A Primer on the Lagrangian Picture of Transport in Porous Media

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Abstract The dominant conceptual paradigm of porous media flow, solute mixing and transport is based on steady two-dimensional (2D) flows that can preclude important transport dynamics. Novel transport phenomena can arise in unsteady and/or three-dimensional (3D) flows at the pore- or Darcy-s scale which can only be truly understood in the Lagrangian frame. These Lagrangian kinematics are governed by Lagrangian coherent structures (LCSs) that include chaotic mixing regions, hold-up regions and transport barriers that are only beginning to be visualised by novel experimental methods. In this primer we review the Lagrangian picture of porous media flow and transport and connect the associated tools and techniques with the latest research findings from pore to Darcy scales. This primer provides an introduction to the tools for porous media researchers to know when to expect complex Lagrangian kinematics, how to uncover and understand LCSs and their impact on solute transport, and how to exploit these dynamics to control solute transport in engineered subsurface flows.

Keywords solute mixing, solute transport, chaotic advection

1 Introduction

Since the pioneering work of [Darcy](1856) regarding the quantitative relationship between fluid pressure gradient and flux through soil columns, interest in the fluid dynamics of porous media systems has grown rapidly. These dynamics govern the transport, reaction and biological activity of solutes, colloids and microorganisms...
in a wide range of porous materials ranging from geological media to biological tissues and engineered structures, and now underpin many vital industries, including biotechnology, energy, agriculture and water supply. All porous media are characterised by complex pore-scale architectures and many also exhibit significant heterogeneities from pore scales to much larger (e.g. regional) length scales, resulting in complex flow and transport dynamics not resolved in Darcy’s original work. Due to these inherent complexities, the conceptual progress of porous media science has not been smooth. Progress has relied upon irregular advances in technology that have enabled greater precision and resolution in observation, which have then provided the data that seeded the next conceptual advance. Today, researchers have unparalleled access to pore-scale data of fluid flow, three-dimensional geometry and surface chemistry, yielding an almost overwhelmingly detailed and rich picture of the process complexity inherent in porous media. The next conceptual advance is imminent.

Fig. 1: Heterogeneous and anisotropic dispersion of a solute plume (imaged near the injection point in a plane oriented normal to the mean flow direction) during the pull phase of a push-pull experiment through randomly packed, index-matched glass beads. The initially ellipsoidal dye cross section at the beginning of the pull phase (given by $\tilde{t} = 0$) diffuses preferentially along directions of high fluid deformation (indicated by white arrows), leading to a highly striated dye signature at later times. Adapted from [Heyman et al. (2021)].

Figure 1 presents an example of the kinds of complex experimental data now available and awaiting interpretation. The figure shows the results of a standard
push-pull experiment at low Reynolds number where the concentration distribution of a fully developed solute plume near the injection point is shown at different times $\tilde{t}$ during the pull phase. The width of the injected plume shown at $\tilde{t} = 0$ has similar dimensions to those of the glass beads used to form the randomly packed porous medium. In the absence of molecular diffusion, reversibility of the push-pull flow would result in the collapse of the solute plume during the pull phase back to the original injection profile shown at $\tilde{t} = 0$. Hence the solute plume shown in Figure 1 represents a residual “diffusive signature” resulting from the irreversible interactions between fluid deformation and solute diffusion. After completion of the pull phase, at $\tilde{t} = 25$, this diffusive signature is observed as an unexpectedly extensive and striated distribution. This distribution indicates the presence of profound anisotropic fluid transport phenomena at the pore scale which are unseen in less-resolved investigations, and cannot be described via a conventional solute dispersion framework. Novel tools and techniques that go beyond the Eulerian paradigm are required to understand, characterise and quantify such transport phenomena.

At the same time, it has also been discovered that quite unexpected transport phenomena can present in naturally occurring flows at the Darcy scale, i.e. well beyond the pore scale. Using a conventional poroelastic Darcian flow model, [Wu et al. (2019)] showed that simply by increasing the compressibility $C$ of the porous medium a range of transport structures of increasing complexity can be generated. Figure 2 depicts the motion of tracer particles (black points and lines) at integer multiples of the tidal forcing period $P$ (for simplicity of exposition) in a 2D model of a compressible heterogeneous aquifer subject to both tidal boundary forcing and a background regional flow. As shown in Figure 2a, for small values of $C$ tracer particles move along curved paths from inland (right) toward the coastal boundary (left). With increasing compressibility (Figure 2b, c), a closed region (where tracer particles are trapped indefinitely) and associated pair of elliptic (E) and hyperbolic (H) periodic points (where tracer particles return to the same location after each flow period) arise in the aquifer, indicating a topological bifurcation and a qualitative change in the aquifer transport dynamics. Above a critical compressibility (Figure 2d), the hyperbolic point (H) and the associated open region bifurcates into a chaotic region (indicated by the scattered points) and a regular region, while the closed region forms an stable “island” with the elliptic point (E) at its centre. This chaotic region exhibits complex solute transport dynamics, including stochastic residence time signatures and accelerated mixing. The above transport structures are not easy to predict, detect or understand using standard Eulerian techniques, yet they exert significant control on solute transport.

