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Direct numerical simulation of hydrodynamic dispersion in open-cell solid foams

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**HIGHLIGHTS**

- Axial Dispersion in open-cell foams scales non-linearly with the Péclet Number.
- Phenomenon equivalent to Taylor dispersion is observed for Darcy flow.
- Non-mechanical dispersion is induced by the appearance of stagnant zones.
- Hydrodynamic dispersion is governed by chaotic advection at high velocities.
- Dispersion coefficients have an inverse dependency on the particle diameter.

**ARTICLE INFO**

Keywords: Dispersion | Numerical study | Immersed boundary method | Open cell foams | Porous media | Volume averaging theory

**ABSTRACT**

Fully resolved simulations of flow and mass transfer in a unit cell of structured open-cell foam catalysts are presented. Numerical studies are conducted on a uniform three-dimensional Cartesian grid where the fluid-solid interface coupling is enforced via a sharp interface Immersed Boundary technique. Several validation cases for the numerical method are presented followed by extensive calculations to quantify hydrodynamic dispersion in open-cell foams. In our study five different porosities of the idealized foam structure, represented by the spatially periodic Kelvin’s unit cell, were considered. Dimensionless dispersion coefficients were calculated for varying Péclet numbers and flow directions using volume-averaging theory. Our numerical studies indicate that Taylor dispersion is the dominant mechanism for structured porous media in the Darcy-Brinkman flow regime.

1. Introduction

Open-cell solid foams have gained considerable interest over the past decades due to their various applications in the chemical industry, ranging from heat exchangers to vapourizers etc. More recently, they have been used as catalyst supports in fixed-bed reactors [1] as they provide a larger external surface area of reactivity per unit volume when compared to classical packing materials (ex. spheres). Open-cell foams, generally made of metals or ceramics, consist of interconnected struts forming a continuous network of randomly oriented or structured polyhedra. In fixed-bed reactors, the base cellular foam structure acts as a support over which the active catalytic material is washcoated. The open-cell network through the bed provides a tortuous flow path which enhances the heat and mass transport within the reactor.

Due to the complex geometrical structure of open-cell foams, most studies concerning transport in solid foams are based on experimental investigations. Numerical studies on complex porous media traditionally rely on coarse-grained models which are governed by volume-averaged transport equations. Generally, the volume-averaged models consider the fluid-solid porous media to be homogeneous [2] and the pore-scale fluid-solid interactions are represented in the model via closure terms [3]. These closure terms may be determined by performing Direct Numerical Simulation (DNS) [4] of the microscopic transport equations by resolving the detailed solid porous structure in a 3-D computational domain and also applying the appropriate fluid-solid interface boundary conditions. Lucci et al. [5] performed pore-scale simulations to study mass transfer in idealized open-cell foams and provided a closure for the Sherwood Number. The effective thermal conductivity of metal foams saturated in a stagnant fluid was studied by Boomsma and Poulikakos [6] and Krishnan et al. [7] by performing DNS using an idealized open-cell foam structure. Das et al. [8] numerically investigated heat transfer in open-cell foams generated using a micro-CT scan of a real foam sample to provide a Nusselt Number correlation. Rickenbach et al. [9] studied catalytic conversion in open-
cell foams using a multi-scale numerical model.

While the number of studies on transport in open-cell foams have increased over the past two decades [10], there exists little literature which addresses the detailed pore-scale interaction between flow and mass transport of solute particles through the fluid. Hydrodynamic dispersion accounts for the spread of a solute tracer through a porous medium due to spatial fluctuations in velocity of the fluid flowing through the media. Taylor [11] was the first to quantify dispersion and concluded that the spread of a solute can be characterized with the help of an ‘apparent diffusion coefficient’ as explained by Aris [12] who extended Taylor’s work to include the effect of molecular diffusion into the expression for ‘dispersion coefficients’. Brenner [13] later extended the Taylor-Aris theory to study dispersion of inert solutes in spatially periodic porous media. This provided a framework to perform computational studies on dispersion in porous media having complex geometries without needing to simulate the entire geometry of the structure. Following the work of Brenner [13], Carbonell and Whitaker [14] derived a framework to calculate dispersion coefficients in spatially periodic media using volume-averaging theory. They showed that their theory is analogous to Brenner’s ‘B-field’ theory and that it also reduces down to the Taylor-Aris theory for cylindrical capillaries. Kuwahara et al. [15] used an approach based on the volume-averaging theory of Carbonell and Whitaker [14] to numerically compute dispersion coefficients in a porous media comprising of arrays of square cylinders. Similar numerical studies have been performed since to study dispersion, primarily using simplified 2-D geometrical structures [16,17].

Direct Numerical Simulations have the distinct advantage to coarse-grained, empirical or semi-empirical models in that the pore-scale interactions of the fluid and solid are elucidated in great detail for visualisation and quantification purposes. It also allows one to perform a systematic parametric study (ex. the effect of porosity) which may be a tedious task when trying to measure dispersion coefficients experimentally using residence time distribution curves [18–20] and also helps capture the transition of the different regimes governing hydrodynamic dispersion as shown later. However, DNS requires the incorporation of the appropriate fluid-solid interface coupling wherein the interface boundary conditions are applied in a fully resolved manner across the entire three-dimensional solid geometry present inside the computational domain. In this numerical study we use the Immersed Boundary Method (IBM) developed by Deen et al. [4] and extended by Deen et al. [8] to ensure the accurate enforcement of the boundary conditions. The IBM employs a non-body conformal Cartesian grid where the fluid and solid phases are solved on a single uniform computational mesh. A general review of the broad range of Immersed Boundary techniques may be found in Deen et al. [21]. The IBM used in this manuscript may be classified under the ghost-cell approach wherein the boundary condition is enforced at the level of the discretized transport equations. A quadratic interpolation is used along the fluid cells neighboring the solid cells to recalibrate the discretized algebraic equations governing the transport in a control volume such that it experiences the effect of the solid in the neighboring cell(s).

In this manuscript we perform Direct Numerical Simulation of flow and mass transfer with the aim to study and quantify hydrodynamic dispersion in structured open-cell foams. A DNS model to quantify stream-wise dispersion based on the volume-averaging theory of Carbonell and Whitaker [14] applicable to spatially periodic porous media is presented in Section (2) along with the details of the geometric structure used to represent the spatially periodic foam cells. The numerical model and the Immersed Boundary Method used is presented in Section (2.3). Section (3) details the validation of the Immersed Boundary Method in application to measuring dispersion in other spatially periodic media. The results obtained on dispersion in open-cell foams are discussed in Section (4) with the conclusions presented in Section (5).

