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Rayleigh-Darcy convection with hydrodynamic dispersion

Baole Wen,1,2,* Kyung Won Chang,2,† and Marc A. Hesse1,2,‡

1Institute of Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX 78712 USA
2Department of Geological Sciences, Jackson School of Geosciences, The University of Texas at Austin, Austin, TX 78712 USA

We investigate the effect of hydrodynamic dispersion on convection in porous media by performing direct numerical simulations (DNS) in a two-dimensional Rayleigh-Darcy domain. Scaling analysis of the governing equations shows that the dynamics of this system are not only controlled by the classical Rayleigh-Darcy number based on molecular diffusion, \( Ra_m \), and the domain aspect ratio, but also controlled by two other dimensionless parameters: the dispersive Rayleigh number \( Ra_d = H/\alpha_t \) and the dispersivity ratio \( r = \alpha_t/\alpha_l \), where \( H \) is the domain height, \( \alpha_t \) and \( \alpha_l \) are the transverse and longitudinal dispersivities, respectively. For \( \Delta = Ra_d/Ra_m > O(1) \), the influence from the mechanical dispersion is minor; for \( \Delta \lesssim 0.02 \), however, the flow pattern is determined by \( Ra_d \) while the convective flux is \( F \sim c(Ra_d) \cdot Ra_m \) for large \( Ra_m \). Our DNS results also show that the increase of mechanical dispersion, i.e. decreasing \( Ra_d \), will coarsen the convective pattern by increasing the plume spacing. Moreover, the inherent anisotropy of mechanical dispersion breaks the columnar structure of the mega-plumes at large \( Ra_m \), if \( Ra_d < 5000 \). This results in a fan-flow geometry that reduces the convective flux.

* wenbaole@gmail.com
† Present address: Geomechanics Department, Sandia National Laboratories, Albuquerque, NM 87123 USA
‡ mhesse@jsg.utexas.edu
I. INTRODUCTION

Convection in porous media controls mass and energy transfer in many natural and engineered applications [1–4]. This subject has received renewed interest due to its potential impact on geological carbon dioxide (CO\textsubscript{2}) storage, which allows large reductions of CO\textsubscript{2} emissions from fossil fuel-based electricity generation [5–7]. After the CO\textsubscript{2} is injected into the deep saline aquifers, it dissolves into the brine and increases the brine density. The dissolution of CO\textsubscript{2} eventually forms a stable stratification and ensures secure long-term storage [8, 9].

The rate of CO\textsubscript{2} dissolution is limited by mass transfer of dissolved CO\textsubscript{2} away from the CO\textsubscript{2}-brine interface. Diffusive mass transport may take millions of years to saturate the brine [10–12]. However, once the diffusive boundary layer of dissolved CO\textsubscript{2} in brine has grown thick enough, it might become unstable and subsequently, convection sets in and forms descending CO\textsubscript{2}-rich plumes. This process greatly increases the CO\textsubscript{2} dissolution rate and significantly reduces the leakage risk of buoyant CO\textsubscript{2} into potable aquifers or into the atmosphere [13].

Dynamics of porous media convection can be studied in either a ‘one-sided’ system where convection is driven by a source of buoyancy on only one boundary, e.g., the solutal convection system [14–20], or a ‘two-sided’ system where both of top and bottom boundaries actively drive the convection, e.g., the thermal convection system [17, 21–25]. These two systems share many common characteristics in convective pattern and transport properties, although dynamics in the former generally evolve over time while there exists a statistically-steady state in the latter [12, 17, 19, 23, 26, 27]. In this study, we focus on the two-sided convective system (Rayleigh-Darcy convection) to perform long-time direct numerical simulations (DNS) for reliable averaged results.

In the absence of mechanical dispersion, the flow pattern and transport flux of convection in porous media are generally thought to be controlled by the molecular Rayleigh number,

\[
Ra_m = \frac{k \Delta \rho g H}{\mu \phi D_m},
\]

where \( k \) is the medium permeability, \( \Delta \rho \) the density change between the fresh and the saturated water, \( g \) the acceleration of gravity, \( H \) the domain height, \( \mu \) the dynamic viscosity of the fluid, \( \phi \) the porosity, and \( D_m \) the molecular diffusion coefficient. At large \( Ra_m \), convection appears in the form of columnar plumes fed continually with a series of proto-plumes generated from the diffusive boundary layer [23, 25]. As \( Ra_m \) is increased, the inter-plume spacing \( \delta \) and the flux \( F \) in the quasi-steady convective regime follow specific power-law scalings of \( Ra_m \), i.e., \( \delta \sim Ra_m^{-\alpha} \) with the positive exponent \( \alpha \leq 0.5 \) [17, 23–26, 28, 29], and \( F \sim c \cdot Ra_m \) [19, 22, 23, 25–27, 29–34], where \( c \approx 0.0068 \) for the two-sided system and \( c \approx 0.017 \) for the one-sided system with fixed CO\textsubscript{2}-water contact at the top boundary [19, 23, 26, 29, 30, 35].

