Mixing, Flow Kinematics and Lamb Surfaces in Darcy Flow

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Abstract Hydrodynamic dispersion is governed by flow heterogeneity and kinematics, which determines the organization of streamlines. The existence Lamb surface constrains the flow kinematics in the same manner as two-dimensional flows.

The existence of Lamb surfaces in three-dimensional Darcy flow has deep implications for the understanding and modelling of transverse mixing and dispersion in heterogeneous porous media. In a series of pioneering studies, Sposito (Wat. Resour. Res., **30** (8), 2395-2401 (1994); Adv. Wat. Res., **24** (7), 793-801 (2001)) argues that steady, isotropic Darcy flow gives rise to Lamb surfaces, two-dimensional material surfaces which contain both streamlines and vortex lines (field lines of the vorticity vector). Hence, the existence of these surfaces renders steady isotropic Darcy as essentially two-dimensional. This topological constraint strongly affects transverse mixing and dispersion because two-dimensional steady and divergence-free flow fields do not admit macroscopic transverse dispersion. In this study, however, we show that Lamb surfaces are not ubiquitous to all steady isotropic Darcy flows. We derive the conditions for when Lamb surfaces exist in isotropic Darcy flow, and discuss the implications of our findings for the kinematics of fluid elements and the transport, mixing and dilution of solutes.

Keywords Darcy flow · fluid deformation · hydrodynamic dispersion

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1 Introduction

The mixing, dispersion and transport of solutes in heterogeneous Darcy flow is central to vast array of engineered and natural processes; from spreading of pollutants in groundwater flows to the mixing of chemical reagents in packed bed reactors and the delivery of pharmaceutical drugs through human tissue. These processes are all governed by the interplay of fluid advection and molecular diffusion - here the advection process acts to organise the evolution and distribution of fluid elements (stirring), whilst the diffusive process continually acts to locally randomise solute molecules (mixing) [8]. As such, mixing, dispersion and transport cannot be properly understood without a deep understanding of the advection process, which is described in terms of the *Lagrangian kinematics* of the flow [24], which seek to answer the question: what is the fate of material elements given knowledge of their initial position and the (Eulerian) properties of the flow?

A complete understanding of the Lagrangian kinematics of Darcy flow is then vital to understand, quantify and predict these processes. For example, the deformation of fluid elements is integral to solute mixing, where the distribution of fluid stretching rates serves as key inputs (along with molecular diffusion) to predictive models for solute mixing and dilution [16, 17, 20], whilst the transport and spreading of fluid elements governs longitudinal and transverse dispersion [5].

The inherent heterogeneity of these porous materials is typically described via a stochastic framework; by characterising the statistical parameters of the hydraulic conductivity at the Darcy scale (spatial correlation structure, conductivity probability distribution, etc) it is then possible to make predictions of transport, mixing and dispersion of solutes with respect to the ensemble of realisations of these random conductivity fields. This is the topic, in essence, of stochastic hydrology. One aim of this field is to develop predictive models for mixing, dispersion and transport in terms of the medium statistical properties that characterise the hydraulic conductivity field.

Due to the stochastic nature of this problem it is then possible to overlook constraints imposed by the Lagrangian kinematics of the flow. It is critical that any stochastic groundwater model may only produce sets of particle trajectories and deformations that are admissible by the Lagrangian kinematics, otherwise there is a real risk of generating spurious predictions that violate these constraints. As the Lagrangian kinematics then govern solute evolution, such violations lead to spurious predictions of solute mixing, transport and dispersion. For two-dimensional divergence-free steady random flows, for example, it was shown that for purely advective transport, transverse dispersion is asymptotically zero [3] as a result of the solenoidal nature of the flow field, which imposes a topological constraints on the Lagrangian kinematics. Stochastic models that do not respect this constraint predict macroscale transverse dispersion. Another important topological constraint refers to the conditions under which chaotic advection can arise. According to the Poincaré-Bendixson theorem, two-dimensional steady flow does not admit chaotic advection. This means, material elements cannot be stretched and folded back on themselves leading to exponential increase of material lines. Thus, one key question regarding these kinematic constraints is whether the kinematics of steady 3d Darcy flow is truly 2d or 3d in nature? In other words, are streamlines in 3d steady flow fields confined to 2d surfaces, so called *Lamb surfaces*. If this is the case, the same topological constraints that apply to 2d flow also apply to 3d flow. Importantly, the existence of such Lamb surfaces then implies that there can be no macroscopic transverse dispersion in 3d, and that there can be no chaotic advection in 3d Darcy flows.

In a series of landmark papers, Sposito [27–29, 31, 30] argues that the kinematics of steady Darcy flow is essentially 2d in nature due to the existence of *Lamb surfaces* [15]; these 2d surfaces are spanned by streamlines and vortex lines (field lines of the vorticity vector) and pack together throughout the flow in a lamellar fashion. As such, streamlines are confined to families of 2d surfaces and so are subject to the same constraints as 2d Darcy flow. Hence if Lamb surfaces exist in Darcy flow, then the Lagrangian kinematics are 2d. Note that the Lamb surfaces do not need to be flat objects, but can be warped in space. The 2d nature refers to the fact that purely advective particle trajectories (streamlines) are confined to a 2d surface with all its consequences for transverse dispersion and the deformation and stretching of material elements.

In this study we examine whether Lamb surfaces do exist in steady, isotropic Darcy flow and consider the implications for mixing, transport and dispersion. In Section 2 we shall briefly demonstrate how the Lagrangian kinematics impact these transport processes, followed by a review of the existence of Lamb surfaces in steady Darcy flows in Section 3. In Section 4 we shall present numerical evidence that shows Lamb surfaces are not ubiquitous to isotropic Darcy flow, and in Section 5 we derive the conditions under which Lamb surfaces do exist in these flows. Finally we discuss the implications of our findings for transport, mixing and dispersion in steady isotropic Darcy flow.

