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# Asymptotic theory of classical tracer transport in inhomogeneous and nonstationary media. Hamilton's formalism

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## Contents



**Abstract. We develop an asymptotic theory of tracer transport due to diffusion and advection, when the diffusivity and advection velocity vary slowly over space and time. The tracer concentration is expressed through a single time integral. The integrand is determined by solving first-order ordinary differential equations, which are similar to Hamilton's equations for a material point in classical mechanics.**

**Keywords:** diffusion, advection, asymptotic form, Hamilton's equations

## 1. Introduction

The problem of tracer transport in inhomogeneous media has a long history and remains relevant today. Existing transport models are obtained using appropriate averaging procedures over small- and moderate-size inhomogeneities. When the medium's characteristics are independent of spatial coordinates and time, theoretical transport models offer analytical solutions for the tracer concentration, at least in asymptotic limits [1–4]. In other cases, solving for the concentration requires cumbersome, time-consuming numerical calculations.

In Ref. [5], one of the present authors proposed a new approach based on the asymptotic description of transport processes, assuming that the medium's structural characteristics depend on spatial coordinates on large scales. This approach is based on considering that, according to all known physical models, the concentration decays exponentially at asymptotically large distances from the domain that contains most of the tracer. This makes the asymptotic problem of tracer transport similar to the geometric optics, allowing it to be reduced to ordinary differential equations of the first order. The solutions can be expressed as integrals over the trajectory of the concentration signal (a quasi-ray). The trajectory is determined by a variational principle, which is analogous to Fermat's principle. The asymptotic theory [5] was then applied to specific transport models [6, 7]. Reference [7] shows that calculations of concentration based on the asymptotic theory of classical diffusion reduce the computational time by two orders of magnitude compared to direct numerical calculations based on the diffusion equation with spatially varying diffusivity.

Note that the method proposed in Ref. [5] describes the case of a stationary inhomogeneous medium. Here, we develop an asymptotic theory of tracer transport in a classical diffusion–advection model in a medium that is not only inhomogeneous but also nonstationary. The problem is formulated in Section 2. Section 3 derives the asymptotic theory and illustrates its results using examples. Section 4 is a summary.

## 2. Problem statement

Tracer transport in a diffusion–advection model is described by the well-known equation

$$\frac{\partial}{\partial t}\, c\,(\mathbf{r}, t) + \big(\mathbf{u}\nabla c\,(\mathbf{r}, t)\big) - \operatorname{div}\big\{D\nabla c\,(\mathbf{r}, t)\big\} = 0\,, \quad \operatorname{div}\mathbf{u} = 0\,. \tag{1}$$

The advecting velocity and diffusivity are functions of the coordinates and time ($\mathbf{u} = \mathbf{u}(\mathbf{r}, t)$, $D = D(\mathbf{r}, t)$). The tracer concentration satisfies the initial and boundary conditions

$$c\,(\mathbf{r}, 0) = N\delta(\mathbf{r})\,, \quad c\,(\mathbf{r}, t)\big|_{|\mathbf{r}|\to\infty} = 0\,, \tag{2}$$

where $N$ is the total number of tracer particles.

Taking into account the exponential decay of concentration at large distances from its main localization domain, the concentration can be conveniently expressed as

$$c\,(\mathbf{r}, t) = A(\mathbf{r}, t)\,\exp\big[-S\,(\mathbf{r}, t)\big]\,. \tag{3}$$

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Our goal is to find an expression for the concentration under the following condition:

$$S(\mathbf{r}, t) \gg 1\,. \tag{4}$$

Due to this condition, the problem acquires a small parameter

$$\xi = \max\left\{ \left(L|\nabla S|\right)^{-1},\quad \left(T\left|\frac{\partial S}{\partial t}\right|\right)^{-1} \right\} \ll 1\,, \tag{5}$$

where $L$ and $T$ are, respectively, the characteristic spatial and temporal scales of the medium.

By substituting expression (3) into equation (1) and exploiting the existence of the small parameter $\xi$ (5), we can derive equations for the exponent $S(\mathbf{r}, t)$ and the pre-exponential $A(\mathbf{r}, t)$.

## 3. Asymptotic theory

**Motion equations.** After substituting expression (3) into equation (1) in zeros-order with respect to the small parameter $\xi$, we obtain an equation for the exponent $S(\mathbf{r}, t)$:

$$\frac{\partial S}{\partial t} + (\mathbf{u}\nabla S) + D(\nabla S)^2 = 0\,. \tag{6}$$

Since this equation corresponds to the zeroth order in the parameter $\xi$, it does not contain the derivatives of the medium parameters ($\mathbf{u}$ and $D$) or second derivatives of $S$. Consequently, equation (6) is a first-order partial differential equation. Its independent variables are the spatial coordinates and time; therefore, its form is an analog of the Hamilton–Jacobi equation for a material point in classical mechanics [8]. As a result, Hamilton's formalism can be conveniently used to solve equation (6).

