



## Non-Fickian mixing: Temporal evolution of the scalar dissipation rate in heterogeneous porous media

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### ABSTRACT

We investigate the temporal scaling properties of mixing in heterogeneous permeability fields with variances ranging from very small ( $\sigma_{\ln K}^2 = 0.01$ ) to very large ( $\sigma_{\ln K}^2 = 9$ ). We quantify mixing by the scalar dissipation rate, which we estimate over a large range of temporal scales. For an initial pulse line injection, we find that moderate and strong heterogeneity induce anomalous temporal scaling of the scalar dissipation rate, which we call non-Fickian mixing. This effect is particularly relevant for upscaling reactive transport as it implies a non-Fickian scaling of reactive transport. Although spreading and mixing are intimately coupled, we find that their scaling properties are not directly related in general. In the non-Fickian mixing regime, the temporal scaling of the scalar dissipation rate depends on the complex spatial distribution of the concentration field that generates transverse mixing. For times larger than the characteristic diffusion time associated with one permeability field correlation length, the heterogeneity of concentration in the plume is attenuated and progressively erased by diffusion. Thus, at large times, the temporal scaling of mixing and spreading can be related through a simple analytical expression.

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### 1. Introduction

Mixing is a fundamental process that drives chemical reactions in fluids [40,11,43,14,15]. Understanding and predicting mixing is a key step for predicting reactive transport as it describes the rate at which reactants will meet. Therefore, it has attracted the attention of researchers across a range of scientific communities. In geophysical flows, mixing finds applications both in porous media flow [30,27,31] and in turbulent flows at various scales as found in oceanic and atmospheric flows [38,47,39]. Heterogeneous velocity fields, which fluctuate at multiple scales, are typical in these applications. The flow heterogeneity generates complex concentration distributions that enhance mixing (e.g., [38,44]).

For transport in heterogeneous porous media, a fundamental difference exists between the concepts of spreading and mixing [29,30]. Spreading describes the spatial extent of a solute plume, while mixing can be seen as the process that increases the actual volume occupied by the solute. Thus, the processes of spreading and mixing may be quantified in terms of (suitably defined) moments of the concentration distribution (e.g., [29,1,16–18]). Mixing can also be seen as the process that smoothes out concentration

contrasts, or in other words homogenizes a given (heterogeneous) concentration distribution. Various measures for quantifying mixing have been proposed. For example, the dilution index is a mixing measure based on entropy concepts [30] that quantifies the volume occupied by the solute. As such it measures the mixing state of a plume. On the other hand, the mean scalar dissipation rate defined from the local concentration gradients quantifies the mixing rate (e.g., [38]). The mixing state and mixing rate evolve with time in opposite directions.

Spreading and mixing are strongly coupled (e.g., [29,30]). Spreading is essentially driven by advective mechanisms and tends to enhance concentration contrasts, which in turn enhance mixing. Various studies on effective mixing and reactive transport for moderately heterogeneous media exist [25–27,22,35,10,21]. These are typically based on perturbation methods and restricted to moderately varying permeability fields. Mixing has not been analyzed for highly heterogeneous permeability fields. The high degree of heterogeneity implies that the large scale spreading of a solute plume is non-Fickian over a large range of times [36,23,4,3,12,34,32,37,50]. Non-Fickian spreading can be characterized by the scaling of the characteristic plume size,  $\sigma_1$ , defined as the standard deviation of the spatial distribution of concentrations:

$$\sigma_1^2(t) = \frac{1}{L_x} \int_{\Omega} d^d x [x_1 - \langle x_1(t) \rangle]^2 c(\mathbf{x}, t). \quad (1)$$

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where  $\langle x_1(t) \rangle$  is the center of mass coordinate of the plume in the direction of mean flow, which here is aligned with the one-direction of the coordinate system  $\Omega$  is the transport domain. The broad interest in non-Fickian spreading contrasts with the paucity of similar work on mixing. The objective of our work is precisely to investigate the relationship between non-Fickian spreading and non-Fickian mixing.

We start by introducing the mixing measure that we consider, the scalar dissipation rate and show that it is related to effective reaction laws. We propose an efficient numerical method to quantify the temporal scaling of the scalar dissipation with high accuracy. Using this method, we quantify the temporal scaling of spreading and mixing. We demonstrate the occurrence of non-Fickian mixing, even for cases that appear to be Fickian from a spreading perspective, and discuss its physical origin.

## 2. The scalar dissipation rate

We consider transport by diffusion and advection in a heterogeneous velocity field. We quantify global mixing by the scalar dissipation rate (e.g., [38,24,27,19,46,6]), which is a global measure of the mixing rate defined as

$$\chi(t) = \int_{\Omega} d^d x D \nabla c(\mathbf{x}, t) \cdot \nabla c(\mathbf{x}, t), \quad (2)$$

where  $D$  is the constant diffusion coefficient,  $c$  is the local concentration and  $d$  is the Eulerian dimension of space. Note that for simplification we do not consider a local dispersion tensor in this study. The methods and analysis presented can however readily be extended to take this into account.