Nevertheless, recent bench-top experiments on solutal convection in porous media show that \( Ra_m \) does not control the convective pattern in typical granular media, because mechanical dispersion is the dominant dissipative mechanism [36]. Mechanical dispersion in porous media is due to non-uniformities in the flow that cause mixing of the solute [37–39]. The mathematical description of hydrodynamic dispersion on the Darcy-scale is a subject of active investigation [40–42], however, here we consider the commonly used Fickian dispersion tensor [43–50]. In an isotropic and homogeneous porous medium, this tensor is described by two parameters: the longitudinal and transverse dispersivities \( \alpha_l \) and \( \alpha_t \), respectively. Therefore, the hydrodynamic dispersion tensor in the fixed Cartesian reference frame can be expressed as

\[
D^* = D_m I + (\alpha_l - \alpha_t) \frac{\mathbf{u}^* \mathbf{u}^*}{|\mathbf{u}^*|} + \alpha_t |\mathbf{u}^*| I,
\]

where \( I \) denotes the identity tensor and the mechanical dispersion scales linearly with the interstitial fluid velocity \( \mathbf{u}^* \). As long as \( |\mathbf{u}^*| \ll D_m / \alpha_t \), \( D^* \approx D_m I \), so that molecular diffusion dominates over hydrodynamic dispersion; when \( |\mathbf{u}^*| \gg D_m / \alpha_t \), however, the mechanical dispersion starts to dominate.

Recent studies by [36, 46–54] indicate that hydrodynamic dispersion significantly affects the flow pattern and mass transport of convection in porous media under certain conditions. The numerical simulations by [47, 48] show that hydrodynamic dispersion enhances the convective mixing and greatly reduces the onset time for convection; however, recent laboratory experiments reveal that the mechanical dispersion coarsens the convective pattern and reduces the increase of convective flux with increasing permeability \( k \) [36, 51]. Particularly, the systematic experiments by [36] illustrate that adjusting \( Ra_m \) via changing the density difference \( \Delta \rho \) or the medium permeability \( k \) may result in distinct convective characteristics due to hydrodynamic dispersion. For fixed \( \Delta \rho \), increasing \( k \) (via choosing a larger glass bead diameter \( d \) as \( k \sim d^2 \)) raises \( Ra_m \) but enlarges the inter-plume spacing \( \delta \); for fixed \( k \), however, \( \delta \) is nearly fixed for increasing \( \Delta \rho \). Secondly, for fixed \( \Delta \rho \), the dissolution flux \( F \) does not increase linearly with \( k \) and is lower than expected at high \( k \); for fixed \( k \), in contrast, \( F \sim c(k) \cdot Ra_m \) with decreasing prefactor \( c \) as \( k \) is increased. Despite this decrease in flux, the vertical velocity, as measured by the speed of the fastest descending fingertip, increases...
approximately linearly with both $\Delta \rho$ and $k$. Some of the above findings contradict the classical predictions made in the absence of mechanical dispersion.

To understand the effect of dispersion on convection, we perform DNS in a two-dimensional (2D), rectangular, homogeneous and isotropic Rayleigh-Darcy domain. We aim to identify the dimensionless parameters governing convection in porous media with hydrodynamic dispersion, determine the scaling law for the quasi-steady convective flux, and quantify the contribution of molecular diffusion and mechanical dispersion to the hydrodynamic dissipation. As mentioned earlier, we focus on a two-sided convective system for long-time averaged results of individual simulations, but the results can be qualitatively applied to the one-sided case due to many common features in convection shared by these two systems [12, 17, 23, 26, 27].

The remainder of this paper is organized as follows. In the next section, we non-dimensionalize the system in a specific way so that the parameters controlling the pattern and the flux, respectively, are decoupled, and describe the numerical method to solve the dimensionless equations. In Sec. III, we present the DNS results in terms of different control parameters, including both the diffusion-dominant and dispersion-dominant limits. In Sec. IV, we analyze how hydrodynamic dispersion affects the convective pattern and flux, apply our results to recent laboratory experiments of solutal convection in bead packs, compare our results with previous numerical investigations in [47, 48], and discuss the limitations of the Fickian dispersion model. Our conclusions are given in Sec. V.

II. PROBLEM FORMATION AND COMPUTATIONAL METHODOLOGY

In previous studies, the dispersivity, $\alpha_d$ or $\alpha_t$, and the molecular diffusivity $D_m$ are combined to define the characteristic length and time scales or the Rayleigh number [47, 48]. In this work, however, we rescale the system using the domain height $H$, the buoyancy velocity $U = k \Delta \rho g / (\mu \phi)$, and the convective timescale $T_c = H / U$. As will be discussed in Sec. IV C, different scales for nondimensionalization may lead to ‘opposite’ conclusions. However, it will be shown below that the scales chosen in this study allow us to decouple the parameters controlling the flow pattern and the flux which simplifies the discussion. Based on these scales, we obtain the dimensionless equations

\[
\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = \nabla \cdot (\mathbf{D} \nabla C),
\]

\[
\mathbf{u} = -\nabla p - C \mathbf{e}_z,
\]

\[
\nabla \cdot \mathbf{u} = 0,
\]

where $C, \mathbf{u} = (u, w)$, and $p$ are the dimensionless forms of concentration, velocity, and pressure, respectively, and $\mathbf{e}_z$ is a unit vector in $z$ (upward) direction. The dimensionless hydrodynamic dispersion tensor is then given by

\[
\mathbf{D} = Ra_m^{-1} \mathbf{I} + Ra_d^{-1} \left[ (r-1) \frac{\mathbf{uu}}{|\mathbf{u}|} + |\mathbf{u}| \mathbf{I} \right],
\]

and characterized by the molecular Rayleigh number $Ra_m = U H / D_m$, defined in Eq. (1) and two additional parameters,

\[
Ra_d = \frac{U H}{\alpha_d U} = \frac{H}{\alpha_t} \quad \text{and} \quad r = \frac{\alpha_t}{\alpha_d},
\]

which are referred to as dispersive Rayleigh number and dispersivity ratio, respectively. Here, $D_t = \alpha_t U$ is the transverse dispersion coefficient, and the definition of the dispersive Rayleigh number is analogous to the definition of $Ra_m$ or the Peclet number based on the longitudinal/transverse dispersion coefficient [55]. Moreover, from the definition, the dissipation by mechanical dispersion increases with decreasing $Ra_d$. This allows us to easily recover the case without mechanical dispersion and to study the limit of high-$Ra_m$ convection.