We will therefore refer to the function $S(\mathbf{r}, t)$ as the action, $\nabla S$ as the momentum $\mathbf{p}$, and $-\partial S/\partial t$ as the Hamiltonian $H(\mathbf{p}, \mathbf{r}, t)$. From equation (6), it then follows that

$$H(\mathbf{p}, \mathbf{r}, t) = (\mathbf{u}\,\mathbf{p}) + D\,\mathbf{p}^2\,. \tag{7}$$

In the time interval $0 < t' < t$, the momentum and the coordinate satisfy the canonical Hamilton equations

$$\frac{\mathrm{d}r_i}{\mathrm{d}t'} = \frac{\partial H}{\partial p_i}\,, \quad \frac{\mathrm{d}p_i}{\mathrm{d}t'} = -\frac{\partial H}{\partial r_i}\,,$$

which, according to (7), take the form

$$\frac{\mathrm{d}r_i}{\mathrm{d}t'} = u_i + 2Dp_i\,, \tag{8}$$

$$\frac{\mathrm{d}p_i}{\mathrm{d}t'} = -p_k\,\frac{\partial u_k}{\partial r_i} - \mathbf{p}^2\,\frac{\partial D}{\partial r_i}\,. \tag{9}$$

The vector integration constant follows from the obvious condition

$$\int_0^t \mathrm{d}t'\,\frac{\mathrm{d}\mathbf{r}(t')}{\mathrm{d}t'} = \mathbf{r}\,, \tag{10}$$

which, using (8), becomes

$$\int_0^t \mathrm{d}t'\,\left[\mathbf{u}\big(\mathbf{r}(t'), t'\big) + 2D\big(\mathbf{r}(t'), t'\big)\mathbf{p}(t')\right] = \mathbf{r}\,. \tag{11}$$

**Action.** According to the canonical formalism [8], the action is

$$S(\mathbf{r}, t) = \int_0^{\mathbf{r}} \mathbf{p}\,\mathrm{d}\mathbf{r}' - \int_0^t \mathrm{d}t' H\big(\mathbf{p}(t'), \mathbf{r}(t'), t'\big)\,. \tag{12}$$

Using (8), we get

$$\mathrm{d}\mathbf{r}' = \frac{\mathrm{d}\mathbf{r}(t')}{\mathrm{d}t'}\,\mathrm{d}t' = \left[\mathbf{u}\big(\mathbf{r}(t'), t'\big) + 2D\big(\mathbf{r}(t'), t'\big)\,\mathbf{p}(t')\right]\mathrm{d}t'\,. \tag{13}$$

Inserting equalities (7) and (13) into expression (12) yields the final result for the action:

$$S(\mathbf{r}, t) = \int_0^t \mathrm{d}t'\,D\big(\mathbf{r}(t'), t'\big)\,\mathbf{p}^2(t')\,. \tag{14}$$

We emphasize that the derivation in this subsection is in accordance with the general theory of first-order partial differential equations [8].

**Pre-exponential and concentration.** The equation for the pre-exponential $A(\mathbf{r}, t)$ is obtained in the first order of the parameter $\xi$ by substituting equality (3) into equation (1) and collecting the terms containing only first derivatives of quantities $A(\mathbf{r}, t)$, $D(\mathbf{r}, t)$ (i.e., $\partial A/\partial t$, $\nabla A$, and $\nabla D$) and second derivatives of $S(\mathbf{r}, t)$ (i.e., $\Delta S$),

$$\frac{\partial A}{\partial t} + (\mathbf{u}\,\nabla A) + 2D(\nabla A\nabla S) + A\,\mathrm{div}\,(D\nabla S) = 0\,. \tag{15}$$

Using the equality that follows from (8),

$$\nabla S = \mathbf{p} = \frac{1}{2D}\left(\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'} - \mathbf{u}\right), \tag{16}$$

and taking into account the property $\mathrm{div}\,(\mathbf{u}(\mathbf{r}, t)) = 0$ and also the equality

$$\frac{\partial A}{\partial t'} + \left(\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'}\,\nabla A\right) = \frac{\mathrm{d}A}{\mathrm{d}t'}\,, \tag{17}$$

we obtain the equation

$$\frac{\mathrm{d}\ln A}{\mathrm{d}t'} = -\frac{1}{2}\,\mathrm{div}\left(\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'}\right). \tag{18}$$