2. Governing equations and numerical details

2.1. Foam geometry

The open-cell foam structure may be ideally represented as a tetra-kaidecahedron or a Kelvin’s unit cell. A similar approach has been used by Krishnan et al. [7]; 22 and Das et al. [6], and the idealized representation is based on the proposition by Lord Kelvin [23] that the minimization of surface area of a foam sample in a given volume attains the shape of a tetra-kaidecahedron or a ‘Kelvin’s unit cell’. An advantage of the Kelvin cell structure is that it may be used as a basic periodic unit cell representation of the macroscopic matrix forming the open-cell foam structure. Also it has been found that the ordered Kelvin cell structure is a justifiable approximation to characterize realistic open-cell foams where the open-cell network has a more random distribution. The closures obtained for heat and momentum transport using the Kelvin cell agree well against the closures obtained by performing DNS on realistic open-cell foam structures [24]. Considering a spatially periodic medium also significantly reduces computational costs as mentioned before, as we require just one Representative Elementary Volume (REV) of the entire porous medium. However, appropriate periodic boundary conditions must be applied to simulate the fully developed profiles for flow and mass. Furthermore, we can also study the effect of different lattice structures by imposing a mean flow in different lattice directions using just one REV.

In this work the Kelvin’s unit cell is constructed with the help of 36 intersecting spherocylinders as shown in Fig. 1. The idealized foam structure contain struts having a cylindrical morphology and the REV consists of 6 square holes and 8 hexagonal holes. In order to create foams having different porosities we may either increase or decrease the ligament diameter (d1) by constraining Lp to be constant within the REV. l1 refers to the length of the ligaments forming the open-cell network as depicted in Fig. 1 and is kept constant with l1 = Lp/2√2. Foams with 5 different porosities (ε) are constructed (0.728, 0.813, 0.864, 0.920 and 0.962). The geometrical details of the Kelvin cells used in this study are presented in Table (1). The porosity of the medium, ε, is the fluid phase volume fraction where

\[ ε = \frac{V_f}{V} \]  

(1)

\[ V_f \] is volume occupied by the fluid within the REV and \( V \) is the total volume of the REV. The characteristic length of the foam sample is defined on the basis of the equivalent particle diameter (d_eq) as used in the Blake-Kozeny equation [25] to characterize pressure drop in porous media, with

\[ d_{eq} = \frac{6V_f}{A_i} \]  

(2)

Fig. 1. A single unit cell of open-cell foams depicted by the Kelvin’s unit cell and its geometrical details. Reproduced with permission from Das et al. [22].
where \( V_f \) and \( A_p \) represent the volume and surface area of the solid within the REV respectively.

### 2.2. Model description

The governing equations are solved on a uniform 3-D Cartesian domain. The mass and momentum balance for an incompressible Newtonian fluid reads

\[
\nabla \cdot \vec{v} = 0
\]

\[
\frac{\partial \rho}{\partial t} + \rho \nabla \cdot (\vec{v} \vec{v}) = -\nabla p + \nabla \cdot \vec{\tau}
\]

where \( \rho \) and \( \mu \) represent the fluid's density and viscosity respectively and \( \vec{\tau} \) is the stress tensor with \( \vec{\tau} = -\mu (\nabla \vec{v} + (\nabla \vec{v})^T) \).

The no-slip boundary condition is enforced along the fluid-solid interface with

\[
\vec{v} = 0 \text{ on } A_s
\]

and as we are considering a spatially periodic media, the flow field will also be spatially periodic such that

\[
\vec{v}(\vec{r} + i) = \vec{v}(\vec{r})
\]

where \( i \) is the position vector of any arbitrary point within the REV and\( i_1 \) represents the lattice vectors that map the periodic REV in 3 dimensions where \( i = 1, 2, 3 \) and \( i_1 \) corresponds to the 3 lattice directions \( (1 0 0), (0 1 0), (0 0 1) \) with \( |i_1| = L_p \).

The governing equation solved for the solute concentration is

\[
\frac{\partial \vec{c}}{\partial t} + \nabla \cdot (\vec{v} \vec{c}) = \nabla \cdot \vec{D} \vec{c} + q
\]

where \( \vec{\phi} \) is the molecular diffusivity of the solute tracer and \( q \) is a homogeneous volumetric source term and can be considered as a tracer input into the fluid to impose a concentration gradient across the REV. The solute is considered to be non-reactive and non-adsorbing, thus the solid phase is assumed to be inert and the fluid-solid interface boundary condition is given by

\[
-\nabla \vec{D} \vec{c} \cdot \vec{n} = 0 \text{ on } A_s
\]

The periodic boundary condition for concentration which satisfies the above system of equations is

\[
c(\vec{r} + i_1) = c(\vec{r}) + V_1 \cdot \nabla \vec{c}/|V_1|
\]

where \( V_1 \cdot \nabla \vec{c}/|V_1| \) refers to the macroscopic concentration gradient across the REV. Upon introducing a tracer source \( q \) into the macroscopic porous medium, the solute spreads across the fluid and under quasi-equilibrium conditions it should satisfy a mass balance across the REV. Following the work of Whitaker [26], the fluid phase averaged concentration within the REV is defined as

\[
\langle \vec{c} \rangle = \frac{1}{V_f} \int_{V_f} c \, dV
\]

Similarly, the interstitial velocity of the fluid in the REV is given by

\[
\langle \vec{v} \rangle = \frac{1}{V_f} \int_{V_f} \vec{v} \, dV
\]

The characteristic lengths of the Kelvin cell used in this study.

<table>
<thead>
<tr>
<th>Porosity (( \alpha ))</th>
<th>( L_p ) (mm)</th>
<th>( l/d_s )</th>
<th>( a_d ) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.962</td>
<td>10</td>
<td>4.50</td>
<td>1.257</td>
</tr>
<tr>
<td>0.920</td>
<td>10</td>
<td>3.00</td>
<td>1.929</td>
</tr>
<tr>
<td>0.864</td>
<td>10</td>
<td>2.25</td>
<td>2.668</td>
</tr>
<tr>
<td>0.813</td>
<td>10</td>
<td>1.875</td>
<td>3.291</td>
</tr>
<tr>
<td>0.728</td>
<td>10</td>
<td>1.50</td>
<td>4.344</td>
</tr>
</tbody>
</table>

Here, \( V_f \) refers to the volume of the fluid over which the variables are being averaged and in this case, is the volume occupied by the fluid within the REV. It must be noted that the constitutive set of equations given by Eqs. (3), (4), (5), (7) and (8) hold true for the entire macroscopic lattice structure while the periodic boundary conditions given by Eqs. (6) and (9) are applicable only across the REV. Following Carbonell and Whitaker [14], it can be assumed that the tracer spreads linearly across the REV thus giving us the balance as follows:

\[
q = \langle \vec{v} \rangle \cdot \nabla \langle \vec{c} \rangle
\]

Using the above relationship we obtain the magnitude of the concentration gradient across the REV

\[
|\nabla \langle \vec{c} \rangle| = \frac{q}{\langle \vec{v} \rangle}
\]

The orientation of the concentration gradient vector is discussed later in Section (2.4). Thus we now have a closed system of equations and boundary conditions which may be solved numerically.