It is worth noting that the dimensionless hydrodynamic dispersion tensor can also be written as

\[
\mathbf{D} = \frac{1}{Ra_h} \left\{ \mathbf{I} \left( 1 + 1/\Delta \right) + \frac{1}{1 + \Delta} \left[ (r-1) \frac{\mathbf{uu}}{|\mathbf{u}|} + |\mathbf{u}| \mathbf{I} \right] \right\}
\]

or

\[
\mathbf{D} = \frac{1}{Ra_m} \left\{ \mathbf{I} + \frac{1}{\Delta} \left[ (r-1) \frac{\mathbf{uu}}{|\mathbf{u}|} + |\mathbf{u}| \mathbf{I} \right] \right\},
\]

where

\[
Ra_h = \frac{U H}{D_m + D_t} = \frac{1}{\frac{1}{Ra_m} + \frac{1}{Ra_d}} \quad \text{and} \quad \Delta = \frac{D_m}{D_t} = \frac{Ra_d}{Ra_m}
\]
represent the effective Rayleigh number based on hydrodynamic dispersion and the ratio of molecular diffusion to mechanical dispersion, respectively. In addition, $1/\Delta = U_\alpha c / D_m$ can also be interpreted as a micro-level Péclet number based on a pore-scale length, i.e. the dispersivity $\alpha_c \sim d/r$. Therefore, diffusion is the dominant dissipative mechanism for $\Delta \gg 1$, so that $Ra_h \approx Ra_m$; similarly, mechanical dispersion is the dominant dissipative mechanism for $\Delta \ll 1$ and $Ra_h \approx Ra_d$.

The flow is assumed to be periodic laterally with an impermeable top and bottom boundaries. Solute concentration along the top and bottom boundaries is unity and null, respectively. Hence, the boundary conditions at the top and the bottom are given by

$$C|_{z=1} = 1 \text{ and } w|_{z=1} = 0; \quad C|_{z=0} = w|_{z=0} = 0.$$  \hspace{1cm} (9)

Note that the problem posed by (3) and (9) is formally identical to the two-sided thermal convection problem in which the domain is heated from below and cooled from above. Here, (3) and (9) are solved numerically using a Fourier-Chebyshev-tau pseudospectral solver developed in [25, 29], the temporal discretization is achieved using a three-step semi-implicit Runge-Kutta scheme [56], and the numerical scheme is parallelized using the Message Passing Interface (MPI). In order to obtain reliable averaged results, the DNS are performed up to $O(10^3)$ convective time units. The dispersivity ratio $r$ can vary from 1 to 30 in various field sites [57], and laboratory experiments and numerical simulations reveal that the transverse dispersivity is usually an order of magnitude less than the longitudinal dispersivity in advection dominated systems [58–62]. Thus, we set $r = 10$ in most simulations, but also explore how $r$ affects both the convective pattern and the flux when mechanical dispersion dominates the hydrodynamic dispersion at $Ra_d = 1000$.

To quantify the flow, we measure the convective flux $F$ at the top wall,

$$F = \left\langle \frac{\partial C}{\partial z} + \frac{Ra_m}{Ra_d} \left| u \right| \frac{\partial C}{\partial z} \right\rangle_{z=1} = F_m + F_d,$$  \hspace{1cm} (10)

where the angle bracket and the overbar denote the long-time and the horizontal averages, respectively, the first term on the right side of (10) represents the flux at the boundary via pure molecular diffusion $F_m$, and the second term represents the flux via mechanical dispersion $F_d$. We also measure the inter-plume spacing $\delta$ by time-averaging the dominant Fourier mode number in the interior, the mean horizontal velocity at the top wall, $\bar{u} = \langle |u| \rangle_{z=1}$, the mean vertical velocity in the interior, $\bar{w} = \langle |w| \rangle_{z=\frac{1}{2}}$, and the magnitude of the time-averaged $w$ extremum value in the interior, $w_m = \langle \max(|w|_{z=\frac{1}{2}}) \rangle$. In our study, these averaged results are all from individual simulations.

### III. RESULTS

To explore the effect of hydrodynamic dispersion on convection, numerical simulations and laboratory experiments can be conducted in different combinations of parameters, e.g. $Ra_h$ and $\Delta$, or density difference $\Delta \rho$ and grain size $d$. In this study, we perform DNS in terms of fixed $(Ra_m, r)$, $(Ra_d, r)$, and $(Ra_m, Ra_d)$, respectively. It will be shown below for fixed $r$, the parameters $Ra_m$ and $Ra_d$ predominantly control the flux and the pattern, respectively, in the dispersion dominated regime. However, in experiments it is difficult to change $Ra_d$ with fixed $Ra_m$ by varying $\Delta \rho$ and $d$, since the variation of grain size changes both $Ra_m$ and $Ra_d$ simultaneously.

