodic point.

The orbits of these particles can be characterised by a winding number $\nu$. When $\nu$ is a rational number given by $\frac{p}{q}$, every point on the described orbit is a periodic point of period $q$. A particle released at such a period-$q$ point moves around the central fixed point for subsequent mappings. The period-$q$ point moves around the central fixed point $p$ times each cycle of $q$ periods. For irrational $\nu$ a point on the orbit will never return exactly to its original position.

The KAM theorem states that under perturbations, rational orbits will break up first and irrational orbits are the most stable. Because points on rational orbits return to their original position after some time, disturbances in the position caused by the perturbations can grow. This is in contrast to irrational orbits where disturbances can average out over time, prohibiting their growth.

Consider an orbit with a rational winding number around a periodic point. Generally $\nu$ changes continuously meaning there will be irrational orbits bounding the rational orbit both on the inside and on the outside. When this rational orbit breaks up as the result of small perturbations, a chain of hyperbolic and elliptic points will appear in the area bounded by the irrational orbits. In this area chaotic dynamics can be observed.
Chapter 3

The pulsed source-sink system

As a first step in investigating chaotic advection in a porous medium the pulsed source-sink system is investigated. This conceptual model, proposed by Jones and Aref (1988), provides a basic look into the chaotic properties of source-sink systems. It also serves as a benchmark to test the simulation code and the search for periodic points.

In this section the advection properties of both a 2D and 3D pulsed source-sink system are investigated by means of numerical simulations. Poincaré maps are constructed, periodic points and manifolds are identified and dye tracing simulations are performed. This provides qualitative information on the advection properties of these source-sink systems. In addition, a velocity perturbation is applied to the system to investigate the effects of inertia and dispersion.

3.1 The two-dimensional pulsed source-sink system

The pulsed source-sink system consists of a source and a sink placed at positions $(-a, 0)$ and $(a, 0)$ respectively, as shown in figure 3.1. In 2D the velocity field $\vec{v}$ produced by a point source is given by

$$\vec{v} = \frac{Q}{2\pi r} \vec{e}_r,$$

where $Q$ is the source strength, with $Q > 0$ for a source and $Q < 0$ for a sink, $r$ is the radial distance to the source or sink and $\vec{e}_r$ the unit vector in the radial direction away from the source or sink.

When a passive tracer is tracked in a flow field its position $\vec{x}$ over time $t$ is governed by

$$\frac{d\vec{x}}{dt} = \vec{v}.$$

In the velocity field of a source or a sink, paths traced out by these particles are straight lines that coincide with so-called streamlines. Streamlines are lines that are tangent to the velocity field at every point on the line. Figure 3.2a shows several of these streamlines for the individual source and sink velocity fields. These lines were obtained by strategically placing tracer particles close to the source and far away from the sink and tracking their paths over time.

To create chaotic dynamics the source and sink operate alternately for time periods of $T/2$, defining $T$ as a full switching period. Tracer particles first follow the streamlines associated with the velocity field of the sink. After a time period $T/2$ the sink is switched off and the source

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becomes operational. Tracer particles then follow the streamlines related to the velocity field of the source. This forcing protocol results in the tracer particles performing a zigzag motion as shown in figure 3.2b.

Figure 3.1: Schematic representation of the pulsed source-sink setup consisting of a source and a sink positioned a distance $2a$ apart on the $x$-axis.

Figure 3.2: (a) Streamlines for the individual source flow (red) and the sink flow (blue). (b) A typical trajectory of a particle in the pulsed source-sink flow released at $(x/a, y/a) = (0.3, 1.2)$. The source and sink are marked by $\oplus$ and $\ominus$, respectively. Black dots show position after full switching periods. Starting position is marked by $\times$.

When a tracer particle is sufficiently close to the sink it is absorbed and would leave the system, hence the tracer particle would reside in the system for only a finite amount of time. This makes the pulsed source-sink system difficult to study using the standard tools of dynamical systems. Therefore the tracer particle is reintroduced at the source after absorption in the previous sink step. In this reinjection procedure, tracer particles are reintroduced in the flow field at the source.
on a streamline mirroring the trajectory associated with the previous (sink) step, as shown in figure 3.2b. Reinjecting particles at the source also relates better to practical applications of groundwater mixing. The distance a tracer particle travels after reinjection at the source depends on the distance travelled by the particle during the previous sink step such that particles that are absorbed first will be reinjected first.

Physically the reinjection procedure described above can be realised using a very long and narrow tube. The fluid is collected in the tube during the sink step. During the source step the bottom of the tube is connected to the source and the fluid is reinjected. This reinjection procedure is equivalent to the procedure used in Jones et al. (1988) and bears great resemblance to the procedures used in systems with different configurations of sources and sinks [Hertzsch et al., 2007].

The 2D pulsed source-sink system has several parameters of interest, namely $T$, $Q$ and $a$, which can be combined into a single dimensionless parameter describing the system completely:

$$\Gamma = \frac{QT}{a^2}. \quad (3.3)$$

The pulsed source-sink model can be described by the composite map $\Phi_T$, i.e.

$$\Phi_T = F_2F_1, \quad (3.4)$$

relating the position $\vec{x}_t$ at time $t$ to the position $\vec{x}_{t+T} = \Phi_T(\vec{x}_t)$ at time $t+T$, where $F_1$ and $F_2$ are the mapping functions describing the sink and source steps, respectively.

In the following analysis, we will determine the characteristics and locations of the periodic points for different $\Gamma$. As hyperbolic points are responsible for the stretching and folding dynamics they serve as an indicator of the mixing properties of the system.

### 3.1.1 Simulation setup

The pulsed source-sink system allows for analytical computation of particle trajectories. An expression for the particle position as a function of time can be obtained by combining the radial component of equation (3.2) with equation (3.1), giving

$$\frac{d\vec{r}}{dt} = \frac{Q}{2\pi r} \vec{e}_r. \quad (3.5)$$

Integration with respect to time gives

$$r^2(t) = r^2(t_0) + \frac{Q}{\pi} t, \quad (3.6)$$

where $r(t_0)$ is the radial distance from the active point source or sink at the start of the respective source or sink step ($t = t_0$). Equation (3.6) together with the reinjection procedure defined earlier were implemented in a Matlab code to perform computer simulations on this system.

### 3.1.2 Identification of periodic points

Periodic points play a vital role in chaotic dynamics. Therefore periodic points are of great interest when investigating a chaotic system. This section describes three methods for finding periodic points.
The first method to be discussed is the symmetry method. This widely applicable method to find periodic points makes use of symmetry relations in the system. As a second approach, a geometrical method is discussed. This method, proposed by Jones et al. (1988), provides much insight into the distribution of periodic points in the pulsed source-sink system. Finally, a numerical method called the Newton-Raphson method, is discussed. This method is fully numerical and no insight into the underlying flow is required as long as the mapping function can be evaluated. The use of these methods is illustrated for the 2D pulsed source-sink system with $\Gamma = 19.1$.

Symmetry method

Coherent flow structures such as periodic points and invariant manifolds can be found by analysing the symmetry properties of the flow [Speetjens, 2001]. These symmetry properties can be identified with relative ease by making use of general insight into the flow topology and boundary conditions without the need of a detailed knowledge of the flow.

Flow field symmetries can arise due to symmetries in the forcing protocol or symmetries in the boundary conditions. Symmetry operators are denoted by $S$ and their associated symmetry planes $I_s$ are defined by

$$S I_s = I_s.$$  

(3.7)

\[ \Phi_T S(x) \]

\[ \Phi_T^{-1} S(x) \]

\(x\)

\(y\)

\(\Phi_T S(x)\)

\(\Phi_T^{-1} S(x)\)

(a) Ordinary reflectional symmetry (b) Time-reversal reflectional symmetry

Figure 3.3: Schematic representation of ordinary reflectional symmetry and time-reversal reflectional symmetry.

Relevant symmetry classes are ordinary reflectional symmetries and time-reversal reflectional symmetries, and are illustrated in figures 3.3a and 3.3b respectively. Systems with ordinary reflectional symmetry obey

$$\Phi_T = S \Phi_T S^{-1},$$  

(3.8)
where $\Phi_T$ again is the mapping associated with the system. Systems with time-reversal reflectional symmetry obey

$$\Phi_T = S\Phi_T^{-1}S^{-1},$$

(3.9)

where the superscript $-1$ denotes time-reversed mapping. Note that symmetry operator $S$ satisfies: $S = S^{-1}$.

Symmetries also apply to periodic points. Consider a period-$k$ point $\vec{x}_p$. By symmetry the point $\vec{x}'_p = S\vec{x}_p$ is also a period-$k$ point, though not necessarily belonging to the same set. This can be shown using equation (2.5) with equations (3.8) and (3.9). For systems with ordinary reflectional symmetry this results in

$$\Phi^k_T Sx_p = S\Phi^k_T SSx_p = S\Phi^k_T x_p.$$  

(3.10)

Similarly, for systems with time-reversal reflectional symmetry:

$$\Phi^k_T Sx_p = S\Phi^{-k}_T SSx_p = S\Phi^{-k}_T x_p.$$  

(3.11)

Periodic points can be observed in two different configurations. First a single periodic point $x_p$ which always has a symmetrical counterpart $Sx_p$ forming the pair $[\vec{x}_p, S\vec{x}_p]$. In the special case that $x_p$ is on the symmetry plane $I_x$ there is no symmetrical counterpart.

In the 2D pulsed source sink model described above, the sink step $F_1$ and the source step $F_2$ permit the following symmetry relations:

$$F_1 = S_y F_1 S_y, \quad F_2 = S_y F_2 S_y, \quad F_1 = S_x F_2^{-1} S_x, \quad F_2 = S_x F_1^{-1} S_x,$$

(3.12)

with $S_x : (x, y, z) \rightarrow (-x, y, z)$ and $S_y : (x, y, z) \rightarrow (x, -y, z)$ representing reflection about the plane $x = 0$ and the plane $y = 0$, respectively. Global symmetries in the forced flow can be found by combining these relations, giving

$$\Phi_T = F_2 F_1 = S_y F_2 S_y S_y F_1 S_y = S_y F_2 F_1 S_y = S_y \Phi_T S_y$$

(3.13)

and

$$\Phi_T = F_2 F_1 = S_x F_1^{-1} S_x S_x F_2^{-1} S_x = S_x (F_2 F_1)^{-1} S_x = S_x \Phi_T^{-1} S_x.$$  

(3.14)

This puts forth the $y$-axis as an axis of time-reversal reflectional symmetry. In addition the system has ordinary reflectional symmetry about the $x$-axis, as shown by:

$$\Phi_T = F_2 F_1 = S_x F_2 S_x S_x F_1 S_x = S_x F_2 F_1 S_x = S_x \Phi_T S_x.$$  

(3.15)

Sets of periodic points that are symmetrical can be localized by making use of this symmetry relation. Periodic points on the symmetry plane $I_x$ can be localized by observing that period-$k$ points return to the symmetry plane after $k$-fold application of the mapping $\Phi_T$. These points are found by mapping a material line $I_s$ on $I_x$ for $k$ periods and searching for intersections with the symmetry plane, hence

$$x_I = I_s \cap \Phi^k_T (I_s).$$

(3.16)

This is illustrated in figure 3.4a where this method is applied to find period-1 points on the symmetry plane $I_x$. The black line corresponds to the material line $I_s$ and the red line corresponds to the
mapping $\Phi_T I_s$. The intersection point is a candidate period-1 point. Mapping of this point confirms that this is a period-1 point.

\begin{figure}[h]
\centering
\includegraphics[scale=0.5]{example.png}
\caption{(a) Example of finding period-1 points using the symmetry method. The material line $I_s$ (black) and the mapped line $\Phi_T I_s$ (red). The intersection ($\times$) is a possible period-1 point. (b) Periodic points (up to order 6) found using the symmetry method, marked the symbols: $\cdot$ for period 1, $\times$ for period 2, $\triangledown$ for period 3, $\square$ for period 4, $\star$ for period 5 and $\ast$ for period 6.}
\end{figure}

Consider the set period-2 points $[\mathbf{x}_p, S\mathbf{x}_p]$ symmetrical about the symmetry plane. A particle released at one of these points returns to its initial position after two applications of the mapping function. During this process the trajectory of the particle needs to cross the symmetry manifold at least twice. By symmetry these crossings occur at $t = T/2$ and $t = 3T/2$. This can be seen in figure 3.5b where the trajectory of a period-2 point is plotted.

The set of period-2 points can now be found by advection of a material line $I_s$ on the symmetry plane $I_x$ by application of the mapping $F_1F_2$, advancing time from $t = T/2$ to $t = 3T/2$. Intersections $G$, of the mapped material line with the symmetry plane are candidates for the point where the trajectory crosses the symmetry plane at $t = 3T/2$. The periodic point can then be found by application of $F_2$ to this point. In summary, off-axis sets of period-2 points can be found by computing

$$G = I_s \cap F_1 F_2 (I_s), \quad x_p = F_2 G. \quad (3.17)$$

This method can be extended to period-$k$ points giving

$$G = I_s \cap (F_1 F_2)^{k/2} (I_s), \quad x_p = F_2 G. \quad (3.18)$$

This method is used to find periodic points of the 2D pulsed source-sink system (up to order 6). The resulting periodic points are shown in figure 3.4b. Many periodic points are found, all in symmetrical sets about the $y$-axis.

\footnote{Observe that in the case of absorption of a particle by the sink and a subsequent reinjection at the source there is a virtual crossing of the symmetry plane. This situation is also considered as a crossing of the symmetry manifold here.}

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Geometrical method

In their work on the 2D pulsed source-sink system Jones and Aref (1988) presented a geometrical way to find periodic points for this system. Here, we closely follow their approach. This method is illustrated using the 2D pulsed source-sink system with $\Gamma = 19.1$.

The reflection of a periodic point $\vec{x}_p$ in the $y$-axis is a periodic point of the same order, as proved in equation (3.11):

$$\Phi^k T S x_{\vec{x}_p} = S x_{\vec{x}_p},$$  \hspace{1cm} (3.19)

where $S_x$ again denotes a reflection about the $y$-axis.

Now, consider a semicircle $C$ (red) with radius $\sqrt{\frac{QT}{4\pi}}$ centered around the source and its mirror image $S_x C$ (blue), centered around the sink, as shown in figure 3.5a. The radii of the semicircles is chosen such that any point $\vec{x}$ on $S_x C$ is mapped to a point on $C$:

$$\Phi_T P = S_x P.$$  \hspace{1cm} (3.20)

Therefore the radius is equal to $\sqrt{\frac{\Delta r^2}{2}}$ with $\Delta r^2 = r^2(t) - r^2(t_0) = \frac{QT}{2\pi}$.

For a period-1 point, equation (3.20) reduces to $P = S_x P$. These points can be identified by searching for the intersection of $C$ with $S_x C$, hence

$$\vec{x}_p = C \cap S_x C.$$  \hspace{1cm} (3.21)

This is shown in figure 3.5a as the crossing of the blue and the red line. This point is verified to be a period-1 point by application of the mapping function. The particle trajectory corresponding to the period-1 point is shown in figure 3.5b.

![Figure 3.5: (a) Finding periodic points using the geometry method, circle C (red), circle S_x C (blue) and the mapping of C (black) (b) Periodic-1 point (•) and periodic-2 points (×) with their respective particle trajectories.](image)

Due to the simplicity of the period-1 trajectory, the position of this point can be calculated analytically with relative ease, using geometrical considerations. By symmetry the period-1 point
is on the $y$-axis $x = 0$. The $y$-position of the period-1 point $y_p$ is essentially the height of the red triangle shown in figure 3.5b. As the lengths of the sides of this triangle are known, this yields

$$\frac{y_p}{a} = \frac{1}{a} \sqrt{\frac{QT}{4\pi} - a^2} = \sqrt{\frac{\Gamma}{4\pi} - 1}. \quad (3.22)$$

Equation (3.22) reveals that the period-1 point moves towards the $x$-axis for smaller $\Gamma$ and eventually vanishes when $\Gamma < 4\pi$. For $\Gamma > 4\pi$ particles cannot travel far enough to reach their initial position after one period. For higher-order points, this method becomes very complex due to the mapping function and nesting of mapping functions. In general it can be noted that as $\Gamma$ is decreased, the radius of the semicircle $C$ decreases and periodic points shift closer to the source and sink, and eventually vanish as particles cannot travel the distance required for the trajectories.

Periodic points of higher order can also be found using geometrical considerations. Consider the symmetrical set of period-2 points $\vec{x}_{p1}$ and $\vec{x}_{p2}$, satisfying

$$\Phi_T \vec{x}_{p1} = \vec{x}_{p2}. \quad (3.23)$$

Because of their symmetry these points must be on the circles $C$ and $S_xC$ according to equation (3.20). If $\vec{x}_{p2}$ is on $S_xC$ then $\vec{x}_{p1}$ is on $C$ and $\vec{x}_{p2}$ can be found using

$$\vec{x}_{p2} = \Phi_T \bigcap S_xC. \quad (3.24)$$

The corresponding period-2 point $\vec{x}_{p1}$ can then be found by simple application of the mapping function. The line $\Phi_T C$ is shown in black in figure 3.5a and shows two intersection points with $S_xC$. The first is the period-1 point found earlier which naturally is a period-2 point as well. The second intersection point is a period-2 point, again this is verified by application of the mapping function. The particle trajectory corresponding to the period-2 points is plotted in figure 3.5b.