### 2.3. The immersed boundary method

The governing equations are solved on a uniform 3-D Cartesian domain using a finite volume approach. The detailed description of the numerical procedure to solve the Navier-Stokes equations can be found in Das et al. [22] which focussed on deriving a pressure-drop correlation for open-cell foams. A transient solver is used for solving the governing equation for concentration with the convective flux being treated explicitly and the diffusive flux being treated fully implicitly. The source in Eq. (7) is uniform and homogeneous and is solved implicitly. The Total Variation Diminishing (TVD) min-mod scheme is used for spatial discretization of the convective flux and central differencing is used for the diffusive flux. The details of the spatial and temporal discretization of the transport equations can be found in Das et al. [8].

The key component of our numerical procedure is the Immersed Boundary (IB) Method [21] which is used to enforce the appropriate fluid-solid interface boundary conditions. The Dirichlet boundary condition for velocity (no-slip) and the Neumann b.c. for concentration are both enforced using the IB technique based on the works of Deen et al. [4] and further extended upon by Das et al. [8]. The algebraic discretized form of the governing equations at a control volume (CV) 'c' can be represented as

\[
a_i \phi_i + \sum_{a b} a_{a b} \phi_{a b} = b_i
\]

where \( \phi \) corresponds to one of the fluid velocity components or concentration. 'nb' indicates the cell-centre of the surrounding CVs. The coefficients 'q' arise upon discretization and are dependent on the fluid properties and grid resolution. All the explicit terms are contained in 'b'. For each 'IB-fluid' cell c, the interface boundary condition is imposed by calibrating the central coefficient \( a_c \), the term \( b_c \), and the neighboring coefficients \( a_{a b} \).

For enforcing the Dirichlet b.c., the value of \( \phi \) at the fluid-solid interface is already known. In Fig. 2a, the IB-fluid cell c neighbors a solid cell w and a fluid cell e. The value of \( \phi \) at the solid surface is a known value, \( \phi_s \), which in the case of velocity is \( v_s = v_f = v_c = 0 \), i.e. the no-slip boundary condition. To enforce the fluid–solid coupling, the transport quantity \( q \) in the solid cell w is first expressed as a linear combination of the neighbouring fluid cells in such a way that \( \phi \) equals \( \phi_s \) at the point on the solid surface indicated by 's'. To incorporate this, a quadratic fit with \( \phi = p\xi^2 + q\xi + r \) is applied along the direction of the stencil under consideration with \( \xi \) being the dimensionless distance measured from the solid cell w. The coefficients \( p, q \) and \( r \) are obtained from the known values of \( \phi \) at the interface (\( \phi = \phi_s, \xi = \xi_s \)) and the 2 fluid nodes, c (\( \phi = \phi_c, \xi = 1 \)) and e (\( \phi = \phi_e, \xi = 2 \)). The dimensionless distance \( \xi \) from the node w to the surface s is calculated analytically as

<table>
<thead>
<tr>
<th>Table 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>The characteristic lengths of the Kelvin cell used in this study.</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>-----------------------------------------------</td>
</tr>
<tr>
<td>0.962</td>
</tr>
<tr>
<td>0.920</td>
</tr>
<tr>
<td>0.864</td>
</tr>
<tr>
<td>0.813</td>
</tr>
<tr>
<td>0.728</td>
</tr>
</tbody>
</table>
In the solid cell node. The length of the second and rearranging the terms, we may express the Neumann and in cell node 2 where probes and are calculated respectively. The values of refer to the positional values of concentration at the are in the direction of the unit vector . Ideally the length of, 2 probes is chosen to be twice the length of the first probe, , using Eq. (22). Similarly, the concentration at the point on the surface can be evaluated using an interpolation technique as described below.

Expanding Eq. (20) up to the second degree using Taylor series with a step size , and rearranging the terms, we may express the Neumann b.c. algebraically as follows

\[ c_i = \frac{1}{3} 4c_i - c_{i-2} \left( \frac{j}{\phi} \right) |\hat{p}_1| \]  

where and refer to the positional values of concentration at the location of and respectively. The values of and are calculated by trilinear interpolation using the concentration field from the previous time-step. Hence, one can estimate the concentration at the fluid–solid intersection point on the surface can be evaluated using an interpolation technique as described below.

In the rare case that a fluid-solid intersection point is in close proximity to another solid cell, the second probe normal to that point may lie inside the solid phase. For such cases a first order interpolation is used where

\[ c_i = c_i \left( \frac{j}{\phi} \right) |\hat{p}_1| \]

It must be noted that the evaluation of is treated explicitly; however the fully implicit implementation of the Dirichlet b.c. framework maintains the stability of the solution. The validity of this Immersed Boundary Method for generic cases has been tested quite thoroughly by Das et al. [8] and more details regarding this can be found there. Further validation of the Immersed Boundary Method as a whole with regard to measuring dispersion is presented in Section (3).

2.4. Longitudinal dispersion

In Section (2.2) we formulated the constitutive set of governing equations and boundary conditions. In this section the task of measuring hydrodynamic dispersion in spatially periodic media is addressed. The methodology to measure dispersion coefficients is based off the works of Deen et al. [14] using volume averaging theory. The method used here is similar to the works of Kuwahara et al. [15] and Alshare et al. [17] who also used volume-averaging theory to study thermal dispersion in idealized 2-D systems.
Hydrodynamic dispersion may be defined as the measure of spatial fluctuations of the concentration of a solute induced by hydrodynamic effects over an ensemble of fluid elements constituting the porous medium. These spatial fluctuations of point concentration are caused by the disturbances of the solute’s velocity when traversing through the complex topology of the porous medium. Mathematically, hydrodynamic dispersion induced over an ensemble of fluid with volume \( V_f \) may be quantified as given by Whitaker [26]:

\[-\langle \bar{v} \bar{v} \rangle^f = \mathbf{D} \cdot \nabla (c) \]

(24)

where \( \bar{v} \) and \( \bar{v} \) represent the spatial deviations of point velocity and concentration across the fluid volume \( (V_f) \) respectively, with

\[ \bar{v} = \bar{v} - \langle \bar{v} \rangle^f, \quad \bar{v} = c - \langle c \rangle^f \]

(25)

We may now employ a mathematical translation to capture expression (24) as a function of the macroscopic concentration gradient as follows

\[-\langle \bar{v} \bar{v} \rangle^f = \mathbf{D} \cdot \nabla (c) \]

(26)

The above translation is commonly seen in turbulence modelling [27] and the assumption is referred to as the gradient diffusion hypothesis. In the above equation, the tensor \( \mathbf{D} \) is the hydrodynamic dispersion tensor and more detailed derivations of the dispersion tensor may be found among the works of Brenner [28]; 13; 14. Of the 9 components of the tensor, the off-diagonal elements are zero for spatially periodic media when the interstitial velocity is parallel to an axis of symmetry[29]. The cross-stream dispersion (lateral dispersion) coefficients though negligible, are generally of the same order \( O(\bar{v}) \) as molecular diffusivity up to Péclet Numbers of \( O(10) \) [30] for gas-solid systems.

