Asymptotic behavior of dilution index in steady Darcy flows through heterogeneous porous media

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Abstract :

The dilution index E is an indicator of mixing of inert solute clouds in heterogeneous porous media. Its maximum value is theoretically known to increase monotonically in steady Darcy flows through isotropic heterogeneous porous media. Our numerical results allow us to test this hypothesis by establishing the relationship between the slope a of maximum dilution index E_{max} and the averaged positive second invariant Q_{av} of deformation tensor $\nabla \mathbf{u}$. The parameters of this relationship depend on molecular diffusion and dimensionality of problem considered.

Keywords : *Heterogeneity, Darcy flow, Second invariant of deformation tensor, Dilution index*

1 Introduction

Studying the transport behavior of inert solutes through heterogeneous geological formations is important for many environmental and hydrogeological problems such as enhanced oil recovery, geothermal energy development, remediation of contiminated groundwater, and carbonate storage (Nowamooz *et al.*, 2013 ; Wang *et al.*, 2014). During the transport of inert solutes in these same geologicial formations, three main mechanisms are involved : advection, molecular diffusion and dispersion. They are responsible for the mixing of inert solutes, combinaison of spreading and dilution that changes the size of inert solute clouds and the water volume occupied by the inert solutes (Dentz *et al.*, 2011 ; Herrera *et al.*, 2017). This physical process can be quantified by the dilution index E, introduced by Kitanidis in 1994. The dilution index E is a quantitative measure of the water volume occupied by inert solutes.

In their work, de Barros *et al.* (2012) have established the relationship between the Okubo Weiss parameter ζ and the dilution index E :

$$E(t) = \frac{4\pi D_m}{\sqrt{\zeta}} \sqrt{\frac{2(\zeta+\omega^2)}{\zeta} cosh(\sqrt{\zeta}t) - \frac{2(\zeta+\omega^2)}{\zeta} - (\omega t)^2} \tag{1}$$

with D_m the coefficient of molecular diffusion and ω the vorticity. This relationship shows that the dilution index E is controlled by the Okubo Weiss parameter ζ, characterizing flow topology. For incompressible flows in two dimensional porous media, the Okubo Weiss parameter ζ can be compared to the second invariant Q of deformation tensor $\nabla \mathbf{u}$ (Okubo, 1970 ; Dimotakis, 2005) :

$$\zeta(\mathbf{x}) = -4det(\nabla \mathbf{u}(\mathbf{x})) = -4Q(\mathbf{x}) \tag{2}$$

with $\mathbf{u}$ the Darcy velocity. Q quantifies the ratio between the vorticity ω and the shear rate τ (Hunt *et al.*, 1988 ; Jeong *et al.*, 1995). When Q is positive, ω dominates over τ. The fluid motion is then dominated by a rotation. Ohterwise the fluid motion is dominated by a contraction or a dilation.

In the case of Gaussian clouds injected in unbounded domains, the maximum value of the dilution index E_{max} can be defined as a function of second moments of solute clouds :

$$E_{max}(t) = (2\pi)^{n/2} exp(n/2)(det(\mathbf{S}(t)))^{1/2} \tag{3}$$

with $\mathbf{S}$ the second order moment tensor and n the dimension of the domain. By revisiting the Borden and Cape Cod experiments, Thierrin and Kitanidis (1994) observed that the maximum dilution index E_{max} should increase monotonically with a slope $a = dln(E)/dt \approx n/(2t)$, but the data did not show that an asymptotic behaviour is reached.

In this work, we verify this hypothesis by establishing the relationship between the slope a of maximum dilution index E_{max} and the averaged positive second invariant Q_{av} of deformation tensor $\nabla\mathbf{u}$.

2 Numerical model PARADIS

Based on the Monte Carlo approach, the numerical model PARADIS has been used to study the influence of heterogeneous hydraulic conductivity fields on macrodispersion in the past (Beaudoin *et al.*, 2013). In this work, the numerical model PARADIS is used to estimate the averaged positive second invariant Q_{av} from the Darcy velocity $\mathbf{u}$ and the maximum dilution index E_{max} from the second order moment $\mathbf{S}$. The model assumptions and numerical schemes, used to estimate the Darcy velocity $\mathbf{u}$ and the second order moment $\mathbf{S}$, are not recalled here.

2.1 Averaged positive second invariant Q_{av}

For an incompressible fluid, the second invariant Q of deformation tensor $\nabla\mathbf{u}$ is given by :

$$Q(\mathbf{x}) = -\frac{1}{2} trace((\nabla\mathbf{u}(\mathbf{x}))^2). \tag{4}$$

A first order central finite difference scheme was used for estimating the components of the deformation tensor $\nabla\mathbf{u}$ on a regular grid. The averaged positive second invariant Q_{av} of deformation tensor $\nabla\mathbf{u}$ is given by :

$$Q_{av} = \frac{1}{\Omega}\int_{\Omega} Q(\mathbf{x})d\Omega \quad \text{with} \quad \Omega = L_x \times L_y \quad \text{in 2D} \quad \text{and} \quad \Omega = L_x \times L_y \times L_z \quad \text{in 3D.} \tag{5}$$

Ω is the surface (in 2D) or the volume (in 3D) of the computational domain.