#### A. Fixed $Ra_m$ and $r$

Figures 1 and 2 show the variation of the convective flow pattern and the corresponding averaged DNS results as a function of $Ra_d$ for $Ra_m = 20000$ and $r = 10$. When the smallest diffusive length scale $1/Ra_m$ is much larger than the pore scale of the medium $d/H$, i.e. $Ra_d \gg r Ra_m$ as $\alpha_t \approx d/r$ [38, 63], the molecular diffusion dominates the hydrodynamics dispersion [19, 23, 36]. Our DNS results reveal that only for $\Delta \equiv Ra_d/Ra_m \gtrsim 10^3$, the convection with mechanical dispersion converges to the classical columnar flow (Figs. 1f and 2).

When $O(1) < \Delta < O(10^3)$, the relatively weak mechanical dispersion slightly increases the plume width and enhances the convective transport, but the flow still retains the columnar structure (Figs. 1c and 2akb). For $\Delta < O(1)$, however, the mechanical dispersion starts to apparently affect the convective pattern and flux: the convection transitions to a fan flow with laterally expanding mega-plumes along the vertical flow direction (Fig. 1b–d), and the convective flux is reduced to approximately 50% of the high-$Ra_d$ value at $\Delta = 0.05$ (Fig. 2a).

Increasing dispersion thickens the diffusive boundary layer (Fig. 1a), smoothly the small-scale plumes near the walls, and stabilizes the flow (Fig. 1b–f). Eventually, the convection becomes steady at $Ra_d = 100$ (Fig. 1b) and the flux is again increased for $\Delta \leq 0.05$ due to the large magnitude of the effective diffusion coefficient, $(Ra_m/Ra_d)|u|$, induced
FIG. 1. Time-averaged horizontal-mean concentration profile $\langle C \rangle$ and snapshots of the concentration field $C$ from DNS at $Ra_m = 20000$ and $r = 10$ for different $Ra_d$. The domain aspect ratio is $L = 5$. In (a), only half of $\langle C \rangle$ is shown due to its antisymmetry about the mid-plane, and the $z$ values on the horizontal axis are non-uniformly spaced to clearly show the structure near the wall. Increasing mechanical dispersion (decreasing $Ra_d$) thickens the diffusive boundary layer, coarsens the flow pattern and stabilizes the flow. Moreover, the convection transitions to a fan-flow structure at $Ra_d < 5000$. by the mechanical dispersion (Fig. 2a). Moreover, it is also seen from Fig. 2(b) and (c) that hydrodynamic dispersion coarsens the flow pattern, given by $\delta$, and the mean buoyancy velocities at the top and in the interior, $\tilde{u}$, $\tilde{w}$ and $w_m$, roughly follow the same trend as the convective flux. It should be noted that the $w$ extremum value, $w_m$, becomes nearly constant for $0.025 \leq \Delta \leq 0.25$ (Fig. 2c).

B. Fixed $Ra_d$ and $r$

Figures 3 and 4 show the convective pattern and the corresponding averaged DNS results as a function of $Ra_m$ for $Ra_d = 1000$ and $r = 10$. The convection basically remains a fan-flow structure at $Ra_d = 1000$ as $Ra_m \to \infty$.
FIG. 2. Averaged DNS results of convection at $Ra_m = 20000$ and $r = 10$ for different $Ra_d$. The domain aspect ratio is $L = 5$. The dashed lines denote the results in the absence of mechanical dispersion and the dashed-dot line separates the fan-flow and the columnar-flow regions. Relatively weak mechanical dispersion slightly enhances the convective transport. However, as convection transitions to a fan-flow structure, the transport flux is significantly reduced. Nevertheless, in the strong-dispersion limit, the flow is stabilized and the flux is increased again due to the large magnitude of the effective diffusion coefficient.

FIG. 3. Time-averaged horizontal-mean concentration profile $\langle C \rangle$ and snapshots of the concentration field $C$ from DNS at $Ra_d = 1000$ and $r = 10$ for different $Ra_m$. For $Ra_m \leq 20000$, the domain aspect ratio is $L = 5$; while for $Ra_m > 20000$, DNS are performed in a small unit $L = 0.5$ where there only exists a single rising and descending mega-plume but the turbulent convection still sustains itself. In (a), only half of $\langle C \rangle$ is shown due to its antisymmetry about the mid-plane, and the $z$ values on the horizontal axis are non-uniformly spaced to clearly show the structure near the wall. For fixed $Ra_d = 1000$ and $r = 10$, the averaged and instantaneous concentration fields become nearly invariant at $Ra_m \gtrsim 50000$ (i.e. $\Delta \lesssim 0.02$).
FIG. 4. Averaged DNS results of convection at $Ra_d = 1000$ and $r = 10$ for different $Ra_m$. $L$ is as in Fig. 3. For fixed $Ra_d$ and $r$, the concentration field $C$, the inter-plume spacing $\delta$ and the buoyancy flow velocity $\mathbf{u}$ become invariant at sufficiently large $Ra_m$. Hence, as $Ra_m \to \infty$ the flux by molecular diffusion, $F_m = \langle \partial_z C \rangle |_{z=1}$, becomes constant, while the flux by mechanical dispersion, $F_d = \langle Ra_m/Ra_d \, |\mathbf{u}| \partial_z C \rangle |_{z=1}$, increases linearly with $Ra_m$. 