2 Lagrangian kinematics and solute evolution

We consider here Lagrangian and kinematics and solute evolution at the Darcy scale. The divergence-free, steady flow field $\mathbf{v}(\mathbf{x})$ is governed by the Darcy equation

$$\mathbf{v}(\mathbf{x}) = -k(\mathbf{x})\nabla\phi(\mathbf{x}), \quad (1)$$

where $k(\mathbf{x})$ is the hydraulic conductivity field and $\phi(\mathbf{x})$ is the velocity potential (or pressure head). Transport is described by the advection-dispersion equation for the solute concentration $c(\mathbf{x}, t)$

$$\frac{\partial c(\mathbf{x}, t)}{\partial t} + \mathbf{v}(\mathbf{x}) \cdot \nabla c(\mathbf{x}) - \nabla \cdot [\mathbf{D}\nabla c(\mathbf{x}, t)] = 0, \quad (2)$$

where porosity is assumed to be constant and absorbed in a rescaled time, $\mathbf{D}$ is the local dispersion tensor. The transport, mixing and macroscale dispersion of a solute plume is governed by the continual interplay of advection and local dispersion, where the former process organises the distribution and deformation of fluid elements (stirring and stretching), the latter randomises the local distribution of solute particles due to a Brownian motion-type process within and between these fluid elements. The motion of solute particles is governed by the Langevin equation

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{v}[\mathbf{x}(t)] + \sqrt{2\mathbf{D}} \cdot \xi(t), \quad (3)$$

where we assume for illustration that local scale dispersion is constant. The Gaussian white noise $\xi(t)$ models for the above mentioned random motion that distributed solute particles within and between fluid elements. The relative importance of advective and dispersive mass transfer is quantified by the Péclet number $Pe = \bar{v}\ell_c/D$ with $\bar{v}$ the average flow velocity, ℓ_c a characteristic velocity correlation scale and D a characteristic local dispersion rate. Whilst the local dispersion process is characterised solely in terms of the hydrodynamic dispersion

tensor, advection can be much more complicated, leading to complex distributions of fluid elements which may be deformed and exhibit a broad distribution of arrival times. This interplay can often lead to non-Fickian “anomalous” transport and dispersion in heterogeneous Darcy flows that cannot be resolved in terms of a conventional (Fickian) macro-dispersion framework [10].

As such, solute evolution (transport, mixing, dispersion) in heterogeneous Darcy flow cannot be understood without insight into the advective template upon which diffusion plays out. This advective template is couched in the Lagrangian frame, as the transform between the Eulerian and Lagrangian frames is defined in terms of solutions to the advection equation for the motion of a fluid element

$$\frac{d\mathbf{x}(t, \mathbf{a})}{dt} = \mathbf{v}[\mathbf{x}(t, \mathbf{a})], \quad (4)$$

where the label $\mathbf{a}$ denotes the initial position $\mathbf{x}(t = 0, \mathbf{a}) = \mathbf{a}$. The organisational role of advection is completely defined by the *Lagrangian kinematics* of the flow, which quantifies the motion and deformation of fluid elements due to the advection process, without regard to the origins and dynamics of the underlying advective velocity field. These kinematics are often subject to constraints on the allowable fluid motions, which arise from principles such as conservation of mass and continuity of fluid deformation.

As such, the Lagrangian kinematics of heterogeneous Darcy flow govern the transport, mixing and dispersion of solute plumes in these flows, and the constraints on these kinematics then limit the classes of allowable solute behaviour. In order to illustrate how the Lagrangian kinematics of a flow impacts solute evolution we consider transverse hydrodynamic dispersion in steady, 2d heterogeneous Darcy flow at high Péclet numbers. Here, the inherent heterogeneity of the porous medium results in convoluted fluid streamlines as they navigate high and low permeability regions, leading to wandering of particles as they are advected with the mean flow direction. As such, a seemingly reasonable approach to modelling transverse hydrodynamic dispersion in this flow is to develop a stochastic model for particle motion (conditioned upon experimental or numerical observations) that is based upon a random walk transverse to the mean flow direction as particles are simultaneously advected with the mean flow. A classical approach borrowed from turbulent diffusion would be to model transverse particle motion as an unbiased random walk as

$$\frac{dy(t)}{dt} = \sqrt{2D_T^*} \xi(t), \quad (5)$$

where the transverse macrodispersion coefficient would be equal to the transverse velocity variance $\sigma_{v_2}^2$ and the advection time scale $\tau_v = \ell_c/\bar{v}$, this means $D_T = \sigma_{v_2}^2 \ell_c/\bar{v}$. However, such a description does not account for the fact that $v_1(\mathbf{x})$ and $v_2(\mathbf{x})$ are not independent, but related through $\nabla \cdot \mathbf{v}(\mathbf{v}) = 0$. This implies that any steady 2d flow may be described in terms of streamlines which cannot cross each other. Whilst these streamlines can diverge or converge momentarily, they cannot do so without bound due to conservation of fluid volume, and this constraint applies to the set of all streamlines. This implies that transverse dispersion is asymptotically going to 0 in the limit $Pe \rightarrow \infty$ and for times larger than the correlation time scale τ_c [9, 3]. As such, the naive stochastic model (5) for 2d transverse hydrodynamic macro-dispersion has failed to incorporate an important constraint on the Lagrangian kinematics which arises from the 2d nature of the flow. Clearly, real 3d porous media flows do exhibit transverse hydrodynamic dispersion, and the above constraint which arises from the 2d idealisation is not immediately obvious. While the example above demonstrates in a fairly obvious way how a simple constraint on the Lagrangian kinematics can manifest

in limiting solute plume evolution, there exist more complex constraints that impose less obvious but equally important limitations on the classes of admissible solute behaviour.