The term of most interest in the dispersion tensor is the stream-wise dispersion (longitudinal dispersion) component \( (D_h) \) which measures the effective transport of the solute along the direction of macroscopic flow. In order to measure longitudinal dispersion, the macroscopic concentration gradient is imposed parallel to the interstitial velocity vector. Hence, the stream-wise dispersion component across a spatially periodic REV is measured as follows

\[ D_h = \frac{-1}{V_f} \left[ \frac{1}{|\nabla (c)|} \int_{V_f} (\bar{v} - \langle \bar{v} \rangle) (c - \langle c \rangle) \cdot \nabla (c) dV \right] \]

(27)

where \( \nabla (c) \) is a unit vector of the macroscopic concentration gradient given by

\[ \nabla (c) = \frac{\nabla (c)}{|\nabla (c)|} \]

(28)

As the gradient is imposed along the direction of macroscopic flow, the unit vector in Eq. (27) will have the same orientation as the interstitial velocity vector. Thereby, the periodic boundary conditions for concentration given by Eq. (9) is thus complete with the gradient in concentration also being applied parallel to the flow profile.

It must be noted that the system of governing equations, boundary conditions, and Eq. (27), used to measure hydrodynamic dispersion are equivalent to the original formulation by Carbonell and Whitaker [14] to measure longitudinal dispersion via volume-averaging theory using their ‘F-field’ equation. The formulation used in this paper is simpler to implement when performing expensive numerical calculations.

3. Verification and validation

The numerical technique and the model to study dispersion in spatially periodic media are thoroughly compared with existing literature. As an elementary verification test, we first study the classical Taylor-Aris dispersion theory to check the implementation of the Immersed Boundary Method and the approach to measure longitudinal dispersion.

3.1. Taylor-Aris dispersion theory

The Taylor-Aris theory describes dispersion of an inert solute in a fluid flowing through a long cylindrical tube. The original formulation by Taylor [11] is the measure of the hydrodynamic contribution to dispersion with the hydrodynamic dispersion found to be equal to \( \frac{1}{2} Pe^2 \). This hydrodynamic dispersion contribution is referred to as Taylor dispersion [31,29] and is calculated using Eq. (27). The ‘effective’ dispersion coefficient \( (D_h^e) \) which is the sum of the contribution of molecular diffusion and the hydrodynamic contribution as derived analytically by Aris [12] is expressed in dimensionless form as follows:

\[ D_h^e = \frac{D_h}{\bar{v}} = 1 + \frac{1}{48} Pe^2 \]

(29)

where the Péclet number is defined as

\[ Pe = \frac{R \bar{u}}{\bar{v}} \]

(30)

with \( R \) being the radius of the tube and the characteristic velocity \( \bar{u} \) being the average velocity of the fluid in the tube.

The above described case was replicated in a 3 dimensional Cartesian domain with the boundary conditions along the walls of the cylinder given by Eqs. (5) and (8) enforced using the Immersed Boundary Method. Periodic boundary conditions given by Eqs. (6) and (9) were applied along the direction of flow. A computational grid of size \( 80 \times 80 \times 80 \) was used with a resolution of 80 cells across the cylinder diameter (\( N = 80 \)) and 80 cells along the longitudinal direction for all cases. A very good agreement was found as shown in Fig. 3 with the dimensionless axial dispersion coefficients plotted for varying Péclet numbers. All data points plotted in Fig. 3 are within 2.20% absolute error from the analytical solution. A grid dependency analysis has been presented in Table (2) for \( Pe = 28.87 \).

3.2. Dispersion in square arrays of cylinders

The numerical model currently used is validated by comparison with numerical results obtained by other researchers. Axial dispersion coefficients were computed for flow through square arrays of cylinders and compared with the results of Edwards et al. [32] and Salles et al. [31].

The simulation domain consists of a single cylinder placed at the centre, with the boundary conditions given by Eqs. (5) and (8) enforced along the interface of the cylinder using the Immersed Boundary Method. Periodic boundaries given by Eqs. (6) and (9) were enforced along the walls of the domain.

The dimensionless dispersion coefficients were measured for varying Péclet numbers and 2 different porosities, \( \varepsilon = 0.590 \) and \( \varepsilon = 0.804 \). The Péclet number is defined as follows

\[ Pe = \frac{d_{cyl} \bar{u}}{\bar{v}} \]

(31)

where \( d_{cyl} \) is the diameter of the cylinder and \( \bar{u} \) is the characteristic velocity wherein for the case of Salles et al. [31] is the interstitial velocity \( (\bar{v}) \). It must be noted that the characteristic velocity used by Edwards et al. [32] to define their Péclet number is the superficial velocity \( (\bar{v}) = \varepsilon (\bar{v}) \) and not the interstitial velocity as described originally in their paper. This discrepancy was acknowledged by the authors in a later publication, Edwards et al. [33].

Edwards et al. [32] measured dispersion coefficients only for flow parallel to the in-line arrangement of the cylinders; i.e., the angle of flow is \( 0^\circ \) along the lattice direction (100). Salles et al. [31] studied dispersion for varying angles of flow through the periodic REV, starting from \( 0^\circ \), lattice direction (100), up to \( 45^\circ \), lattice direction (110).

Dimensionless dispersion coefficients \( (D_h^e) \) were measured for in-line arrays of cylinders at Stokes flow and varying Péclet numbers (by varying the Schmidt number) and compared with the results of Edwards et al. [32].
et al. [32] and Salles et al. [31] for flow along the directions \{100\} and \{110\}. As seen in Fig. 4, a satisfactory agreement is observed with Salles et al. [31] while an excellent match is obtained with the results of Edwards et al. [32]. All simulations portrayed in Fig. 4 were performed with a spatial resolution of 80 grid cells across the cylinder diameter ($N = 80$).

Edwards et al. [32] also measured dispersion coefficients for certain cases of finite Reynolds numbers. We once again find an excellent match with their results as shown in Table (3). Furthermore, a less stringent grid resolution is required for lower Schmidt numbers as depicted in the table when compared to the Stokes flow cases simulated in the former. This is attributed to the usage of uniform grids for our numerical technique.