Additionally it can be noted that the black line, which is the mapping of $C$, is much longer than $C$, which is the result of the exponential divergence of nearby trajectories. The black line consists of two segments, an inner and an outer segment. The inner segment is connected to the source and is the result of the part of the line $C$ that is absorbed and reinjected upon application of $\Phi_T$ in equation (3.24). The outer segment of $\Phi_T C$ is not reinjected.

This method can be generalised to period-$k$ points giving

$$\vec{x}_{p}^k = \Phi_T^n C \cap \Phi_T^{-m} S_xC, \quad (3.25)$$

where $n$ and $m$ are the integers $0, 1, 2, ...$ such that $k = n + m + 1$. Figure 3.6a shows the semicircle $C$ and its corresponding mappings. The mirror image $S_xC$ of the semicircle $C$ is also shown. Owing to the successive mapping of the semicircle $C$, the mappings of the semicircle become longer and longer due to the exponential divergence of nearby trajectories. Absorption and subsequent reinjection causes these mappings to break up in several segments which result in multiple crossings of the mapped lines with $S_xC$. It should be noted that this method can only find periodic points with a set member on the semicircles $C$ or $S_xC$. For $k > 2$ this is not guaranteed.
Figure 3.6: (a) Semicircle $C$ with is respective mappings to order 5, and semicircle $S_x C$ (b) Periodic points (up to order 6) found using the geometry method. $\cdot$ for period 1, $\times$ for period 2, $\nabla$ for period 3, $\Box$ for period 4, $\star$ for period 5 and $\ast$ for period 6.

Figure 3.6b shows that the periodic points found using the symmetry method are organised in branch-like structures. These branches coincide with the semicircle $C$ and $S_x C$ and their successive mappings. This is illustrated in figure 3.6b with the blue line. All periodic points found with this method have a set member on $C$. This is a direct consequence of equation (3.25). Some intersections result in higher-order periodic points than expected. For example, some sets of period-12 points (not shown in figure 3.6b) are found when looking for period-6 points. This is caused by the fact that the intersection point $P$ of $S_x C$ with $\Phi^{k-1}_T C$ does not necessarily has to be the mapped point $\Phi^{k-1}_T S_x P$. This is why the existence and the properties of the periodic points found by the geometry method should always be verified.

Some differences can be observed when comparing the results from the symmetry method with the results from the geometry method, especially for higher-order periodic points. However, many of the periodic points found with both methods do coincide. The geometry method was not able to detect the set of period-5 points and the two sets of period-6 points that were detected using the symmetry method. These sets have no point on the semicircle $C$ or its mappings (up to order 4) and could not have been detected using the geometry method. In contrast with the geometry method, the symmetry method was not able to detect a set of period-6 points as well as a set of period-5 points. This is most likely caused by the amount of mappings involved. Every mapping of the line $I_s$ stretches the line. This line breaks up into segments and this makes some intersections harder to detect. This especially holds for hyperbolic periodic points as local stretching rates are very high.

The geometry method provides an instructive way to identify periodic points of the pulsed source-sink system. However, just like with the symmetry method, there is no guarantee that all periodic points will be found with this method. The periodic points found with this method have a set member on $C$, but there are some sets of periodic points that fall outside of this category. Moveover, due to the stretching of the mapped semicircle $C$ the search for higher-order periodic points becomes computationally more demanding.
The Newton-Raphson method

Following equation (2.5) a periodic point $\vec{x}_p$ satisfies

$$\Phi^k_\vec{f}(\vec{x}_p) - \vec{x}_p = 0. \quad (3.26)$$

Close to a periodic point this equation does not hold and a small difference is present in the position of the point $\vec{x}$ and its mapping:

$$\Phi^k_\vec{f}(\vec{x}) - \vec{x} = f(\vec{x}). \quad (3.27)$$

The function $f(\vec{x})$ is a measure of the error in the position of the periodic point. Periodic points can be identified by numerically searching for points where

$$f(\vec{x}) = 0. \quad (3.28)$$

These points are found using the Newton-Raphson iteration method. This method is illustrated in figure 3.7. The method takes an initial guess $x_0$ for the root of the function and calculates the root of the tangent $x_1$ of the function at the initial point. This root of the tangent is an approximation of the root of the function. This approximation is then used to find the next improved approximation of the root $x_2$, using a tangent at the previously obtained point $x_1$. This process is repeated in subsequent iterations until the approximation of the root of the function satisfies a predetermined error tolerance.

Figure 3.7: Newton-Raphson iteration scheme for finding roots of functions. Source http://www-rohan.sdsu.edu/~jmahaffy/courses/f00/math122/lectures/newtons_method/newtonmethod.html

In 3D problems the iteration is dependent on the Jacobian $\vec{J}_f(\vec{x})$ of the function $f(\vec{x})$:

$$\vec{x}_{n+1} = \vec{x}_n - f(\vec{x}_n) \vec{J}^{-1}_f(\vec{x}_n), \quad (3.29)$$
where $\bar{x}_n$ denotes subsequent approximations of the root. The Jacobian $\bar{J}_f$ in equation (3.29) relates to the Jacobian $J$ of the mapping function $\Phi_T$ from equation (2.7) via

$$\bar{J}_f(\bar{x}) = \bar{J}(\bar{x}) - \bar{I}, \quad (3.30)$$

where $\bar{I}$ refers to the identity matrix.

The Newton-Raphson method is able to identify periodic points from initial guesses. By setting up a grid of initial points the flow domain can be scanned for periodic points. However, there is no guarantee that all periodic points will be found. When a periodic point is found, members of the same set can be recovered by straightforward mapping, as used before.

For the pulsed source-sink system a grid of initial guess points is defined, covering half of the domain and spaced 0.1 apart, as shown in figure 3.8a. Only half of the domain needs to be scanned due to the $S_x$ symmetry, as discussed earlier. The resulting periodic points, and their mirror images are shown in figure 3.8b.

![Figure 3.8: (a) Grid of initial guess points for the Newton-Raphson iteration scheme. (b) Periodic points (up to order 6) found using the Newton-Raphson method. · for period 1, × for period 2, ▽ for period 3, □ for period 4, * for period 5 and * for period 6.](image)

Figure 3.8 shows that various periodic points are found. These periodic points are not restricted to the domain covered by the grid of initial guess points. All of the periodic points found using the geometry method and the symmetry method are recovered by the Newton-Raphson method as well. Some additional periodic points are found too.

The two period-1 points located on the $x$-axis were not found using the other two methods. However, in the geometry method there is an indication of these points since the material lines $\Phi_T^{k-1}C$ pile up near the point $(x/a, y/a) = (0.7215, 0)$, which suggests this point is a hyperbolic point. The symmetry method is not able to detect these points because it is a period-1 point off the symmetry plane $I_x$. Refining the grid of initial points did not lead to additional periodic points within the domain covered by the points. This means that the grid spacing of 0.1 is sufficient for the intended purpose.

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While giving less insight into the occurrence of periodic points, the Newton-Raphson method provides the fastest and most reliable method for finding periodic points in the 2D pulsed source-sink system.

### 3.1.3 Parameter variation

**$\Gamma = 19.1$**

Much information on the pulsed source-sink system can be obtained from Poincaré sections. Figure 3.9 shows a Poincaré section for $\Gamma = 19.1$. The Poincaré section was constructed by mapping 201 evenly spaced points on the $y$-axis between $y = 0$ to $y = 2$ for $t = 10000T$.

![Figure 3.9: Poincaré section for $\Gamma = 19.1$. The green $\oplus$ and $\ominus$ mark the source and sink positions respectively.](image)

Figure 3.9 shows a large amount of tracers diverging from their original location. These tracers describe large curved paths from the source to the sink. In the far field, away from the source and sink, the particles describe paths that resemble particle trajectories in a dipole flow (when the source and sink are operational at the same time), which will be discussed later. The large curved paths eventually return to the sink, except for the special case that a particle is the $x$-axis and on the left side of the source. Figure 3.9 shows that the pulsed source-sink system spreads out patches of fluid, away from the source and sink.

To investigate the chaotic advection near the pulsed source-sink system, further analysis will concentrate on the domain close to this system. Figure 3.10 shows a close up of figure 3.9 on the region close to the source and sink. Periodic points found in section 3.1.2 are superimposed on the Poincaré sections. Tracers in elliptic islands are coloured red.
Figure 3.10: Poincaré section for $\Gamma = 19.1$. Trajectories in elliptic islands are coloured red. Periodic points are marked by black symbols: $\cdot$ for period 1, $\times$ for period 2, $\nabla$ for period 3, $\Box$ for period 4, $\star$ for period 5 and $\ast$ for period 6.

The Poincaré section in figure 3.10 clearly shows symmetry with respect to the $y$-axis, consistent with the analysis in section 3.1.2. A large elliptic island is observed around the period-1 point on the $y$-axis at the location predicted by equation (3.22). The period-1 elliptic island contains several higher-order periodic points. A set of period-11 and period-17 islands can be observed in the outer regions of the period-1 island in the form of little oval shapes. The existence of these islands can be explained by the KAM theorem. Two sets of period-6 points are located around the period-1 island. These period-6 points are arranged in a ring with alternating elliptic and hyperbolic points. Small elliptic islands are observed around the elliptic points. The ring of period-6 points is a remnant of an elliptic orbit corresponding to the period-1 island, as predicted by the KAM theorem. These structures can also be observed in figure 3.11 where a close up of part of the period-1 elliptic island is shown.
Figure 3.11: Close up of the Poincaré section for $\Gamma = 19.1$. Tracers in elliptic islands are coloured red. Periodic points are marked by black symbols: $\cdot$ for period 1 and $\ast$ for period 6.

The Poincaré section in figure 3.10 also shows many other higher-order periodic points, arranged in branches, at larger distances from the source and sink. Mapping of tracer particles initially located at these periodic points shows that most of these periodic points are of the hyperbolic type. As noted in section 3.1.2, many more higher-order (>6) periodic points can be found. These points are not shown in the figure.

The large surface area of the period-1 island inhibits chaotic advection as this is a non-chaotic region and particles released within the island are trapped in this region. This is illustrated in figure 3.12a where a blob of tracer particles is followed for several periods of the source-sink flow. Figure 3.12a shows the deformation of a blob of material positioned inside the elliptic island. The material orbits the period-1 point and stays inside the elliptic island. The originally square blob is somewhat deformed over time. This is the result of slight changes in winding number at different radii from the periodic point.

In contrast, a blob placed just outside the period-1 island is not confined to the island as shown in figure 3.12b. The blob is stretched into a thin curved line. At the same time the blob is cut into segments as a result of particles being absorbed and reinjection multiple times. In addition, the simulation shows that the pulsed source-sink system pushes away fluid towards larger distances from the origin.
Figure 3.12: Blob tracing simulations. Panel (a) shows snapshots of the blob released within the period-1 elliptic island. Panel (b) shows snapshots of the blob released just outside the period-1 elliptic island. Colours indicate snapshots at different times. The perimeter of the period-1 elliptic island is marked by the black line.
The Poincaré section for $\Gamma = 13.6$ is shown in figure 3.13. Periodic points are obtained using both the symmetry method and the Newton-Raphson method and are also shown in figure 3.13. Some additional particles (red) are added off the $y$-axis to highlight the structure of the period-2 elliptic islands.

As for the case $\Gamma = 19.1$ clear symmetry is observed with respect to the $y$-axis. Again a period-1 point is observed on the $y$-axis. Its position corresponds to the theoretical prediction given by equation (3.22). This periodic point is of the elliptic type, which is clear from the elliptic island surrounding it. Again higher-order periodic points are observed in branch-like configurations coinciding with the semicircle $C$ and its mappings, as discussed in section 3.1.2. Because the radius of the semicircle $C$ is smaller for smaller $\Gamma$ periodic points are located closer to the source and sink.
This is the direct result of the fact that when $\Gamma$ decreases the distance a particle travels each switching period $T$ decreases.

In light of the geometrical considerations regarding periodic points, many of the periodic points for different settings of $\Gamma$ can be directly linked to similar periodic points for other values of $\Gamma$. This feature is illustrated by comparing the composition of the branches of periodic points in the Poincaré sections.

In addition to a change of location, the set of period-2 hyperbolic points observed in the case of $\Gamma = 19.1$ is found to be elliptic for $\Gamma = 13.6$. The corresponding elliptic islands contain a set of period-10 elliptic islands similar to the period-11 and period-17 points found for $\Gamma = 19.1$.

$\Gamma = 10.4$

For $\Gamma = 10.4$ again a Poincaré section is constructed and periodic points are found, using the same methods as before, see figure 3.14. Again, some additional red particles are added to highlight the island structures.

The period-1 elliptic island seen in the cases $\Gamma = 19.1$ and $\Gamma = 13.6$ has been destroyed, as predicted by equation (3.22) since $\Gamma = 10.4 < 4\pi$. In general the surface area of elliptic islands is greatly reduced, mainly due to the absence of the period-1 island. The period-1 hyperbolic points that were found on the $x$-axis in the cases $\Gamma = 19.1$ and $\Gamma = 13.6$ are also destroyed. The distance travelled by a tracer particle during a switching period is too small for period-1 points to exist.

The set of period-2 points located on the semicircle $C$ and on its mirror image $S_xC$ is still present. These points have moved closer to the source and the sink compared to the cases $\Gamma = 19.1$ and $\Gamma = 13.6$, due to the smaller radius of $C$. The period-2 points are elliptic and an elliptic island is observed around these points. A set of period-6 hyperbolic points is located at the sharp edges of these islands. The manifolds of the period-6 hyperbolic points are most likely connected, shielding the island from the chaotic sea.

Two sets of period-5 hyperbolic points are located on the $x$-axis. These points undergo several absorptions and reinjections every cycle. Note that one period-5 point of each set virtually coincides with either the source or sink. Additionally there is a set of period-5 elliptic points with elliptic islands located near the $x$-axis.

Similar to the cases $\Gamma = 19.1$ and $\Gamma = 13.6$ higher-order periodic points appear in branch-like structures coinciding with the semicircle $C$ and its mappings. Every branch contains the same configuration of periodic points as the corresponding branches in the cases $\Gamma = 19.1$ and $\Gamma = 13.6$. This suggests that, although the semicircles $C$ become smaller, the basic topology of the intersections of $C$ with its mappings is largely unchanged.
Figure 3.14: Poincaré section for $\Gamma = 10.4$. Tracers in elliptic islands are coloured red. Periodic points are marked by black symbols: · for period 1, × for period 2, ▽ for period 3, □ for period 4, ⋆ for period 5 and * for period 6.

Figure 3.15 shows the Poincaré section for $\Gamma = 6.5$. Periodic points are again superimposed on the Poincaré section. A distinct difference with the previous cases is the size of the period-2 islands. For $\Gamma = 6.5$ these islands take up a significant amount of space. In addition to the size of the island, the location of the period-2 points have changed. The period-2 points again are located closer to the source and the sink, which conforms to the general trend for decreasing $\Gamma$.

This trend is also visible in the branch-like structure of the higher-order periodic points relatively far away from the source and sink. These branches have moved towards the $x$-axis. Again the configuration of the periodic points on these branches is unchanged.
Figure 3.15: Poincaré section for $\Gamma = 6.5$. Tracers in elliptic islands are coloured red. Periodic points are marked by black symbols: $\cdot$ for period 1, $\times$ for period 2, $\nabla$ for period 3, $\Box$ for period 4, $\star$ for period 5 and $\ast$ for period 6.

In addition to the period-2 islands a set of elliptic period-3 points is found. This set of period-3 points corresponds to the set period-3 hyperbolic points for $\Gamma = 10.4$ at $(x/a, y/a) = (0, 1.21)$, $(x/a, y/a) = (-0.84, 0.89)$ and $(x/a, y/a) = (0.84, 0.89)$. A set of hyperbolic period-6 points is found connected to the period-3 islands. These points could be the result of the destruction of elliptic orbits as described by the KAM theorem.

The sets of period-5 points found near the $x$-axis for $\Gamma = 10.4$ are not recovered in the current case. However, careful inspection of the structures in the Poincaré section close to the $x$-axis suggest possible higher-order hyperbolic points on the $x$-axis.

Concluding on the analysis with various $\Gamma$ a clear trend is observed in the organisation of the periodic points. Periodic points of the pulsed source-sink system are organised in branch-like structures. These branches are related to the semicircles $C$, $S_xC$ and their respective mappings. As $\Gamma$ is decreased the radius of $C$ decreases and the branches of periodic points are located closer to the source and the sink. In other words, as $\Gamma$ decreases the distance a tracer travels each period...
is decreased. This results in the destruction of some periodic points of lower-order, as observed with the central period-1 point when decreasing $\Gamma$ from 13.6 to 10.4. In addition a change from hyperbolic to elliptic nature is observed for low order periodic points when $\Gamma$ is decreased, as illustrated by the sets of period-2 and period-3 points.