2.2 Maximum dilution index E_{max}

The dilution index E is given by :

$$E(t) = exp[\mathbf{S}(t)] \quad \text{with} \quad S_{ij}(t) = \frac{1}{M}\int_{\Omega}(x_i(t) - \bar{x}_i(t))(x_j(t) - \bar{x}_j(t))dM \tag{6}$$

where S_{ij} is an element of the second order moment tensor $\mathbf{S}$, M is the total mass of injected inert particles, x_i (or x_j) is the coordinate of the location $\mathbf{x}$ of a particle in the direction i (or j).

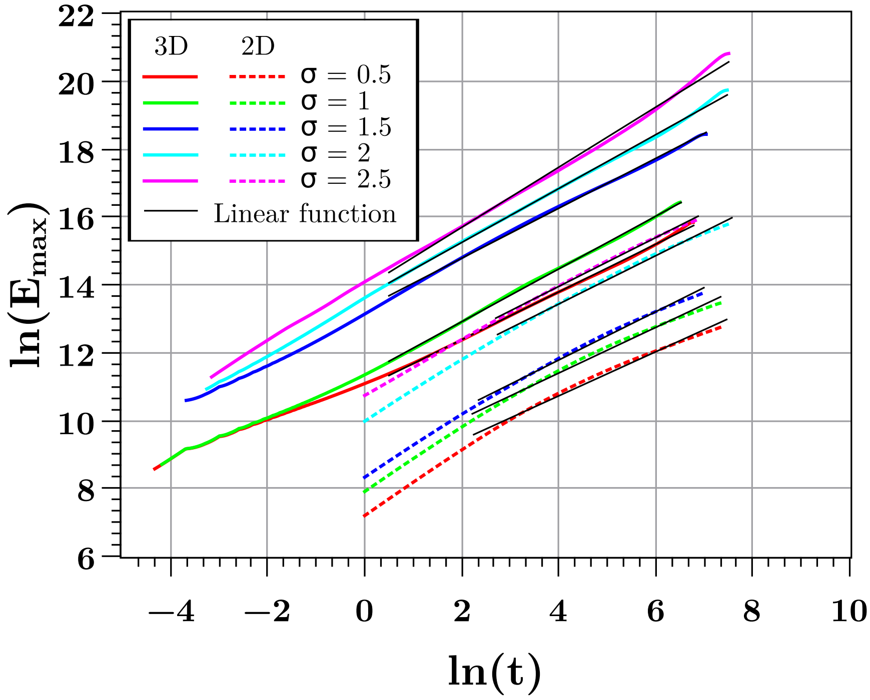

FIGURE 1 – Logarithm of maximum dilution index $ln(E_{max})$ as function of logarithm of time $ln(t)$ for various values of the hydraulic conductivity variance σ^2 with a Peclet number Pe = 20 in 2D and 3D.

3 Numerical results

In Figure 1, the logarithm of the maximum dilution index $ln(E_{max})$ is plotted as a function of the logarithm of time $ln(t)$ for various values of the hydraulic conductivity variance σ^2 with a value of Peclet number Pe = 20 in 2D and 3D. For $ln(t) > 3$, we can observe a monotonically increasing characterized by a constant slope, noted a, in 2D and 3D. a is indicated in the figure with a linear function (black solid line). This behavior is in agreement with the concept of dilution index, proposed by Kitanidis (1994). We can also observed that the dimensionality of the problem studied affects the value of the maximum dilution index E_{max}. E_{max} is higher in 3D than in 2D. The heterogeneity of the porous medium also has the same effect. E_{max} increases with σ^2 in 2D and 3D. These two findings have already been shown in the laboratory by Ye *et al.* (2015). Figure 2 presents the slope a as a function of the averaged positive second invariant Q_{av} of the deformation tensor $\nabla \mathbf{u}$ for various values of Peclet number Pe. In 2D and 3D, the behaviour of a is given by a power function (black solid line) :

$$a = a'(Q_{av})^{b'}. \tag{7}$$

Figure 3 shows the coefficients a' and b' as functions of Peclet number Pe. a' is given by an inverse function, $1.54/Pe + 0.73$ in 2D and $4.16/Pe + 0.93$ in 3D. b' seems to be a constant depending on the dimensionality of problem studied, 0.03 in 2D and 0.08 in 3D. The effect of molecular diffusion on the dilution has been identified in the past (Kapoor *et al.*, 1998 ; Rolle *et al.*, 2014). The maximum dilution index E_{max} decreases with the Peclet number Pe. The solute is more dilute for large values of diffusivity. This effect is taken into account with an inverse correlation between the parameter a' of the previous equation and the Peclet number Pe.