(Fig. 3b–f). In particular, the inter-plume spacing $\delta$ is nearly invariant when $\Delta \lesssim 0.2$ (Fig. 4b); the mean velocities $\bar{u}$ and $\bar{w}$ are roughly unchanged after $\Delta \lesssim 0.05$ (Fig. 4c); and the time-averaged horizontal-mean concentration profile $\langle C \rangle$ becomes almost fixed for $\Delta \lesssim 0.02$ (Fig. 3a), so that at the top and the bottom, the flux due to molecular diffusion (i.e. $F_m$) levels off (Fig. 4a). In short, at sufficiently large $Ra_m$, the flow pattern and the averaged system quantities (i.e. $\langle C \rangle$, $\delta$, $\bar{u}$, $\bar{w}$ and $w_m$) are independent of $Ra_m$.

Actually, as $Ra_m \to \infty$, the hydrodynamic dispersion tensor (4) reduces to

$$D \to Ra_d^{-1} \left[ (r - 1) \frac{\mathbf{uu}}{|\mathbf{u}|} + |\mathbf{u}| \mathbf{I} \right],$$

so that $Ra_d$ becomes the only parameter controlling the dynamics of the system for fixed $r$. Thus, at large $Ra_m$ the concentration field $C$ and the buoyancy velocity $\mathbf{u}$ are determined solely by the dispersive Rayleigh number $Ra_d$, as confirmed by our DNS data. Once $C$ and $\mathbf{u}$ become invariant in the limit of $Ra_m \to \infty$, $F_m \sim c_1$ and $F_d \sim c_2 \cdot Ra_m$ with the constants $c_1$ and $c_2$ determined by $Ra_d$, as shown in Fig. 4(a).

C. Fixed $Ra_m$ and $Ra_d$

In this section we explore how the dispersivity ratio affects the convective pattern and flux at $Ra_m = 20000$ and $Ra_d = 1000$, corresponding to $\Delta \sim 0.05$ where the reduction of the flux by dispersion is strongest (Fig. 2a). In the fixed domain, constant $Ra_d$ implies invariant transverse dispersivity, so increasing the dispersivity ratio $r$ only strengthens the longitudinal dispersivity.

As in Fig. 3(a) where $Ra_d$ is also fixed, when mechanical dispersion is the dominant dissipative mechanism varying $Ra_m$ or $r$ only slightly changes the boundary-layer thickness (Fig. 5a), which is predominantly controlled by the strength of transverse dispersivity (see detailed analysis in Sec. IV A). At $r = 1$, the hydrodynamic dispersion tensor $D$ is heterogeneous but isotropic, the high-$Ra_m$ convection remains a columnar structure (Fig. 5b), and the convective
FIG. 5. Time-averaged horizontal-mean concentration profile $\langle C \rangle$ and snapshots of the concentration field $C$ from DNS at $Ra_m = 20000$ and $Ra_d = 1000$ for different $r$. The domain aspect ratio is $L = 5$. In (a), only half of $\langle C \rangle$ is shown due to its antisymmetry about the mid-plane, and the $z$ values on the horizontal axis are non-uniformly spaced to clearly show the structure near the wall. When mechanical dispersion is the dominant dissipative mechanism at $Ra_d = 1000$, i.e. $\Delta \ll 1$, the high-$Ra_m$ convection in porous media remains a columnar structure at $r = 1$, but transitions to a fan-flow structure at $r > 1$. Flux is increased compared with that in the absence of mechanical dispersion (Fig. 6a). After adding isotropic velocity-dependent mechanical dispersion, the diffusion boundary layer is thickened so that more saturated water is advected downward/upward by columnar flows from the upper/lower layer. For $r > 1$, however, $D$ is both heterogeneous and anisotropic, and the convection transitions to a fan-flow structure (Fig. 5c-e). Increasing $r$ monotonically enlarges the inter-plume spacing $\delta$ (Fig. 6b) and decreases the convective flux and buoyancy velocity (Fig. 6a,c). Finally, for $r \geq 10$ the dynamics of the system become nearly invariant. Similar results have been observed in the one-sided convection problem [36].

D. Pattern formation and transport flux in the $(Ra_m, Ra_d)$ parameter space

In advection dominated systems, the dispersivity ratio, $r \sim O(10)$, is generally fixed [58–62]. A natural question concerns how the mechanical dispersion affects convection in the $(Ra_m, Ra_d)$ parameter space at $r = 10$. For $\Delta > O(1)$, the influence from the mechanical dispersion is minor, so that both the convective pattern and flux are mostly controlled by $Ra_m$; for $0.02 \lesssim \Delta < O(1)$, both the molecular diffusion and the mechanical dispersion are important to convection, e.g. they equally affect the flux at $\Delta \approx 0.05$; and for $\Delta < 0.02$, the mechanical dispersion dominates.
FIG. 6. Averaged DNS results of convection at $Ra_m = 20000$ and $Ra_d = 1000$ for different $r$. The domain aspect ratio is $L = 5$. In the absence of mechanical dispersion, the flux $F \approx 138$ at $Ra_m = 20000$, so the mass transport is enhanced after adding isotropic, velocity-dependent dispersion ($r = 1$). Increasing $r$ enlarges the inter-plume spacing and decreases the convective flux and buoyancy velocity. For $r \geq 10$, the averaged results become nearly invariant.

