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# Simplified numerical model for clarifying scaling behavior in the intermediate dispersion regime in homogeneous porous media

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ABSTRACT

The dispersion of solute in porous media shows a non-linear increase in the transition from diffusion to advection dominated dispersion as the flow velocity is raised. In the past, the behavior in this intermediate regime has been explained with a variety of models. We present and use a simplified numerical model which does not contain any turbulence, Taylor dispersion, or fractality. With it, we show that the non-linearity in the intermediate regime nevertheless occurs. Furthermore, we show that the intermediate regime can be regarded as a phase transition between random, diffusive transport at low flow velocity and ordered transport controlled by the geometry of the pore space at high flow velocities. This phase transition explains the first-order behavior in the intermediate regime. A new quantifier, the ratio of the amount of solute in dominantly advective versus dominantly diffusive pore channels, plays the role of 'order parameter' of this phase transition. Taylor dispersion, often invoked to explain the supra-linear behavior of longitudinal dispersion in this regime, was found not to be of primary importance. The novel treatment of the intermediate regime paves the way for a more accurate description of dispersion as a function of flow velocity, spanning the whole range of Péclet numbers relevant to practical applications, such as ground water remediation.

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## 1. Introduction

Transport of dissolved solutes in pore fluids in homogeneous porous media results from the synergy between advection and diffusion [1,2]. Despite its importance in many applications and fields of research (e.g., groundwater remediation), this process is not yet understood in full detail. Flow through a porous medium causes an increased effective diffusion of the solute, termed dispersion, due to variations in flow velocity within and between the individual pore channels and due to the tortuous pathways the fluid follows through the pores. The corresponding dispersion coefficients are commonly applied in models based on the advection–diffusion equation (ADE) to describe spreading of solute in porous media, for example pollutant plumes in ground water, although one should be aware that the ADE is only valid under rather restrictive conditions [3]. Although it is generally agreed that dispersion increases with flow velocity, there is no agreement on the exact relationship between the dispersion coefficient and controlling parameters, such as flow velocity, pore geometry, fluid viscosity, etc. [4].

To study solute transport in homogeneous porous media, a sample of fluid-filled porous material is subjected to an external pressure head in a specific direction (taken to be the $x$-direction). This results in a fluid flow velocity $v_0$ through the medium, usually expressed in terms of the Péclet number, $\mathrm{Pe} = v_0 G/D$, where $G$ is a typical microscopic length scale (grain size), and $D$ a ('molecular') diffusion coefficient (of the solute in the fluid). Then, the dispersion of an initially concentrated distribution of solute is studied as it is advected through the medium, while simultaneously experiencing diffusion.

The observed longitudinal ($D_x$) and transverse ($D_y$) dispersion as a function of Péclet number (flow velocity) is often described by a disjunct set of up to five dispersional regimes [5,2,6,7], using a separate functional relationship (sometimes referred to as 'correlation') between Péclet number and dispersion, $D_{x,y}(\mathrm{Pe})$, in each regime. Typically, the following regimes are discerned, although the boundaries between the regimes vary somewhat between authors: (i) The molecular diffusion regime ($\mathrm{Pe} < 0.1 - 0.3$); (ii) the transition regime ($0.1 - 0.3 < \mathrm{Pe} < 5$); (iii) the major regime (also known as the power law regime [8]) ($5 < \mathrm{Pe} < 250 - 4000$); (iv) the

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mechanical dispersion regime ($250 - 4000 < \mathrm{Pe}$); (v) the high Pe number regime, sometimes called the inertial or turbulent regime. Here, we are concerned with laminar flow only. We will jointly refer to regimes (ii) and (iii) as the 'intermediate regime', i.e., intermediate between the diffusive and mechanical dispersion regimes.

Quite often, the dispersion in each regime is described by a power law, i.e., $D_{x,y}(\mathrm{Pe}) \propto \mathrm{Pe}^{\alpha_{x,y}}$. Not surprisingly, for regime (i), $\alpha_{x,y} = 0$, while for regime (iv), $\alpha_{x,y} = 1$. However, in the intermediate regime, exponents differing from these limiting values have been reported to fit experimental data, which has given rise to speculation about their origin [9,7]. Reported values for $\alpha_x$ are $1.2 - 1.3$ ([9] and references therein; [7]), while those for $\alpha_y$ are typically around $0.5 - 0.7$ [10–12].

Recently, a simplified heuristic model was proposed to replace this disjunct description of dispersion by a single, unified expression [13,14]. The model assumes that the advective and diffusive transport mechanisms compete in the pore channels. Then, as the mean flow velocity (or pressure head) is increased, transport in more and more pore channels along the solute flow path through the medium will be advection-dominated. By making a simple assumption regarding the growth of the ratio between advection and diffusion dominated channels as the flow is increased, an expression for the net dispersion was derived. The expression successfully describes experimental data for dispersion in homogeneous porous media over the full range of Péclet numbers in laminar flow (regimes (i)–(iv)). In particular, it reproduces faster than linear growth of the longitudinal dispersion with Péclet number in the intermediate regime, corresponding to an apparent exponent $\alpha_x > 1$. It was claimed that this behavior could be understood from the statistical behavior of tracers in the pore channels.