Similar to transverse dispersion, fluid deformation in all steady 2d flows is limited in that it can only be at most algebraic in time (i.e., the length $\ell(t)$ of a material element can only grow as $\ell(t) \sim t^\alpha$), as a consequence of the Poincaré-Bendixson theorem. Conversely, steady 3d flows can involve chaotic advection, whereby fluid elements deform exponentially in time (i.e. $\ell(t) \sim \exp(\lambda t)$) [24, 12]. As such, stochastic models for fluid deformation [11, 19] must recover the correct scaling (i.e. algebraic or exponential) for fluid deformation as a primary consideration prior to attempting to estimate or model the exponents α or λ . Similar to transverse dispersion, the rate of fluid deformation is governed by the Lagrangian kinematics. Here the difference between exponential and algebraic stretching of fluid elements is determined by whether or not the Lagrangian kinematics (particle trajectories) are regular or chaotic.

The questions as to what is the fate of streamlines and how do material elements deform in steady 3d Darcy flow are fundamental to prediction of mixing, dispersion and transport in these systems [33, 16, 17, 34]. Stochastic models for these phenomena must be conditioned to the correct Lagrangian kinematics (as admitted by the Darcy equation), otherwise spurious phenomena (such as non-zero transverse hydrodynamic dispersion in steady 2d flow) can result from model predictions. Key items here are the identification of kinematic constraints of 3d Darcy flow and quantification of their impact on transport processes.

In a series of studies, Sposito [27–29, 31, 30] argues that the fact that the helicity density in 3d Darcy flow is 0, implies the existence of *Lamb surfaces* [15]; these 2d surfaces are spanned by streamlines and vortex lines (field lines of the vorticity vector) and pack together throughout the flow field in a lamellar fashion. As such, streamlines are confined to families of these 2d surfaces. Sposito [30] shows that as a consequence, advection is non-chaotic and behaves in this sense as steady 2d flow. As outlined above, transverse dispersion is 0 for purely advective transport in steady 2d flow. Thus, one may argue that the same holds for isotropic Darcy flow. In the following sections we shall examine whether Lamb surfaces do exist in and draw conclusions as to the kinematics of steady isotropic Darcy flow and its consequences for mixing and transverse dispersion.

3 Lamb Surfaces in Steady Isotropic Darcy Flow

Steady flow in isotropic, heterogeneous porous media at the Darcy scale is commonly modelled via the Darcy equation (1) Whilst steady, these flow can exhibit significant structural complexity due to the strong spatial fluctuations in the hydraulic conductivity. The Lagrangian kinematics of these flows govern the transport, dispersion and mixing of solutes and associated processes such as chemical reactions and biological activity. One important kinematic characteristic of isotropic Darcy flow is that the vorticity

$$\omega(\mathbf{x}) \equiv \nabla \times \mathbf{v}(\mathbf{x}) = -\nabla k(\mathbf{x}) \times \nabla \phi(\mathbf{x}), \quad (6)$$

is everywhere perpendicular to the velocity $\mathbf{v}$, as reflected by the helicity density [23] (henceforth simply denoted as helicity) which is identically zero for steady, isotropic Darcy flow

$$h(\mathbf{x}) \equiv \mathbf{v}(\mathbf{x}) \cdot \omega(\mathbf{x}) = k(\mathbf{x}) \nabla \phi(\mathbf{x}) \cdot (\nabla k(\mathbf{x}) \times \nabla \phi(\mathbf{x})) = 0. \quad (7)$$

The helicity density $h(\mathbf{x})$ measures the degree of local helical motions of the fluid (leading to the formation of helical windings of streamline bundles), and the global helicity $H \equiv \int_{\Omega} h(\mathbf{x}) d\Omega$ over the flow domain Ω is a measure of the knottedness of vortex lines.

Sposito [27,30] argues that the helicity-free structure of steady isotropic 3d Darcy flow (7) admits the existence of Lamb surfaces, lamellar 2d material surfaces that permeate through the entire flow domain and contain both streamlines and vortex lines. As these 2d surfaces are material, they render the kinematics of steady, isotropic Darcy flow essentially equivalent to that of a steady 2d flow. Hence these surfaces have significant implications for dispersion and mixing (beyond those of the helicity-free condition), as for steady flow they imply zero transverse hydrodynamic dispersion.

Lamb surfaces were first discovered by Lamb [15], who proved their existence in steady, inviscid, incompressible flow, followed by more technical proofs by Poincaré [26] and Arnol'd [2], which were further generalised to fluids with uniform entropy fields by Kozlov [14]. Sposito [28] shows that a condition for the existence of Lamb surfaces is that vortex lines are *material*, i.e. sets of streamlines that emanate from a given vortex line are themselves spanned by a single vortex line downstream. As such, the vortex lines and streamlines span a single 2d surface, the Lamb surface. The condition for vortex lines to be material is that the curl of Lamb vector [15,32]

$$\ell(\mathbf{x}) \equiv \boldsymbol{\omega}(\mathbf{x}) \times \mathbf{v}(\mathbf{x}), \quad (8)$$

is everywhere parallel to the vorticity vector,

$$\boldsymbol{\omega}(\mathbf{x}) \times (\nabla \times \ell(\mathbf{x})) = \mathbf{0}, \quad (9)$$

a condition known as the Helmholtz-Zorawski condition [32]. In practice, this condition is quite restrictive, and it only applies to homogenous, isotropic Darcy flows, i.e. potential flows, where $k=\text{constant}$. A less restrictive condition for the existence of Lamb surfaces is that the Lamb vector must be everywhere perpendicular to its curl

$$(\nabla \times \ell(\mathbf{x})) \cdot \ell(\mathbf{x}) = 0, \quad (10)$$

a condition termed *complex lamellar* (CL) by Kelvin [13], which is akin to the Lamb vector itself being helicity-free. According to Brand [6], any continuously differentiable vector field is everywhere parallel to a set of such surface normals if and only if it is everywhere perpendicular to its curl. This is certainly the case for the velocity field $\mathbf{v}(\mathbf{x})$, as it is everywhere perpendicular to its vorticity, as reflected by the zero-helicity condition (7), and the streamlines conform to stream-surfaces which are everywhere perpendicular to iso-potential surfaces. Similarly, the CL condition on the Lamb vector (10) ensures the existence of Lamb surfaces which are spanned by both streamlines and vortex lines. Sposito [30] argues that the CL condition (10) arises as a direct result of the topological constraints imposed by the steady isotropic Darcy flow equation (1), hence Lamb surfaces are ubiquitous to such flows and their kinematics are 2d in character. In the following Section we test this assertion against highly-resolved numerical solutions of steady, isotropic heterogeneous 3d Darcy flow.