From the above examples it is clear that conventional Darcy- and pore-scale tools and techniques in the Eulerian frame (that are so well suited to many practical problems in industry today) are unlikely to be of much use in understanding and quantifying the detailed transport and mixing dynamics involved in such highly resolved systems. A conceptual advance is required to push the science further, and this requires consideration of the Lagrangian kinematics of these flows to elucidate the underlying transport structure. This underlying transport structure governs processes ranging from solute mixing and pollutant dispersion, to chemical reactions and biological activity. The natural language of these kinematics is couched in terms of dynamical systems (chaos) theory, and in this paper we introduce the key concepts in this field required to understand solute transport in porous media.
Fig. 2: Bifurcation of transport structures in heterogeneous, poroelastic Darcy flow as a function of increasing medium compressibility $C$. With increasing compressibility $C$, the transport structure bifurcates from open trajectories (a) to a closed region (b,c) with elliptic (E) and hyperbolic (H) periodic points and stable ($w_{1D}^s$) and unstable ($w_{1D}^u$) manifolds. At large $C$ the hyperbolic point (H) bifurcates to a chaotic mixing region and part of the closed region persists (d). Adapted from Wu et al. (2019).

from a Lagrangian perspective. This primer on so-called “chaotic advection” is deliberately superficial to provide an overview of the field rather than a detailed exposition, and the interested reader is directed the referenced works for greater detail. As we will see in the following sections, dynamical systems theory brings with it a rich set of concepts and tools relevant to modern porous media, and it already has a (relatively short) history in the subject.

Taking a broad (and deliberately highly selective) overview of porous media research, we may form a timeline of key concepts and breakthroughs in transport in porous media, depicted in Figure 3. The timeline shows the recent application of dynamical systems concepts to the field, in green. The dynamical systems entries are disproportionately over-represented in the timeline as each of the other research themes have accrued many thousands of articles over the decades while there are still only a handful of dynamical systems articles in the porous media literature.
However we contend that the new tools and techniques provided by dynamical systems theory may facilitate rapid advances in our understanding of flow and transport in porous systems, for the following reasons.

Fig. 3: Timeline of porous media research showing some key research themes and scales of investigation, and emphasizing a recent articles on the dynamical systems approach to understanding transport in porous media (green).

(1) Darcy (1856); (2) Einstein (1905); (3) Lamb (1932); (4) Polubarinova-Kochina (1938); see Zlotnik and Emikh (2007); (5) Leverett (1941), see Parker (1989); (6) Terzaghi (1943); (7) Scheidegger (1954); (8) Saffman (1959); (9) Scheidegger (1961); (10) Bear (1961, 2021); (11) Gelhar (1974); (12) Gelhar et al. (1979); (13) Lichtner (1985); (14) Spanne et al. (1994); (15) Weeks and Sposito (1998); (16) Metcalfe et al. (2009); (17) Mays and Neupauer (2012); (18) Cho et al. (2019); (19) Lester et al. (2013b); (20) Trefry et al. (2019).

It is now well recognized that several classes of porous media flows give rise to complex transport phenomena that cannot be understood via conventional Eulerian analysis (Weeks and Sposito, 1998). The dynamical systems theory approach provides a convenient framework for detecting and classifying kinematic features in the Lagrangian frame that can control fluid mixing, segregation and discharge in porous media. These kinds of transport phenomena describe complex Lagrangian structures which engender potentially profound impacts on solute migration and reaction (Toroczkai et al., 1998; Tél et al., 2005; Valocchi et al., 2019). Coupled with appropriate stochastic methods (such as random walks and non-local transport theories), this Lagrangian frame can be used to develop quantitative predictions of solute transport, mixing and reaction that resolve the complex dynamics observed in Figures 1 and 2.

Early conceptual work by Ottino (1989); Jones and Aref (1988); Sposito (2001, 2006) and others (Lester et al., 2009, 2010b; Metcalfe et al., 2010a, 2010b; Trefry et al., 2012) has led to the prediction, observation and engineering of complex Lagrangian structures in saturated porous media at the Darcy (Zhang et al., 2009; Metcalfe et al., 2010a) and field (Cho et al., 2019) scales. Complex Lagrangian structures have also been predicted to occur in natural environments (Trefry et al., 2019; Wu et al., 2019), e.g. compressible Darcian systems where engineered pumping activity is absent. Dynamical
systems concepts have also been used to link the topology of pore-scale architectures with pore-scale solute mixing and macroscopic transport phenomena (Lester et al., 2013b, 2014b, 2016b), resulting in fundamental upscaling behaviours conditioned on the details of pore-scale Lagrangian structures. These mechanisms have recently been confirmed via direct experimental observations of pore-scale mixing (Souzy et al., 2020; Heyman et al., 2021, 2020), leading to the highly striated solute distributions shown in Figure 1. Dynamical systems approaches also shed new light on other fluid-borne phenomena (Tel et al., 2005) and thus Lagrangian dynamics underpin the transport, spreading, clustering and reactivity of solutes, colloids and microorganisms in porous media. Hence it is natural to seek new learnings from the Lagrangian picture of dynamical systems theory.

But what is dynamical systems theory, what can it tell us about the fundamental characteristics of flow, and how can it be applied to porous media systems? We attempt to answer these questions in the remainder of this paper. Our approach is to provide clear and concise definitions of key dynamical terms and concepts, illustrated by examples from the recent research literature, so that the reader is armed with the basic tools and knowledge to consider future applications of this powerful theory in the context of porous media.

2 What is Chaotic Advection?

Chaotic advection is the science at the intersection of fluid mechanics and nonlinear dynamical systems (Aref et al., 2017). In this case the phase space (coordinates of interest) of the dynamical system is the physical space that the fluid occupies, whether at the pore- or Darcy-scale, and either in a 2-dimensional (2D) approximation or the full 3-dimensional (3D) space.

Hence chaotic advection is concerned with the trajectories of the dynamical system given by the collective motion of all fluid particles—where “particle” refers to a conceptual massless tracer particle—given by the Lagrangian kinematics of the flow. The main point in this section is that particular structures in the flow—collections of points, lines, surfaces—organize the Lagrangian transport in the entire flow, and transport can only truly understood in the Lagrangian frame. These Lagrangian coherent structures (LCS)—such as those shown in Figure 2—form the "skeleton" of the flow that organises global transport (MacKay, 1994), even in the presence of random processes such as diffusion. And to understand or design transport in porous media flows—be it of heat, of chemical or biological species, of matter, in fact, of all interactions mediated by the flow—it is important and useful to find, classify, and elucidate these LCS. Broadly interpreted these Lagrangian structures consist of attracting regions, repelling regions, hold up regions, and the distinguished pathways that connect one critical region to another.