The interest of the scalar dissipation rate as a mixing measure can be understood from the work of de Simoni et al. [14,15], which we briefly summarise here. Consider the transport of two reacting species of concentrations  $c_1(x, t)$  and  $c_2(x, t)$ , which react in equilibrium to produce a third immobile component  $c_3(x, t)$ . The governing equations can be written as

$$\frac{\partial c_i}{\partial t} + \mathbf{v}(\mathbf{x}) \cdot \nabla c_i = D \nabla^2 c_i + r(\mathbf{x}, t), \quad i = 1, 2 \quad (3)$$

and

$$\frac{\partial c_3}{\partial t} = -r(\mathbf{x}, t), \quad c_1 c_2 = K_c, \quad (4)$$

where  $\mathbf{v}(\mathbf{x}, t)$  is the velocity field,  $D$  is the diffusion coefficient, assumed to be identical for all components,  $r(\mathbf{x}, t)$  is the equilibrium reaction rate and  $K_c$  is the chemical equilibrium constant. A conservative component for this reactive transport system can be defined as  $c(\mathbf{x}, t) = c_1(\mathbf{x}, t) - c_2(\mathbf{x}, t)$ . Subtracting the transport equations (3) for  $c_1$  and  $c_2$ , it can be shown that  $c$  satisfies the pure advection diffusion equation, which is the same as (3) but with  $r = 0$ . This shows that  $c$  is indeed conservative.

Using (4) and the definition of  $c$  allows us to solve for  $c_1(c)$  and  $c_2(c)$ . Substituting the latter in (4), while using the fact that  $c$  is conservative yields

$$r_2(\mathbf{x}, t) = \left( \frac{d^2 c_2}{dc^2} \right) D \nabla c \cdot \nabla c, \quad (5)$$

where the first term  $d^2 c_2 / dc^2$  is called the chemical factor and depends on the specifics of the reaction (stoichiometry and equilibrium constant). The second term  $D \nabla c \cdot \nabla c$ , called the mixing factor, is exactly the integrand of the scalar dissipation rate defined in (2). From (5) we can define the global reaction rate as:

$$R_2(t) = \int_{\Omega} d^d x \frac{d^2 c_2}{dc^2} D \nabla c \cdot \nabla c. \quad (6)$$

When the chemical factor varies little over the range of  $c(\mathbf{x}, t)$  considered [21,42], it can be assumed to be almost constant and thus the global reaction rate is directly proportional to the scalar dissipation rate. Note however that when the chemical factor varies strongly with the mixing ratio such a global measure is not sufficient for predicting reactions [49,5]. In general, if the scalar dissipation rate temporal scaling is anomalous, i.e. the mixing process is non-Fickian, the reaction rate temporal scaling is also expected to be anomalous. Thus, understanding the scaling behavior of the scalar dissipation rate is an important first step for upscaling reactive transport.

One of the main difficulties in evaluating the scalar dissipation rate and reactions for that matter is the numerical calculation of the concentration gradients in Eqs. (2) and (6). The concentration field can vary sharply over small distances, particularly for highly heterogeneous velocity fields. An accurate quantification of concentration gradients requires a very fine discretization for Eulerian numerical schemes, where numerical dispersion can induce errors, or a very large number of particles for random walk approaches. Concentration gradients are very sensitive to numerical noise in the concentration field. To circumvent this issue, Fernandez-Garcia et al. [21] proposed an interpolation procedure to obtain a smooth concentration field from a limited number of particles. While appealing and useful in practice, such interpolation methods must be conducted with caution as they can lead to smoothing of actual gradients. A lack of resolution of these gradients can seriously compromise the ability of any model to accurately predict mixing and reactions [2].

Global mixing measures such as the scalar dissipation rate can be determined without the computation of the local concentration gradients. Instead one can evaluate the scalar dissipation rate from the integral of the squared concentration (e.g., [38]), defined as

$$M(t) = \int_{\Omega} d^d x c^2. \quad (7)$$

For advective–diffusive transport in a domain with no solute flux boundary conditions, the scalar dissipation rates can be expressed as

$$\chi(t) = -\frac{1}{2} \frac{dM}{dt}. \quad (8)$$

The equivalence of expressions (8) and (2) can be seen by multiplying the advection–diffusion equation in (4) for  $r(\mathbf{x}, t) = 0$  by  $c$  and integrating over space, using the divergence theorem. This is detailed in Appendix A. Notice that  $M(t)$  should not be confused with spatial or temporal moments of concentration. It quantifies the variability of the concentration values at a given time and not the temporal or spatial extent of the plume.

We now illustrate that calculating the scalar dissipation rate using Eq. (8) is significantly better than calculating it from local gradients of concentration (Eq. (2)). We solve the advection–diffusion equation for a homogeneous medium and an initial line injection using a particle tracking method. We take a permeameter geometry with homogeneous velocity  $v$  and diffusion coefficient  $D$ . Snapshots of the calculated concentration distributions are shown in Fig. 1. The time is normalized by the characteristic diffusion time over one pixel  $\tau_D = \Delta x^2 / D$  (here we take  $\tau_D = 3$ ), where  $\Delta x$  is the pixel size. The local concentration is normalized by the total mass so that  $\int_{\Omega} d^d x c(\mathbf{x}) = 1$ . For such system, the analytical solution for the scalar dissipation rate is obtained by replacing the ADE solution in Eq. (2), which yields,

$$\chi_{1D}(t) = \frac{C_0^2 L_y t^{-3/2}}{8\sqrt{2\pi D}}, \quad (9)$$

where  $C_0$  is the initial concentration and  $L_y$  is the size of the domain in the transversal direction.

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