SHOW HERE THAT THE EXISTENCE OF LAMB SURFACES IMPLIES THAT TRANSVERSE DISPERSION IS 0.

4 Numerical Results

4.1 3D Heterogeneous Flow

To numerically test for the existence of Lamb surfaces in heterogeneous, isotropic 3d Darcy flow, we performed high-resolution simulations of these flows with a Gaussian hydraulic

Fig. 1 Fluid streamlines and isosurfaces of (a) log-conductivity field $\ln k$ and (b) potential ϕ from high-resolution finite-difference solution (128^3 grid) of the heterogeneous Darcy field. (bottom) Typical fluid streamline (black) with orthogonal vorticity vectors ω (red) and Lamb vectors ℓ (blue) computed from high-resolution finite-difference solution.

Fig. 2 Typical fluid streamline (black) with orthogonal vorticity vectors ω (red) and Lamb vectors ℓ (blue) computed from high-resolution finite-difference solution.

conductivity field with correlation length $\lambda = 1/8$, mean conductivity $\langle k \rangle = 1$ and log-variance $\sigma_{\ln k} = 1$ over the domain $\mathcal{D} : \mathbf{x} = \{x_1, x_2, x_3\} \in [0, 1] \times [0, 1] \times [0, 1]$, subject to periodic boundary conditions transverse to the mean flow direction and fixed-head conditions at the inlet ($x_3 = 0$) and outlet ($x_3 = 1$) planes. To ensure our results are mesh-independent, we use a series of finite-difference (FD) grids with increasing spatial resolution with grid dimensions 64^3 , 128^3 , 256^3 and 512^3 that correspond respectively to 8, 16, 32 and 64 grid points per correlation length-scale. A FD method is used to solve the head ϕ on these grids to a numerical divergence error of machine precision (10^{-16}) with respect to the FD stencil. A cross-section of a typical conductivity field $k(\mathbf{x})$, potential solution $\phi(\mathbf{x})$ and associated streamlines for the 128^3 grid is shown in Figure 1.

To generate continuous solutions from the finite-difference solutions, we then compute the hydraulic conductivity $k(\mathbf{x})$ and head $\phi(\mathbf{x})$ field as C_5 -smooth 3d spline interpolations based upon the finite difference grid data. The primitive variables k , ϕ are then used to analytically compute the velocity, vorticity, Lamb vector and derivatives thereof using equations

Fig. 3 (a) Histogram of the relative divergence error d in (12) for the 64^3 (red), 128^3 (green), 256^3 (blue) and 512^3 (grey) FD grids and (b) scatter plot of complex lamellar angle θ_{cl} against divergence d in (12) for the 128^3 grid.

(1), (6), (8). Throughout the remainder of this paper we shall work exclusively with these interpolated values only. From these primitive variables, we compute all combinations of the dot products of $\mathbf{v}$, $\boldsymbol{\omega}$, $\boldsymbol{\ell}$ over 10^6 random points in the domain. As expected we find these dot products are all within machine precision $\varepsilon = 10^{-16}$ throughout the domain, i.e.

$$|\mathbf{v}(\mathbf{x}) \cdot \boldsymbol{\omega}(\mathbf{x})| < \varepsilon, \quad |\mathbf{v}(\mathbf{x}) \cdot \boldsymbol{\ell}(\mathbf{x})| < \varepsilon, \quad |\boldsymbol{\ell}(\mathbf{x}) \cdot \boldsymbol{\omega}(\mathbf{x})| < \varepsilon, \quad (11)$$

rendering the velocity $\mathbf{v}$, vorticity $\boldsymbol{\omega}$ and Lamb vectors $\boldsymbol{\ell}$ everywhere orthogonal, as illustrated in Fig. 2. Whilst the divergence of the flow is order machine precision ε with respect to the FD stencil, the relative divergence error

$$d(\mathbf{x}) \equiv \frac{\nabla \cdot \mathbf{v}}{\sqrt{\mathbf{D} : \mathbf{D}}} = \frac{-k(\mathbf{x}) \nabla^2 \phi(\mathbf{x}) - \nabla k(\mathbf{x}) \cdot \nabla \phi(\mathbf{x})}{\sqrt{\mathbf{D} : \mathbf{D}}}, \quad (12)$$

(where $\mathbf{D} = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^\top)$ is the rate of strain tensor) is significantly larger when computed with respect to the interpolated primitive variables, as shown for 10^6 random points illustrated in Figure 3(a). As expected, the divergence error reduces with increasing mesh resolution, where the standard deviation σ_d of the relative divergence error d reduces from $\sigma_d = 0.0182$ for the 64^3 grid to $\sigma_d = 0.00151$ for the 512^3 grid. In the following sections we shall show the whilst the divergence errors are still significant, the relevant model predictions have converged for the 512^3 grid, hence we shall consider these results as being mesh independent.