In fluids, including porous media flows from pore to regional scales, the Lagrangian trajectories are the trajectories of fluid particles. From it’s initial condition the trajectory of every fluid particle is given by the kinematic equation

\[
\frac{dx}{dt} = V_x \quad \frac{dy}{dt} = V_y \quad x(t = 0) = x_0 \quad y(t = 0) = y_0
\]

(1)

here written in 2D with the fluid particle location \((x, y)\) moved passively by the fluid velocity vector field \((V_x, V_y)\). Deceptively simple, the kinematic equation can
be taken as the elementary definition of velocity or as defining a nonlinear dynamical system in which a given velocity field generates the Lagrangian trajectories of the fluid tracer particles. Hence these trajectories provide a coordinate transform between the Eulerian \((x, y)\) and Lagrangian \((x_0, y_0)\) frames. In keeping with the idea of building from simplest concepts first, the kinematic equation \((1)\) has no diffusion/dispersion, however such physics can be readily incorporated. By deceptively simple we mean that equation \((1)\) can generate complex trajectories even for simple velocity fields. An example will illustrate a simple case and expose selected hidden LCS.

Referring to figure 4, our example is a 2D, time-periodic Stokes flow in a box of fluid. This is amongst the simplest settings in which to observe LCSs. One sidewall steadily slides for half the period and drives a simple vortex flow as in figure 4a during the other half period, the opposing wall steadily slides in the opposite direction (figure 4b). A video of a similar experiment is also available (Jana et al., 2015).

In figure 4c two blobs of fluid are marked red or blue, and figures 4d–4f show the advection only evolution of the blobs after the indicated number of periods. The evolution of the two blobs is markedly different because their deformation is being controlled by different types of LCS. The blue blob was deliberately put into a hold-up region and undergoes a shear-like deformation that yields (at most) linear stretching, and every three periods it returns close to its initial condition. In 2D, time-periodic flows material starting in a hold-up region is truly cut off from the rest of the flow; these regions are called elliptic islands because the material inside the island rotates around an elliptic point (such as that shown in Figure 2(c,d)), and the net deformation around these periodic points is a simple rotation. In 3D or non-periodic flows hold-up regions may not be completely cut off from the rest of the flow, but are still delineated by surfaces of minimal flux across them that keeps material close for long periods of time.

The red blob, on the other hand, is rapidly deformed into a highly ramified and extended filament. The red blob was deliberately placed near a hyperbolic point (shown in Figure 4g), where the net fluid deformation over one flow period consists of repelling (stretching) in two directions and attracting (compressing) in the two orthogonal directions (as shown in figure 2c,d)). In this simple example these hyperbolic points encapsulate both the attracting and repelling LCSs; moreover, in this case the distinguished pathways between attracting and repelling regions begins and ends at the same point, which is denoted a homoclinic connection. In general in 2D periodic flows heteroclinic connections, where the repelling and attracting points are different, are typical. Here the hyperbolic point and its homoclinic connection strongly deforms the red blob through repeated stretching and folding. This in turn generates exponential growth of the red blob’s interfacial area, even though the blob remains confined inside a finite volume of fluid.

That the chaotic part of a flow generates small-scale structure in the spatial distribution of material (the red blob) is why chaotic advection is associated with
mixing. The chaotic part of the flow quickly evolves any smooth initial distribution into a complex pattern of filaments or sheets, depending on the dimensionality of the system, which converges at an exponential rate to a fractal structure. When the characteristic length scale of the blob becomes small enough, this structure can then be smoothed by diffusion, manifesting as accelerated mixing. This rapid
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reduction of length scale and these augmented transport characteristics are purely effects of the simple kinematic equation (1).

Figure 4g illustrates several ways to bring out the Lagrangian structure that are commonly used in the dynamical systems literature. The black dots are a “stroboscopic map” of tracer particles similar to that used in figure 2. Take a small set of initial conditions (a line of particles at \( x = 0.5 \) in figure 4g), and for each fluid particle evolve its trajectory and place a dot to mark the particle’s location after every period. Continue for many periods and such maps visualise the long term Lagrangian structure. For instance, in figure 4g the stroboscopic map clearly partitions the fluid region into three elliptical island regions and a chaotic “sea”, the dense jumble of particle locations seemingly without structure. This common technique is also often called a Poincaré section (Aref et al., 2017).

The blue and red lines in figure 4g are structures termed respectively stable manifolds and unstable manifolds, which are associated with the central hyperbolic periodic point (Ottino, 1989). The stable manifold is most repelling material curve, while the unstable manifold is the most attracting material curve. While the stable and unstable manifolds are time inverses of each other, we focus on the red unstable manifold and note how much it resembles the deformed red blob, particularly the deformed red blob after 6 periods (figure 4f). This is no coincidence. The unstable manifold is a fractal structure that fills the chaotic sea, and material starting near the central hyperbolic point is stretched along the unstable manifold and eventually converges to the unstable manifold. The unstable manifolds of other hyperbolic points, if they exist, interweave together to form the chaotic seas. The unstable manifold is the fundamental mixing pattern (or “mixing template”, see Aref et al. [2017]). Technically to generate chaotic advection requires transverse intersection of the unstable and stable manifolds, and manifold interaction is in fact the generic mechanism behind—and topological condition for—chaos in both steady and time-periodic flows.