the hydrodynamic dispersion: the flow pattern is determined by $Ra_d$, e.g. $C = C(Ra_d)$, $\delta = \delta(Ra_d)$ and $u = u(Ra_d)$, while the flux is predominantly controlled by $Ra_m$, i.e. $F = F_m + F_d \sim c_1(Ra_d) + c_2(Ra_d) \cdot Ra_m \sim c_2(Ra_d) \cdot Ra_m$. Since $\Delta$ represents the ratio of molecular diffusion coefficient to transverse dispersion coefficient, in this study it is used to characterize when the mechanical dispersion becomes the dominant dissipative mechanism at given $Ra_m$ or $Ra_d$. However, the parameter $\Delta$ couples both the media and fluid properties, and determines neither the flow pattern nor the convective flux in the macro level. Our DNS results and analysis indicate that in dispersion-dominated regime (i.e. $\Delta < 0.02$), $Ra_d$ and $Ra_m$ are more effective parameters controlling the pattern and the flux, respectively, throughout the domain.

IV. DISCUSSION

A. Effects of dispersion on convective pattern and flux: mechanisms

Our DNS results and analysis above reveal that at sufficiently large $Ra_m$, the convective pattern is determined by the dispersive Rayleigh number $Ra_d$: the convection appears in the form of columnar flow at $Ra_d > 100 \cdot Ra_d$, where mechanical dispersion dominates the dissipation ($\Delta \ll 1$). Here we only show the variations of $c_1$ and $c_2$ as a function of $Ra_d$ for $Ra_d \leq 1000$ due to the expensive computations (Fig. 7). Our study above shows that the pattern of convection is determined by $Ra_d$ for $\Delta \ll 1$. Increasing dispersion (i.e. decreasing $Ra_d$) thickens the diffusive boundary layer and decreases the concentration gradient at the wall, thereby monotonically decreasing $c_1$, i.e. $c_1 \sim Ra_d^{0.74}$, as shown in Fig. 7(a). Moreover, for $Ra_d \leq 1000$ the prefactor $c_2$ increases with decreasing $Ra_d$ due to the large magnitude of the effective diffusion coefficient $(Ra_m/Ra_d)|u|$, i.e. $c_2 \sim Ra_d^{-0.51}$, as shown in Fig. 7(b).

We note that these scalings may not hold at large $Ra_d$, where the determination of $c_1(Ra_d)$ and $c_2(Ra_d)$ requires more systematic numerical simulations at extremely high $Ra_m$ (to ensure $\Delta \ll 1$).
FIG. 7. Variations of the prefactors (a) $c_1$ and (b) $c_2$ as a function of $Ra_d$ in the limit of $Ra_m \to \infty$ at $r = 10$. The solid lines denote the best power-law fit to the DNS data (circles). For each $Ra_d$, DNS are performed up to $Ra_m \sim 1000 \cdot Ra_d$ to determine $c_1$ and $c_2$.

FIG. 8. Schematics showing the distribution of the hydrodynamic dispersion tensor in the form of ellipses. (a): columnar flow in the absence of mechanical dispersion; (b): fan flow with mechanical dispersion. The arrows denote flow direction. In (a), $D^* = D_m I$ is homogeneous and isotropic; in (b), the anisotropy of the hydrodynamic dispersion leads to an asymmetry between the rising and the descending mega-plumes near the walls.

The mass conservation of the incompressible flow requires

\[ u^*_w \sim w^*_r \] near the wall. Hence, in advection dominated systems the inherent anisotropy of the mechanical dispersion, i.e. $\alpha_l \gg \alpha_t$ or $r \gg 1$, leads to $D^*_{xx,w} \gg D^*_{xx,r}$, and therefore the inter-plume spacing increases faster with dispersion than the plume width. This asymmetry results in the fan-flow structure and reduces the transport efficiency.

Below we show how the hydrodynamic dispersion affects the boundary-layer thickness and the convective flux using scaling analysis. In the absence of mechanical dispersion, the balance between advection and diffusion across the near-wall region yields the dimensional boundary-layer thickness

\[ \epsilon^* \approx \frac{D_m}{w^*} = \frac{U}{w^*} \cdot \frac{D_m}{U} = \frac{1}{w} \cdot \frac{H}{Ra_m} \sim \frac{H}{Ra_m}, \] (12)

since the dimensionless vertical buoyancy velocity $w$ converges to a constant value at sufficiently large $Ra_m$ [23]. And

the dimensional convective flux transported through the upper and lower boundary layers is

\[ F^* \approx D_m \frac{\Delta C}{\epsilon^*} \approx w^* \Delta C, \] (13)

where $\Delta C$ is the concentration difference between the fresh water and the saturated water. As the flux by pure molecular diffusion is $F^*_m \approx D_m \Delta C / H$, the dimensionless convective flux (i.e. the ratio of the transport in the place of the wall boundary layer) is

\[ F^* \approx D_m \frac{\Delta C}{\epsilon^*} \approx w^* \Delta C. \]
assuming increases Rayleigh number is \( [12, 17, 23, 26, 27] \). Qualitative predictions for the one-sided case due to many common features in convection shared by these two systems and analysis to those experiments. Although our DNS are performed in the two-sided system, they may provide in distinct convective characteristics due to hydrodynamic dispersion. In this section, we apply above DNS results media by [36] indicate that adjusting 

\[
\epsilon = \frac{\epsilon^*}{H} \approx \frac{1}{R_d}.
\]

Therefore, increasing dispersivity thickens the diffusive boundary layer. However, the form of the convective flux in Eq. (13) is not changed, because the reduction of flux due to the increment of boundary-layer thickness is made up by the simultaneous increment of effective diffusion coefficient. Since the buoyancy velocity is only determined by \( R_d \) as \( R_m \to \infty \) (Figs. 2c and 4c), Eq. (14) becomes

\[
F \approx w R_m \sim c(R_d) \cdot R_m.
\]

Namely, the convective flux is predominantly controlled by \( R_m \), but the prefactor is determined by \( R_d \).