To test for the existence of Lamb surfaces in this flow we then choose a subset (comprising 6,274, 21,016, 78,410 and 291,727 points for the 64^3 , 128^3 , 256^3 and 512^3 grids respectively) of the points used to compose Figure 3(a) for which the magnitude of the relative divergence d is smaller than the cutoff value $|d| < 10^{-4}$, and compute the complex lamellar condition (10) at these points. To test the CL condition (10) we define the CL dot product

$$\alpha_{CL}(\mathbf{x}) \equiv (\nabla \times \boldsymbol{\ell}(\mathbf{x})) \cdot \boldsymbol{\ell}(\mathbf{x}), \quad (13)$$

and the CL angle as

$$\theta_{CL}(\mathbf{x}) \equiv \arccos \left(\frac{(\nabla \times \boldsymbol{\ell}(\mathbf{x})) \cdot \boldsymbol{\ell}(\mathbf{x})}{\|(\nabla \times \boldsymbol{\ell}(\mathbf{x}))\| \|\boldsymbol{\ell}(\mathbf{x})\|} \right), \quad (14)$$

Fig. 4 (a) Histogram of the complex lamellar angle θ_{CL} in (12) for the 64^3 (red), 128^3 (green), 256^3 (blue) and 512^3 (grey) FD grids.

Fig. 5 Scatter plot of relative divergence d and the vortex-line acceleration term $a_1 \equiv \frac{1}{2} \omega \cdot \nabla ||\mathbf{v}||^2$, (b) Histogram of a_1 for the 64^3 (red), 128^3 (green), 256^3 (blue) and 512^3 (grey) FD grids.

where $\alpha_{\text{CL}} = 0$, $\theta_{\text{CL}} = \pi/2$ everywhere for the Lamb vector to be complex-lamellar. The resultant scatter plot for the CL angle $\theta_{\text{CL}}(\mathbf{x})$ is shown in Figure 3(b), which depicts significant deviations from the complex-lamellar condition $\theta_{\text{CL}} = \pi/2$ (10) for the Lamb vector for all FD grids used. The distribution of CL angles appear to converge to a uniform distribution in the limit of infinite mesh resolution, indicating that the complex lamellar condition (10) is violated throughout the domain.

Furthermore, there appears to be no correlation between the deviations from $\theta_{\text{CL}} = \pi/2$ and the relative divergence $d(\mathbf{x})$, hence it appears unlikely that these deviations can be attributed to point-wise divergence errors associated with the interpolation of primitive variables. As such, it appears that the CL condition does not hold generically for steady isotropic Darcy flow, nor are the Lamb vectors complex-lamellar. This is in contrast with the derivation of Sposito [30], who claims that the CL condition (10) is satisfied as a direct consequence of the Darcy equation (1).

A second independent numerical test for the existence of Lamb vectors arises from consideration of the change in velocity along vorticity lines, which evolves according to the kinematic identity [4]

$$\frac{D\mathbf{v}}{Dt} = \frac{1}{2} \nabla ||\mathbf{v}||^2 + \boldsymbol{\omega} \times \mathbf{v}, \quad (15)$$

where D/Dt denotes the Lagrangian derivative. Sposito [30] argues that moving points in a steady isotropic Darcy flow are only accelerated along streamlines or Lamb vector field lines, but their velocity remains constant along vorticity lines, i.e. $\boldsymbol{\omega} \cdot D\mathbf{v}/Dt = 0$. This as-

Fig. 6 Scatter plot of relative divergence d and the potential second derivative $\phi_{1,2} \equiv \partial^2 \phi / \partial \xi_1 \partial \xi_2$, (b) Histogram of $\phi_{1,2}$ in (18) for the 64^3 (red), 128^3 (green), 256^3 (blue) and 512^3 (grey) FD grids.

section may be tested by taking the dot product of the vorticity vector with equation (15), yielding

$$\boldsymbol{\omega} \cdot \frac{D\mathbf{v}}{Dt} = \frac{1}{2} \boldsymbol{\omega} \cdot \nabla ||\mathbf{v}||^2 + \boldsymbol{\omega} \cdot (\boldsymbol{\omega} \times \mathbf{v}), \quad (16)$$

where the latter term on the right hand side is identically zero due to orthogonality of the velocity, vorticity and Lamb vectors, i.e. $\boldsymbol{\omega} \cdot \boldsymbol{\ell} = 0$.

However, we find the velocity along any given vorticity is not constant, and the acceleration $a_1(\mathbf{x}) \equiv \frac{1}{2} \boldsymbol{\omega} \cdot \nabla ||\mathbf{v}||^2$ is non-zero throughout the flow domain across the various FD grids, as shown in Figure 5(a). As for the CL angle $\theta_{CL}(\mathbf{x})$, we find that the acceleration $a_1(\mathbf{x})$ is uncorrelated with the relative divergence $d(\mathbf{x})$ (Figure 5(b)), indicating that deviations from $a_1 = 0$ are not governed by divergence errors due.

The non-zero acceleration a_1 can be shown to be generated by the second derivative of the velocity gradient by expanding a_1 as

$$\frac{1}{2} \boldsymbol{\omega} \cdot \nabla ||\mathbf{v}||^2 = k^2 \boldsymbol{\omega} \cdot \nabla \nabla \phi \cdot \nabla \phi, \quad (17)$$

where we have used $(\nabla \phi \times \nabla k) \cdot (\nabla \phi \nabla k) = \mathbf{0}$. If we denote the orthogonal coordinate system (ξ_1, ξ_2, ξ_3) where the coordinate directions correspond respectively to the orthogonal vectors $\mathbf{v}, \boldsymbol{\omega}, \boldsymbol{\ell}$, then as $k^2 > 0$, then $a_1 \neq 0$ corresponds to

$$\phi_{1,2} \equiv \frac{\boldsymbol{\omega}}{||\boldsymbol{\omega}||} \cdot \nabla \nabla \phi \cdot \frac{\nabla \phi}{||\nabla \phi||} = \frac{\partial^2 \phi}{\partial \xi_1 \partial \xi_2} \neq 0. \quad (18)$$

Thus the second order partial derivative $\phi_{1,2}$ which quantifies the change in velocity gradient $\nabla \phi$ along the vorticity direction is directly responsible for acceleration along vortex lines, invalidating the existence of Lamb surfaces. We compute $\phi_{1,2}$ over the flow domain for the FD grids and, as shown in Figure 6(a), we find it is uncorrelated with the relative divergence error d . Figure 6(b) shows the distribution of $\phi_{1,2}$ for 10^6 randomly placed points over the flow domain for the 64^3 , 128^3 , 256^3 and 512^3 FD grids, indicating that $\phi_{1,2}$ is indeed non-zero throughout the flow domain in the mesh-independent limit.