The general trend of periodic points moving closer to the source and sink for smaller $\Gamma$ results in a higher density of periodic points for smaller $\Gamma$. This trend suggest better mixing in the area close to the source and sink, in systems with low $\Gamma$, if all the peridic points where hyperbolic in nature. However, the change from hyperbolic to elliptic nature for decreasing $\Gamma$ causes a reduction in the amount of hyperbolic points as well as a increased surface area of elliptic islands. Considering the currently investigated cases, these two effects are best balanced in the system with $\Gamma = 10.4$ as the total area of the elliptic islands is relatively small and many hyperbolic points are located close to the source and sink.

### 3.1.4 Manifolds

As discussed in section 2.2.3 stable and unstable manifolds originating from hyperbolic points play a key role in chaotic systems. To increase insight into the pulsed source-sink system, part of the manifolds corresponding to the hyperbolic period-1 points are identified for $\Gamma = 19.1$.

The hyperbolic period-1 points are located on the $x$-axis at $(x/a, y/a) = (\pm 0.7215, 0)$, as shown in figure 3.10. The eigenvector directions corresponding to the two periodic points can be obtained by linearising the flow around the periodic point, as summarised in equation (2.7). The eigenvector directions are indicated by the red and black arrows in figure 3.16. The period-1 point on the negative $x$-axis stretches material along the $x$-axis and compresses material on the $y$-axis. The period-1 point on the positive $x$-axis has its stretching direction parallel to the $y$-axis and compresses material along the $x$-axis.

![Figure 3.16: The position of the hyperbolic period-1 points and the orientation of their stable (red) and unstable (black) manifolds near the periodic point. The hyperbolic periodic-1 points marked by](image)

Figure 3.16: The position of the hyperbolic period-1 points and the orientation of their stable (red) and unstable (black) manifolds near the periodic point. The hyperbolic periodic-1 points marked by
Manifolds can be found by tracing a short material line close to the corresponding periodic point in the main stretching and compressing directions. On the unstable manifold particles move away from the periodic point, hence this manifold can be found by mapping forward in time using $\Phi^k_T$. Particles on the stable manifold move towards the periodic point, these manifolds can be found by reversed time mapping using $\Phi^{-k}_T$.

The initial material line positioned near the periodic point is $10^{-8}$ long and consists of $10^5$ tracer particles. As time progresses this line will be stretched and additional points will be added to maintain a smooth line. When two subsequent tracer particles are spaced more than $10^{-3}$ length units apart new particles will be added. The amount of added particles depends on the spacing between the tracer particles so that the spacing will not exceed $10^{-3}$ length units. Particles are added using a linear interpolation scheme.

The resulting manifolds for the period-1 point on the positive $x$-axis are shown in figure 3.17. The figure shows that the stable manifold (red) on the left of the period-1 point, connects the two hyperbolic period-1 points. Apparently particles that move away from the periodic point on the left move towards the periodic point on the right. On the right side of the period-1 point on the positive $x$-axis the stable manifold is connected to the sink.

![Figure 3.17: Stable (red) and unstable (black) manifolds corresponding to the hyperbolic period-1 point located at $(x/a, y/a) = (0.7215, 0)$ for $\Gamma = 19.1$.](image)

The unstable manifold branches out upwards as well as downwards. The resulting manifolds are symmetrical due to equation (3.20). Only the positive $y$-plane is shown here. Due to various absorptions and reinjections the unstable manifold is cut into segments. First there is a large arch starting at the hyperbolic point on the right side and ending at the source, enclosing the period-1 elliptic island. Keep in mind that structures are deformed due to the scaling of the axis. Several loops of the unstable manifold are enclosed within, curling up around the edges of the large arch. This feature nicely illustrates the stretching and folding dynamics vital to chaotic advection. Further tracing of the manifold leads to more and more loops enclosed within the center arch.

In addition, some structures arise at the right side of the sink. These structures occur due to material on the far left side of the main arch not being absorbed by the sink and subsequently being pushed further to the right by the source. The small arch structures are caused by the small loops within the large arch. Further tracing of the manifold will lead to more and more of these small arch structures.

On the far left of figure 3.17 long curved lines are observed in groups. The most right group of these lines originates from the structures on the far right of the source. The groups more to the left are subsequent mappings of this most right group.

![Figure 3.18: Blob tracing simulation. A blob of tracer particles positioned in a loop of the manifold is mapped for five switching periods. Colours indicate different times, as shown in the legend.](image-url)
The connection between the manifolds and mixing can be observed in figure 3.18 where a blob of tracer particles is set up in one of the loops of the manifold. The blob of particles is traced for five periods. The figure shows that particles inside the loops are mapped to neighbouring loops. This is the essence of the stretching and folding dynamics underlying chaotic behaviour.

To obtain the stable manifold corresponding to the hyperbolic period-1 point on the negative $x$-axis a material line needs to be traced backwards in time. Due to the symmetry relation in equation (3.16) this stable manifold corresponds to the mirrored version of the unstable manifold shown in figure 3.17.

To illustrate the existence of heteroclinic points the manifolds of both hyperbolic period-1 points are plotted together in figure 3.19. The figure focuses only on the part of the manifolds between the source and the sink.

![Figure 3.19: Stable (red) and unstable (black) manifolds corresponding to the hyperbolic period-1 points, located at $(x/a, y/a) = (\pm 0.7215, 0)$.](image)

The figure above shows many crossings of the unstable and stable manifolds of the hyperbolic period-1 points. The existence of these heteroclinic points is a strong indication of chaotic dynamics. Recall that further tracing of the manifolds will lead to more and more loops contained within the central arch structure. These additional loops will produce more and more heteroclinic points.
3.1.5 Perturbed flow

To investigate the effects of fluid inertia and dispersion on the pulsed source-sink system the velocity field $\vec{u}_0$ from equation 3.1 is perturbed with a small perturbation $\vec{u}'$ giving

$$ \vec{u} = \vec{u}_0 + \vec{u}' \quad (3.31) $$

In the investigation of chaos near the surface of a periodically forced rotating sphere, Moharana (2013) found invariant surfaces to be linked together upon application of a small time-dependent perturbation. These invariant surfaces were connected via tubes that form upon the breakup of a periodic line. These effects are qualitatively similar to the effects found by Speetjens (2001) in the investigation of chaotic dynamics in a cylindrical domain with a moving bottom wall, where the effects of inertia were investigated by solving the actual governing equations including inertia using sophisticated software.

The similarity of the results using a perturbed velocity field with the results obtained by solving the actual governing equations suggest that application of a small perturbation on the velocity field is able to mimic the effect of fluid inertia. This is independent on the details of the perturbation, as long as it is small with respect to the unperturbed velocity field [Moharana et al., 2013]. Due to the very low Reynolds number in typical groundwater flows, fluid inertia is of little importance in these systems. However, the effect of dispersion might be mimicked in the same way.

The perturbation applied to the source and sink velocity fields is given by

$$ \vec{u}' = \frac{\epsilon}{(x - x_0)^2 + g(t)^2(y - y_0)^2} \left[ \frac{g(t)(y - y_0)}{g(t)(x - x_0)} - \frac{1}{g(t)} \right], \quad (3.32) $$

with

$$ g(t) = 1 + \kappa \sin(t), \quad (3.33) $$

where $\epsilon$ and $\kappa$ are parameters to control the amplitude and time dependency of the perturbation, respectively. The parameters $x_0$ and $y_0$ control the position of the centre of the perturbation. During the source step the perturbation is centered around the source and during the sink step the perturbation is centered around the sink. This perturbation closely resembles the perturbation used by Moharana et al. (2013). It can be shown that the applied perturbation maintains mass conservation $\nabla \cdot \vec{v} = 0$ of the velocity field.

Simulation setup

To obtain particle trajectories, the perturbed velocity fields of the source and sink need to be integrated according to equation (3.2). Since no analytical solution can be found for these integrals, the velocity field needs to be integrated numerically to obtain particle trajectories. The numerical integration is performed in a Matlab using an ordinary differential equation solver. The numerical integration code was verified using the unperturbed pulsed source-sink system and was able to reproduce particle trajectories with an accuracy of $O(10^{-8})$. The error analysis of the simulation code is discussed in Appendix A.
Time-independent perturbation

Poincaré sections for the time-independent perturbation ($\kappa = 0$) are shown in figure 3.20, where several values of $\epsilon$ are considered at $\Gamma = 19.1$. The corresponding unperturbed case ($\epsilon = 0$) is shown in figure 3.10. The Poincaré maps are obtained by mapping 51 points on the $y$-axis for $1000T$. The Newton-Raphson method was used to identify periodic point up to order 3. These points are plotted in figure 3.20. Higher-order periodic points where not investigated due to the increase in the required computational power.

Elliptic orbits gradually break up as the result of the applied perturbation. For small per-
turbations ($\Upsilon = 0.01$, panel (a) and (b)) the shapes of the elliptic islands change. For larger perturbations the elliptic orbits break up, leaving only part of the original elliptic island intact for $\epsilon = 0.1$ (panel d).

Note that the period-1 points found on the $x$-axis in the unperturbed case move away from the $x$-axis, as shown in figure 3.20. This is the result of the perturbation inducing a non-zero vertical velocity on the $x$-axis.

Figure 3.21: Close-ups of the central period-1 elliptic island in the Poincaré sections for selected $\epsilon$ for $\Gamma = 19.1$ and $\kappa = 0$. The Poincaré sections of three particles initially on the top edge of the elliptic island are marked red to illustrate the breakup of elliptic orbits.

The mechanism of the breakup of elliptic orbits is illustrated in figure 3.21, where the Poincaré sections of three points at the outer edge of the period-1 island are highlighted in red for several values of $\epsilon$. Figure 3.21a shows that for small perturbations the shape of the period-1 elliptic island is slightly deformed compared with the unperturbed case from figure 3.10. For slightly larger
perturbation strength a chain of hyperbolic and elliptic periodic points appears in place of some elliptic orbits, shown in figure 3.21b. Increasing the perturbation strength $\epsilon$ further, results in chaotic bands appearing in place of the chains of periodic points, as shown in figure 3.21c. These bands slowly dissolve into the chaotic sea upon further increase of the perturbation strength, as seen in figure 3.21d. This effect can be observed at the outer edges of the period-1 elliptic island. These results confirm the effect of small perturbations on elliptic orbits as predicted by the KAM theorem.

Interestingly, the hyperbolic period-2 points become elliptic upon perturbing the system (see figure 3.20). In the unperturbed case the pair of period-2 points is hyperbolic but, as figures 3.20b to 3.20d shows, these points become elliptic upon stronger perturbation of the system. This is emphasized by the elliptic islands around these points, as highlighted in figures 3.20b to 3.20d by placing several red tracers near the elliptic period-2 points and following them for $100T$. These islands are formed for small $\epsilon$ where the period-1 island structure undergoes its most dramatic shape change. The transformation of the period-2 points from hyperbolic to elliptic is also seen in the unperturbed case when $\Gamma$ was decreased. For larger $\epsilon$ the elliptic islands around the period-2 points also break down in a similar fashion as the central period-1 island.

**Time-dependent perturbation**

Application of a small time-dependent perturbation on the velocity field has been shown to produce equivalent effects on the dynamics as fluid inertia [Moharana et al., 2013] and might also be used to simulate the effects of dispersion. Therefore a time-dependent ($\kappa \neq 0$) perturbation is applied to the velocity fields of the source and sink.

Figure 3.22 illustrates the effect of a time-dependent perturbation on the source sink-system for several values of $\kappa$ with constant $\epsilon$. Again the Poincaré sections are constructed from 51 points on the $y$-axis for $0 < y < 2$ and following them for $1000T$.

Figure 3.22a shows a structure closely resembling the period-1 elliptic islands seen in the unperturbed pulsed source-sink system. Positioning a tracer at the centre of this structure reveals the central period-1 point, located at $(x/a, y/a) = (0, 0.7215)$ in the unperturbed case in no longer a periodic point in the strict sense of equation (2.5). When a tracer is released at the location of the former periodic point, corresponding to the unperturbed case, the Poincaré section shows a complicated but regular pattern around this point. The tracer does not return to its original position but does returns to a small region. For increasing amplitudes, $\kappa$ the deviations of the tracer from its initial location become larger, as seen in figures 3.22b to 3.22d.

Figure 3.22a shows six darker spots surrounding the central structure discussed above. These darker spots are the remnants of period-6 elliptic islands, as observed in the unperturbed case. Similar to the case of the original elliptic period-1 point, a tracer released at the position of a former period-6 point associated with the unperturbed case, does not return exactly to its initial position after $6T$. On larger timescales ($t > 100T$) these tracers leave the neighborhood of the original period-6 points and exhibit chaotic motion. In contrast with the original period-1 structure, the remnant structure corresponding to the period-6 elliptic islands is entirely destroyed for larger perturbations, as shown in 3.22b to 3.22d.
Figure 3.22: Poincaré sections for selected $\kappa$ for $\Gamma = 19.1$ and $\epsilon = 0.01$. The symbols $\oplus$ and $\ominus$ denote source and sink position. One particle inside the period-1 elliptic island is labeled red in the Poincaré section to visualise the dynamics of a single point.

The process of the destruction of elliptic islands is illustrated in Figure 3.22 by the red-labeled particle. The tracer shows elliptic orbits transforming into bands, seen in figure 3.22a. These bands gradually grow in width for increasing $\kappa$, as shown in figures 3.22b to 3.22d. Also note that these bands overlap but particles remain in the specific band. For large values of $\kappa$ these bands eventually break up and dissolve into the chaotic sea.

These results show great resemblance with the results from Speetjens (2001) who observed similar effects of inertia on invariant surfaces, referred to as adiabatic surfaces, in their work. This resemblance further indicates that a time-dependent perturbation mimicks the effects of inertia.
3.2 The three-dimensional pulsed source-sink system

Although the 2D pulsed source-sink system is a useful model to study some basic phenomena of chaotic advection in potential flows, various applications involve a 3D domain. The 3D advection problem is investigated using a 3D version of the pulsed source-sink system.

In the 3D case, the velocity field due to a point source of strength $Q$ is given by

$$\vec{v} = \frac{Q}{4\pi \rho^2} \vec{e}_\rho,$$  \hspace{1cm} (3.34)

again with $Q > 0$ for a source and $Q < 0$ for a sink. Here $\rho$ is the radial distance to the source and $\vec{e}_\rho$ the unit vector in the radial direction away from the source. The 3D pulsed source-sink system is best described in a cylindrical coordinate system $\vec{e}_r, \vec{e}_\theta, \vec{e}_x$, with $r = y^2 + z^2$ and $\theta = \arctan \frac{z}{y}$. Because $\vec{v}_\theta = 0$ particles are confined to 2D planes of constant $\theta$. This essentially reduces the system once again to essentially 2D dynamics.

The 3D pulsed source-sink system can be described by the dimensionless parameter

$$\Pi = \frac{QT}{a^3}. \hspace{1cm} (3.35)$$

3.2.1 Simulation setup

Integrating the advection equation (3.2) using the velocity field from equation (3.34) results in the following expression for the displacement of a tracer particle as function of time:

$$r^3(t) = r^3(t_0) + \frac{3Q}{4\pi} t.$$  \hspace{1cm} (3.36)

Similar to the 2D case, $r(t_0)$ is the radial distance from the point source or sink at $t = t_0$. Together with the reinjection rule, equation (3.36) is implemented into a Matlab code that calculates the discrete time evolution of particles in the 3D pulsed source-sink system.

To compare the 3D case with the 2D case values for $\Pi$ are chosen such that the period-1 point, if existent, is at the same position. From equation (3.22) and (3.36) $\Pi$ and $\Gamma$ relate via

$$\Pi = \frac{16\pi}{3} \left( \frac{\Gamma}{4\pi} \right)^{\frac{3}{2}}. \hspace{1cm} (3.37)$$

The $\Pi$-values investigated and their corresponding 2D setting of $\Gamma$ are shown in table 3.1.

<table>
<thead>
<tr>
<th>$\Gamma$</th>
<th>$\Pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>19.1</td>
<td>$10\pi$</td>
</tr>
<tr>
<td>13.6</td>
<td>$6\pi$</td>
</tr>
<tr>
<td>10.4</td>
<td>$4\pi$</td>
</tr>
<tr>
<td>6.5</td>
<td>$2\pi$</td>
</tr>
</tbody>
</table>

Table 3.1: Conversion table showing corresponding values of $\Pi$ and $\Gamma$. 