Fig. 5: Diagram of when Darcy flows have the potential for chaos, depending on whether the conductivity \( K \) is homogeneous, heterogenous, or heterogenous and anisotropic, and whether the flow is steady or unsteady in time. Steady flows generally do not admit chaos, except when \( K \) is sufficiently complex. Chaos is possible in all unsteady cases.
So far, we have given a very brief overview through one particular example of how Lagrangian critical regions, consisting of attracting, repelling, and hold-up regions along with the distinguished connections between critical regions, organize the Lagrangian transport of passive fluid particles. An immediate question is then where does this kind of transport occur in porous media flows? The answer is wherever there are sufficient degrees of freedom (DOFs) in the fluid velocity field, be that as an upscaled continuum flow or in pore spaces, chaotic advection is the norm rather than the exception. The sufficient DOFs for chaos in continuous systems is three, meaning that 3D steady or 2D unsteady flows can possibly exhibit chaotic advection (Speetjens et al., 2021), whereas steady 2D flows are intrinsically non-chaotic. Thus we must reconsider steady 2D flow as being representative of many porous media flows at both the pore- and Darcy-scales.

Consider first the Stokes flow in pore spaces discussed in section 3. Here the 3D pore spaces intrinsically have many hyperbolic points in the skin friction field of the solid matrix surface (Lester et al., 2013b) that generically generate chaotic fluid trajectories. Suggestive of this generic chaos is the similarity of the stretched and folded solute plume in the experiment of figure 7(c) with the stretched and folded filaments of figure 4. However, in 3D periodic or non-periodic flows not all of the organizing LCSs are as well characterised mathematically or experimentally as they are in 2D; there is a richer set of of Lagrangian structures and connections between them that one can investigate and use (Haller, 2015; Speetjens et al., 2021).

These mechanisms also apply to evolution of the diffusive dye blob shown in Figure 1, which is most clearly elucidated by first considering the push phase through the bead pack as a complex steady 3D flow. Unlike the time-periodic 2D flow considered figure 4, there do not exist periodic points and lines in this flow, but there still exist stable and unstable manifolds (attracting and repelling LCS) that organise transport and impart exponential stretching of fluid elements. The diffusive dye shadows the unstable manifold of the push flow, and diffuses transverse to this structure in a filamentous manner whilst being stretched exponentially along the backbone of the unstable manifold. Eventually these filaments merge together via diffusion, leading to a well-mixed state. However, for the push-pull flow, the flow is reversed before this state is reached. Due to reversal the stable and unstable manifolds are exchanged, and the dye blob now evolves along the stable manifolds of the push flow, leading to the highly striated structures shown in Figure 1 for different reversal times $\bar{t}$. While the original dye blob would be recovered upon flow reversal for non-diffusive dyes, for diffusive dyes, the irreversible nature of diffusion means that resultant dye structure contains artifacts from the stretching history of the blob, and so provides a diffusive snapshot of the stable manifolds of the push flow.

Similarly, the Poincaré sections shown in Figure 2 clearly illustrate the LCS of the time-periodic poroelastic Darcy flow, where elliptic and hyperbolic points, elliptic islands and stable and unstable manifolds are shown. In this case, Lagrangian transport is trivial for small values of the medium compressibility $C$ (Figure 2(a)), but with increasing compressibility a topological bifurcation occurs, leading to formation of elliptic and hyperbolic points (Figure 2(b,c)). Under a further increase of the medium compressibility (Figure 2(d)), the stable and unstable manifolds form a heteroclinic connection (not shown), and a chaotic sea forms around the elliptic island. These LCS govern the transport of both non-diffusive and diffusive
species in this time-periodic poroelastic Darcy flow, and can lead to trapping of solutes, regions of accelerated mixing and transport that cannot be observed without elucidation of the LCS. In general, the tools and techniques associated with chaotic advection are necessary to understand solute transport in a wide range of porous media applications.

For Darcy type flows figure 5 is a guide. Now steady flows, even in 3D, are non-chaotic unless the conductivity field is sufficiently complex. The constraint that causes this is discussed in section 4. Unsteady Darcy flows in either 2D or 3D can always be made chaotic if one has control over the time-dependent flow forcing. In natural Darcy flows, time-dependent forcing can unleash chaotic fluid trajectories, but as illustrated in Figure 2 the transition to chaotic behaviour is dependent upon the details of the system at hand.

To end this section we point out one more feature of figure 4, our simple prototype chaotic flow: the typical Lagrangian picture consists of both hold-up regions (fluid somewhat or completely isolated from the rest of the domain) and well-mixed regions (generated by the manifold interactions of the attracting and repelling regions). Applications of porous media flows often require maximizing one or the other of isolating fluid or mixing it. It is not always easy to find the particular flow forcing sequence that will maximize fluid isolation or mixing. However, it can be done, and figure 12 shows an experiment designed to confine fluid in a Darcy flow, while figure 13 shows a field experiment designed to maximize mixing of emplaced fluid. General tools to take a porous media flow and quickly tailor it for a particular purpose is an area of ongoing research.

3 Chaos in Pores

The conventional picture of pore-scale fluid flow and solute dispersion follows a steady 2D paradigm as shown in the top part of Figure 6, which is reproduced from Bear and Verruijt (1987). This 2D conceptual image illustrates the main features that govern solute transport, including mechanical dispersion due to (a) strong flow velocity gradients between grains, (b) flow separation around grains and (c) molecular diffusion of the solute. Although these solute transport mechanisms have been elaborated significantly from many contributions over the past few decades, it is often not recognized that the 2D nature of this conceptual image itself imposes severe constraints upon the admissible fluid dynamics, which in turn impacts our mental picture of solute transport. Although conceptual, these 2D topological constraints implicitly skew our understanding of the true 3D mechanisms which drive solute transport and sometimes lead us to neglect other important phenomena which may occur in 3D domains.

