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# Research papers On the effect of solute release position on plume dispersion

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## ABSTRACT

Associated with Taylor dispersion, in this paper we analyze how the vertical position of a point-source solute release will affect the transport process in laminar open channel flow, through obtaining and applying analytical solution by the two-scale perturbation analysis (Wu and Chen, 2014, J. Fluid Mech., 740, 196–213), which is verified and supported by results from numerical simulations. Based on multi-dimensional spatial concentration distribution of the solute plume, we resort to the previously proposed criterion for identifying the stage of solute transport characterized by the dispersion-dominated (Taylor dispersion) regime, focusing on the relative uniformity of concentration distribution across a given family of curved surfaces (Wu et al., 2016, Sci. Rep., 6, 20556). The most important finding is that for the solute transport transition into the dispersion-dominated regime, the necessary time is about 50% more for the case of solute release at free water surface compared with that at the channel bed, which is substantial under typical physical parameters. Other effects of release position include affecting the displacement of the solute plume centroid, the value of the maximum mean concentration, and non-Gaussian properties regarding the form of the streamwise distribution of the mean concentration.

#### 1. Introduction

Taylor dispersion (Taylor, 1953) is a concept describing an enhanced streamwise diffusion of the transported species, which is contributed by the combined action of flow shear and molecular diffusion. To date, the concept has found broad applications in different fields including environmental science and engineering, biomedical engineering, and chemical engineering (e.g. Bello et al., 1994; Bruant et al., 2002; Chen et al., 2012; Fischer, 1976; Fischer et al., 1979; Ghosal, 2006; Ng and Yip, 2001; Spurny et al., 1969; Stone et al., 2004; Wang and Huai, 2018; Wang and Chen, 2017a; Wang and Chen, 2017b; Wu and Chen, 2014a; Wu et al., 2012; Zeng, 2010; Zeng et al., 2015; Zeng et al., 2014).

The streamwise distribution and evolution of the mean concentration of the solute plume has been discussed as a key issue of the Taylor dispersion (Taylor, 1953). This is essentially related to the form of Taylor dispersion model, an effective diffusion equation for the mean concentration, since Taylor's initiative (Taylor, 1953). The later contribution of Aris (1956) on the method of concentration moment has also been regarded as classic, due to its capability of providing exact statistical information for the concentration distribution associated with different orders of moments, especially when there is no exact solution found for the governing convection-diffusion equation for the shear-induced solute transport in flows. At the same time, direct explorations on the asymptotic solutions (Chatwin, 1970; Latini and Bernoff, 2001; Lighthill, 1966; Phillips and Kaye, 1996; Vrentas and Vrentas, 2000) for the concentration distribution have been made, and different analytical methods were proposed such as the expansion of the mean concentration (Gill, 1967; Gill and Sankarasubramanian, 1970; Wu et al., 2015), delay-diffusion equation (Smith, 1982; Smith, 1983), homogenization technique (Mei et al., 1996; Ng, 2006; Ng and Yip, 2001), Lyapunov-Schmidt technique based exact averaging model (Ratnakar and Balakotaiah, 2011; Ratnakar et al., 2012), and so on. Some results have also been verified by numerical simulations of the transport process (Houseworth, 1984; Shankar and Lenhoff, 1991; Stokes and Barton, 1990).

On the other hand, systematically studying the transverse (or crosssectional) concentration distribution was the effort that has been made very recently (Wu and Chen, 2014b), aiming at getting more information on the physical process of solute transport. Analytically, Wu and Chen (2014b) extended the extensively applied homogenization technique (Mei et al., 1996; Ng, 2006; Ng and Yip, 2001) on introducing the longitudinal (streamwise) correction functions and modifying the Taylor dispersion model with solutions of the higher-order perturbation problems. The transverse concentration distribution was then analyzed based on a more accurate description for the skewed streamwise distribution of the mean concentration. By considering the process of approaching transverse uniformity of concentration distribution,

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importantly it is found that the time scale needed is much greater than that for approaching streamwise normality, the latter of which is generally taken as the time for Taylor dispersion model to be applicable at the scale of  $R^2/D$  (*R* is a characteristic length such as the tube radius, and *D* is the molecular diffusion coefficient). This result actually rectified some common mistake in recognition (Latini and Bernoff, 2001) that the concentration should be uniformly distributed over the cross-section at Taylor dispersion stage of solute transport (Wu and Chen, 2014b).

To give a sound description for the transverse concentration distribution patterns, a family of curved transverse surfaces were chosen in a further study (Wu et al., 2016). It was found that the concentration actually distributed uniformly across the proposed surfaces at the time scale of  $R^2/D$ . Thus, the slow asymptotic process of approaching transverse uniformity (Wu and Chen, 2014b) is simply the result of the decreased streamwise concentration gradient over time. Combining analytical and numerical results, approaching uniform distribution across the curved surfaces is also shown to be a remarkable criterion for identifying the dispersion-dominated process (Taylor dispersion regime), during which the analytical solution by Wu and Chen (2014b) is valid. It should be noted that the applicability of Taylor's model can be determined by considering the vanishing of some non-Gaussian properties of the streamwise distribution of the mean concentration (Chatwin, 1970; Wu and Chen, 2014b), however, there is still no common criterion for transition to the dispersion-dominated process.