<table>
<thead>
<tr>
<th>$Pe$</th>
<th>$D^*_f$ (Analytical)</th>
<th>Grid Size</th>
<th>$D^*_f$ (Numerical)</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>28.87</td>
<td>18.364</td>
<td>$40 \times 40 \times 40$</td>
<td>17.478</td>
<td>$-4.82%$</td>
</tr>
<tr>
<td>$-$</td>
<td>$-$</td>
<td>$80 \times 80 \times 80$</td>
<td>17.997</td>
<td>$-1.99%$</td>
</tr>
<tr>
<td>$-$</td>
<td>$-$</td>
<td>$120 \times 120 \times 120$</td>
<td>18.153</td>
<td>$-1.15%$</td>
</tr>
</tbody>
</table>

3.3. Dispersion in cubic arrays of spheres

Gunn and Pryce [34] experimentally investigated dispersion through a fixed bed packed with cubic arrays of spheres. The packing consisted of inert glass spheres having an in-line arrangement through the bed, thus replicating a spatially periodic medium with a bed porosity of $\varepsilon = 0.48$. The solute tracer was Argon with the convecting fluid being air. They studied the dispersion of Argon for varying Reynolds numbers by tabulating the respective Péclet numbers ($Pe_c$) measured for the case. They defined their Péclet number as follows

$$Pe_c = \frac{k^2/\nu}{D^*_f}$$

$$D^*_f = \frac{D^*_f(Edwards \ et \ al. [32])}{D^*_f(N = 20)}$$

$$D^*_f(N = 40)$$

$$D^*_f(N = 80)$$

Fig. 4. Dimensionless dispersion coefficients, $D^*_f$, against the Péclet number $Pe$, for Stokes flow in square arrays of cylinders. The present simulation results are validated with results from Edwards et al. [32] and Salles et al. [31].
where \( d_{sp} \) is the diameter of the sphere and \( D_1 \) is the axial dispersion component and the characteristic velocity being the interstitial velocity. With the Schmidt number of Argon fixed to be 0.77 (\( Sc = 0.77 \)), we may reconstruct the dimensionless axial dispersion coefficient (\( D^* = D_1 / \mathcal{D} \)) as a function of the Péclet number dimensioned using the molecular diffusivity as follows

\[
P_{em} = \frac{\nu_{eq} / d_{sp}}{\mathcal{D}}
\]

(33)

Our simulation domain consists of a single sphere enclosed completely on all 6 sides, replicating the periodic cubic packing of spheres. This inherently creates a packing of porosity \( \varepsilon = 0.48 \). A grid resolution of 80 cells across the sphere diameter was used for cases simulated in Fig. 5. The dimensionless dispersion coefficients (\( D^*_m \)) were calculated for varying Péclet numbers (\( P_{em} \)) and fixed Schmidt number (\( Sc = 0.77 \)), and compared with the results of Gunn and Pryce [34]. A very good agreement was found with the experimental values as shown in Fig. 5. Similar agreements were also observed by Salles et al. [31] and Koch et al. [29] when comparing their results against that of Gunn and Pryce [34].

4. Results and discussion

The system of equations described in Section (2.2) were solved in a cubic 3 dimensional computational domain. The REV consists of a unit cell of the idealized representation of the foam structure described in Section (2.1). We have considered 5 different porosities and 3 different flow directions for each porosity. 8 different flow rates were investigated for each direction and porosity, thus resulting in a cumulative total of 120 simulations. All simulations were performed on a mesh of size 200 × 200 × 200. The grid independence analysis is given in Appendix A. It must be noted that for all cases considered here the Schmidt Number was taken to be 1, where

\[
Sc = \frac{\nu}{\mathcal{D}} = 1
\]

(34)

with \( \nu \) referring to the kinematic viscosity of the carrier fluid. The particle Reynolds number of the system is defined as follows

\[
Re_p = \frac{\nu_{eq} / d_{eq}}{\nu}
\]

(35)

and the particle Péclet number as

\[
P_{ep} = \frac{\nu_{eq} / d_{eq}}{\mathcal{D}}
\]

(36)

with \( P_{ep} = Re_p \) for all cases investigated in this section. All results of the stream-wise (longitudinal) dispersion component, \( D^*_\parallel \), computed using Eq. (27), are non-dimensionalized by the molecular diffusivity of the tracer (\( \mathcal{D} \)), where the ‘dispersion coefficients’ \( D^*_\parallel \) are defined as

\[
D^*_\parallel = \frac{D_\parallel}{\mathcal{D}}
\]

(37)

The 3 different flow directions (across the periodic REV) studied in this section are shown in Fig. 6. The concentration gradient is imposed parallel to the direction of flow wherein the interstitial velocity vector

![Fig. 6. Orientation of the velocity and concentration gradient vectors considered in this study: (a) (100) (b) (110) (c) (111). Reproduced with permission from Das et al. [22].](image-url)
Fig. 7. Dimensionless dispersion coefficients $D^*$ as a function of the particle Péclet number $P_{ep}$ for different flow directions. Trend lines have been added to qualitatively illustrate the different regimes governing hydrodynamic dispersion.
Fig. 8. Dimensionless dispersion coefficients $D^*$ as a function of the REV Péclet number $Pe_{REV}$ for different flow directions.
is tangential to the planes \{100\}, \{110\} and \{111\} denoted using Miller Indices. The lattice directions considered, \{100\}, \{110\}, and \{111\}, are all planes of mirror (reflectional) symmetry. However, it is observed that hydrodynamic dispersion is greatly influenced by the orientation of the lattice structure as discussed later.

4.1. Effect of flow rate

Fig. 7 contains the master plots of the simulation results where the dispersion coefficients (\(D_p\)) are plotted as a function of the particle Péclet number (\(Pe_p\)) for different porosities and the 3 different flow directions. In general, we observe that hydrodynamic dispersion increases as the interstitial velocity in the porous medium increases, as seen in Fig. 7. This trend is not always monotonic and the exceptions to this are discussed in a later subsection. In order to measure stream-wise dispersion we impose a concentration gradient parallel to the direction of flow. The contours showing the spread of the tracer solute for different flow orientations and Péclet numbers are shown in Figs. 9–11. As the velocity in the porous medium increases, the velocity fluctuations are enhanced due to the enhanced drag experienced by the carrier fluid from the fibers. The amplified velocity disturbances cause the solute particles to be pushed in the lateral direction and then convected further downstream. As the solutes are being convected downstream, molecular diffusion triggers some of the solute particles to diffuse across the velocity streamlines enhancing dispersion. This combined contribution of convection and diffusion towards dispersion is analogous to Taylor dispersion in cylindrical capillaries. The analogy may be drawn based on 2 factors:

i. The velocity profile in ordered media such as Kelvin cells and cylindrical tubes is deterministic and spatially periodic
ii. Molecular diffusion will contribute towards hydrodynamic dispersion (\(-\langle \nabla C \rangle/'\)) independent of the Péclet number. If molecular diffusion is neglected, the hydrodynamic contribution term, \(-\langle \nabla C \rangle/'\), will be indeterminate irrespective of the velocity magnitude [29]. This arises from a situation when a solute particle travels along a specific streamline across the entire macroscopic porous medium without ever changing its trajectory.

The exception to the above 2 points arise when the velocity profile is uncorrelated within its original (initial) position or trajectory, or if there exist regions of closed streamlines. According to Koch et al. [29],

\(\|\)
dispersion in ordered porous media scales quadratically with the Péclet number equivalent to Taylor’s theory. The dimensionless hydrodynamic dispersion coefficient $D_a = a Pe^2$ where $a$ is a coefficient whose value depends on the structure of the porous media. For cylindrical capillaries, $a = \frac{1}{48}$ [11] and $a = \frac{1}{105}$ [35] for infinitely long parallel plates (Hele-Shaw Cells).