An important topological constraint that applies to all steady 2D flows is that streamlines cannot cross over each other and separating streamlines that pass either side of a grain must eventually recombine. Hence, the separation distance between neighbouring streamlines may only fluctuate as they move downstream, and cannot grow or shrink without bound. In mathematical terms, this topological constraint means that fluid elements in steady 2D flow may only grow at most algebraically with time (due to e.g. shear between grains), which in turn places limitations on the rates of dispersion and mixing in such flows (Le Borgne et al. 2015). This constrained streamline behaviour in steady 2D flow also limits trans-
verse dispersion as molecular diffusion is the only mechanism by which solutes can spread transversely to the mean flow direction. Conceptually, and in the absence of molecular diffusion, solute molecules simply follow initial streamlines and so cannot spread transversely, hence mechanical transverse dispersion is zero in 2D. Experimental observation of this 2D splitting-recombination phenomenon is shown in the bottom part of Figure 6, where the solute plume in the 2D porous medium splits and recombines several times, yet the net transverse dispersion is limited and is governed by the solute molecular diffusivity.
Fig. 7: (a) Numerically reconstructed streamlines from PIV experiments of steady 3D flow within a random glass bead pack illustrating complex braiding motions of tracer particles. Adapted from Souzy et al. (2020). (b) Braiding motion of three streamlines (red, yellow, cyan) with downstream distance $l$ in a chaotic steady 3D flow. Due to the braiding motion of these streamlines, a material line (purple) connecting the yellow and cyan streamlines must grow exponentially with downstream distance. Adapted from Boyland et al. (2000). (c) Experimental images of a steady solute dye plume at various cross-sections (transverse to the mean flow direction) at distance $x$ downstream from the injection point. The cross-sectional length $L$ of the plume grows exponentially with $x$ due to stretching and folding of fluid elements. Adapted from Heyman et al. (2020).

Although it is tempting to conceptualise steady flow through 3D porous architectures as an extrusion of the dynamics indicated in Figure 6, these topological constraints do not apply to 3D steady flows, as the additional degree of free-
dom associated with the third spatial dimension removes the restriction that a fluid streamline is bounded by its neighbours, with the result that the streamline may wander freely throughout the fluid domain, as shown in Figure 7(a). Thus, in steady 3D flows neighbouring streamlines may diverge without bound as they are advected downstream, leading to wholly new transport mechanisms (such as chaotic advection) which are not readily apparent in conventional dispersion models. This freedom also admits the braiding of streamlines as depicted in Figure 7(a) that is associated with exponential growth of transverse material lines.

The origin of chaotic advection in 3D pore-scale flows can be traced back to stagnation points that arise on grains or at pore boundaries in all porous media (Lester et al., 2013a) that generate persistent exponential stretching of fluid elements. Conversely, in steady 2D flows, such local fluid stretching at stagnation points is cancelled out at downstream reattachment points. The persistent exponential stretching in 3D leads to the highly striated and filamentous solute distributions transverse to the mean flow direction shown in Figure 7(c). Thus, flow separation and persistent exponential stretching of material elements is wholly responsible for the complex steady solute plume structures observed in 3D pore-scale flows. Conversely, these dynamics are inadmissible in steady 2D flow, and so tend to be neglected in conventional modelling frameworks.

The impact of pore-scale chaotic advection extends beyond accelerated solute mixing, and also acts to augment longitudinal dispersion (Lester et al., 2014a,c), chemical reactions and biological activity (Tel et al., 2005) and transport of colloids and micro-organisms (Haller, 2011). As the Pélet number $Pe$ which characterises the relative timescales of advection to diffusion is typically small in pore-scale flows, it is commonly assumed that diffusion is rapid compared to advective transport and so chaotic advection has minimal impact. However, it has been shown (Heyman et al., 2020) that exponential fluid stretching results in incomplete solute mixing at the pore scale even for small Pélet numbers ($Pe > 5$), hence chaotic advection acts to augment diffusive mixing and transport across a wide range of pore-scale systems.

Heyman et al. (2021) has recently developed a novel method to characterise pore-scale chaotic mixing in opaque porous media based on the push-pull flow shown in Figure 1. This method has been used to recover the extent of chaotic mixing in model systems such as glass beads, as well as to estimate the extent of chaotic mixing in natural systems such as randomly-packed gravel. Thus this technique has the potential to characterise chaotic mixing across a broad range of natural porous media, ranging from granular matter to biological pore networks. The concept of biological tissue as porous networks than can host chaotic mixing applies to a range of systems including living brain tissue (Reichold et al., 2009) (Figure 8a), vascular networks (Ghaffarizadeh et al., 2015) (Figure 8b) and lung alveoli (Tsuda et al., 2002, 2011).

Conversely, Turuban et al. (2018, 2019) shows that highly ordered and engineered porous materials such as crystalline lattices of uniform spheres can exhibit a broad range of pore-scale mixing dynamics ranging from non-chaotic to chaotic mixing that is stronger than that exhibited by any known random system. These mixing dynamics strongly depend upon the orientation of the crystalline axes with respect to the mean flow direction. Zhao (2012) have used disordered engineered porous metal foams (Figure 9) to develop compact heat exchangers that accelerate heat transfer by generating chaotic mixing in the pore space. These advances
Fig. 8: Micro-circulation in living tissue as physiological instance of transport in porous networks: (a) impact of vascular occlusion (arrow) on global through flow (from bottom) in somatosensory cortex in rat brain visualised by simulated flow rate (red/blue: relatively larger/lower flow rate; green: unaffected region) (adapted from (Reichold et al., 2009)); (b) impact of tumor cells (green) on oxygen distribution via vascular network (red) visualised by simulated oxygen levels (yellow/blue: healthy/hypoxic) in grey cross section (inset) (adapted from (Ghaffarizadeh et al., 2015)).

illustrate the potential for chaotic mixing principles to assist the development of novel porous materials exhibiting tuneable mixing and transport properties, with myriad industrial and medical applications.