B. Application for recent laboratory experiments of solutal convection in bead packs

As described in the introduction section, the laboratory experiments on (one-sided) solutal convection in porous media by [36] indicate that adjusting \( R_m \) via changing the density difference \( \Delta \rho \) or the grain size \( d \) may result in distinct convective characteristics due to hydrodynamic dispersion. In this section, we apply above DNS results and analysis to those experiments. Although our DNS are performed in the two-sided system, they may provide qualitative predictions for the one-sided case due to many common features in convection shared by these two systems [12, 17, 23, 26, 27].

In granular media, the mechanical dispersion is proportional to grain size, \( \alpha_t \sim d \), so that the appropriate dispersive Rayleigh number is \( R_d \) \( \approx \nu H/d \) [38, 63]. In experiments of [36], increasing \( d \) from 0.8 mm to 4 mm simultaneously increases \( R_m \) from \( 1.4 \cdot 10^4 \) to \( 5.0 \cdot 10^4 \) (\( \Delta \rho = 9.3 \text{ kg/m}^3 \)) but decreases \( R_d \) from 3750 to 750 (\( H = 30 \text{ cm} \) and assuming \( r = 10 \)), thereby reducing \( \Delta \) from 0.3 to \( 1.5 \cdot 10^{-3} \) (Fig. 9a). As shown in Fig. 9, most of the experiments

![Graph](image-url)
Many studies of porous media convection [46–49]. In this case, mechanical dispersion can be described by the standard pattern and the convective flux.

Moreover, for fixed $d$, the prefactor $c_2(R_d)$ is constant so that the convective flux, $F \sim c_2 \cdot R_m$, increases linearly with $\Delta \rho$; while for fixed $\Delta \rho$, $F$ is lower than expected at higher $d$ since the flow pattern transitions from columnar flow to fan flow as $R_d$ declines (Fig. 2a). However, this reduction in $F$ is accompanied only by a slight reduction in $w_m$ (Fig. 2c), which is consistent with the experimental observation that the speed of the fastest fingers increases approximately linearly with both $\Delta \rho$ and $k$ [36, 51].

**C. Comparison with previous numerical simulations**

As mentioned in the introduction section, previous investigations of [47, 48], utilizing the same Fickian dispersion model, reveal that hydrodynamic dispersion greatly reduces the onset time for convection and enhances the convective mixing. This seems to ‘contradict’ our numerical simulation results, which indicate that the hydrodynamic dispersion may change the flow pattern and significantly reduce the convective flux (Figs. 1 & 2). Below we show that this discrepancy is mainly due to different non-dimensionalizations and their interpretation. It should be noted that in those studies the dispersivity and buoyancy velocity are defined differently by scaling the porosity.

In [47], the longitudinal dispersivity $\alpha_l$ is introduced to characterize the timescale $\tilde{T} = (D_m + \alpha_l U)/U^2$. For stronger dispersion, i.e. increasing $\alpha_l$, the timescale $\tilde{T}$ is simultaneously increased, thereby resulting in a smaller dimensionless time $\tilde{t} = t^* / \tilde{T}$ (where $t^*$ is the dimensional time). Thus, as the dispersion is increased, the onset time, evaluated using $\tilde{t}$, can be significantly reduced at fixed molecular Rayleigh number $R_m$ and dispersivity ratio $r$, due to the increase of $\tilde{T}$. How hydrodynamic dispersion affects the onset of convection is beyond the scope of this contribution, but it is necessary to use the same characterize scales for comparison.

In [48], the molecular diffusivity $D_m$ and the longitudinal dispersivity $\alpha_l$ are combined to define the dimensionless parameters, namely,

$$\tilde{R}_a = \frac{UH}{D_m + \alpha_l U}, \quad \tilde{S} = \frac{\alpha_l U}{D_m + \alpha_l U}, \quad \tilde{\alpha} = \frac{\alpha_l}{\alpha},$$

where $\tilde{R}_a$, $\tilde{S}$ and $\tilde{\alpha}$ are, respectively, the effective Rayleigh number, the dispersion strength and the dispersivity ratio. Hence, these parameters are related to our work via

$$R_m = \frac{\tilde{R}_a}{1 - \tilde{S}}, \quad R_d = \frac{\tilde{R}_a}{\tilde{\alpha} \tilde{S}}, \quad r = \frac{1}{\tilde{\alpha}}.$$

The range of parameters for numerical simulations in [48] is shown in table I. For most of those simulations, the ratio of molecular diffusion to mechanical dispersion $\Delta > 1$, so that the mechanical dispersion is relatively weak. The simulation results in [48] reveal that with increasing $\tilde{S}$ from 0 to 0.7 at $\tilde{R}_a = 500$ and $\tilde{\alpha} = 0.2$, the dispersion enhances the mixing and reduces the onset of convection (see in particular their Figs. 5–10).