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3.2.2 Periodic points

The symmetry considerations discussed in the 2D case still hold for the 3D case. Because the dynamics of the 3D pulsed source-sink model is confined to 2D planes and the symmetry properties of the system are not changed, periodic points can be found using the same methods as for the 2D case. For the 3D pulsed source-sink system the Newton-Raphson method is used to find periodic points. The same grid of initial points is used as in the 2D case. The resulting periodic points are shown in figure 3.23 and may be compared to the 2D case for $\Gamma = 19.1$ shown in figure 3.10.

Due to the rotational symmetry about the $x$-axis the periodic points found in the 3D case are actually periodic lines. These periodic lines are circles with the $x$-axis as a centre. Any elliptic islands present in the 3D system forms a 3D torus. Within the torus 2D elliptic orbits are found.

![Figure 3.23: Periodic points up to order 6, found by the Newton-Raphson method for $\Pi = 10\pi$. Periodic points are marked by black symbols: · for period 1, × for period 2, ▽ for period 3, □ for period 4, * for period 5 and * for period 6.]

A period-1 point is found on the $y$-axis at $y = 0.7215$. This is the same point with the same
position as for the 2D case and is the result of the settings of $\Pi$ chosen to compare the 2D and 3D cases. The amount of periodic points surrounding the central period-1 point is increased compared with the 2D case. This might be explained by the fact that the change in the velocity field induces changes in the locations of the mappings of the semicircle $C$.

Comparing the 2D and 3D cases it is clear the periodic points are organized in similar, branch-like structures. These branch-like structures in the 3D case also coincide with semicircles $C$ and their respective mappings, where the radius of the semicircles $C$ and $S_2 C$ has been adapted for the 3D case. In light of the geometrical considerations for finding periodic points, many of the periodic points in the 3D case can be directly linked to similar periodic points in the 2D case. This is illustrated by comparing the composition of periodic points on the branch-like structures. In general the periodic points in the 3D case are closer to the origin than for the 2D case and are confined to a smaller area. This is the result of the velocity field being dependent on $r^{-3}$ instead of $r^{-2}$ as for the 2D case. This causes the velocity to decrease faster with increasing distance from the source and sink. Hence particles will travel shorter distances every switching period. An exception to this rule is found close to the source and sink. Because $\Gamma$ is defined such that the central periodic-1 point is in the same position the velocity field close to the source and sink must be larger to accommodate particles to travel this trajectory. Similar to the 2D case, geometry considerations predict many periodic points of order 7 and higher further away from the source and sink. These points will also show branch-like structures.

### 3.2.3 Parameter variation

Poincaré sections are constructed to investigate the chaotic dynamics near the source and sink. These Poincaré sections are constructed in the same manner as for the 2D case, where periodic points are superimposed on the Poincaré sections. In some cases additional particles are added to highlight the structure of elliptic islands.

For $\Pi = 10\pi$ the resulting Poincaré section is shown in figure 3.24. This case may be compared to the 2D case for $\Gamma = 19.1$ as shown in figure 3.10. The Poincaré section shows a similar structure as found in the 2D case with a large elliptic island surrounding the central period-1 point. A key difference with the 2D case is that the period-2 points are of the elliptic type in the 3D case. This is evident from the elliptic islands surrounding these points. This difference might be explained by the fact that the velocity field in the 3D case is dependent on $r^{-3}$. This causes tracers at larger distances from the source and sink than the elliptic period-1 point, to travel shorter distances each period $T$. A decrease in travel distance caused the hyperbolic period-2 points in the 2D case to become elliptic points.
Figure 3.24: Poincaré section for $\Pi = 10\pi$. Trajectories in elliptic islands are coloured red. Periodic points are marked by black symbols: $\cdot$ for period 1, $\times$ for period 2, $\triangledown$ for period 3, $\boxdot$ for period 4, $\star$ for period 5 and $\ast$ for period 6.

Decreasing $\Pi$ results in shorter distances traveled by particles per period $T$. Similar to the 2D case this will lead to periodic points moving closer to the origin as shown in figures 3.25a-3.25c. Some periodic points disappear while new periodic points are created. As $\Pi$ is decreased, less and less similarities are observed between the 2D and the 3D case. This is caused by the inherent difficulty to compare the 2D and 3D cases. The choice of the comparable values of $\Gamma$ and $\Pi$ is quite arbitrary.

Despite difficulties in comparing the 2D and 3D cases, many similarities can be observed and the branch-like structures in the periodic points is still present, forming the backbone in the structures seen in the Poincaré sections. In addition, the 3D case clearly illustrates that as $\Pi$ decreased, more and more periodic points become elliptic, as observed in the 2D case as well.

Finally it can be noted that the chaotic sea in figure 3.25c appears darker blue than figures 3.25b and 3.25a. This is due to the higher density of blue points caused by the fact that the trajectories are confined to a smaller area near the source and sink.
Figure 3.25: Poincaré sections corresponding to (a) $\Pi = 6\pi$, (b) $\Pi = 4\pi$ and (c) $\Pi = 2\pi$. Periodic points (up to order 6) found using the Newton-Raphson method and superimposed on the Poincaré sections. ⋅ for period 1, × for period 2, ▽ for period 3, □ for period 4, ⋆ for period 5 and ⋆ for period 6.
3.2.4 Perturbed flow

Similar to the the 2D case presented in section 3.1.5 a small perturbation is applied to the 3D pulsed source-sink system to investigate the influence of inertia and dispersion on the dynamics. The perturbation is applied to the velocity fields of the source and the sink according to equation (3.31). The velocity perturbation \( \vec{u}' \) is given by

\[
\vec{u}' = \epsilon e^{-\left(\frac{(x-x_0)^2+(y-y_0)^2+g(t)^2(z-z_0)^2}{2}\right)} \begin{bmatrix}
g(t)(y - y_0)(z - z_0) & g(t)(x - x_0)(z - z_0) \\
g(t)(x - x_0)(y - y_0) & -\frac{2}{g(t)}(x - x_0)(y - y_0)
\end{bmatrix},
\]

(3.38)

with

\[ g(t) = 1 + \kappa \sin(t), \]

(3.39)

where \((x_0, y_0, z_0)\) is the location of the source or sink that is operational.

Simulations with this perturbed velocity field are performed by extending the numerical integration code from the 2D case to accommodate an additional dimension.

Results

Poincaré sections for the 3D perturbed pulsed source-sink system are constructed for the case of \( \Pi = 10\pi \) by tracing a line of tracer particles on the positive \( y \)-axis for 1000\( T \). Figure 3.26a shows the \((x, r)\)-projection of the resulting Poincaré section. This figure shows coherent structures instead of the period-1 elliptic island in the unperturbed case, as shown in figure 3.24. The elliptic orbits are transformed into bands. In contrast with the time-dependent perturbation in 2D these bands appear as the result of the time-independent perturbation and show a very regular pattern. This pattern might be the result of the rotational motion about the \( x \)-axis. This rotating motion slightly changes the mapped position of tracer particles. Inside elliptic islands this results in deviations from elliptic orbits. As the perturbation is only dependent on the position this results in complex but regular motion inside the elliptic islands.

The dynamics in the \((y, z)\)-plane is illustrated in figure 3.26b where the \((y, z)\)-projection of the Poincaré section is plotted for two tracer particles. The red tracer particle is released within the period-1 elliptic island and describes a well defined and regular circular motion about the \( x \)-axis. The blue tracer particle is released just outside the period-1 elliptic island and shows a more elaborate motion in the \((y, z)\)-projection. The particle also rotates about the \( x \)-axis. Additionally it moves towards larger \( r \) where the motion is governed by the perturbation in the velocity field and its trajectory is completely unrelated to the source-sink flow.

No significant differences are observed in the time-dependent perturbation (not shown) compared with the time-independent case. A possible explanation is that the effects caused by the time-independent perturbation are much larger than the additional effects caused by the time-dependency of the perturbation.
Figure 3.26: Projections of the 3D Poincaré section for $\Pi = 10\pi$ with $\epsilon = 0.02$ and $\kappa = 0$. (a) Close up of the $(x, r)$-projection of the area near the source and sink. (b) $(y, z)$-projection of the Poincaré section constructed from 2 particles. The red tracer particle is released within the period-1 elliptic island. The blue particle is released just outside the period-1 elliptic island.

Concluding the study of the 3D pulsed source-sink system, symmetry considerations reduced the 3D system into an essentially 2D system that is rotationally symmetric about the $x$-axis. In the 2D planes, comparable dynamics were observed to the 2D pulsed source-sink system. In general the periodic points are located closer to the source and sink for the 3D case compared with the 2D case. However, care should be taken in comparing the 2D and 3D cases. Perturbing the 3D system also showed comparable results in the 2D planes. In the direction of rotation about the $x$-axis the perturbation resulted in regular motion about the $x$-axis. It is unlikely that this effect resembles the effects caused by weak fluid inertia or dispersion and might be explained by the symmetry in the perturbation function.

The pulsed source-sink system provided insight into chaotic advection in a potential flow. The organisation of the periodic points was understood using geometrical considerations. In addition, it was shown that the pulsed source-sink system pushes fluid away from the region close to the source and sink. For these reasons the next section will focus on more realistic systems consisting of pulsed dipoles.
Chapter 4

Dipole systems

The pulsed source-sink system, described in section 3, is a relatively simple system that gives much insight into the concept of chaotic advection. A system consisting of multiple sources and sinks might increase the efficiency of the mixing process.

When a source and a sink, separated by some distance, are operated at the same time a so-called dipole is created. The fluid moves from the source towards the sink. This configuration is shown in figure 4.1a where the source and sink now operate simultaneously. Streamlines of the dipole flow are plotted in the figure as well. In 2D, the velocity field due to a dipole consisting of a source at
\( (x, y) = (x_0, y_0) \) and a sink at \( (x, y) = (x_1, y_1) \) is given by
\[
\vec{v} = \frac{Q}{2\pi} \left( \frac{1}{(x-x_0)^2 + (y-y_0)^2} \begin{bmatrix} x-x_0 \\ y-y_0 \end{bmatrix} - \frac{1}{(x-x_1)^2 + (y-y_1)^2} \begin{bmatrix} x-x_1 \\ y-y_1 \end{bmatrix} \right). \tag{4.1}
\]

Similar to the flow caused by a single source or sink, the time-independent dipole flow does not exhibit chaotic behaviour. To create chaotic behavior a second dipole is introduced in the system as shown in figure 4.1b. By operating the two dipoles sequentially the system may become chaotic.

As a result of the sequentially operated dipoles, some tracer particles may be absorbed by a sink. For the same reasons as described in section 3.1, the particles that are absorbed by a sink are reintroduced into the system. In contrast to the pulsed source-sink system the reinjection in the dipole system takes place immediately. The absorbed particles are reinjected at the source of the dipole. This reinjection takes place on the same streamline, consistent with the reinjection rule used in the pulsed source-sink system.

Two different schemes of sequentially operated dipoles are investigated: the ‘switched dipole’ and the ‘rotated dipole’. In the former case, a vertically oriented dipole is alternated with a horizontally oriented dipole. Hence a full period of this system is composed of two forcing steps. The individual dipoles operate for equal duration \( \tau = \frac{T}{2} \) where \( T \) is a full period. The switched dipole system is discussed in section 4.2. The rotated dipole system consists of four equal forcing steps each period. Moving from one step to the next the orientation of the dipole is rotated by 90 degrees about the centre of the dipole. The first two steps are identical to the forcing steps in the switched dipole system. The third and fourth forcing steps are essentially equal to the first and second step, respectively, only the source and sink have switched positions. Each forcing step of the rotated dipole flow takes \( \tau = \frac{T}{4} \). Since the rotated dipole system has four forcing steps and the switched dipole system has two forcing steps, a period \( T \) of the rotated dipole system takes twice as long when the time duration of the individual steps \( \tau \) are the same as for the switched dipole system. The rotated dipole system is discussed in section 4.3. In both the switched dipole system and the rotated dipole system, the source and sink of each individual dipole are separated by a distance \( 2a \).

Similar to the case of the source-sink system the relevant parameters \( Q, \tau, a \) can be combined into a single dimensionless variable \( \Upsilon \). The parameter \( \Gamma \) used for the 2D pulsed source-sink system can also be used for the dipole systems, but changing \( T \) into \( \tau \) allows for a better comparison of the two dipole systems. In addition, multiplying \( \Gamma \) with \( \frac{3}{4\pi} \) results in
\[
\Upsilon = \frac{3Q\tau}{4\pi a^2}. \tag{4.2}
\]

Using the pre-factor \( \frac{3}{4\pi} \) causes \( \Upsilon = 1 \) when a tracer is able to travel exactly the shortest path from the source to the sink of a dipole each time step \( \tau \), as shown in appendix B. This shortest path corresponds to the straight line connecting the source and sink (see figure 4.1a). When \( \Upsilon > 1 \) tracers on the straight line travel longer distances each time step, when \( \Upsilon < 1 \) tracers on the straight line travel shorter distances each time step.

### 4.1 Simulation setup

As no analytical solution can be obtained for the system of equations (4.1) and (3.2), this system is integrated numerically to obtain particle positions as function of time. The integration takes place in Matlab with the same code as for the perturbed source-sink flow described in section 3.1.5.
4.2 Switched dipole system

The switched dipole system consists of two dipoles operated sequentially to produce a time dependent velocity field. The dipoles are oriented along the $x$-axis and $y$-axis, as shown in figure 4.1b. First the vertically oriented dipole (blue) is operational for a time period $\tau$, followed by the horizontally oriented dipole (red), operational for an equal amount of time. The horizontally oriented dipole is followed again by the vertically oriented dipole and the sequence repeats itself. A typical trajectory of a tracer in the switched dipole system is shown in figure 4.2.

Figure 4.2: Typical trajectory of a tracer particle in the switched dipole system for two periods, with $\Upsilon = 1$. The initial position $(x/a, y/a) = (0.4, -0.7)$ is marked by $\times$. The symbol $\cdot$ marks the position of the tracer after full periods $T$.

4.2.1 Symmetry analysis

The analysis of the source-sink system described in section 3.1.2 showed that identifying flow field symmetries greatly simplifies the search for periodic points. The current analysis of the symmetries in the switched dipole system is similar to the symmetry analysis of the pulsed source-sink system. Consider the mapping

$$\Phi_T = F_2F_1,$$  \hspace{1cm} (4.3)

where $F_1$ and $F_2$ describe de mapping functions for the separate dipole steps. Using this approach the following symmetry relations can be distinguished:

$$F_1 = S_xF_1S_x, \quad F_1 = S_yF_1^{-1}S_y, \quad F_1 = RF_2R^{-1},$$ \hspace{1cm} (4.4)

$$F_2 = S_yF_2S_y, \quad F_2 = S_xF_2^{-1}S_x, \quad F_2 = R^{-1}F_1R,$$ \hspace{1cm} (4.5)
where $R$ denotes a 90 degree counterclockwise rotation about the origin.

Global symmetries in the forced flow can be found by combining these relations, giving

$$\Phi_T = F_2 F_1 = R^{-1} F_1 R R F_2 R^{-1} = R^{-1} S_y F_1^{-1} S_y R R S_x F_2^{-1} S_x R^{-1}. \tag{4.6}$$

Using $RR = S_y S_x$ this results in

$$\Phi_T = R^{-1} S_y F_1^{-1} F_2^{-1} S_x R^{-1} = S_{-xy} \Phi_T^{-1} S_{-xy}, \tag{4.7}$$

where $S_{-xy} = S_x R^{-1} = R^{-1} S_y$ describes the symmetry operator corresponding to a reflectional symmetry about the line $y = -x$.

Equation (4.6) expresses the time-reversal reflectional symmetry of the switched dipole system in the line $y = -x$. Hence, periodic points of this system will also be configured symmetrically about this line, as proved by equation (3.11).

### 4.2.2 Periodic points

Periodic points of the switched dipole system are identified using the Newton-Raphson iteration scheme discussed in section 3.1.2. The search for periodic points is restricted to period-1 points. The symmetry of the system from section 4.2.1 permits a reduction of the search area to half of the domain. The grid of initial points used for the Newton-Raphson scheme is plotted in figure 4.3a. The points are spaced 0.1$a$ apart and cover the area close to the sources and sinks of the dipole systems.

![Figure 4.3](image_url)

*Figure 4.3: (a) Grid of initial points for the Newton-Raphson iteration scheme. (b) Period-1 points (·) of the switched dipole system, found using the Newton-Raphson method for $\Upsilon = 1$.***
Three period-1 points are identified for $\Upsilon = 1$. These points are shown in figure 4.3b. The period-1 point at the centre of the dipole system can be understood from the fact that when $\Upsilon = 1$ particles can travel a full distance of $2a$ during each forcing step when located on the line connecting the active source and sink of the dipole. Hence a particle located at the origin will be mapped to the origin after each separate forcing step. The particle trajectory corresponding to this period-1 point as well as the trajectories of the two other period-1 points are plotted in figure 4.4a.