4 Chaos in Darcy Flows

4.1 Steady Darcy Flows

At scales much larger than the pore scale, it is neither practical nor desirable to resolve the detailed pore-scale flows described in the previous section. Under the assumption that the characteristic length scale \( L \) of material properties or pressure fluctuations at the Darcy scale is much larger than the characteristic pore scale \( \ell \), fluid flow in porous media is described by Darcy’s law, which arises from a formal upscaling of the Stokes equation at the pore scale

\[
\mu \nabla^2 \mathbf{v} - \nabla p = 0, \quad \nabla \cdot \mathbf{v} = 0, \quad \mathbf{x} \in \Omega_f,
\]

coupled with the no-slip boundary condition

\[
\mathbf{v} = 0, \quad \mathbf{x} \in \partial \Omega_f,
\]

where \( \mu \) is the fluid viscosity, \( \mathbf{v} \) and \( p \) respectively are the pore-scale velocity and pressure. The fluid-filled pore space is denoted by the domain \( \Omega_f \), and the pore
Fig. 9: Transport in engineered porous media illustrated by a compact heat exchanger based on metal foam: (a) typical metal foam (Fe-Cr-Al-Y alloy) for heat-transfer purposes (reproduced from Zhao (2012)); (b) simulated cooling of hot fluid flow entering (from the left) metal foam with cold top and adiabatic bottom visualised by temperature of foam surface and streamlines (blue/red: min/max) and velocity magnitude (blue/red: zero/max) in planar cross-sections (adapted from Hugo et al. (2011)).

boundary $\partial \Omega_{fs}$ denotes the boundary between the fluid domain and the solid matrix $\Omega_s$.

Upscaling of these equations via either volume averaging, method of moments or multiscale expansions recovers Darcy’s law, an empirical law that links the macroscopic (averaged) Darcy flux $\mathbf{q} \equiv \langle \mathbf{v} \rangle$ to the macroscopic pressure field $P \equiv \langle p \rangle$ as

$$\mathbf{q} = -\frac{K}{\mu} \cdot \nabla P, \quad \nabla \cdot \mathbf{q} = 0, \quad \mathbf{x} \in \Omega. \quad (4)$$

Here $K$ is the permeability tensor (and $K/\mu$ is known as the hydraulic conductivity tensor) and $\Omega = \Omega_f \cup \Omega_s$ denotes the porous medium that is comprised of both the fluid-filled pore-space $\Omega_f$ and the solid matrix $\Omega_s$. As such, this upscaling process effectively removes the pore boundary $\partial \Omega_{fs}$ and the associated no-slip condition $\mathbf{v} = 0$ at the fluid-solid interface, and the permeability tensor $K$ accounts for the flow resistance that is associated with this no-slip condition. In this way, the permeability tensor $K$ may be considered as a closure model for the Darcy equation (4) as a result of upscaling Stokes flow at the pore scale. For many classes of porous media, the permeability is isotropic and so may be represented by the scalar value as $K = k \mathbf{I}$, and Darcy’s law simplifies to

$$\mathbf{q} = -\frac{k}{\mu} \nabla P, \quad \nabla \cdot \mathbf{q} = 0, \quad \mathbf{x} \in \Omega. \quad (5)$$

As the pore boundary is key to the generation of pore-scale chaos, omission of this boundary in the upscaling process also omits the dynamics associated with pore-scale chaos. Thus the impacts of pore-scale mixing upon solute dilution, dispersion
Fig. 10: (a) Complex of pressure $P$ (grey) and streamfunction $\psi_1$ (red), $\psi_2$ (blue) isosurfaces for a steady heterogeneous, isotropic 3D Darcy flow. Streamlines arise as the intersection of 2D topologically planar streamsurfaces, and so cannot exhibit braiding motions characteristic of chaotic flow. Adapted from Lester et al. (2021b).
(b) Knotted fluid particle trajectories (white lines) and isoconductivity surfaces (coloured surfaces) in a steady anisotropic 3D Darcy flow. Adapted from Cole and Foote (1990).

and transport must be incorporated via appropriate upscaled models. Indeed, for homogeneous porous media where the isotropic permeability $k$ is constant, steady 3D Darcy flows are irrotational (as the vorticity is identically zero: $\omega \equiv \nabla \times \mathbf{q} = -k/\mu(\nabla \times \nabla P) = 0$), and so must also be non-chaotic as there is no mechanism for the creation of chaos-inducing structures known as homoclinic and heteroclinic transverse connections. Similarly, even for strongly heterogeneous porous media with isotropic permeability, i.e. $k = k(x)$, steady Darcy flow is non-chaotic as the helicity density defined (Moffatt, 1969) as the dot product of Darcy flux and vorticity is identically zero:
\[
 h(x) \equiv \mathbf{q} \cdot \omega = k/\mu^2 \nabla P \cdot (\nabla P \times \nabla k) = 0. \tag{6}
\]

The helicity density is a measure of the topological complexity of a flow, and it can be shown (Arnol’d, 1965) that all steady helicity-free flows are non-chaotic.

In a series of studies Sposito (1997, 2001, 2006) argued that the helicity-free condition (6) gives rise to Lamb surfaces (Lamb, 1932) that are spanned by streamlines and vorticity lines of the flow, and provide strong topological constraints on streamline motion. Lester et al. (2019) showed that Lamb surfaces only exist for trivial isotropic 3D Darcy flows, however it has since been established (Lester et al., 2021b) that the helicity-free condition admits a pair of coherent streamfunctions (Zijl, 1986) $\psi_1(x)$, $\psi_2(x)$. These streamsurfaces $\psi_i(x) = \text{constant}$ are “foliated” (stacked together) throughout the flow as non-intersecting 2D lamellae.

The intersection of these 2D streamsurfaces then form the 1D streamlines of the flow, which are topologically equivalent to straight lines. As shown in Figure 10,
even if the conductivity field is strongly heterogeneous, these 1D streamlines must be confined to these topologically planar 2D streamsurfaces and so are topologically equivalent to parallel straight lines. Thus, 1D streamlines in steady isotropic flow cannot undergo the braiding motions (shown in Figure 7b) that are characteristic of chaotic mixing. Thus, no matter how heterogeneous, steady isotropic 3D Darcy flows have trivial flow topology akin to that of steady 2D flow. Lester et al. (2021a) show that this simplified flow topology leads to algebraic rates of fluid deformation, solute mixing and dispersion in isotropic 3D Darcy flow, and so these phenomena are qualitatively very similar to those of steady 2D Darcy flow.