Fig. 7 Streamlines (black) and isosurfaces of (a) log-conductivity $\ln k$ and (b) potential ϕ for the extruded heterogeneous media $k(\mathbf{x}) = k(x_1, x_2)$. For this flow Lamb surfaces correspond to iso-conductivity surfaces and vortex lines (not shown) wrap around the iso-conductivity surfaces.

Fig. 8 Distribution of (a) the divergence error $d \equiv \nabla \cdot \mathbf{v}$ and (b) of CL dot product α_{CL} for flow in extruded porous media.

4.2 Quasi-2d Heterogeneous Flow

In contrast to the results in Subsection 4.1, Lamb surfaces can occur in 3d Darcy flows which are inherently 2d in nature. One clear example is flow in 3d heterogeneous porous media which is invariant in one direction or more, such as stratified media. In this subsection we consider several examples where Lamb surfaces can arise in these quasi-2d Darcy flows. First, we consider flow in 2d extruded porous media with hydraulic conductivity which is invariant in the same direction as the pressure gradient, i.e. $k(\mathbf{x}) = k(x_2, x_3)$. A typical log-conductivity field and potential distribution is shown in Fig. 7, along with streamlines of the flow. For this simple flow Lamb surfaces do exist and correspond to isosurfaces of hydraulic conductivity (which are topological cylinders) as these surfaces are oriented parallel to streamlines (which line in the x_1 direction) and are also wrapped by vortex lines (in the direction perpendicular to the flow direction). We also find the divergence error on the interpolated velocity over 10^5 random points is less than 10^{-10} (Fig. 8(a)), and the CL condition

Fig. 9 Streamlines (black), vortex lines (red) and isosurfaces of (a) log-conductivity $\ln k$ and (b) potential ϕ for the extruded heterogeneous media $k(\mathbf{x}) = k(x_1, x_2)$. For this flow Lamb surfaces correspond to extrusion of streamlines parallel to vortex lines (red lines) which are straight lines oriented in the x_3 direction.

is fulfilled over all of these points to within α_{CL} less than 10^{-12} as shown in Fig. 8(b). These results are expected as the velocity potential $\phi(\mathbf{x}) = \phi(x_1)$ only varies with the longitudinal coordinate so the flow is essentially 2D.

Similarly, flow in extruded 2d porous media where the hydraulic conductivity is invariant in a direction perpendicular to the pressure gradient (i.e. $k(\mathbf{x}) = k(x_1, x_2)$) also yields Lamb surfaces. As shown in Figure 9, this flow admits vortex lines which are straight lines oriented in the x_3 direction, and so Lamb surfaces arise as streamlines which are extruded in the x_3 direction. Similar to the previous case, the computed relative divergence d of this flow (not shown) throughout the flow domain is everywhere less than 10^{-10} and the complex-lamellar dot product α_{CL} (not shown) is everywhere less than machine precision.

Similar to the flows above, Sposito [31] considers tracer advection in a quasi-2d flow given by flow in a stratified aquifer (where the conductivity varies only in the vertical direction, i.e. $k = k(x_3)$) driven by a pressure gradient that is oriented at an oblique angle to the depositional layers in the stratified medium, i.e.

$$\nabla\phi = -J_1\hat{\mathbf{e}}_1 - \frac{q_3}{k(x_3)}\hat{\mathbf{e}}_3, \quad (19)$$

where J_1 represents a constant pressure gradient, q_3 is a constant flux and $\hat{\mathbf{e}}_i$ is the unit vector in the x_i coordinate direction. From (19), the fluid flux, vorticity and Lamb vector are then

$$\mathbf{v} = k(x_3)J_1\hat{\mathbf{e}}_1 + q_3\hat{\mathbf{e}}_3, \quad (20)$$

$$\boldsymbol{\omega} = \frac{dk}{dx_3}J_1\hat{\mathbf{e}}_2 = \hat{\boldsymbol{\omega}}\hat{\mathbf{e}}_2, \quad (21)$$

$$\boldsymbol{\ell} = \boldsymbol{\omega}q_3\hat{\mathbf{e}}_1 - \boldsymbol{\omega}k(x_3)J_1\hat{\mathbf{e}}_1, \quad (22)$$

and the Lamb surfaces correspond to level sets of the function $H(\mathbf{x}) = H(x_1, x_3)$, where

$$\nabla H = q_3\hat{\mathbf{e}}_1 - k(x_3)J_1\hat{\mathbf{e}}_3. \quad (23)$$

Sposito [31] identifies that the function H plays the role of a streamfunction in the planar 2d flow (in the x_1x_3 -plane) described by (20) as

$$\frac{\partial H}{\partial x_1} = q_3 \quad \frac{\partial H}{\partial x_3} = -\omega k(x_3)J_1 \quad \frac{\partial H}{\partial x_2} = 0. \quad (24)$$

Hence Lamb surfaces in this 3d flow are streamlines in the x_1x_3 -plane which are extruded in the x_2 direction. Through a rotation of coordinate frame, this flow has the same structure as the example above for flow in extruded 2d porous media where the conductivity field is invariant in a coordinate direction perpendicular to the mean flow gradient, i.e. $k = k(x_1, x_2)$.