The numerical results obtained for the present case on Kelvin cells show that a quadratic dependency is indeed achieved with the particle Péclet number ($Pe_p$) in the Darcy-Brinkman flow regime for $Pe_p < 20$ [22]. The dimensionless dispersion coefficients are plotted against the particle Péclet number for the 5 different porosities considered for $Pe_p < 20$ in Fig. 12. The curve-fit analyses shows that $D_a$ scales as $Pe_p^2$ with the dispersivity coefficient ‘a’ having different values for different porosities and different orientations of the porous matrix. The contour plots for low Péclet numbers depicted in Figs. 9a, 10a and 11a indicate that the tracer solute is spread homogeneously across the entire REV sampling all points within the fluid phase. This uniform smearing of the solute may be attributed to the absence of closed velocity streamlines at low Péclet numbers.

For $Pe_p > 20$ it is observed that dispersion does not scale quadratically anymore with $Pe_p$ as seen in Fig. 7. The dispersion coefficients do not follow the same slope as observed in Fig. 12 for the Darcy-Brinkman flow regime ($Pe_p < 20$), with $D_a$ scaling lesser than $Pe_p^2$ for $Pe_p > 20$, coinciding with the transition into the Forchheimer flow regime [22]. This deviation from the $Pe_p^2$ dependency at moderately high Reynolds Numbers ($Re_p = Pe_p$) is attributed to the onset of the phenomenon termed as boundary layer dispersion by Koch and Brady [36]. For $Re_p > 20$, when inertial effects predominate viscous effects, regions of closed streamlines are observed. Stagnation zones start to appear at junctures where different struts intersect, stemming from the no-slip boundary condition imposed along the solid interface. The tracer solute particles which enter into these stagnant zones get trapped within and may only escape through molecular diffusion. Fig. 13 pictorially highlights regions in open-cell foams where boundary layer dispersion is prominent. As the solid phase is considered to be impermeable, the solutes are concentrated along the sharp hydrodynamic boundary layers. Additionally, as convective transport overshadows diffusive transport ($Pe_p > 20$), the time-scale over which the solutes escape from the boundary layers is much slower than the advection of solutes in the bulk stream. Boundary layer dispersion is probably a unique feature of consolidated porous media as it is quite evident even in the dilute limit. The interconnected network of ligaments generate regions of sharp
bends across the continuous solid phase which may not be seen in the dilute limit of unconsolidated porous media consisting of spheres or cylinders. The Koch and Brady [36] theory indicates that this non-mechanical contribution to hydrodynamic dispersion scales as a function of \( Pe \ln Pe \) which is qualitatively much different to the \( Pe^2 \) dependency of Taylor dispersion. The cumulative effect of Taylor dispersion and boundary layer dispersion at high Péclet numbers causes the hydrodynamic dispersion coefficient (\( D_p \)) to scale non-linearly but not quadratically with the Péclet number. Thus justifying the dependency observed for high Péclet numbers in Fig. 7, with \( D_p \) indicating a dependency lesser than the \( Pe^2 \) formerly observed in the Darcy-Brinkman regime.

At \( Re \approx 100 \) the flow profile transitions from a steady velocity field to a dynamic one. The behavior is initially quasi-steady with small oscillations [22] observed inside the inertial core and at \( Re \approx 200 \) the flow is fully unsteady. At the onset of dynamic flow (\( Re \sim 100 \)) it is observed that the velocity streamlines are periodic in time; i.e., the streamlines repeat themselves across the REV over a sample period of time. This enables the dispersion coefficient to be evaluated by averaging over the sample time period. Figs. 14 and 15 portray the quasi-steady behavior of the concentration profile. The concentration contour snapshots in Figs. 14 and 15 were taken 2500 and 3000 time-steps apart respectively, with the dispersion coefficient values also similar at the time the snapshots were taken. For \( Pe > 150 \) it is seen that the flow field oscillations increase greatly with the quasi-steady behavior breaking down. The enhanced velocity fluctuations result in good back-mixing of the solutes and the tracer is spread more evenly across the entire REV. A similar behavior is observed for dispersion in Taylor-Couette flows [37] when the symmetric Taylor vortices break to form wavy vortices. When this transition occurs, the quasi-steady patterns disappear with the solute now being spread in a chaotic manner. The ‘chaotic advection’ [38] of solutes which occurs as a result of this transition into wavy Taylor vortex flows causes the solutes which are trapped inside the vortex cores to escape and spread in a random manner across the domain. A similar phenomenon is captured here for dispersion in open-cell foams where the solutes trapped along the boundary layers are now advected across the REV in a chaotic manner. This is shown in Fig. 16 where 4 snapshots were taken 500 time-steps apart for \( Pe \approx 216 \). No quasi-steady patterns were observed with each snapshot depicting an uncorrelated transport of the solutes. In Fig. 7 it
is also observed that the slope which dispersion coefficients follow for $P_e > 150$ is qualitatively much different to the dependencies observed previously. According to Koch et al. [29], chaotic advection is a mechanical contribution to hydrodynamic dispersion and is independent of molecular diffusion unlike Taylor dispersion or boundary layer dispersion. This mechanical dispersion effect arises from a velocity field which is not correlated to its initial flow-path.

### 4.2. Effect of porosity

The general trend observed from the plots in Fig. 7 indicate that dispersion increases as the porosity (fluid phase volume fraction, $\varepsilon$) increases. Similar observations were made by Hutter et al. [19] in their experimental study of dispersion in metal foams. They claimed that dispersion coefficients increased with increasing the pore size of the metal foams for the same mass flow rate. This observation is also backed by the theoretical analysis of Koch and Brady [36] who provided an asymptotic solution for dispersion coefficients in the dilute limit ($\varepsilon \to 1$) for a bed of fibrous media. It is interesting to note here that dispersion coefficient correlations for classical fixed beds consisting of spherical particles have an inverse dependency on porosity. This is based on the correlation proposed by Koch and Brady [39] for a dilute bed of randomly packed spheres. Parthasarathy et al. [40] also observed that their numerically calculated dispersion coefficients for
ceramic open-cell foam structures increased with decreasing porosity. However, Parthasarathy et al. [40] used a different length scale to characterize the Péclet number as compared to the particle Péclet number ($Pe_p$) used here. This is the primary reason for the difference in dependencies.