In this paper, the most typical initial condition of instantaneous point-source release is considered for laminar open channel flow, the idealized flow regime of which is the foundation for models of many natural systems, such as in fractures or rivers, and has been discussed extensively in literature (e.g. Wang et al., 2012). In some recent progress, Fu et al. (2016) considered the case of solute release at the free water surface of wetland flows by the obtained concentration moments, exploring how the centroid of the solute plume travels downstream and thus affects the concentration distribution. Here, we further study the effects of vertical release position referring to the multi-dimensional spatial concentration distribution patterns of the solute plume (Wu et al., 2016), based on the analytical framework of Wu and Chen (2014b). Since the plane-source solute release (Wu and Chen, 2014b) can be seen as the superposition of point-source releases at different cross-sectional positions, analysis based on a more fundamental initial condition for the transition to the dispersion-dominated regime is promising to reveal more physical insights for the solute transport process. This paper is organized as follows. In section 2, the modeled system and the analytical method are introduced briefly, followed by the determination of the two unknown functions required in the analytical solution under the framework of concentration moments. In section 3, detailed discussions on the effects of solute release position are provided by comparisons between analytical and numerical results whereas section 4 presents the conclusions.

### 2. Methods

The analytical solution by the proposed two-scale perturbation analysis, as discussed by Wu and Chen (2014b), captures certain non-Gaussian properties of the streamwise distribution of the mean concentration for only part of the initial stage of the solute transport. It is now understood that the solution becomes valid when the transport process enters the so-called "dispersion-dominated" regime (Wu et al., 2016). That is, the transport is dominated by the mechanism of Taylor dispersion, but the streamwise distribution of the mean concentration can deviate evidently from the Gaussian curve predicted by the onedimensional Taylor dispersion model.

To understand the validity of Taylor dispersion model, conventionally we can observe the process of approaching normality for the mean concentration (Chatwin, 1970; Wu and Chen, 2014b), which can be achieved based on the analytical solution by the proposed twoscale perturbation analysis. On the other hand, to acquire detailed information for the transition to dispersion-dominated regime, numerical simulations for the transport process are to be performed providing the vertical concentration distribution patterns, which serves as a validation for the analytical solution while at the same time can be examined by the proposed criterion regarding a family of curved surfaces for the uniform concentration distribution (Wu et al., 2016). We follow the same numerical procedure as that performed previously for solute transport in laminar tube flow (Wu et al., 2016), which solves the governing convection-diffusion equation by the finite element method.

#### 2.1. Analytical solution by two-scale perturbation analysis

In this paper, combining analytical and numerical approaches, the effects of position of a point-source solute release are discussed for the laminar open channel flow, which is a most idealized case enabling theoretical analysis with important implications extended to solute transport in natural rivers with turbulent flows (Taylor, 1953; Taylor, 1954). A sketch for the configuration is given as Fig. 1. The channel is of depth *H*. In a Cartesian coordinate system the origin *O* is set at the bed surface, with longitudinal (streamwise) *x*-axis and vertical *z*-axis. An instantaneous point source release is considered at a vertical position  $z_0$  at the very beginning of the solute transport.

The transport process is governed by a convection-diffusion equation:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} + D \frac{\partial^2 C}{\partial z^2},\tag{1}$$

where *C* is the concentration, *t* is the time, *u* is the flow velocity as a function of *z*, and *D* is the molecular diffusion coefficient.

The initial release of solute at a height of  $z_0$  with mass Q can be given as

$$C(x, z, t)|_{t=0} = Q \,\delta\left(\frac{x}{H}\right)\delta\left(\frac{z}{H} - \frac{z_0}{H}\right),\tag{2}$$

where  $\delta(\cdot)$  is the Dirac delta function.

The boundary conditions at the channel bottom of z = 0 and the free water surface of z = H can be expressed as

$$\frac{\partial C}{\partial z}\Big|_{z=0} = \frac{\partial C}{\partial z}\Big|_{z=H} = 0.$$
(3)

Since the amount of release is finite, the upstream and downstream conditions are

$$C(x, z, t)|_{x=\pm\infty} = 0.$$
(4)

By introducing the following dimensionless parameters:

$$\psi = \frac{u}{\langle u \rangle}, \ \tau = t / \frac{L}{\langle u \rangle}, \ \xi = \frac{x}{L} - \tau, \ \zeta = \frac{z}{H},$$
  
$$\epsilon = \frac{H}{L}, \ \text{Pe} = \frac{\langle u \rangle H}{D}, \ \Omega = C/Q,$$
(5)

where L is a length characterizing the longitudinal scale of the solute plume, and the angle brackets define the vertical average operation, for example,

$$\langle u \rangle \equiv \int_{0}^{1} u \, d\zeta \tag{6}$$

**Fig. 1.** Sketch for the instantaneous point-source solute release in laminar open channel flow. The release is shown as a solid circle at the vertical position of  $z = z_0$  in the channel.

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