![Figure 4.4: (a) Trajectories corresponding to the three period-1 points found for the switched dipole system with $\Upsilon = 1$. Period-1 points are marked with . (b) Streamlines of the individual dipole steps showing the overlap of streamlines on the circle with radius $a$ centered around the origin.](image)

The trajectories corresponding to the two other period-1 points are similar due to the symmetry properties of the flow. Both points are located on the circle of radius $a$ connecting all the sources and sinks. The streamlines of the individual dipoles overlap on this circle, as shown in figure 4.4b. This causes the particle trajectory corresponding to the two period-1 points to consist of two overlapping segments. First the particle released at the period-1 point is forced upwards by the vertically aligned dipole. The particle is subsequently moved down again by the horizontally aligned dipole. Important to note is that a particle released at this point is never absorbed by a sink. Mapping of tracers released at these period-1 points reveal that these points are hyperbolic in nature.

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4.2.3 Poincaré section

The confining properties of this system are clearly observed in a Poincaré section. A Poincaré section for this system is constructed by mapping a single particle located at \((x/a, y/a) = (0, 0.7)\) for 10000\(T\). For \(\Upsilon = 1\) this results in the Poincaré section shown in figure 4.5. The particle seems to be confined to a circle with radius \(a\) centered around the origin. This feature can be understood by considering the streamlines of the individual dipole steps, as shown in figure 4.4b. As the streamlines overlap on a closed circle this circle acts as a transport barrier. Particles released within the region enclosed by the circle are trapped in this region. This is an interesting property as pollutants, microorganisms and other material can be prevented from leaving the enclosed area and spread out.

![Poincaré section](image)

*Figure 4.5: Poincaré section for \(\Upsilon = 1\) constructed by mapping the point \((x/a, y/a) = (0, 0.7)\) for 10000\(T\). Two additional particles (red) are added to the Poincaré section to highlight the structure of elliptic islands. Sources and sinks are marked by \(\oplus\) and \(\ominus\), respectively; period-1 points are marked by \(\cdot\).*
Figure 4.5 shows some structure around the period-1 point located at the origin. This structure is not the result of an elliptic island but is caused by the fact that particles near this period-1 point slowly move around the hyperbolic period-1 point. The Poincaré section is constructed for a single particle and only a few instances occurred where particle came close to the period-1 point. The two other period-1 points are also shown on the bounding streamline. Mapping of a tracer released close to these points shows that these points are also hyperbolic. Notice also the area within the bounding streamlines to be relatively uniformly covered with points, implying that the tracer particle generally visits every part on the circle equally often. In addition to the empty spot at the origin, other empty spots are observed within the bounding streamlines. Mapping of tracers released in these areas shows these structures are the outlines of two sets of elliptic islands corresponding to elliptic period-3 points, as illustrated in figure 4.5 by the red tracers.

When a particle is released outside of the confining circle it stays outside this circle. Far away from the bounding streamline the system of switched dipoles behaves as a stationary dipole. Particles describe large, curved trajectories in the Poincaré section, from the lower left quadrant to the upper right quadrant. This can be seen in figure 4.6 where an additional particle (shown in red) is included in the Poincaré section for $\Upsilon = 1$.

![Figure 4.6: Poincaré section the same case as shown in figure 4.5 but now an additional particle (red) is added in the exterior region. This particle is initially located at $(x/a, y/a) = (0.75, -0.75)$.](image)

### 4.2.4 Parameter variation

When $\Upsilon$ is changed the distance particles travel during each forcing step will change. Similar to the pulsed source-sink system this changes the location and nature of the periodic points in the system. In this section three additional settings of $\Upsilon$ are discussed and compared with the case $\Upsilon = 1$. Poincaré sections are constructed using a single tracer released at the same position as before. Periodic points are also identified using the same methods as for $\Upsilon = 1$. The resulting data is shown in figure 4.12 where the case $\Upsilon = 1$ is plotted again for comparison.
Figure 4.7: Poincaré sections for selected Υ constructed by mapping the point \((x/a, y/a) = (0, 7)\) for 10000T. ⊕ and ⊖ denote source and sink position. Period-1 points are marked by ⋅.

All the Poincaré sections show symmetry about the line \(y = -x\) as predicted by the symmetry analysis in section 4.2.1. In addition, the particle remains confined within a circle of radius \(a\) centered at the origin.

The case \(Υ = 1\) was characterized by a hyperbolic period-1 point located at the origin and two hyperbolic points on the bounding streamline. When \(Υ\) is increased slightly two elliptic period-1 points are found surrounded by large elliptic islands, as shown in figure 4.7a. In addition, two
hyperbolic period-1 points are found located near the origin and close to the elliptic islands. The existence of these four period-1 points can be explained by the fact that for larger Υ tracers can travel larger distances.

When Υ is decreased particles can no longer travel the full distance from the source to the sink of a dipole in one forcing step. This leads to the destruction of all period-1 points for which the particles are absorbed by a sink each period. For example the central period-1 point is absent for Υ = 0.90, as seen in figure 4.7c. In addition, the period-3 islands observed for Υ = 1 are destroyed as well.

Further decrease of Υ results in the formation of empty spots in the Poincaré sections, as seen in figure 4.7d. These empty spots correspond to elliptic islands of higher-order periodic points. Mapping of tracers in these empty spots confirms the existence of two sets of period-4 islands and a set of period-5 islands. For small Υ particle trajectories follow a relatively smooth path from bottom right to the top left of the domain. This can be explained by the positions of the sources and sinks. This movement is also observed for the particles released in the periodic islands. Figure 4.7d also shows two hyperbolic period-1 points. In addition, a white channel is seen joining these points. This channel acts as a transport barrier and no particle can cross this channel, as will be discussed in the next section.

Particles released at the period-1 points on the bounding streamline are not absorbed by a sink. The corresponding periodic points remain intact upon changing Υ. When Υ is decreased these points move toward the left while remaining on the bounding streamline. In the limit of Υ → 0 these points converge to the points \((x/a, y/a) = \left(\frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}\right)\) and \((x/a, y/a) = \left(-\frac{1}{2}\sqrt{2}, -\frac{1}{2}\sqrt{2}\right)\). The limiting case of Υ → 0 can be understood as a very fast switching between the two dipoles. In this case particles approximately behave as if the two dipoles are operational at the same time, as shown in figure 4.8. The Poincaré section again shows the transport boundary connecting the two hyperbolic periodic points on the bounding streamline.

Figure 4.8: Poincaré section for Υ = 0.09. Constructed from a single particle, initially located at \((x/a, y/a) = (0, 0.7)\). Period-1 points are marked by ·.
4.2.5 Manifolds

The existence of a transport barrier along the white channel in figures 4.7d and 4.8 is confirmed by tracing the manifolds associated with the hyperbolic period-1 points on the bounding streamline in the case $\Upsilon = 0.27$. These manifolds are found using the same methods used for the pulsed source-sink system, described in section 3.1.4.

The unstable manifold of the left period-1 point is directed towards the period-1 point on the right. Due to the time-reversal reflectional symmetry of the system the stable manifold of the period-1 point on the right is the mirrored version of the unstable manifold of the period-1 point on the left. These manifolds are shown in figure 4.9 where the right panel is a close up of the region near the period-1 point on the right.

![Figure 4.9](image)

*Figure 4.9: (a) Manifolds traced for the hyperbolic period-1 point on the bounding streamline in the case $\Upsilon = 0.27$. The red line denotes the unstable manifold of the period-1 point on the left and the black line denotes the stable manifold of the period-1 point on the right. (b) A close up of the manifold structure near the period-1 point on the right.*

The unstable manifold of the period-1 point on the left (red) and the stable manifold of the period-1 point on the right (black) overlap for a large part. As a manifold cannot be crossed by a tracer, this part acts as a transport barrier. Close to the two hyperbolic points the manifold show the characteristic oscillating structures with many heteroclinic points, responsible for the stretching and folding dynamics. When a transport barrier develops between the two period-1 points on the bounding streamline, the confined area is divided into two regions. Particles will remain in one region until they are absorbed.
4.2.6 Blob tracing simulation

The mixing capabilities of the switched dipole system are visualised by following a blob containing a large amount of tracers. A square blob of 10000 tracer particles, covering an area of $0.1a \times 0.1a$, is placed inside the chaotic region in the confining circle. The individual tracer particles are mapped for $10T$ using $Y = 1$. The initial and final distributions of tracer particles are shown in figures 4.10a and 4.10b, respectively.

![Figure 4.10: Advection of a square blob of tracer particles. (a) Initial configuration (b) configuration after $10T$.](image)

Figure 4.10 shows the distribution of the square blob of tracer particles after $10T$. Due to the chaotic motion the blob is spread out over much of the confined area. Stretching and folding effects can be observed with the presence of the stacked filamentary structures. Comparing the Poincaré section in figure 4.5 with the distribution of spread tracers it is clear that the tracers do not spread into the elliptic islands. This is in line with the expectations on the non-chaotic nature of elliptic islands, discussed in section 2.

4.2.7 Perturbed flow

To investigate the effects of dispersion on the switched dipole system, a perturbation is applied to the velocity fields of each forcing step. For each source and sink the perturbation given by equation (3.32) is added to the velocity field. Similar to the pulsed source-sink system, both time-dependent and time-independent perturbations were studied. Figure 4.11 shows typical Poincaré sections for each of these cases.

Application of a perturbation to the velocity fields of the switched dipole system results in similar dynamics as observed in the perturbed source-sink system. Elliptic islands corresponding to periodic points gradually break down as the amplitude of the perturbation is increased, as
evident by comparing figures 4.11a and 4.7a. In addition, a time-dependent perturbation results in the transformation of elliptic orbits into partially overlapping bands, as seen in figure 4.11b. Also note the blue particle is not confined to the circle joining the sources and sinks.

![Figure 4.11: Poincaré sections for perturbed flow of the switched dipole system with $\Upsilon = 1.08$. The Poincaré sections are constructed for a single particle (blue), initially located at $(x/a, y/a) = (0, 0.7)$ additional particles (red) were added at positions inside the elliptic island of the unperturbed case. (a) Time-independent perturbation, with $\epsilon = 0.01$ and $k = 0$. (b) Time-dependent perturbation with $\epsilon = 0.01$ and $k = 0.006$.](image)

### 4.3 Rotated dipole system

In this section the rotated dipole system, introduced at the start of this chapter, is investigated. The positions of the subsequent dipoles are related via a 90 degree clockwise rotation about the origin, as shown in figures 4.12a to 4.12d.

![Figure 4.12: Schematic time evolution of the rotated dipole system. The system is composed of four sequential dipole steps per period $T$, each step takes $T/4$. Sources and sinks are marked with ⊕ and ⊖, the arrows indicate the direction of the flow.](image)
Particles follow the streamlines of the dipole that is active. Hence, particle trajectories are composed of segments of these streamlines from different dipoles. Typical particle trajectories for $\Upsilon = 1$ are shown in figure 4.13.

![Figure 4.13: Typical particle trajectories for the rotated dipole system. Sources and sinks are marked by $\circ$. Trajectories are indicated by the black lines. Trajectories are constructed for $\Upsilon = 1$ with initial conditions (a) $\left(\frac{x}{a}, \frac{y}{a}\right) = (-0.3, 0)$ and (b) $\left(\frac{x}{a}, \frac{y}{a}\right) = (-0.6, -0.7)$ (marked by $\times$).](image)

Similar to the switched dipole system, particles can be absorbed by a sink and are subsequently reinjected at the source of the same dipole. Figure 4.13a shows a particle being absorbed and reinjected several times each period. In addition, other particle trajectories are not subject to absorption and reinjection, as shown in figure 4.13b.
4.3.1 Symmetry analysis

Similar to the switched dipole system, the search for periodic points in the rotated dipole system is simplified greatly by analysing the symmetry properties of the system. The rotated dipole system is composed of four steps and can be described by the composite map

$$\Phi_T = F_4 F_3 F_2 F_1,$$

(4.8)

where $F_1$, $F_2$, $F_3$ and $F_4$ describe the mapping functions for the separate dipole steps. Various symmetry relations between the individual steps can be distinguished, including

$$F_1 = S_y F_1^{-1} S_y, \quad F_1 = RF_4^{-1} R^{-1}, \quad F_2 = S_y F_2 S_y, \quad F_2 = RF_3 R^{-1},$$

(4.9)

$$F_3 = S_y F_3^{-1} S_y, \quad F_3 = RF_2^{-1} R^{-1}, \quad F_4 = S_y F_4 S_y, \quad F_4 = RF_1 R^{-1}.$$  

(4.10)

Combining these relations leads to a symmetry relation of the total system. Making use of $RR^{-1} = I$, with $I$ the identity operator, this yields

$$\Phi_T = RF_1 R^{-1} RF_2^{-1} R^{-1} RF_3 R^{-1} RF_4^{-1} R^{-1} = RF_1 F_2^{-1} F_3 F_4^{-1} R^{-1},$$

(4.11)

and,

$$\Phi_T = RS_y F_1^{-1} S_y F_2^{-1} S_y F_3^{-1} S_y F_4^{-1} R^{-1} = RS_y F_1^{-1} F_2^{-1} F_3^{-1} F_4^{-1} S_y R^{-1}.$$  

(4.12)

Finally defining the operator $S_{xy} = RS_y = S_y R$ as a reflectional symmetry about the line $y = x$ this reduces to

$$\Phi_T = S_{xy} F_1^{-1} F_2^{-1} F_3^{-1} F_4^{-1} S_{xy} = S_{xy} \Phi_T^{-1} S_{xy},$$

(4.13)

proving time-reversal reflection symmetry of the rotated dipole system about the line $y = x$.

The rotated dipole system can be linked to the switched dipole system by recognising that the first two forcing steps of the rotated dipole system are identical to the switched dipole system. The two additional forcing steps in the rotated dipole system can be linked to the first two with a 180 degree rotation $R^2$ giving

$$\Phi_T^{RDF} = F_4 F_3 \Phi_T^{SDF} = R^2 \Phi_T^{SDF} R^2 \Phi_T^{SDF},$$

(4.14)

where RDF and SDF refer to the rotated dipole system and the switched dipole system respectively. Consequently, any pair of period-$k$ points of the switched dipole system that has an $R^2$ symmetry will result in a period-$k$ point in the rotated dipole system with the same $Y$. 

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4.3.2 Periodic points

Periodic points are found using the Newton-Raphson method. Again the search is restricted to period-1 points. Symmetry considerations allow a reduction in the search area. A grid of initial points spaced $0.1a$ apart is used for the Newton-Raphson method. This grid is shown in figure 4.14a. The resulting periodic points are shown in figure 4.14b.

Figure 4.14b shows many period-1 points for $\Upsilon = 1$. The larger part of these points is located within the confining circle. First point to notice is the period-1 point located at the origin. As this point was invariant under the action of every single forcing step in the switched dipole system, the addition of two extra steps does not destroy this point.

![Figure 4.14: (a) Grid of initial points for the Newton-Raphson iteration scheme. (b) Period-1 points found using the Newton-Raphson method for $\Upsilon = 1$.](image)

Two period-1 points are identified on the confining circle. In addition, some period-1 points are found close to this circle. The trajectory for a period-1 point close to the confining circle is shown in figure 4.15a for the point labelled 2. The particle initially moves upward and is absorbed by the sink at $(x/a, y/a) = (0, 1)$ and is subsequently re-injected at the source at $(x/a, y/a) = (0, -1)$. After the first forcing step the particle ends up at a position that is the 90 degree clockwise rotation of its initial position. In subsequent forcing steps this procedure is repeated until the particle comes back to its initial position after a full period of the system.
Figure 4.15: Trajectories for selected period-1 points for \( \Upsilon = 1 \). The numbering of the points corresponds to the numbering in figure 4.14b. Period-1 points are marked with \( \times \). Positions of tracers after each forcing step are marked by \( \cdot \). Trajectories are shown by the red and blue lines.

Several period-1 points are found located inside the confined area. Two distinct types of trajectories can be identified here. Some trajectories of particles released at the period-1 points are not subject to absorption, for example the period-1 point labelled 6 in figure 4.15b. Other trajectories are related to particles subject to absorption and reinjection, illustrated by the trajectory corresponding to the point labelled 1 in figure 4.15a. Additionally several points are located outside the confining circle. Typical trajectories are shown in figure 4.15b corresponding to points labelled 3 to 5.

Symmetry is a key part of the trajectories of particles released at periodic points. All the trajectories shown in figure 4.15 show a time-reversal reflectional symmetry about the \( y \)-axis (e.g. point number 6) or have a time-reversal reflectional counterpart (e.g. points number 5 and 3). These periodic points exploit the symmetry of the individual dipole steps. In section 4.3.1 it was shown that the rotated dipole system possesses a time-reversal reflectional symmetry about the line \( y = x \). All the periodic points and their corresponding particle trajectories have a symmetrical counterpart.
4.3.3 Poincaré section

A Poincaré section for $\Upsilon = 1$ is constructed by mapping the point $(x/a, y/a) = (0, 0.7)$ for 10000$T$. This results in the Poincaré section shown in figure 4.16.