The topological simplicity of steady isotropic Darcy flows can be broken in a number of ways, leading to the possibility of more complex flow topology and chaotic mixing. First, if the Darcy flow is unsteady, the trajectories of fluid tracer particles are no longer confined to the streamlines of the steady flow and so the flow topology can be much richer and possibly chaotic (Weeks and Sposito, 1998). Second, if the permeability tensor is anisotropic and heterogeneous, i.e. \( K(x) \), then the helicity density is non-zero in general:

\[
h(x) \equiv \mathbf{q} \cdot \mathbf{\omega} = (\mathbf{K} \cdot \nabla P) \cdot (\nabla \times \mathbf{K}) \cdot \nabla P \neq 0.
\] (7)

The breaking of this topological constraint means that the coherent streamfunctions \( \psi_1, \psi_2 \) no longer exist and so streamlines are no longer confined to topologically planar 2D streamsurfaces but rather are free to wander throughout the flow domain. This topological freedom opens the possibility for the braiding of streamlines (as shown in Figure 7b), exponential stretching of material elements and chaotic motion. This potential topological complexity is reflected in Figure 10b, which shows clear evidence of knotted and braided streamlines that are characteristic of chaotic mixing. Several studies (Cirpka et al., 2015; Chiogna et al., 2014, 2015; Ye et al., 2015) have observed complex mixing dynamics and streamline structure in anisotropic Darcy flows, however the signatures of chaotic mixing (such as positive Lyapunov exponent or non-trivial flow topology) are yet to be positively identified in these flows. At the Darcy scale, chaotic mixing is anticipated to have a profound impact upon solute mixing, transport and dispersion and so the uncovering of these dynamics and their link to the structure of the anisotropic permeability tensor is currently an important open problem in groundwater hydrology.

At regional scales much larger than the Darcy scale, it is often not computationally feasible to completely resolve the heterogeneous permeability field, and so often upscaling techniques such as block or effective conductivity are employed (Sanchez-Vila et al., 2006). In many cases the locally isotropic (scalar) permeability field \( k(x) \) at the Darcy scale is statistically anisotropic (in that the correlation structure is orientation-dependent due to e.g. geological layering etc), and in these cases, conventional upscaling techniques (Sanchez-Vila et al., 2006) result in an upscaled permeability field \( K^* \) which is tensorial. Cirpka et al. (2015) and Chiogna et al. (2014) have shown that although the fully resolved Darcy-scale flow is helicity-free and has trivial mixing dynamics, the upscaled regional flows can have non-zero helicity and complex streamline motion. In contrast to upscaling from the pore scale to the Darcy scale, where pore scale chaotic dynamics are omitted via the upscaling process, these results suggest that upscaling from the Darcy scale to regional scales may introduce chaotic dynamics that are not apparent at the Darcy scale. As upscaling is essentially a coarse-graining process that results
in a loss of information, it argued that these chaotic dynamics are a non-physical artefact of the employed upscaling methods employed. This is a research area that requires further investigation and may call for *topologically consistent* upscaling methods that preserve the Lagrangian topology of the fully resolved Darcy-scale flow.

### 4.2 Transient Darcy Flows

It understood that transient Darcy flows can not only accelerate transport and dispersion (Dentz and Carrera, 2005; Cirpka and Attinger, 2003), but in certain cases can also admit a range of qualitative transport behaviours that may not otherwise occur in their steady counterparts (Weeks and Sposito, 1998). These transport dynamics are critical to the transport and fate of solutes and colloids in both natural and engineered systems, from seasonal and tidal forcing in coastal aquifers, through to transport through biological tissues and porous engineered structures. Due to the unsteady nature of these flows, it is difficult to detect and understand the corresponding transport structures in the Eulerian frame, whereas the Lagrangian frame facilitates detection and classification of the kinematic features that can control complex fluid mixing, dispersion, reaction, segregation and discharge phenomena at the Darcy scale. Together, these kinds of transport phenomena describe complex Lagrangian structures which engender potentially profound impacts on solute migration and reaction (Toroczkai et al., 1998; Tel et al., 2005; Valocchi et al., 2019). Building on early conceptual work by Jones and Young (1994), Ottino (1989), Sposito (2001, 1997) and others (Piscopo et al., 2013; Lester et al., 2009; 2010a; Metcalfe et al., 2010b; Trefry et al., 2012b; Mays and Neupauer, 2012; Lester, 2016), groundwater researchers are now able to predict, observe and engineer complex Lagrangian structures in saturated porous media at the laboratory (Zhang et al., 2009; Metcalfe et al., 2010b; Bagtzoglou and Oates, 2007) and
field \cite{Cho2019} scales, with quantified benefits for mixing and reactivity enhancement.

\cite{Zhang2009} clearly demonstrated (Figure 11) that a significant increase in reaction rate and yield can be achieved when engineered chaotic mixing flows are introduced in laboratory-scale experiments. Taking this idea further, \cite{Metcalfe2012} and \cite{Trefry2012} used a novel pumping arrangement based upon the reoriented potential mixing (RPM) flow \cite{Metcalfe2010,Lester2009} to demonstrate control of solute transport at the mesoscale (Figure 12), alternating between confinement of a solute plume and accelerated mixing and release. \cite{Cho2019} then demonstrated that chaotic mixing could be also used at the field scale to accelerate solute transport and mixing (Figure 13), with obvious applications in pollutant remediation and resource extraction.