Although we have shown that the relatively weak mechanical dispersion slightly enhances the convective transport (Fig. 2a), in [48] the increment of flux and the reduction of onset time are because the corresponding molecular Rayleigh number $R_m$, which controls the convective flux, increases simultaneously with $\tilde{S}$ from 500 to 1667 (table I). Moreover, based on their simulation results at $\tilde{S} = 0.7$ and $\tilde{R}_a = 500$ for $\tilde{\alpha} = 0.1, 0.2, 0.5 & 1$, it is concluded in [48] that the dispersivity ratio has a very weak impact on the convective pattern and flux (see in particular their Figs. 11–13), which ‘contradicts’ our DNS results in Sec. III C.

This discrepancy is actually due to different ranges of parameters: the numerical simulations in [48] generally focus on the moderate-$R_m$ and weak-dispersion regime, while our DNS results indicate that at high $R_m$ and for strong mechanical dispersion (e.g. $R_m = 20000$ and $R_d = 1000$), the dispersivity ratio significantly affects both the flow pattern and the convective flux.

**D. Non-Fickian dispersion**

The DNS and analysis presented here are performed in the framework of the classical Fickian dispersion model. This relatively simple model can treat homogeneous porous media under certain conditions, and is therefore used in many studies of porous media convection [46–49]. In this case, mechanical dispersion can be described by the standard...
dispersion tensor, given by (4). This model ignores non-Fickian anomalous behavior, such as the scale dependence and solute tailing, which is commonly observed in solute transport experiments and field observations [40].

However, mathematical formulations that capture such anomalous behavior are typically particle based and hence not amendable to the DNS approach employed in most convection studies. We are not aware of any attempts to model convection in porous media with anomalous dispersion, in fact to date most numerical studies ignore dispersion entirely. Therefore, even the effect of the Fickian model on the dynamics of convection in porous media are poorly understood.

Hence, this study explores the first-order effect of hydrodynamic dispersion on the convective transport in porous media. Above we have argued that simulations based on the standard model of mechanical dispersion give results that are consistent with experiments performed in homogeneous bead packs [15, 36]. It appears that the key characteristics of mechanical dispersion required to explain these experimental data are its velocity and grain size dependence. Anomalous behavior is not evident in these experimental observations, which may be due to the relative homogeneity of the bead packs, the constant geometry of the experiments and the quasi-steady convective dynamics.

### V. CONCLUSIONS

We study the effect of dispersion on convective mixing in the 2D Rayleigh-Darcy scenario, where a statistical steady state can be obtained. Our DNS results and analysis reveal that the dynamics of this system in a sufficiently wide domain are controlled by three parameters: the molecular Rayleigh number, $Ra_m$, the dispersive Rayleigh number, $Ra_d$, and the dispersivity ratio, $r$. If mechanical dispersion is the dominant dissipative mechanism, for fixed $r$ the dimensionless convective flux is predominantly controlled by $Ra_m$, while the convective pattern is determined by $Ra_d$. This implies that convective flux and pattern are decoupled during porous media convection with dispersion. Moreover, when mechanical dispersion dominates the hydrodynamic dispersion, for fixed $(Ra_m, Ra_d)$ both the flow pattern and the flux are significantly affected by $r$: the high-$Ra_m$ convection remains a columnar structure at $r = 1$, but transitions to a fan-flow structure at $r \gg 1$ which reduces the convective flux.

Here we confirm that the linear flux scaling, $F \sim Ra_m$, also holds in the presence of hydrodynamic dispersion. However, this is only true if $Ra_d$ remains constant (e.g. same media property), since $Ra_d$ determines the prefactor of the scaling law. In practice, $Ra_m$ and $Ra_d$ commonly change together, because changes in grain size affect both permeability and dispersivity. This makes it difficult to observe the linear flux scaling in bead packs, where the flux does not increase linearly with permeability.

More specifically our simulations in advection dominated systems ($r = 10$) show the following:

- For $\Delta = Ra_d/Ra_m > O(1)$, molecular diffusion dominates the hydrodynamic dispersion, although relatively weak mechanical dispersion slightly enhances the convective transport.
- For $0.02 \lesssim \Delta < O(1)$, both the molecular diffusion and the mechanical dispersion significantly affect the convective pattern and flux.
- For $\Delta < 0.02$, mechanical dispersion dominates the hydrodynamic dispersion: the flow pattern is determined by $Ra_d$, e.g. $C = C(Ra_d)$, $\delta = \delta(Ra_d)$ and $u = u(Ra_d)$, while the flux is predominantly controlled by $Ra_m$, e.g. $F \sim c(Ra_d) \cdot Ra_m$.
- In the limit of $Ra_m \to \infty$, the flow still exhibits the columnar structure for $Ra_d > 5000$; however, for $Ra_d < 5000$ the convection transitions to the fan-flow structure, due to the inherent anisotropy of mechanical dispersion, which reduces the convective flux.

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<th>$\tilde{\alpha}$</th>
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<th>$r$</th>
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TABLE I. Range of parameters for numerical simulations in [48].
We note that the above criterions may vary quantitatively in other (e.g. the one-sided) convective systems, and many characteristics shown here are unlikely to be observed in the Hele-Shaw experiments, due to the absence of transverse mechanical dispersion [64].

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