![Poincaré section](image)

Figure 4.16: Poincaré section for $\Upsilon = 1$ constructed by iterating the point $(x/a, y/a) = (0, 0.7)$ for 10000$T$. Sources and sinks are marked by $\circ$ and period-1 points are marked by ·.

A large island is situated around the period-1 point in the origin. This is confirmed by simulation of a tracer trajectory in the island, as shown in the figure. A second island containing several period-1 points is observed in the confining circle. An elliptic period-1 point with a small elliptic island is found at the center of this island, as shown in figure 4.17. Surrounding this small elliptic period-1 island is a chain of period-1 points of alternating elliptic and hyperbolic kinds. The existence of this structure is attributed to the KAM theorem.
Figure 4.17: Poincaré section for Υ = 1 showing the structure of the elliptic islands using several tracer particles (red). Sources and sinks are marked by ◦ and period-1 points are marked by ·.

The dynamics outside the confining circle is shown in figure 4.18. Two large elliptic islands can be observed, these islands correspond to the period-1 points shown in figure 4.14b. In addition, an indentation of the confining circle is observed. This indentation indicates the existence of an additional elliptic island.

Figure 4.18: Poincaré section for Υ = 1 constructed by mapping a particle released at (x/a, y/a) = (−0.3, 1) for 10000T. Sources and sinks are marked by ◦ and period-1 points are marked by ·.
4.3.4 Parameter variation

As with the switched dipole system, smaller $\Upsilon$ result in smaller distances travelled by particles each dipole step. This will result in a change in periodic points and elliptic islands. For the rotated dipole system several values of $\Upsilon$ are investigated by identifying period-1 points and construction of Poincaré sections. The resulting data is shown in figure 4.19.

![Figure 4.19: Poincaré sections for selected $\Upsilon$ constructed by mapping the point $(x/a, y/a) = (0, 0.7)$ for 10000$T$. Period-1 points are marked by ∙.](image)

For $\Upsilon < 1$, particles will travel smaller distances during each forcing step. In contrast with the switched dipole system, the rotation of the dipole positions in the rotated dipole flow still allows period-1 points to exist inside the confining circle, as shown in figure 4.19a where three elliptic islands can be observed surrounding period-1 points.

For $\Upsilon > 1$, particles are able to travel a larger distance than the distance between the source and sink of a dipole. This can result in multiple instances of absorption and reinjection during each forcing step. Many features seen in the case of $\Upsilon = 1$ remain visible for $\Upsilon = 1.26$. Notice the large elliptic island at the bottom left of the confining circle is preserved, though somewhat decreased in size. This island corresponds to particles moving in the confining circle with orbits similar to particle number 6 in figure 4.15b. Additionally an elliptic period-1 point is observed not far from the origin. This point results from the central period-1 point for $\Upsilon = 1$. For increasing $\Upsilon$ this point moves away from the origin. The curved trajectories take more time and the particle is able to return to its initial position after a single dipole step.

In conclusion, two different systems of sequentially operated dipoles have been studied: the switched dipole flow and the rotated dipole flow. Both these systems showed a confinement of particles within a circle connecting the sources and sinks. Periodic points were identified using the Newton-Raphson method. Much more periodic points were observed in rotated dipole systems.
compared with the switched dipole systems. This observation holds for both hyperbolic and elliptic points.

The switched dipole system showed less elliptic islands than the rotated dipole system. The case \( \Upsilon = 0.9 \) for the switched dipole showed no elliptic islands at all. Based on the amount of hyperbolic period-1 points, the rotated dipole flow appears to be a more efficient mixer at the cost of more surface area of elliptic islands and an doubling of the time required to mix.

The simulations with a perturbed velocity field show the break up of elliptic islands and the broadening of elliptic orbits. These results are very similar to the results obtained for the pulsed source-sink system. The perturbed flow simulations are performed on the switched dipole system only. However, the similarity between the switched dipole system and the rotated dipole system indicates that identical results can be obtained for the rotated dipole system.
Chapter 5

Experiments

In this section the possibilities of making a translucent artificial porous medium are investigated and tested in the laboratory. The model porous medium will be used in a future study of the fundamental transport properties of porous media flow, such as dispersion. In addition, a large-scale model porous medium may be used to experimentally investigate mixing properties of a periodically forced flow inside a porous medium, as was investigated numerically in chapters 3 and 4.

The model is made translucent to allow measurements on fluid flow inside the porous medium by advanced optical techniques, which are based on tracing particles through the porous medium. The model porous medium consists of a large number of translucent spheres with a diameter of 1-10mm, submerged in a liquid as shown schematically in figure 5.1.

![Figure 5.1: Schematic representation of the RIM artificial porous medium allowing tracer particles (black dot) to be observed using optical techniques, in this case a camera.](image)

When a ray of light passes a material interface its direction will change, as shown in figure 5.2. This refraction of light depends on the indices of refraction $n_1$ and $n_2$ of the two materials on the interface, as described by Snell’s law

$$n \sin(\theta) = \text{constant},$$

(5.1)
where $\theta$ is the angle of the ray of light with respect to the interface normal, as shown in figure 5.2.

![Figure 5.2: Light refraction at a material interface. An incident light ray under an angle $\theta_i$ in a material with index of refraction $n_1$ is refracted at a material surface. The refracted ray of light travels on with an angle $\theta_r$ inside the second material with index of refraction $n_2$. Angles are measured with respect to the interface normal (dashed line).](image)

To allow a clear and undistorted view of the flow inside our translucent model porous medium, refraction of light needs to be minimised. Therefore the index of refraction of the liquid in the model needs to match the index of refraction of the spheres. The technique of using refractive index matched (RIM) materials for optical flow measurements has been used in numerous applications [Dijksman et al., 2012]. The basic principle of the RIM technique is the same in all these cases. However, the requirements on the match of the refractive index are different with different applications. When doing flow experiments with relative simple geometries a light ray only encounters a small amount of refractive surfaces. In contrast, in the case of RIM porous media and particle suspensions, a much larger number of refractive surfaces are encountered, increasing demands on the refractive index match.

First an overview of the literature regarding experiments on RIM porous media is presented. This overview is followed by a discussion of the methods and setups used in the current investigation on producing a RIM porous medium. This chapter ends with the results obtained from this investigation.
5.1 Literature overview

Several authors report on experiments using a RIM artificial porous medium setup. These setups are listed in table 5.1. This section provides an overview of these setups and discusses the methods that are used to obtain a refractive index match, the materials used and the optical techniques that are applied to measure inside the porous medium.

5.1.1 Methods

To create an RIM artificial porous medium the index of refraction of the solid phase (the spheres) needs to match with the index of refraction of the liquid phase. Several methods have been developed to match these indices of refraction.

The refractive index of some liquids can be tuned by mixing them with other liquids with a different index of refraction. The index of refraction of glycerol for example can be changed by mixing it with water, as applied by Kong et al. (2010). As the index of refraction of glycerol is higher than that of water, increasing the amount of water in the mixture will decrease the index of refraction. This method can be applied to other liquids too. For example a mixture of different oils can be used to create a liquid with a specified index of refraction, as applied Yarlagadda et al. (1989). Mixing different components to create a liquid phase with an index of refraction that matches the solid phase in an RIM setup provides a robust way to make an RIM setup. In practice, small adaptations to the index of refraction of the liquid are difficult once the spheres are added. Additional fluid is hard to mix due to the small velocities inside the model porous medium, especially for setups using more viscous fluids.

The second way to obtain a RIM setup is based on the fact that the index of refraction of most materials changes with temperature. The index of refraction of liquids is usually more sensitive to temperature changes than the index of refraction of solids. Therefore the index of refraction of the solid and liquid phases in an RIM setup can be matched by adjusting the temperature of the RIM setup [Moroni and Cushman, 2001]. As the index of refraction changes only slightly with temperature (in the order of $10^{-4} K^{-1}$ [Dijksman et al., 2012]) the index of refraction of the liquid phase can only be tuned by a small amount. Therefore this method can be applied only when the initial indices of refraction of the liquid and solid phase are almost equal. However, this method does provide an accurate way to fine tune an RIM setup.

A third method to obtain a refractive index matched system is similar to the temperature method but uses variation in wavelength of light instead of temperature. The index of refraction of a material varies with the wavelength of the light passing though. The wavelength dependency is different from material to material and can therefore be used to match the index of refraction of the liquid phase with the solid phase. This method is described in Stohr et al. (2003).

Changing the temperature or changing the composition of the liquid phase will also effect other properties of the setup such as viscosity and density. A combination of the techniques described above can be applied to create RIM setups with a prescribed viscosity or density.

5.1.2 Solid phase materials

The choice of materials for index matching depends on many factors. Naturally the index of refraction and transmittance are most crucial but also temperature dependence of optical properties, availability, toxicity, price, chemical properties and factors concerning storage and handling play a
role. The choice of the solid phase mostly depends on index of refraction and optical transmittance of the material. The solid phase materials used in RIM porous media setups are listed in table 5.1. For the solid phase in artificial porous media several glasses as well as the plastic PMMA are used. Of all the solid materials, PMMA appears to be used the most, possibly because it is lighter than glass.

Most often, the solid phase in the artificial porous medium consists of spheres with sizes between 0.4 mm and 19 mm, because of their symmetry and commercial availability with well-defined properties. However some authors used crushed grains, rods or equilateral cylinders as a solid phase. The size of the porous medium varies and is largely dependent on the size of the solid phase grains and the application. Porous media are reported consisting of about 4 − 10 layers for larger grain sizes (> 0.5mm). Porous media with smaller grains have been reported with up to 200 layers.

5.1.3 Liquid phase materials

Besides the refractive index, viscosity is important when considering the liquid phase. In order for the physical effects to scale properly the Reynolds number needs to be the same in the laboratory model as it is in actual groundwater flow. The Reynolds number defined in equation (2.2) gives the ratio of inertial to viscous forces. The Reynolds number is dependent on the diameter of the solid phase grains, the characteristic velocity $v$ of the flow and the kinematic viscosity $\nu$ of the RIM liquid. As the characteristic velocity in a laboratory setup is limited by practical considerations such as the duration of the experiment and unwanted side effects of tracer particles, the kinematic viscosity of the RIM liquid needs to be considered in combination with the size of the solid phase grains. Typical Reynolds numbers for groundwater flow vary but in general they are much smaller than 1 [Bear and Cheng, 2010]. Therefore, the kinematic viscosity needs to increase when the scale of the model is increased. This is why many RIM liquids listed in table 5.1 have a viscosity several times higher than that of water.

Many artificial porous media reported in the literature use a mix of two liquids to match the index of refraction of the solid material. A mixture of Dow Corning oils is used most often as they are commercially available in different types with different indices of refraction and viscosities [Stöhr et al., 2003]. Other mixtures include a combination of ESSO oils and a glycerol-water mixture. Some artificial porous media use temperature to match the index of refraction of the solid and the liquid material. Additionally the temperature method is often used to fine tune a refractive index match obtained using the mixing method.

5.1.4 Optical techniques used

The main reason for producing an RIM porous medium is to allow optical measurements to be performed inside the medium. Several optical techniques are used in the literature. These methods are described below.

- PIV: In Particle image velocimetry (PIV) the fluid is seeded with tiny particles. Flow velocities are obtained by correlating subsequent snapshots of 2D planes in the flow [Northrup et al., 1993].

- PTV: Particle tracking velocimetry (PTV) is a technique that tracks individual tracer particles over time. From the positions of these particles Lagrangian data as well as a velocity field
can be constructed. Measurements with multiple cameras allow for 3D measurements [Monica et al., 2009].

- LDA: A laser Doppler anemometer (LDA) uses the doppler shift of laser light to obtain velocity data. Motion of tracer particles in the flow causes a shift in the frequency of laser light incident on the fluid [Yarlagadda and Yoganathan, 1989].

To avoid problems due to light scattering at the solid-liquid interfaces within the artificial porous medium, fluorescent tracer particles are often used in the PIV and PTV techniques. These fluorescent tracer particles emit light when illuminated by light of a specific frequency. The fluorescent light emitted by tracer particles travels less distance inside the porous medium compared with light from outside the porous medium that is reflected by the tracer particles. The decreased travel distance of the light inside the porous medium reduces the amount of solid-liquid interfaces encountered by the light and hence, reduces scattering effects.

<table>
<thead>
<tr>
<th>Solid</th>
<th>( n_r )</th>
<th>Liquid</th>
<th>Viscosity ((\text{mm}^2\text{s}^{-1}))</th>
<th>Grain size</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda lime glass</td>
<td>±1.52</td>
<td>Cargile oil type DF</td>
<td>–</td>
<td>3mm, 20 layers</td>
<td>Structure measurements using fluorescent dye and a laser sheet [Slotterback et al., 2008]</td>
</tr>
<tr>
<td>Borosilicate glass</td>
<td>±1.5</td>
<td>Paraffin 23.5°C</td>
<td>33.5</td>
<td>6 – 10mm, 12 – 20 layers</td>
<td>3D particle tracking [Lachhab et al., 2008]</td>
</tr>
<tr>
<td>Duran glass</td>
<td>1.473</td>
<td>Mixture of Dow Corning oils 550 and 556 20°C</td>
<td>42.5</td>
<td>2.5mm, ±38 layers</td>
<td>3D flow measurements using PIV [Stöhr et al., 2004]</td>
</tr>
<tr>
<td>PMMA</td>
<td>1.4885</td>
<td>Mixture of Dow Corning oils 550 and 556 19.8°C</td>
<td>–</td>
<td>3.1mm, ±14 layers</td>
<td>3D particle tracking [Rashidi et al., 1996]</td>
</tr>
<tr>
<td>PMMA</td>
<td>1.49</td>
<td>Mixture of Dow Corning oils 550 and 556</td>
<td>95</td>
<td>0.6mm, ±8 layers</td>
<td>3D flow measurements [Stöhr et al., 2003]</td>
</tr>
<tr>
<td>PMMA</td>
<td>–</td>
<td>Mixture of Dow Corning 550 and 200</td>
<td>–</td>
<td>12.7mm, 7 layers</td>
<td>fluid velocity measurements using laser anemometry [Johnston et al., 1975]</td>
</tr>
<tr>
<td>PMMA</td>
<td>1.4905</td>
<td>Mixture of Union Carbide L42 and Dow Corning 550 13.8°C</td>
<td>–</td>
<td>0.5 – 9.4mm, 4 – 10 layers</td>
<td>flow velocity measurements using PIV and a laser sheet [Northrup et al., 1991a]</td>
</tr>
<tr>
<td>PMMA</td>
<td>–</td>
<td>Cargile oil 5610 24°C</td>
<td>1.4</td>
<td>9.5mm, 10 layers</td>
<td>Measurement of velocity profiles using 3D-PTV [Dill et al., 1995]</td>
</tr>
<tr>
<td>PMMA</td>
<td>–</td>
<td>Dibutyl Phthalate (C16H22O4)</td>
<td>–</td>
<td>–</td>
<td>Measurement of velocity profiles using PIV [Amini and Hassan, 2012]</td>
</tr>
<tr>
<td>PMMA</td>
<td>1.4905</td>
<td>Mixture of Dow Corning 550 and Union Carbide L42</td>
<td>–</td>
<td>–</td>
<td>Velocity measurements using LDA [Amini and Hassan, 2012]</td>
</tr>
<tr>
<td>PMMA</td>
<td>–</td>
<td>paracymene 15°C</td>
<td>118</td>
<td>7mm 7 layers</td>
<td>velocity and structure measurements [Huang et al., 2008]</td>
</tr>
<tr>
<td>Solid</td>
<td>n_r</td>
<td>Liquid</td>
<td>Viscosity $(mm^2 s^{-1})$</td>
<td>Grain size</td>
<td>Application</td>
</tr>
<tr>
<td>---------------</td>
<td>-----</td>
<td>---------------------------------------------</td>
<td>---------------------------</td>
<td>------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Pyrex</td>
<td>1.474</td>
<td>Glycerol $23^\circ C$</td>
<td>–</td>
<td>4–19mm, 10–20 layers</td>
<td>Investigating dispersion of air bubbles using 3D-PTV [Moroni and Cushman, 2001] [Moroni et al., 2003] [Monica et al., 2009]</td>
</tr>
<tr>
<td>Pyrex</td>
<td>1.474</td>
<td>Mixture of Dow Corning oils 556 and 550</td>
<td>40–70</td>
<td>$D = 3$mm class rods, ±18 layers</td>
<td>Velocity measurements using a laser doppler anemometer [Yarlagadda and Yoganathan, 1989]</td>
</tr>
<tr>
<td>Pyrex</td>
<td>–</td>
<td>Mixture of ESSO MARCOL 82 and PRIMOL 352</td>
<td>34–230</td>
<td>±10mm, ±10 layers</td>
<td>Velocity measurements using particle tracing [Saleh et al., 1992]</td>
</tr>
<tr>
<td>Pyrex</td>
<td>1.474</td>
<td>Mixture of Dow Corning 556 and 550</td>
<td>–</td>
<td>–</td>
<td>Velocity measurements using LDA [Amini and Hassan, 2012]</td>
</tr>
<tr>
<td>Pyrex</td>
<td>1.474</td>
<td>Mixture of Sohio MDI-57 oil and mineral seal oil</td>
<td>–</td>
<td>–</td>
<td>Velocity measurements using LDA [Amini and Hassan, 2012]</td>
</tr>
<tr>
<td>Fused Silica</td>
<td>1.457</td>
<td>Mixture of glycerol and water</td>
<td>132</td>
<td>0.4 – 2mm crushed grains, ±200 layers</td>
<td>Structure analysis of air plume using the reflection of a laser sheet [Kong et al., 2011] [Kong et al., 2010]</td>
</tr>
<tr>
<td>Fused Silica</td>
<td>1.46</td>
<td>Mixture of Dow Corning oils 556 and 200</td>
<td>21</td>
<td>0.6 – 1.0mm, ±50 layers</td>
<td>3D flow measurements [Stöhr et al., 2003]</td>
</tr>
<tr>
<td>Fused Silica</td>
<td>1.46</td>
<td>$ZnCl_2$ (aq) solution</td>
<td>4</td>
<td>0.6 – 1.0mm, ±50 layers</td>
<td>3D flow measurements [Stöhr et al., 2003]</td>
</tr>
<tr>
<td>Fused Quartz</td>
<td>1.4584</td>
<td>Tetraethylenglycol $23.5^\circ C$</td>
<td>–</td>
<td>equilateral cylinders, $D = L = 7$mm</td>
<td>Velocity measurements by particle tracing [Stephenson and Stewart, 1986]</td>
</tr>
<tr>
<td>Fused Quartz</td>
<td>1.4584</td>
<td>Tetrahydroxypyrane-2-methanol $20^\circ C$</td>
<td>–</td>
<td>equilateral cylinders, $D = L = 7$mm</td>
<td>Velocity measurements by particle tracing [Stephenson and Stewart, 1986]</td>
</tr>
<tr>
<td>Fused Quartz</td>
<td>1.4584</td>
<td>Mixture of cyclooctane and cyclooctene $20^\circ C$</td>
<td>–</td>
<td>equilateral cylinders, $D = L = 7$mm</td>
<td>Velocity measurements by particle tracing [Stephenson and Stewart, 1986]</td>
</tr>
<tr>
<td>Super absorbent polymer</td>
<td>–</td>
<td>water</td>
<td>0.893</td>
<td>±5–20mm</td>
<td>Structure measurements [Iskander, 2010]</td>
</tr>
</tbody>
</table>