It implies that

$$A(\mathbf{r}, t) = \frac{B}{t^{3/2}}\,\exp\left[-Q(\mathbf{r}, t)\right], \tag{19}$$

where

$$Q(\mathbf{r}, t) = \frac{1}{2}\int_0^t \mathrm{d}t'\left(\mathrm{div}\left(\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'}\right) - \frac{3}{t'}\right). \tag{20}$$

Here, we took into account that at relatively short times, when the medium can be considered homogeneous and stationary, one can approximately write

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'} \cong \frac{\mathbf{r}}{t'}\,, \quad \mathrm{div}\left(\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'}\right) \cong \frac{3}{t'} \quad \text{for} \quad t' \to 0\,. \tag{21}$$

The quantity $B$ is the integration constant, found by comparing equality (19) for $t' \to 0$ with the known expression for the concentration in the same limit

$$c(\mathbf{r}, t) \cong \frac{N}{(4\pi D_0 t)^{3/2}}\,\exp\left[-\frac{\mathbf{r}^2}{4D_0 t}\right]: \qquad B = \frac{N}{(4\pi D_0)^{3/2}}\,, \quad D_0 \equiv D(0, 0)\,. \tag{22}$$

Inserting expression (22) into (19) and then (19) into (3) yields the final asymptotic expression for the tracer concentration in diffusive–advective transport in an inhomogeneous, nonstationary medium:

$$c(\mathbf{r},t) = \frac{N}{(4\pi D_0 t)^{3/2}} \exp\left[-S(\mathbf{r},t) - Q(\mathbf{r},t)\right]. \tag{23}$$

The quantities $\mathbf{p}(t')$ and $\mathrm{d}\mathbf{r}/\mathrm{d}t'$ that enter the expressions for $S(\mathbf{r},t)$ and $Q(\mathbf{r},t)$, which are given by expressions (14) and (20), respectively, are found by solving Hamilton's equations (8) and (9), taking into account relationship (10).

**Particular cases.** We illustrate the results of the asymptotic theory developed here for three particular cases.

*Homogeneous and stationary medium* ($\mathbf{u}, D = \text{const}$).

Solving the system of equations (8)–(10) yields expressions for the momentum and velocity:

$$\mathbf{p}(t') = \frac{\mathbf{r} - \mathbf{u}t}{2Dt}, \quad \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'} = \frac{\mathbf{r}}{t}.$$

Inserting these expressions into formulas (10) and (20) and then inserting these formulas into (23) yields the well-known solution to problem (1), (2) in a homogeneous and stationary medium:

$$c(\mathbf{r},t) = \frac{N}{(4\pi Dt)^{3/2}} \exp\left[-\frac{(\mathbf{r}-\mathbf{u}t)^2}{4Dt}\right]. \tag{24}$$

*Homogeneous and nonstationary medium without advection* ($\mathbf{u} = 0,\ D = D(t)$).

Equations (9) and (10) lead to the following expressions for the momentum and velocity:

$$\mathbf{p}(t') = \frac{\mathbf{r}}{2K(t)}, \quad \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'} = \frac{D(t')}{K(t)}\,\mathbf{r}, \tag{25}$$

where

$$K(t) = \int_0^t \mathrm{d}t'\, D(t'). \tag{26}$$

Substituting expressions (25) into (14) and (20) and then inserting these equations into (23), we obtain the expression for the concentration,

$$c(\mathbf{r},t) = \frac{N}{\big(4\pi K(t)\big)^{3/2}} \exp\left[-\frac{\mathbf{r}^2}{4K(t)}\right], \tag{27}$$

which is an exact solution for $\mathbf{u} = 0$ and $D = D(t)$.

*Stationary inhomogeneous medium without advection* ($\mathbf{u} = 0,\ D = D(\mathbf{r})$).