Hydrodynamic dispersion is a measure of the spatial fluctuations of the microscopic convective flux ($\vec{v} \cdot \vec{f}$) and is thus strongly dependent on the velocity fluctuations induced by the porous solid in the bed. Intuitively it would seem that $D_0^* \rightarrow 0$ as the solid phase fraction reaches 0 ($\varepsilon \rightarrow 1$). This is true because the velocity fluctuations diminish as the volume of solids decrease. At $\varepsilon = 1$, each point in the microscopic velocity field equals the macroscopic superficial velocity, $\langle \vec{v} \rangle = \varepsilon \langle \vec{v} \rangle'$, thus giving $\langle \vec{f} \rangle' = 0$. This trend is observed in our simulation results if we were to redefine the Péclet Number. Now we introduce a new REV Péclet number, $Pe_{REV}$, where

$$Pe_{REV} = \frac{\varepsilon^2 D_0^*}{\mu L^*}$$

The flow characteristics of the foam can be understood by observing the concentration and velocity contour plots (Fig. 13). The regions highlighted in red circles indicate zones of stagnation where solutes are trapped and can only escape through molecular diffusion.
The characteristic velocity used here is the superficial velocity and $L_p$ is the length of the periodic REV. The Péclet number is now normalized such that it is independent of the porosity of the solid media. Here, the characteristic length is the same for all porosities and only dependent on the volume over which we are averaging. Upon plotting the dispersion coefficients as a function of $Pe_{REV}$, we observe that the trend is reversed and dispersion is now decreasing as the solids volume fraction within the REV decreases, as seen in Fig. 8. The characteristic length used by Parthasarathy et al. [40] to define their Péclet number is the axial mixing length which scales linearly with the REV length ($L_p$), hence showing the same trend. The axial mixing length is based on the ‘cell mixing theory’ of Aris and Amundson [41] and extended by Prausnitz [42]. It is the length of an arbitrary unit cell over which the concentration gradient appears to have been diffused in a Fickian manner. This mixing ‘cell’, mainly used in anisotropic media, is essentially the REV for isotropic porous media.

In the previous subsection we established that $D^*_{app} = aPe_p^2$ for $Pe_p < 20$. Furthermore, in Fig. 12 it is seen that the dispersivity coefficient $a$ is proportional to the porosity of the medium, with the value of $a$ increasing as the porosity increases. According to the Koch and Brady [36] theory, the dependency of dispersion on porosity may be explained via the concept of hydrodynamic screening. They postulated that the velocity fluctuations induced by the cylindrical struts in a dilute fibrous bed decay only at large distances relative to the strut. The distance at which the velocity disturbances decay from the strut due to the ‘screening’ effect provided by the neighboring struts is termed the Brinkman Screening Length. Furthermore, the Koch and Brady [36] analysis yields that the coefficient $a$ for Péclet numbers dimensioned using the particle diameter such as $Pe_p$ is a function of the permeability of the medium. More specifically, the Brinkman length is the square root of the permeability ($\chi$) of the porous medium, and $\chi$ increases in the dilute limit. The permeability of open-cell foams as derived previously by Das et al. [22] is:

$$\chi = 0.0142 \frac{\varepsilon^{1.38} d_{eq}^2}{(1-\varepsilon)^{1.38}}$$

(39)

Thus it is quite evident from the above equation that the screening length ($\chi$) scales linearly with the particle diameter and has a strong non-linear dependency with porosity. In the dilute limit ($\varepsilon \rightarrow 1$), the Brinkman length increases as the porosity increases, causing the velocity fluctuations to decay at comparatively larger distances, thus justifying the sharp increments in the value of $a$ for decreasing values of $d_{eq}$.

![Concentration contour plots depicting the periodic behavior of hydrodynamic dispersion for flow along (100) direction, $\varepsilon = 0.962$. The contour snapshot (b) was taken 2500 time-steps after (a).](image1)

![Concentration contour plots depicting the periodic behavior of hydrodynamic dispersion for flow along (110) direction, $\varepsilon = 0.962$. The contour snapshot (b) was taken 3000 time-steps after (a).](image2)
as seen in Fig. 12. This relationship may not be fully evident for un-consolidated media where the dilute limit can easily be reached by decreasing the fiber density or decreasing the number of particles in the bed by keeping the diameter (size) of the particle constant. However, for a consolidated porous medium such as the one in consideration, the equivalent particle diameter ($d_{eq}$) has to be decreased in order to increase the porosity ($\varepsilon$) of the medium. Koch and Brady further claim that the screening length $\ell_s$ is the appropriate characteristic length for dimensionalizing the Péclet number. The numerical results obtained here however do not reflect this and it may be due to the fact that their analysis is restricted to the Stokes flow regime, while all simulations performed here are for $Re_p > 1$. Beyond the Stokes flow limit, it is also clear that the permeability of the medium does not have a linear relationship with the interstitial velocity\[22\]. Nevertheless, the isotropy of the medium allows us to reconstruct the correlation for hydrodynamic dispersion in a manner such that the dispersivity coefficient $\alpha$ is exempt from having any dependencies on porosity. Thus we define a new Péclet number $\mathcal{P}_e$ as a function of the porosity of the medium as follows

$$\mathcal{P}_e = \frac{[(\theta)]_1}{\mathcal{P}_{eq}} = \frac{\theta_{25}}{(1-\varepsilon)^{0.345}} = Pe_p \frac{\theta_{25}}{(1-\varepsilon)^{0.345}}$$

(40)

Fig. 17 contains the plots of the dispersion coefficients as a function of the new Péclet number $\mathcal{P}_e$. We observe that all the data points superimpose on to a master curve for a given lattice direction in the Darcy-Brinkman flow regime. The new dispersivity coefficient $\bar{\alpha}$ is now independent of the porosity of the medium and is a constant value differing for different lattice directions. The below correlation was obtained for $0 < \mathcal{P}_e < 25$ using a non-linear regression fit with an average deviation of 7.18%.

$$D_\parallel^* = \bar{\alpha} \mathcal{P}_e^2$$

(41)

The values of the new dispersivity coefficient $\bar{\alpha}$ for the 3 directions considered are given in Table (4).

4.3. Effect of flow direction

From Fig. 12 it is evident that hydrodynamic dispersion magnitude is highest for flow along the $\{111\}$ lattice vector. The dispersion magnitude for flow along $\{110\}$ is only a bit smaller compared to $\{111\}$, while for the $\{100\}$ case it is almost threefolds less in magnitude compared to the $\{111\}$ case for the same $Pe_p$.

For the $\{100\}$ case, a jet-like feature is observed at $Pe_p \approx 50$ (Fig. 9c) which flows right through the uniformly aligned square holes of the Kelvin cell. This jet flows unobstructed through the entire macroscopic porous matrix advecting most of the solutes in its core, very similar to the shear driven Taylor dispersion. The effect of boundary layer dispersion is minimal owing to the straight flow-path experienced by the carrier fluid. The drag experienced by the fluid is least in this direction [22], hence justifying the least magnitude of dispersion.

The unobstructed jet of fluid is absent for the $\{110\}$ case due to the angled alignment of the hexagonal holes of the Kelvin cell. However, 2
Fig. 17. Dimensionless dispersion coefficients $D^*$ as a function of the new Péclet number $\mathcal{P} = \frac{P e_{0.25}(1 - \theta)^{0.345}}{c_{\text{avg}}}$ for different flow directions.
measure hydrodynamic dispersion was presented in Section (3). Dispersion coefficients were numerically calculated using volume-averaging theory [14] for the isotropic Kelvin cell. A total of 120 simulations were performed to study the effect of porosity, flow rate and orientation of the macroscopic lattice structure by considering 5 different porosities (0.728 \( \leq \epsilon \leq 0.962 \)) and varying Pécelt numbers (1 < Pe < 280).