Another class of quasi-2d Darcy flows which admit Lamb surfaces is axisymmetric flows, which may be described in terms of cylindrical coordinates (r, θ, z) , where the conductivity field $k = k(r, z)$ and velocity potential $\phi = \phi(r, z)$ are functions of the radial r and axial z coordinates and are independent of the azimuthal angle θ . In this case, the streamlines of the flow are confined to planes of constant azimuthal angle θ , and the vorticity vector only has components in the θ direction. Hence vortex lines of the flow manifest as circular orbits with fixed r, z . As such, Lamb surfaces in axisymmetric Darcy flows arise as surfaces of revolution of streamlines of the flow. These streamsurfaces are the axisymmetric analogue of the Lamb surfaces in the extruded domain shown in Figure 9(b). These Lamb surfaces correspond directly to level sets of the Stokes streamfunction $\Psi(r, z)$ for axisymmetric flows, which is related to the fluid velocity field as $\mathbf{v} = \nabla \times \Psi(r, z)\hat{\mathbf{e}}_\theta$.

One specific example of axisymmetric Darcy flow is (otherwise uniform) flow over a spherical inclusion, where the conductivity field $k = k(\rho)$ is only a function of the spherical radius $\rho = \sqrt{r^2 + z^2}$. To render the associated gradients well-defined, we assume that the conductivity field varies smoothly over a small distance in the ρ -direction near surface of the inclusion (rather than discontinuously as is often considered), and the conductivity is constant elsewhere. In this flow, the streamlines are confined to (r, z) planes and are perturbed by the inclusion as they travel downstream, whilst the vortex lines wrap around in circular orbits of constant (r, z) . As the conductivity only varies local to the surface of the spherical inclusion, the vortex lines are also confined to this region. Similarly, the Lamb surfaces for this flow are also confined to this region, and manifest as sphere-like “shells” near the surface of the spherical inclusion.

These examples indicate that whilst Lamb surfaces do not arise in all heterogeneous, isotropic 3d Darcy flows, there do exist certain quasi-2d flows that do admit Lamb surfaces. Whilst the results in this Section provide specific examples of Lamb surfaces occurring in quasi-2d flow, these examples do not provide a means of determining whether Lamb surfaces may occur in a specific flow. In the following Section we derive the conditions under which Lamb surfaces do and do not occur in steady, isotropic Darcy flow.

5 Conditions for Existence of Lamb Surfaces

To derive the conditions for the existence of Lamb surfaces in steady isotropic Darcy flow, we consider the analytic conditions for which the complex-lamellar condition (10) holds on the Lamb vector. Kelvin [13] and Piaggio [25] show that any continuous vector field $\mathbf{g}(\mathbf{x})$ is complex-lamellar if and only if the vector field can be expressed as

$$\mathbf{g}(\mathbf{x}) = p(\mathbf{x})\nabla q(\mathbf{x}), \quad (25)$$

for continuously differentiable scalars $p(\mathbf{x}), q(\mathbf{x})$. Hence the velocity vector $\mathbf{v}(\mathbf{x})$ for steady isotropic Darcy flow (1) is always helicity-free (7). The conditions for the Lamb vector

$\ell(\mathbf{x})$ to be complex-lamellar (and thus for Lamb surfaces to exist) may then be derived by expanding (8) in terms of the hydraulic conductivity $k(\mathbf{x})$ and potential $\phi(\mathbf{x})$. We first expand the Lamb vector in terms of these primitive variables as

$$\ell(\mathbf{x}) = a(\mathbf{x})\nabla\phi(\mathbf{x}) + b(\mathbf{x})\nabla k(\mathbf{x}), \quad (26)$$

where

$$a(\mathbf{x}) = -k(\mathbf{x})(\nabla k(\mathbf{x}) \cdot \nabla\phi(\mathbf{x})), \quad (27)$$

$$b(\mathbf{x}) = k(\mathbf{x})(\nabla\phi(\mathbf{x}) \cdot \nabla\phi(\mathbf{x})). \quad (28)$$

We also note that the CL condition may be expressed as

$$(\nabla \times \ell(\mathbf{x})) \cdot \ell(\mathbf{x}) = (a(\mathbf{x})\nabla b(\mathbf{x}) - b(\mathbf{x})\nabla a(\mathbf{x})) \cdot \omega(\mathbf{x}) = 0. \quad (29)$$

As such, the Lamb vector is complex-lamellar if and only if one or more of the following conditions holds:

1. $a(\mathbf{x}) = 0$,
2. $b(\mathbf{x}) = 0$,
3. $a(\mathbf{x}) = mb(\mathbf{x})$,
4. $\nabla\phi(\mathbf{x}) = \mathbf{0}$,
5. $\nabla k(\mathbf{x}) = \mathbf{0}$,
6. $\nabla\phi(\mathbf{x}) = n(\mathbf{x})\nabla k(\mathbf{x})$,
7. $a(\mathbf{x})\nabla k(\mathbf{x}) = b(\mathbf{x})\nabla n(\mathbf{x})$,
8. $b(\mathbf{x})\nabla\phi(\mathbf{x}) = a(\mathbf{x})\nabla n(\mathbf{x})$,
9. $a(\mathbf{x})k(\mathbf{x}) = b(\mathbf{x})\phi(\mathbf{x})$.

Here m is an arbitrary constant and $n(\mathbf{x})$ is an arbitrary scalar function. Condition (1) corresponds to the potential gradient being everywhere orthogonal to the conductivity gradient, which arises in e.g. stratified flow, or in the extruded domain case with fixed head BCs considered in the previous section. Conditions (2) and (4) only hold if there is no potential gradient, and so are considered a trivial case. Conditions (3) and (6) require the conductivity gradient to be everywhere parallel to the potential gradient everywhere, a trivial case. Condition (5) corresponds to homogeneous Darcy flow. Conditions (7-9) correspond to specialised flows where the conductivity field and/or boundary conditions must satisfy specialised forms that will not be satisfied for random heterogeneous fields.