To clarify the origin of this purported statistical behavior, presumed quite generic for porous media, here we study a highly simplified model for porous media consisting of a network of (pore) channels [15,16]. In order to obtain a clear vision of the impact of the statistical behavior mentioned above on dispersion, the model we chose for this study is as minimalistic as possible, removing any physical mechanisms, such as turbulence and Taylor dispersion (see Section 2 below), that might affect these statistical properties. Thus, along the network connections, transport is one-dimensional and strictly diffusive and/or advective. The effective longitudinal and transverse dispersion coefficients are extracted from the final numerical solution, after evolving the system in time. It will be shown that this model does indeed reproduce the dispersion regimes and produces exponents $\alpha_{x,y}$ very similar to those obtained in experiments on actual porous media. In this way, the minimum ingredients giving rise to the observed dispersional behavior are identified. Furthermore, we will extract statistical information regarding the microscopic transport process that will elucidate the origin of the observed behavior.

Clearly, the model has only limited validity for the modeling of real systems. However, we emphasize that this is not its purpose. Rather, the model is constructed to discriminate sharply between qualitatively and quantitatively different physical mechanisms. Discrimination is achieved by the combination of several assumptions, namely: (a) Highly complex three-dimensional porous materials are modeled by a simple two-dimensional network of infinitely thin connections linking nodes. (b) Fluid flow through the system is imposed and not influenced by the presence of the solute; in other words, the solute fraction is assumed to be infinitesimally small. (c) The fluid flow itself is incompressible, which is a reasonable assumption even in a realistic porous system when the fluid chosen is water or similar. (d) The solute is passively transported by the fluid and is not assumed to be subject to independent transport equations (i.e., the solute has no inertia and it is not reactive).

This simplified model is used to study the effect of network topology on dispersion. The philosophy of our approach is similar to that of [9,8]. Here, however, we render the model minimalistically. The objective is to expose the essential ingredients for description of solute transport in porous media. An important aspect of the model is the use of continuum transport equations for the solute. This effectively corresponds to using of an infinite number of tracers, which leads to high accuracy results (not easy to obtain using tracers [17]). Another important aspect is that the numerical model is specifically designed to handle the wide spread of flow velocities in individual channels, typical of general porous media.

## 2. The motivation of the simplified model approach

To motivate the model, we briefly review the main mechanisms thought to cause dispersion in porous media [5,15,2].

### 2.1. Mechanical dispersion

Fluid flows through a network of pore channels; we will only consider laminar flow. Then, fluid flow is determined completely by the applied pressure head and the boundary conditions, e.g., no-slip boundary conditions at the channel walls. An important observation is that the whole problem of obtaining the fluid flow in the complex geometry and with given boundary conditions is *linear* in the applied pressure head: raising the head by a factor $f$ will lead to an increase of fluid velocity by the same factor $f$ everywhere.

Tracers are released into this fluid flow in a small region in space and time, and the tracer cloud is advected passively by the flow. We assume that the tracers are infinitesimal and massless (no inertia) so that they do not interact with each other, do not affect the flow, and follow the flow lines in the absence of diffusion. Further on, we will also consider the effect of (molecular) diffusion, but first we discuss pure flow effects. Tracers (and the fluid itself) cannot leave the network (particle conservation), except at the edge of the model network.

The tracer cloud, traveling through the network, will spread out due to the complex distribution of connections between nodes (leading to a complex flow pattern). Note that this statement implicitly assumes that the flow through the network is such that the tracer cloud will actually spread out, i.e., that tracers may follow alternative paths leading to different net traveled distances from the point of injection—this excludes, e.g., homogeneous flows ($v =$ constant over all space) from the analysis.

After some time $t$, sufficiently large for initial transient effects to die out, but not so large that tracers are lost from the system, the size of the tracer cloud can be estimated by its spread

$$\langle d_x^2 \rangle = \langle (x - \langle x \rangle)^2 \rangle. \tag{1}$$

Here, $x$ indicates the set of $x$-coordinate values of the tracers, and the angular brackets imply a mean over all tracers. Similar expressions hold for the spread in the other coordinate directions. The corresponding effective dispersion coefficient can be estimated from

$$D_v^x = \frac{\langle d_x^2 \rangle}{t} \tag{2}$$

in the $x$ direction, and similar for the other coordinate directions, assuming that the initial size of the tracer cloud is infinitesimally small. Note that we call this dispersion coefficient *effective*, as the tracer distribution may deviate from a Gaussian shape in specific pore geometries. Deviations from Gaussianity may indicate that the ADE is an unsatisfactory model for global dispersional behavior [3]. In spite of this, the foregoing effective dispersion coefficient can always be evaluated in finite-size systems at finite times.

As noted, an increase of the pressure head by a factor $f$ increases the flow velocity everywhere by that same factor, $v' = fv$. As we

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