The increase in flow-rate enhances hydrodynamic dispersion due to the amplified velocity fluctuations. The increase in dispersion is monotonic for cases when the interstitial velocity is tangential to the (100) and (110) planes of the Kelvin cell lattice structure. The increase is not found to be monotonic for the (111) case due to the complex flow-path experienced by the carrier fluid. There exists a transitional regime for the (111) case where dispersion decreases at the onset of dynamic flow and then increases sharply owing to chaotic advection induced by the highly unsteady flow. At low Péclet numbers dispersion increases quadratically with the Péclet Number for Pe < 20 indicating Taylor dispersion like phenomena. For Pe > 20, the solutes get trapped along the hydrodynamic boundary layers due to the appearance of stagnant zones. The trapped solutes may only escape through molecular diffusion contributing to dispersion via a non-mechanical phenomenon termed as boundary layer dispersion.

The extensive numerical analysis indicates that hydrodynamic dispersion increases relative to the particle diameter (\(O(\sqrt[3]{\epsilon})\)) with increasing porosity (\(\epsilon\)). However the total magnitude of dispersion across the bed decreases with decreasing solids volume. The direct dependency of dispersion on porosity in dilute fibrous beds having a cylindrical morphology was earlier predicted theoretically by Koch and Brady [36]. A correlation was proposed to measure Taylor dispersion as a function of a new Péclet number, \(\mathcal{P}\), which is non-dimensionalized to capture the open-cell structure characteristics as a whole. The correlation is valid in the Darcy-Brinkman flow regime (0 < \(\mathcal{P}\) < 25) and \(\mathcal{Sc} \approx 1\) with an average deviation of 7.18%. The transition of flow into the Forchheimer regime results in inertial effects which causes boundary layer dispersion followed by the unsteady chaotic advection. It was found to be extremely cumbersome to numerically quantify the subtle effects of boundary layer dispersion and the behavior of chaotic advection. Thus no correlation is proposed to measure these two effects, while their trends may be observed in Fig. 7.

The non-linear scaling of dispersion with the particle Péclet number indicates that dispersion is an important feature of mass transport in open-cell foams, even at high Reynolds numbers. The inverse dependency of dispersion on the particle diameter is a unique feature in dilute fibrous beds. This allows one to construct highly porous catalyst supports of open-cell foams in reactors without inhibiting the micromixing of the reactants. The added advantage of lower pressure-drops at high porosity [22] is further evidence that open-cell foams are attractive as catalyst supports compared to spherical particles in fixed bed reactors.

**Acknowledgement**

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### Appendix A. Appendix

The grid independence analysis is presented in Table (5) for measuring dispersion in open-cell solid foams. A grid independence analysis is presented for dispersion in the most dense foam considered of porosity 0.728. The analyses indicates that the mesh of 200 × 200 × 200 used for all

<table>
<thead>
<tr>
<th>Lattice Direction</th>
<th>(\mathcal{I})</th>
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<tbody>
<tr>
<td>(100)</td>
<td>0.00442</td>
</tr>
<tr>
<td>(110)</td>
<td>0.01377</td>
</tr>
<tr>
<td>(111)</td>
<td>0.01611</td>
</tr>
</tbody>
</table>

streams of fluid, each at the entrance and exit regions of the cell join together at the inertial core to form one small jet at the center of the cell. The inertial core advects much of the solute, nonetheless, boundary layer dispersion is quite prominent at high Péclet Numbers as seen in Fig. 10. As the Péclet number increases the highly unsteady flow-field causes a thorough mixing of the solutes across the REV and most of the solutes are pushed into the stagnant zones seen in Fig. 11d. The velocity and concentration field is fully steady and the corresponding dispersion coefficient value was calculated to be \(D_\theta^f \approx 478\). At Pe \(\approx 81\), the flow profile is quasi-steady and the time-averaged dispersion coefficient was found to be \(D_\theta^m \approx 184\). The concentration contour plot for Pe \(\approx 94\) for \(\epsilon = 0.920\) seen in Fig. 11d indicates that there is good micro-mixing of the solutes in the recirculation zones. However, the global mixing of the solutes across the REV is poor thus resulting in a decrease in dispersion. This is complimented by the fact that Taylor dispersion is essentially negligible due to the absence of an advective jet. The hydrodynamic dispersion at Pe \(\approx 81\) for \(\epsilon = 0.962\) is purely mechanical with the solute particle unable to sample points across the REV due to the negligible role of molecular diffusion, hence justifying the decrement from the Pe \(\approx 40\) case where diffusion is still prevalent. As the Péclet number increases further (Pe \(\approx 175\)) the highly unsteady flow-field causes a thorough mixing of the solutes across the REV resulting in a dramatic increase in hydrodynamic dispersion (\(D_\theta^m \approx 668\)). The non-monotonic behavior of dispersion in porous media has also been observed in other systems such as densely packed beds [30] and Taylor-Couette systems [43] and is not unique to the case studied here.

5. Conclusion

Pore-scale simulations were performed to study the effect of momentum transfer on the mass transport of a passive tracer in open-cell foams. The Navier-Stokes equations and the species balance equation were solved on a uniform three-dimensional Cartesian grid. The solid phase was an idealized spatially periodic representation of open-cell foams described by a Kelvin’s unit cell. The Kelvin’s cell was artificially constructed within the computational domain using 36 spherocylinders. The fluid-solid interface coupling given by the no-slip boundary condition and the zero-flux boundary condition were enforced using a second order accurate Immersed Boundary Method. The implementation of the IBM was described in detail in Section (2.3). The validation of the Immersed Boundary technique and the model to support investigational purposes of the Netherlands. This work was carried out on the Dutch national e-infrastructure with the support of SURF Cooperative. The authors thank SURF SARA (www.surfsara.nl) and NWO for the support in using the Cartesius supercomputer.

### Table 4

Values of the new dispersivity coefficient \(\mathcal{I}\) appearing in Eq. (47).

<table>
<thead>
<tr>
<th>Lattice Direction</th>
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<td>(111)</td>
<td>0.01611</td>
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Table 5

<table>
<thead>
<tr>
<th>$P_D$</th>
<th>$D_D (100 \times 100 \times 100)$</th>
<th>$D_D (200 \times 200 \times 200)$</th>
<th>$D_D (320 \times 320 \times 320)$</th>
</tr>
</thead>
<tbody>
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<td>1.013</td>
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<td>0.00642</td>
<td>0.00657</td>
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<tr>
<td>273.69</td>
<td>145.27</td>
<td>172.48</td>
<td>186.57</td>
</tr>
</tbody>
</table>

simulations differs by less than 2.5% compared to the finer grid (320 $\times$ 320 $\times$ 320) for low Péclet Numbers and less than 8% for the extreme cases at high Péclet Numbers.

Appendix B. Supplementary data

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.cej.2018.10.017.

References