Complex Lagrangian structures have also been predicted to occur in natural groundwater environments, i.e. Darcian systems where engineered pumping activity is absent. Using a conventional Darcian confined flow model in two dimensions (vertically averaged), \cite{Trefry2019} showed computationally that complex Lagrangian structures arose where aquifer heterogeneity and compressibility were combined with sinusoidal boundary forcing. This analysis was extended by \cite{Wu2019} to consider wide ranges of relevant parameter values, highlighting that the spectra of natural ocean tides around the globe provides significant potential to induce Lagrangian complexity in coastal aquifer flows; other important hydraulic parameters are the aquifer compressibility (as depicted in Figure 2), diffusivity and heterogeneity. These complex mixing dynamics have also been shown \cite{Trefry2020} to extend to more realistic (and complex) scenarios where the boundary forcing is comprised of several superposed periodic modes. Since the basic ingredients of porous media heterogeneity, compressibility and time-dependent forcing arise in other geophysical, industrial and biological systems, the above rich set of transport structures that determine fluid residence times, solute segregation, mixing and reaction can also arise in a wide range of other porous media applications.

5 Conclusions

Complex transport dynamics such as chaotic advection abounds in porous media flow. It is inherent to almost all pore-scale flows, and also arises under many scenarios at the Darcy and regional scales. These complex Lagrangian kinematics differ from conventional mixing dynamics in that fluid deformation is exponential in time, and the underlying dynamics often cannot be fully understood in the Eulerian frame. More than just a quantitative change, exponential fluid stretching profoundly augments solute mixing and transport, chemical reactions and biological activity in porous media. Hence the impacts of chaotic advection are typically not captured by conventional methods of modelling transport in porous media, and so unfamiliar tools and techniques are required to visualise, understand, quantify and, in engineering applications, ultimately control and exploit this phenomenon.

Hitherto this Lagrangian paradigm has not been widely appreciated within the community of practitioners of flow and transport in porous media, and this article unabashedly hopes to address that. This is not to say that chaotic advection, or more precisely transport mediated by Lagrangian coherent structures, is a magic
Fig. 12: Mesoscale solute confinement experiment. (a) A 1.5m diameter cylindrical cavity is filled with glass beads, and three pillars of salt (centre). A series of fluid injection and extraction ports around the perimeter (b) facilitate different rotated potential mixing (RPM) flows to be generated. (c) Repeat switching between confinement and mixing protocols of the RPM flow correlate well with regions of high and low salt concentration exiting the device. Adapted from Trefry et al. (2012a).

bullet that solves all outstanding problems the field. On the contrary, we merely state that students and practitioners should be aware of this transport modality when circumstances warrant, and include appropriate techniques amongst the arsenal of methods (stochastic methods, upscaling techniques, uncertainty analysis) to understand and analyse transport in porous media. However, these circumstances are not rare, rather they are common in porous media flows. In fact, chaotic dynamics are the norm rather than exception, and so arise in most situations except for those where kinematic constraints explicitly forbid it. For historical reasons the mental picture cultivated for porous media transport excluded chaotic advection, but now the dynamical systems point of view of transport should be in your toolkit.
One important conceptual tool is the advective template of the flow which is given by the evolution of non-diffusive fluid tracer particles, and so explicitly resolves the system Lagrangian kinematics, associated coherent structures and topology. For any particular application of porous media flow, this advective template necessarily provides an incomplete description of the system as almost always there will be additional physical phenomena such as dispersion, diffusion, chemical reactions and biological activity, all of which interact nonlinearly with the advective template. We argue, however, that for every application knowledge of the underlying advective template is in and of itself useful and informative as this forms the organising structure upon which all additional fluid-borne phenomena play out. It is for this reason that we have focused this primer mainly on the advective template, yet nearly everywhere else in the porous media flow literature it is neglected. We note that many additional tools and techniques applicable to porous media can be found in the dynamical systems (chaos) literature in general and chaotic advection in particular.

Although deliberately limited in scope, several key messages are conveyed in this primer. First, chaotic advection is common to many porous media applications across all length scales. Second, these complex kinematics qualitatively augment associated fluid-borne phenomena, neither of which can be fully understood without utilisation of appropriate tools and techniques. Third, there exist easily identifiable kinematic constraints in particular applications that explicitly preclude chaotic advection, and chaos is expected when these constraints are absent. Fourth, fundamental studies of chaotic advection point toward development of novel classes of porous hierarchical materials (from pore to Darcy scales) with tuneable transport properties. Fifth, saturated porous media may now be regarded as a reaction vessel whose mixing state can be manipulated to promote reactivity or segregation according to purpose. Finally, many natural systems exhibit chaotic advection and complex transport due to unsteady forcings inherent to these systems.
A new way of looking at a problem opens up myriad new and interesting research questions. Key knowledge gaps in the field include: (i) Development and application of methods for characterisation of chaotic advection in all real (i.e. not model) natural and engineered porous materials, (ii) how the kinematics of steady 3D flow at the pore-scale influence macroscopic fluid mixing and chemical transport in saturated porous media, (iii) how to develop upscaled models of dispersion and dilution which capture these processes, (iv) design rules for engineered porous materials with tuneable transport properties, (v) development of topologically consistent upscaling methods for Darcy flows that do not introduce spurious kinematics, (vi) merging of chaotic advection methods with stochastic methods and conventional approaches to transport in porous media. This topological approach to fluid physics at the pore scale is a relatively new area and opportunities abound for further development. Another knowledge gap is how these concepts may be extended to real porous architectures via the development of stochastic models for the evolution of the fluid deformation tensor conditioned upon computer tomography imaging of the pore space and computational fluid dynamics simulations. Finally, more experiments are needed looking for the effects of chaotic advection across porous media applications.

Our goal with this paper is to implant in the reader the chaotic way of thinking and to generate some familiarity with the requisite mathematical apparatus. By this route we hope to open up new ways of designing porous media reaction technology and new understandings of ecological and biological porous transport. Let us know if we have succeeded.

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