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5.2 Setup

For our RIM porous medium a glycerol-water mixture is used as the liquid phase. The glycerol-water mixture is relatively harmless and can be cleaned easily. The relatively high viscosity of glycerol ensures the Reynolds number remains small despite the larger scale of the laboratory setup. For the solid phase of our RIM porous medium borosilicate glass spheres are used with a diameter of 9 mm. Relevant properties of the liquid and solid components of the RIM porous medium are listed in table 5.2.

The Biot-Arago equation relates the index of refraction of a mixture $n_{\text{mix}}$ to the individual indices of refraction of the mixture components $n_1$ and $n_2$: \begin{equation} n_{\text{mix}} = \phi_1 n_1 + \phi_2 n_2, \end{equation}
where $\phi_1$ and $\phi_2$ denote the volume fractions of the mixture components [Heller, 1965]. These volume fractions are defined as \begin{equation} \phi_i = \frac{V_i}{V_{\text{tot}}}, \end{equation}
with $V_i$ the volume of the mixture component $i$, and $V_{\text{tot}}$ the total volume of the mixture. For the glycerol-water mixture this results in \begin{equation} n_{\text{mix}} = \phi_g n_g + \phi_w n_w = \phi_g n_g + (1 - \phi_g) n_w, \end{equation}
where $\phi_g$ and $\phi_w$ denote the volume fractions of the glycerol and water components, respectively. The second relation follows from $V_{\text{tot}} = V_w + V_g$.

**Table 5.2: Properties of the RIM setup components: glycerol, water and borosilicate glass spheres.**

<table>
<thead>
<tr>
<th>Component</th>
<th>Index of refraction</th>
<th>Density ($g/cm^3$)</th>
<th>Viscosity ($mm^2 s^{-1}$)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glycerol</td>
<td>1.47399</td>
<td>1.2636</td>
<td>1200</td>
<td>SDA, 1990</td>
</tr>
<tr>
<td>Water</td>
<td>1.333</td>
<td>0.997</td>
<td>0.893</td>
<td>Stöhr et al., 2003</td>
</tr>
<tr>
<td>Borosilicate glass spheres</td>
<td>1.4642</td>
<td></td>
<td></td>
<td>Sigmund Linder, 2011</td>
</tr>
</tbody>
</table>

Mixtures are prepared using a scale to measure the mass of glycerol and water. Using this method volume fractions can be controlled within an error of $2.5 \cdot 10^{-4}$, and RIM liquids can be made within an error of $4 \cdot 10^{-4}$ in the refractive index (for volumes of 100ml).

As a starting point the index of refraction of the batch of glycerol used in the RIM experiments is measured using a custom refractometer. The refractometer measures the deflection of a laser beam upon refraction by a small cuvette containing a sample of the glycerol. The batch of glycerol had an index of refraction of $1.46666 \pm 0.00001$ (at room temperature). This is slightly lower than the index of refraction of pure glycerol, as found in table 5.2. The difference in index of refraction is caused by the impurity of the batch of glycerol that is used. Due to the hygroscopic nature of glycerol water is absorbed from the air. An estimate of the optimal volume fraction of glycerol for the matching of the glycerol-water mixture to the borosilicate spheres can be obtained using the measured index of refraction of the glycerol batch in combination with the refractive indices of
water and the glass spheres, as found in table 5.2. Using equation (5.4) a theoretical best match of refractive index is found at a volume fraction $\Phi_g = 98.2\%$.

The quality requirements for index matching depend on the application. When more refractive surfaces are involved a closer index match needs to be obtained. Experiments have shown that for about 15 to 25 particle layers an index match to at least 0.003 is needed [Dijksman et al., 2012]. Due to natural variations of index of refraction within products or collections of products the refractive index of the liquid phase always needs to be fine tuned to match that of the solid phase.

The use of glycerol as the main component in the RIM liquid requires some care to be taken during experiments. Glycerol is a hygroscopic fluid, which means it absorbs water from the air [SDA, 1990]. As a result the index of refraction of the glycerol is lowered. Therefore glycerol should be stored in an airtight environment and additional fine tuning of the RIM liquid is required every month or so. During experiments RIM liquids should be closed off from air as well.

5.2.1  Refractive index matching of a single sphere

For optimisation of the refractive index matching, a variation of the setup used by Dijksman et al. (2012) and Averbakh et al. (1997) is used, as shown in figure 5.3. In this setup a laser (1) shines on a concave lens (2) to produce a horizontal light sheet (3). The light sheet is passed through a large cuvette (7) containing the RIM liquid and a sphere (5). The sphere is fixed in place using a small nut (6). For fine tuning of the optical setup the cuvette is placed on a small platform that can be translated in the vertical direction. Differences in refractive index between the RIM liquid and the sphere will cause refraction of the laser sheet within the cuvette. This refraction is visualised on a white screen (9) and monitored by a camera (8).

The sphere inside the RIM liquid essentially acts as a lens. The sphere acts as a positive lens when the index of refraction of the liquid is lower than the index of refraction of the sphere. When the index of refraction of the liquid is higher than the index of refraction of the sphere, the sphere acts as a negative lens. In the case that the liquid matches the index of refraction of the sphere no
refraction occurs at the surface of the sphere and light rays are unaffected.

The matching of the index of refraction between the RIM liquid and the sphere is measured by the amount of distortion in the laser sheet. Therefore the laser sheet is passed through the sphere at four different heights and the image of the laser sheet at the screen is measured. The root mean square difference is measured between this image and a reference image of the laser sheet only passing though the RIM liquid. The root mean square (RMS) difference $\delta$ between the measured image $I_m$ and the reference image $I_r$, both of size $(M, N)$, is given by

$$\delta = \sqrt{\frac{1}{MN} \sum_{i=1}^{M} \sum_{j=1}^{N} (I_m(i,j) - I_r(i,j))^2}.$$  \hspace{1cm} (5.5)

When the RMS difference is lowest the laser sheet is least affected by the sphere.

The distortion of the laser sheet is measured at four different heights $h_1$ to $h_4$, as shown in figure 5.4. Multiple heights are used to account for irregularities within spheres. The RMS differences of the laser sheet image for the four heights are summed to obtain a global quantity $\Delta = \sum_{i=1}^{4} \delta_i$, which is used as a measure of the refractive index match.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure5.4.png}
\caption{Schematic representation of the different heights of the laser sheet with respect to the sphere. Relative vertical distances of the laser sheets are: $h_1 = 0$, $h_2 = -0.28\text{mm}$, $h_3 = -1.26\text{mm}$ and $h_4 = -3.12\text{mm}$.}
\end{figure}

Several glycerol-water mixtures are prepared varying with varying volume fractions of glycerol. The volume fractions are chosen close to the theoretically predicted fraction of best match.
5.2.2 Shadowgraph experiments

To investigate optical inhomogeneities in translucent materials such as glycerol and glass the shadowgraph method is used. Small optical inhomogeneities cause light to refract inside a translucent material. This refraction can be observed by looking at the shadow of an object [Settles, 2001]. Due to the refraction caused by optical inhomogeneities darker and lighter spots appear in the shadow of the material. These variations in light intensity of the shadow provide a qualitative measure on the optical inhomogeneities of a material.

Shadowgraph measurements are performed using the setup shown in figure 5.5. An approximate point source of light is created by passing light from a lamp through a small diaphragm. The light is subsequently passed through a small tank containing a glass sphere submerged in an RIM mixture of glycerol and water. The shadow cast by the sphere on a white screen is recorded by a camera.

![Figure 5.5: Schematic top view of the shadowgraph setup. The setup consists of a camera (1), a light source (2), a diaphragm (3), a small tank filled with the RIM liquid and a glass sphere (4) and a white screen (5)](image)

Figure 5.5: Schematic top view of the shadowgraph setup. The setup consists of a camera (1), a light source (2), a diaphragm (3), a small tank filled with the RIM liquid and a glass sphere (4) and a white screen (5)
5.2.3 Evaluation of the refractive index match

Once an optimal composition of the glycerol-water mixture is determined using a single sphere, the refractive index match is tested using multiple spheres. The setup used to test the refractive index match on multiple spheres is shown in figure 5.6. Five spheres, positioned in a straight line are placed inside a small tank containing the RIM liquid. A screen containing a regular array of small dots is placed right behind the tank. A camera is setup to focus on the dotted screen while looking through the small tank.

![Schematic representation of the setup](image)

Figure 5.6: Schematic representation of the setup used to evaluate the index match on multiple spheres. The setup consists of a camera (1), a small tank filled with the RIM liquid (2), 5 spheres ordered in a straight line (3), a screen containing dots (4), a small table (5) a light source (6).

Temperature and wavelength of light influence the refractive index. The experiments discussed above are performed at room temperature \((20\pm2)^{\circ} \text{C}\). In the experiments a red laser is used as well as a ‘white’ halogen lamp. Results will show that the variation in wavelength of the light appears to have little effect on the refractive-index match.
5.3 Results

A laser sheet is passed through a glass sphere submersed in glycerol-water mixtures of varying composition, as discussed in section 5.2.1. A typical set of images of the laser sheet is shown in figure 5.7 where the screen image of the laser sheet passing though the sphere at four different vertical levels is recorded.

At $z = h_1$ the laser sheet is slightly effected by the sphere, as seen in the screen image of the laser sheet. As the laser sheet passes though the sphere, the screen image of the laser sheet is changed. For $z = h_2$ a slight bump is observed in the line in the screen image of the laser sheet. Additionally a white spot is observed above the laser line. This white spot is caused by reflection at the sphere surface. For $z = h_3$ and $z = h_4$ the laser sheet is refracted by the sphere causing a vertical shift in the line observed in the screen image of the laser sheet. Additionally distortions are observed in the part of the line that is refracted by the sphere. These distortions are most likely caused by variations in index of refraction within the sphere. The outer edges of the refracted part of the line on the screen bend upwards. These line segments are again caused by reflection at the surface of the sphere.

![Figure 5.7: Typical screen images of the laser sheet that is passed though the sphere that is submersed in a glycerol-water mixture that nearly matches the index of refraction of the sphere. The laser sheet is passed through the sphere at four vertical levels $h_1$ to $h_4$.](image)

Results from the laser sheet method, to match the index of refraction of the liquid to the spheres, are shown in figure 5.8 where the summed RMS differences in the images of the laser sheet are plotted as a function of the volume fraction of glycerol in the RIM liquid.
Figure 5.8: Measured root mean square difference in the image of the laser sheet, as function of the volume fraction glycerol. Measurements are marked by +. The red line joins the measurement points to visualise the overall pattern.

A clear minimum is observed in the summed RMS difference $\Delta$ at $\phi_g = 0.9815$. At this minimum, a best match in index of refraction was obtained resulting in minimal distortions of the laser sheet image. The optimal value of the volume fraction of glycerol is in close agreement with the theoretically predicted value of 98.2% from section 5.2. At the optimal index match the summed RMS difference $\Delta$ is not reduced to 0. The main reason for this is the distortion of the refracted part of the laser line, as shown in figure 5.7c and 5.7d.

The distortions in the screen images of the laser line passing through the sphere are most likely caused by variations in index of refraction inside the spheres. These optical inhomogeneities are investigated further using the shadowgraph method. Shadowgraph images of a single sphere at a near index match with the RIM liquid reveal the probable cause of the distortions in the laser light by the sphere. This is shown in figure 5.9 where a typical shadowgraph result is shown.

Figure 5.9: A typical shadowgraph image of a single sphere in an RIM liquid showing optical inhomogeneities within the sphere.
Figure 5.9 shows dark and light lines appear in the shadow of the sphere. These lines follow curved paths from one side of the sphere to the opposite side of the sphere. Additional experiments show that these lines cannot be washed off using water or acetone, indicating that the lines are not caused by a dirty surface. Scratching the surface of the sphere does not change the pattern observed. This indicates the lines are not caused by scratches or imperfections on the surface of the sphere. A possible explanation of the lines observed in the shadowgraph results is optical inhomogeneity within the sphere. This inhomogeneity can be caused by stresses within the glass that occur during the production process as well as inhomogeneity of the composition of the glass.

The optimal composition of the RIM liquid results in minimal refraction of light by the sphere. This effect can be evaluated by looking a dotted screen behind the RIM setup, as discussed in section 5.2.3. The resulting image is shown in figure 5.10 and shows the sphere has very little effect on the image of the dotted screen. The position of the sphere is indicated with the white arrows.

![Figure 5.10: View of a dotted screen while looking through a single sphere in an RIM liquid with φ = 98.15%. The position of the sphere is indicated by the white arrows.](image)

Figure 5.10 reveals little of the distortions. This is in contrast with the distortions that are observed for the laser lines passing through the spheres and the shadowgraph images. This might be caused by the fact that the dotted screen method is less sensitive to small variations compared with the laser sheet method and the shadowgraph method. Close inspection of figure 5.10 does reveal some very slight variations in contrast in the dotted screen image behind the sphere.

Looking through multiple layers of spheres reduces the quality of the image behind it. This is shown in figure 5.11a where the dotted screen is placed behind a line of three spheres. The
refractive index of the glycerol-water mixture matches well with the borocilicate spheres as the distance between the dots behind the spheres and the distance between the dots next to the spheres is virtually equal. Comparing the results from three spheres (figure 5.11a) with one sphere (figure 5.10) it is clear that more spheres show more distortions.

Figure 5.11b shows the dotted screen behind six spheres. The dots behind the spheres are hardly visible. However it seems that the distance between the dots is almost equal to the distance between the dots next to the spheres. This indicates the refractive index of the liquid matches well with that of the spheres. The dots behind the row of six spheres are hardly visible and the image seems to be blurred. This might be caused by light scattering due to differences in index of refraction in the spheres, as observed in figure 5.9.

\[ \text{Figure 5.11: Images of a dotted screen behind a line of spheres submerged in a RIM liquid (a) three spheres in a row, (b) six spheres in a row} \]

In light of the results seen in figure 5.11 a reduction in optical inhomogeneity of the glass spheres is desired. After consultation with the manufacturer a set of ultra-pure borosilicate spheres was ordered. Before testing the spheres in the laboratory, stresses inside the spheres were reduced by heating the spheres. During the production process of the spheres stresses can develop inside the glass. These stresses might cause small optical inhomogeneities. To reduce the stresses inside the spheres, they are heated to a temperature just below their melting point. At this temperature the glass becomes softer, allowing the stresses in the spheres to resolve.