As such, Lamb surfaces only exist in steady, isotropic 3d Darcy flow in the following (non-trivial) cases: (i) homogeneous media, (ii) heterogeneous media with a conductivity field that is invariant in one direction and where the potential gradient is either normal or parallel to the conductivity gradient. These somewhat restrictive conditions mean that the majority of steady, isotropic 3d Darcy flows do not admit Lamb surfaces, and so may involve truly 3d Lagrangian kinematics. Thus only a small subset of these flows involve Lagrangian kinematics which are 2d. This has important implications for the modelling of mixing, transport and dispersion in steady isotropic Darcy flows as 2d simulations are constrained have zero transverse hydrodynamic macrodispersion, which can be non-zero in truly 3d Darcy flow.

Whilst the presence of Lamb surfaces is a *sufficient* condition for 2d Lagrangian kinematics, the absence of Lamb surfaces is not a *necessary* condition for 3d Lagrangian kinematics. Indeed, there may exist other constraints on steady, isotropic Darcy flow which render the Lagrangian kinematics 2d which are unrelated to Lamb surfaces. This question is beyond the scope of the present study which is only concerned with Lamb surfaces.

It is also important to note that whilst the majority of steady, isotropic Darcy flows are 3d, they all involve smooth and regular (i.e. non-chaotic) Lagrangian kinematics due to the inherent helicity-free nature of these flows. Breaking of this constraint via either introduction of time-dependent flow [1, 24] or anisotropic hydraulic conductivity [34] is necessary for the attainment of chaotic advection.

6 Conclusions

We use numerical and theoretical methods to consider the question of whether the Lagrangian kinematics of steady, isotropic Darcy flow are 2d or 3d in nature. These kinematics have important implications for the understanding, quantification and modelling of dispersion, mixing and transport in heterogeneous porous media. We specifically test for the existence of *Lamb surfaces* in these flows which are 2d material surfaces first postulated by Lord Kelvin in 1884 [13] that are spanned by both streamlines and vortex lines. The existence of Lamb surfaces in steady, isotropic Darcy flow was proposed by Sposito over a series of studies [27, 28, 31, 30] based upon the helicity-free nature (i.e. the vorticity is everywhere perpendicular to the velocity) of these flows. As Lamb surfaces are material, they strongly constrain the Lagrangian kinematics of these flow, rendering them essentially 2d. As Lamb surfaces confine streamlines to 2d surfaces within the flow, their existence renders transverse macrodispersion *zero*, same as for 2d Darcy flow.

We show through both highly-resolved numerical simulations and theoretical analysis that Lamb surfaces are not ubiquitous to all steady, isotropic Darcy flows. Whilst Lamb surfaces are shown to exist for certain quasi-2d flows, numerical simulations (in the mesh-independent limit) of generic heterogeneous 3d Darcy flows do not admit Lamb surfaces. This is due to violation of the complex-lamellar condition on the Lamb vector (given by the cross product of the velocity and vorticity vectors), which is satisfied for any continuously differentiable vector field that this vector field must be everywhere perpendicular to its curl. Whilst the velocity fields of all steady isotropic Darcy flows are complex-lamellar, the existence of Lamb surfaces is dependent upon the *Lamb vector* of these flows being complex-lamellar.

Kelvin [13] and Piaggio [25] show that the complex lamellar condition for any vector field is satisfied if and only if the vector field can be represented as the product of an arbitrary scalar function multiplied by the gradient of another arbitrary scalar function. We expand the Lamb vector in terms of its primitive variables (the hydraulic conductivity and flow potential), and show that this condition is only satisfied for non-trivial or highly specialised steady isotropic Darcy flows which are either (i) homogeneous or (ii) the potential gradient is everywhere orthogonal or everywhere parallel to the conductivity gradient. This second condition is achieved for flows which are clearly already 2d in nature, whereas Lamb surfaces do not exist for arbitrary 3d Darcy flows.

Another implication of the existence of Lamb surfaces is that the fluid speed is constant along vortex lines [30]. We show conclusively that this acceleration is everywhere non-zero for heterogeneous Darcy flow, and this acceleration is directly related to the second derivative of the flow potential with respect to the velocity and vorticity direction. As this second derivative is non-zero for generic heterogeneous Darcy flows, this provides further evidence that Lamb surfaces are not inherent to such flows.

These results have significant implications for the understanding of transport, mixing and dispersion in steady, isotropic Darcy flows as the existence of Lamb surfaces renders the Lagrangian kinematics of these flows as essentially 2d, confining streamlines of these

flows to 2d lamellar material sheets that do not intersect. The finding that Lamb surfaces are not generic to steady, isotropic Darcy flows indicates that the Lagrangian kinematics of these flows may not be truly 2d.

It is important to note that this finding does not necessarily prove that such flows are truly 3d as there may exist different constraints (i.e. aside from the existence of Lamb surfaces) which render these flows 2d.

The absence of helicity in steady, isotropic Darcy flow render the Lagrangian kinematics of the flow non-chaotic [2, 29], i.e. streamlines do not form a space-filling tangle of chaotic orbits and the length $\ell(t)$ of fluid material elements cannot grow exponentially with time [1, 24] as $\ell(t) \sim \exp(\lambda t)$, but rather grow algebraically as $\ell(t) \sim t^\alpha$. Note this restriction does not necessarily hold for Darcy-scale flow in anisotropic porous media, as described by the tensorial Darcy equation $\mathbf{v}(\mathbf{x}) = -\mathbf{K}(\mathbf{x}) \cdot \nabla \phi(\mathbf{x})$, where $\mathbf{K}(\mathbf{x})$ is the anisotropic hydraulic conductivity tensor. Such flows can give rise to non-zero helicity density and chaotic streamlines, as observed numerically [7] and experimentally [34]. Similarly, at the pore-scale, even homogeneous media can generate helical flow trajectories and chaotic streamlines [21], with significant impacts upon mixing [20] and dispersion [22, 18]. As such, the topological constraint of zero helicity density imparts significant constraints upon the Lagrangian kinematics of steady, isotropic Darcy flow. In this study we have firmly established that these flows are not 2d due to Lamb surfaces. An attempt to answer this question more broadly is the subject of future investigation.

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