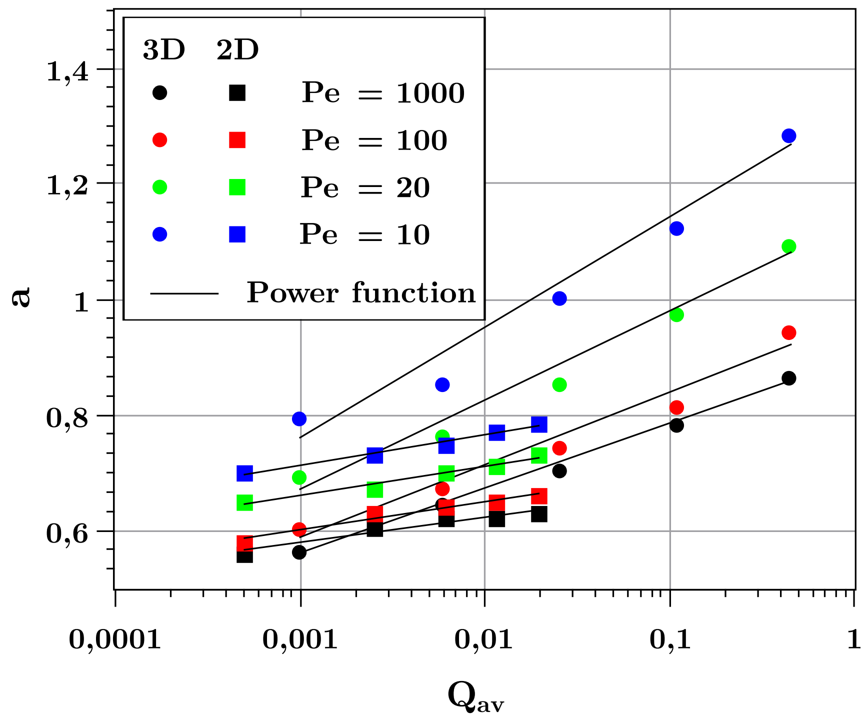

FIGURE 2 – Slope a characterizing the monotone increasing of maximum dilution index E_{max}, as function of averaged positive second invariant Q_{av} of deformation tensor $\nabla\mathbf{u}$ for various values of Peclet number Pe in 2D and 3D.

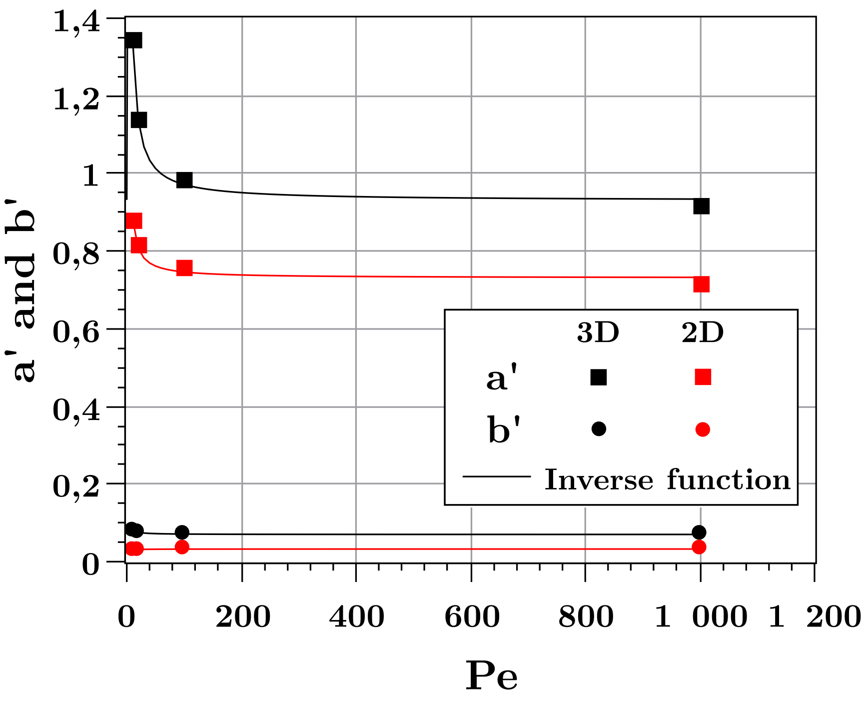

FIGURE 3 – Coefficients a' and b' of the relationship between the slope a and the averaged positive second invariant Q_{av} of deformation tensor $\nabla\mathbf{u}$ as functions of Peclet number Pe in 2D and 3D.

4 Conclusions

Mixing of inert solute clouds in steady Darcy flows through exponentially correlated lognormal hydraulic conductivity fields K was characterized by the maximum dilution index E_{max}. In his concept of dilution, Kitanidis (1994) showed theorically that this physical quantity should increase monotonically. The slope a of this monotonic increase was numerically determined. The relationship between the slope a and the averaged positive second invariant Q_{av} of deformation tensor $\nabla \mathbf{u}$ was etablished. In 2D and 3D, a power function relates the slope a and the averaged positive second invariant Q_{av} of the deformation tensor $\nabla \mathbf{u}$. The parameters of this power function depend on the Peclet number Pe and the dimensionality of the problem studied. These conclusions are specific to the model conditions studied.

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