Three different temperature treatments have been applied to sets of five spheres. These spheres are tested and compared using the dotted screen setup. Additionally a set of the original batch of spheres and an untreated set of ultra pure spheres are included in the comparison. The sets of spheres are aligned in rows according to figure 5.13b. Set 1 contains the batch of untreated ultra pure spheres. Set 5 contains the untreated original batch of spheres as used in the previous experiments. The sets 2 to 4 contain the temperature treated spheres. Different temperature treatments where applied to each of these sets of spheres, the time of the treatment increased with increasing set number.

In the production of glass, material is heated to high temperatures. Glass is produced in a liquid form and subsequently cooled down. During the decrease in temperature the material becomes less and less viscous. At the same time a temperature gradient exists in the material due to the fact that
the outside has a lower temperature than the inside. This induces stresses and density differences within the glass.

At some point in the cooling process the viscosity of the glass changes rapidly and becomes so high that stresses and density differences cannot be relieved any more. This point is referred to as the transition temperature. In order to minimise these stresses and density differences in the glass the material needs to be cooled very slowly after heating.

Stresses and density differences inside the borosilicate spheres are minimised using this method. Following the suggestions of the manufacturer of the glass spheres three different protocols for heating and cooling down have been tested:

- **Set 2**: The glass is heated to the transformation temperature provided by the manufacturer using the glass composition. $T_{\text{trans}} = 586^\circ C$. After being heated in an oven the glass is slowly cooled down. The cooling process takes place by shutting down the oven and keeping it closed. Cooling down to room temperature takes about 5 hours.

- **Set 3**: The glass is heated to $600^\circ C$, slightly above the transition temperature provided by the manufacturer. The glass is maintained at this temperature for 5-15 min before cooling it down using the same process as with set 2.

- **Set 4**: This procedure, based on measurements, is suggested by the major glass manufacturer Schott [Schott, 2012]. The procedure involves heating the glass to $550^\circ C$ before cooling it down in a controlled fashion. The cooling down consists of a few steps involving different temperature gradients as shown in figure 5.12.

![Figure 5.12: Protocol proposed by Schott. Red lines indicate minimum temperatures.](image-url)
Figure 5.13: (a) Schematic top view of the experiment, showing the 5 sets of spheres. (b) View of the dotted screen behind 5 rows of 5 spheres. In every row the glass spheres received different treatments.

The results of the comparison of the different sets of spheres is shown in figure 5.13a. It is clear that the row of five spheres shows significantly less distortions of the dotted screen compared with the experiment using six spheres, shown in figure 5.11b. In addition to the reduction of the number of spheres, this effect could be caused by the use of a different tank in the setup. The use of this new tank enables better control of lighting conditions. Comparing the sets of spheres, only small differences are observed. The set containing the original spheres (far left) shows some of the blurring effects also observed in figure 5.11b. This blurring effect is reduced in the ultra-pure spheres. The temperature treated ultra-pure spheres show less distortions than the untreated spheres, set number 4 appears to show the best results.

Temperature treatment of the spheres positively affects the quality of images behind the spheres. To investigate if the improvement can be related to a reduction of optical inhomogeneities shadowgraph images are recorded of a single sphere from each of the sets shown in figure 5.13. The shadowgraph images are recorded with the spheres in the same RIM liquid as used for the experiments from figure 5.13a. As the light from the diaphragm results in a small spot of light the shadows are recorded in separate images. Only the lighting conditions where adjusted slightly to be able to observe a clear shadow. The results are shown in figure 5.14.
The shadowgraph images show no clear trend with respect to the inhomogeneities. The large variation in patterns observed in the shadows is most likely not caused by the temperature treatment as these variations are also observed in sets of untreated spheres. Temperature treatment of the spheres did positively affect the quality of the image of dots. As the shadowgraph technique is a qualitative method and comparison of experimental results in figure 5.14 is difficult and one can argue that the shadowgraph method is not suited to evaluate the reduction of optical inhomogeneities. However, the shadowgraph results still show inhomogeneities of the temperature treated spheres, indicating there is room for improvement for future setups.
Chapter 6

Conclusion and Discussion

In this project the chaotic advection properties of several systems of sequentially operated sources and sinks were investigated. These systems might ultimately be used to enhance the natural remediation of contaminated groundwater.

Three different systems of sources and sinks were considered using numerical simulations of particle trajectories. An elementary system composed of an alternately pulsed source and sink was investigated in 2D as well as 3D. More realistic systems consisting of periodically reoriented dipoles were also investigated: the switched dipole and the rotated dipole flow. The mixing properties of these systems were explored by identifying the location and nature of periodic points which are essential to chaotic advection. Poincaré sections of individual tracers were computed to support the analysis.

The pulsed source-sink system

The pulsed source-sink system could be described by a single dimensionless parameter $\Gamma$, relating to pulsing time, the strength and separation distance of the source and sink. Periodic points up to order 6 where identified using three complimentary methods. Although the symmetry method is a general method applicable in many chaotic systems, it was not able to find all periodic points and provided little insight into the general structure of the periodic points. The geometrical method for finding periodic points provided much insight into the structure of the periodic points. This method was tailored specifically for the pulsed source-sink system but may not be applicable to other chaotic systems. Both the symmetry method and the geometrical method make use of mapped material lines which requires extensive computational power. The Newton-Raphson method is an iterative method to find periodic points. This method provided the most reliable method for finding periodic points while providing little structural insight. The Newton-Raphson method can be applied to a large range of chaotic systems and requires similar computational power as the other two methods. All the methods used for finding periodic points do not guarantee that all periodic points will be found.

Periodic points where observed in branch-like structures symmetrical about the $y$-axis. Generally, higher-order periodic points are located further away from the source and sink. The branch-like structures were explained using geometrical considerations. This allowed direct comparison of the periodic points found for various settings of the system. When $\Gamma$ is decreased, periodic points move closer to the source and sink. When decreasing $\Gamma$ further some lower-order periodic points are destroyed. Very small $\Gamma$ finally results in many of the periodic points becoming elliptic, thereby
inhibiting chaotic motion. In this case the system behaves similar to a stationary dipole, which does not exhibit chaotic dynamics. The analysis of the pulsed source-sink system was supported by the identification of manifold structures and simulations of blobs of tracers.

The application of a perturbation to the velocity field resulted in the breakup of elliptic orbits and the change of the elliptic orbits into partially overlapping bands. This effect was also observed by Speetjens (2001) when simulating chaotic advection at small Reynolds numbers. The results obtained in the 2D case support the use of a small perturbation to simulate the effects of weak inertia. This method might also be used to simulate the effects of dispersion. However, this assumption has to be tested with experimental results. The magnitude of the observed effects varies with the strength of the applied perturbation. As no comparative material is available for dispersion and low Reynolds number flows in this system there is no direct link between the strength of the perturbation and the amount of dispersion and Reynolds number of the flow. Therefore conclusions can only be drawn on the qualitative effects.

Due to symmetry, the dynamics of the 3D pulsed source-sink system was essentially 2D. All of the features of the 2D pulsed source-sink system where recovered for the 3D case as well. An important difference between the 2D and the 3D case is that periodic points are generally closer to the source and sink as a result of the stronger decay of the velocity field over the distance from the source and sink. This feature results in a higher density of hyperbolic points near the source and sink and may result in better mixing compared with the 2D case. In comparing the 2D and 3D cases, a relatively arbitrary link between the parameters Γ and Υ was made. Therefore care should be taken when drawing conclusions from this comparison.

In applying a velocity perturbation to the 3D pulsed source-sink system, effects similar to the 2D case were observed within the 2D ($x - r$)-planes. In the direction perpendicular to these planes rotational motion was observed. This rotational motion is purely caused by the applied velocity perturbation. It is unlikely this effect resembles the effects caused by inertia as the direction of rotation is strongly dependent on the applied perturbation.

The dipole systems

Two systems consisting of periodically reoriented dipoles were investigated, the switched dipole system and the rotated dipole system. Similar to the pulsed source-sink system, a single dimensionless parameter Υ could be defined that described the system. Both of these systems showed confinement of particles within a circle connecting the sources and sinks of the individual dipoles. This is an important property since this prevents the spreading of material to a larger area.

The switched dipole system contained several periodic points. In general, lowering Υ reduced the number of lower-order periodic points, similar to the pulsed source-sink system. At very small values of Υ the system showed more elliptic islands and behaved like a stationary flow. This was again similar to the pulsed source-sink system. For Υ > 1 the central period-1 point breaks up into four period-1 points. This sequence reoccurs every time Υ passes an integer. Considering the mixing characteristics, the case of Υ = 0.9 showed no elliptic regions, hence chaotic advection occurs over the entire circular domain. The case of Υ = 1.08 showed the most hyperbolic period-1 points and might be the most efficient mixer.

The rotated dipole system showed a significant increase in the number of period-1 points compared with the switched dipole system. A possible cause of this is the rotational behaviour of the forcing. This results in a more symmetrical system with more opportunities for coherent struc-
tures. Similar to the case of the switched dipole system, the amount of period-1 points decreased for decreasing $\Upsilon$. When $\Upsilon$ was decreased further, more elliptic islands were observed. Based on the number of hyperbolic period-1 points the rotated dipole system mixes better than the switched dipole system, at the cost of more elliptic regions and a doubling of the time involved.

During the investigation of the chaos in systems of sources and sinks the mixing properties were evaluated using the amount of hyperbolic periodic points as these are the points that induce the stretching and folding dynamics. Several remarks can be made with respect to this assumption. As it may be that more hyperbolic points cause more stretching and folding dynamics in some regions, elliptic periodic points inhibit mixing. These point are surrounded by non-chaotic islands where no mixing occurs. A more complete measure of the mixing properties should take the surface area of the elliptic islands into account. A second remark can be made considering the hyperbolic character of the periodic points. Some hyperbolic points have larger eigenvalues and induce stronger motion around them. This might lead to more stretching and folding, hence more efficient mixing. Finally the order of the periodic points might be considered. Is it fair to say that in general a period-1 point induces stronger stretching and folding than a period-2 or period-3 point? Effectively all points in a closed chaotic system are periodic points with very high periods.

These questions can be investigated by comparing the number of periodic points, their eigenvalues and their order with a measure for the stretching in chaotic systems such as an average Lyapunov exponent. The Lyapunov exponent provides a local measure of the deviation of nearby particles and hence the stretching of material in a chaotic system. While providing a good measure for the mixing properties, the Lyapunov exponent does not give any insight into the cause of the stretching and the structure of the chaos.

A point of discussion considering the practical applicability of the systems described above is the reinjection procedure. In all the systems of sources and sinks that are investigated a reinjection rule is applied. An absorbed particle is reinjected on a mirroring streamline in the pulsed source-sink system and on the same streamline for the dipole systems. The question is whether this rule is realistic. Aref and Jones (1988) discussed this subject in their study of the pulsed source-sink system and found completely different dynamics when the reinjection rule is changed. For some variants of the reinjection rule regular motion was obtained. Practically the reinjection on the same streamline can be realised when connecting the source and the sink with tubes. If the flow through the tubes is laminar the same streamline rule could be approximated. The direct reinjection without time delay, as applied in the dipole systems can also be realised approximately as the time required to transfer material from the source to the sink through tubing is much shorter than the time required for the material to be transported through the groundwater system.

**Experiments**

The laboratory experiments for constructing an RIM artificial porous medium focused on using borosilicate glass spheres in combination with a mixture of water and glycerol. The index of refraction of the glycerol-water mixture was tuned to within 0.001 index points. With this setup single spheres where made practically invisible. When multiple spheres are considered larger distortions were observed. These distortions where attributed to optical inhomogeneities inside the glass, observed in shadowgraph measurements. Temperature treatment of the glass spheres resulted in a reduction of the distortions but shadowgraph measurements still show optical inhomogeneities. In addition, lighting conditions are important.

Using the current materials a line of at least five spheres can be accurately matched. RIM porous
media setups in literature show experiments with at most 15 layers of particles of comparable size as the spheres used here. The amount of particle layers is limited by the transmittance of the glass, the optical homogeneity of single spheres and the optical homogeneity within a group of spheres. The current setup might be improved by further investigation and reduction of the inhomogeneities observed in the shadowgraph images. These effects might be further reduced by hotter or longer temperature treatments of the glass. A quantitative method for measuring these inhomogeneities would be beneficial. Finally other solid phase materials such as pyrex and PMMA should be tested for optical inhomogeneities. These materials can be matched using a mixture of Dow Corning oils.
Bibliography


Appendix A

Error analysis of the simulation code

In this section the error of the simulation code is discussed. Chaotic systems have the property that nearby points diverge exponentially fast. This means that when performing simulations on chaotic systems, small computational errors result in larger and larger errors over time. In the simulations on the systems of sources and sinks this will result in errors in particle trajectories. This problem is a consequence of the fundamental unpredictability of chaotic systems.

Following [Soulvaiotis et al., 1995] three different types of errors can be identified:

- **Time integration errors:** This type of error is caused by numerical integration of the velocity field to obtain particle positions.

- **Round-off errors:** The finite precision of computer calculations is the cause of these errors. Although the error caused by this effect on a single computation is very small the divergence of nearby points can cause significant errors over time.

- **Discretization errors:** These are the errors associated with the velocity field used in the integration. When a velocity field is obtained from numerical simulations or the velocity is known only at specific grid points, errors are made in the simulation. Because analytical expressions are available for the velocity fields of the systems used in this project, this type of error is avoided.

The effect of these errors on the simulations is difficult to determine as no true solution is available. However, an analytical solution is available for the source-sink system. This only leaves us with the round-off errors associated with the computer precision. An indication of the integration errors can be obtained using the source-sink system by varying the accuracy of the integration scheme and comparing the results with analytically obtained results.

For numerical integration of the velocity field the standard Matlab differential equation solver ode45 is used. The standard Matlab solver was used because of its relative speed and accuracy over a custom programmed integration scheme. Additionally the Matlab solver provided a straightforward implementation into the simulation code. This solver uses a fourth-order Runge-Kutta integration scheme.
Figure A.1: Time evolution of the RMS error in the position calculated by numerical integration with different levels of error tolerance (shown in the legend). The error is calculated with respect to the position obtained using analytical computation using equation (3.6) with $\Gamma = 19.1$ and $(x_0, y_0) = (-0.5, 1)$

Figure A.1 shows the RMS error in the position of a tracer particle over time. The RMS error is calculated using the results from the analytical simulation code as a reference. Several error tolerance settings are tested for the Matlab ode45 solver. The tolerances are shown in the figure legend.

The resulting time evolution of the error clearly shows that lower error tolerance setting of the numerical integration results in smaller errors, as expected. Additionally the figure shows that no matter how small the error tolerances are, the divergence of nearby points results in the total error to become very large over time.

For larger timescale than shown in the figure the error still rises and results in an RMS error that is larger than 1 after $t = 60T$ with an error tolerance setting of $10^{-8}$.

The errors described above are related to the position of a tracer particle over time. In the simulations on the systems of sources and sinks the interests are on periodic points and Poincaré sections.

Considering Poincaré sections the errors described above can cause elliptic orbits to become slightly fuzzy. As the errors can be regarded as perturbations, the KAM theorem predicts the breakup of elliptic orbits due to simulation errors. The basic structure however is maintained.

The search for periodic points is based on particle positions. In the cases that the Newton-Raphson iterations scheme is used, the error is restricted by computational speed. The error tolerance of this scheme is set at $10^{-4}$. As this error tolerance is much larger than the errors made by the integration schemes with a small amount of timesteps.
Appendix B

Calculation of the transfer time

In this section the time needed for a tracer to travel the shortest path form the source to the sink of a dipole is calculated. This so-called transfer time $\tau$ can be calculated analytically using equations (3.2) and (4.1). The transfer time is compared with $\Upsilon$ to show the physical meaning of this dimensionless parameter.

Without loss of generality consider the dipole consisting of a source at $(x, y) = (-a, 0)$ and a sink at $(x, y) = (a, 0)$. The shortest travel path is the straight line connecting the source and sink, hence in this case $y(t) = 0$ and $v = v_x$. This reduces the velocity along the particle path to

$$v = \frac{Q}{2\pi} \left( \frac{1}{x + a} - \frac{1}{x - a} \right).$$

Reorganising gives

$$v = \frac{Q}{2\pi} \left( \frac{-2a}{(x + a)(x - a)} \right).$$

The velocity is related to the position via equation (3.2), giving

$$v = \frac{dx}{dt} = \frac{Q}{2\pi} \left( \frac{-2a}{x^2 - a^2} \right).$$

Separation of variables results in

$$dt = -\frac{\pi}{aQ} \left( x^2 - a^2 \right) dx.$$

Integration of both sides finally results in an expression for the transfer time $\tau_0$

$$\tau = -\frac{\pi}{aQ} \int_{-a}^{a} \left( x^2 - a^2 \right) dx = \frac{4\pi a^2}{3Q}.$$

Substitution of $\tau_0$ into the expression for $\Upsilon$ shows that

$$\Upsilon = \frac{3Q\tau_i}{4\pi a^2} = \frac{\tau}{\tau_0},$$

hence $\Upsilon = 1$ when $\tau = \tau_0$. 

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