In this case, the Hamiltonian is constant, and, according to (14) and (17), the action is

$$S(\mathbf{r},t) = Ht. \tag{28}$$

Let $l$ be the length along the trajectory line of the concentration signal, which is defined by the velocity $\mathrm{d}\mathbf{r}(t')/\mathrm{d}t'$, starting at $\mathbf{r}(0) = 0$ and ending at $\mathbf{r}(t')|_{t'=t} = \mathbf{r}$. There is an obvious kinematic relationship

$$\int_0^{\mathbf{r}} \frac{\mathrm{d}l}{|\mathrm{d}\mathbf{r}(t')/\mathrm{d}t'|} = t. \tag{29}$$

Here and below, the integration over the length $l$ is performed along the concentration signal trajectory. From relationships (7) and (8), we find the absolute value of the velocity

$$\left|\frac{\mathrm{d}\mathbf{r}(t')}{\mathrm{d}t'}\right| = 2\sqrt{HD\big(\mathbf{r}(t')\big)}, \tag{30}$$

which, upon substituting (30) into equality (29), leads to the Hamiltonian

$$H = \frac{1}{4t^2}\left(\int_0^{\mathbf{r}} \frac{\mathrm{d}l}{\sqrt{D(\mathbf{r})}}\right)^2,$$

and, according to (28), the action

$$S(\mathbf{r},t) = \frac{\psi^2(\mathbf{r})}{4D_0 t}, \tag{31}$$

where

$$\psi(\mathbf{r}) = \int_0^{\mathbf{r}} \mathrm{d}l\, n(l), \tag{32}$$

and

$$n(l) = \sqrt{\frac{D_0}{D(l)}}. \tag{33}$$

We now derive the equation for the trajectory line of the concentration signal. Let $\mathbf{v} = \mathbf{v}(l)$ be the unit vector tangent to this line. Using the obvious equalities

$$\frac{\mathrm{d}l}{\mathrm{d}t} = \left|\frac{\mathrm{d}\mathbf{r}(t')}{\mathrm{d}t'}\right| \quad \text{and} \quad \mathbf{v} = \frac{\mathbf{p}}{p},$$

we have

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}l} = \frac{1}{2Dp}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathbf{p}}{p}\right). \tag{34}$$

Developing the derivatives in this equation with the help of equation (9) (for $\mathbf{u} = 0$), we obtain the equation

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{1}{n}\big(\nabla n - \mathbf{v}(\mathbf{v}\,\nabla n)\big). \tag{35}$$

Expression (31) for the action (the exponent in formula (3)) and the equation for the trajectory of the concentration signal (35) coincide with those found in Ref. [7] for stationary inhomogeneous media.

Now, we only need to express the quantity $Q(\mathbf{r},t)$, defined by (20), in the terms of the asymptotic theory for a stationary inhomogeneous medium (32), (33). Using the obvious relationships that follow from (28), (30), and (31),

$$\begin{gathered} \mathrm{d}\psi = n\,\mathrm{d}l, \ \frac{\mathrm{d}l}{\mathrm{d}t'} = \left|\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'}\right|, \ \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'} = \mathbf{v}\left|\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t'}\right|, \\ \mathrm{d}t' = \frac{\mathrm{d}\psi}{2\sqrt{HD_0}}, \quad t' = \frac{\psi}{2\sqrt{HD_0}}, \quad n^{-1}(\mathbf{v}\nabla) = \frac{\mathrm{d}}{\mathrm{d}\psi}, \end{gathered} \tag{36}$$

we transform expression (20) to

$$Q(\mathbf{r},t) = \frac{1}{2}\int_0^{\mathbf{r}} \mathrm{d}\psi\left(\mathrm{div}\left(\frac{\mathbf{v}}{n}\right) - \frac{2}{\psi}\right). \tag{37}$$

Inserting expressions (31) and (37) into formula (23) yields an asymptotic expression for the concentration in the classical tracer transport in a stationary inhomogeneous medium,

$$c(\mathbf{r}, t) = \frac{N}{(4\pi D_0 t)^{3/2}} \exp\left[-\frac{\psi^2(\mathbf{r})}{4D_0 t} - \frac{1}{2}\int_0^{\mathbf{r}} \mathrm{d}\psi \left(\operatorname{div}\left(\frac{\mathbf{v}}{n}\right) - \frac{2}{\psi}\right)\right], \tag{38}$$

found earlier in Ref. [7].

## 4. Conclusion

This paper presents an asymptotic theory for the tracer transport in an inhomogeneous nonstationary medium in the diffusion–advection regime. This theory is based on the idea that the concentration has an exponential structure at asymptotically large distances from the primary tracer localization domain. The concentration is expressed in terms of a single time integral. The integrand is determined by solving a system of two first-order ordinary differential equations, which are analogous to Hamilton's equations in the classical mechanics of a material point.

It is expected that solving for tracer transport in inhomogeneous, nonstationary media based on the proposed asymptotic theory will substantially reduce computational time (by two and more orders of magnitude) compared to the direct numerical integration of the second-order partial differential equation.

One of the applications of the developed theory can be the analysis of long-term transport processes in geological structures to estimate the reliability of radioactive waste deposition.

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