

MODEL FOR HETEROGENEOUS DIFFUSION

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ABSTRACT. A reversible kinetic equation for Brownian particles is introduced when the turning frequency and the collision kernel are spatially heterogeneous. We derive an anisotropic diffusion equation by taking the singular limit of the kinetic equation and then balancing out its curvature effect. We see that an extra information such as the turning frequency or waiting time is also needed together with the diffusivity to model a diffusion phenomenon correctly if the environment is spatially heterogeneous. A thought experiment is introduced to test the validity of diffusion laws. We observe that diffusion models with diffusivity alone fail the test and the anisotropic model driven in the paper passes the test.

1. INTRODUCTION

We consider a heterogeneous *reversible* kinetic equation,

$$(1.1) \quad p_t + \frac{1}{\epsilon} \nabla \cdot (\mathbf{v}_\alpha p) = \frac{\mu(\mathbf{x})}{\epsilon^2} \int_A \left(q(\alpha, \mathbf{x}) p(\alpha', \mathbf{x}, t) - q(\alpha', \mathbf{x}) p(\alpha, \mathbf{x}, t) \right) d\alpha',$$

where A is the index set of a collection velocity vector fields,

$$V = \{\mathbf{v}_\alpha : \mathbf{R}^n \rightarrow \mathbf{R}^n \mid \alpha \in A\},$$

$p(\alpha, \mathbf{x}, t)$ is the fractional density of particles moving along a velocity field \mathbf{v}_α , p_t is its partial derivative with respect to the time variable t , $q(\alpha, \mathbf{x})$ is the probability for a particle to take the velocity field \mathbf{v}_α after a collision at position \mathbf{x} , and $\mu(\mathbf{x})$ is the turning (or collision) frequency at \mathbf{x} . The concept of *revertibility* is introduced in Section 4.1 which is another theoretical contribution of the paper. If all \mathbf{v}_α 's are constant vector fields, the equation returns to the classical heterogeneous kinetic equation. Furthermore, if the two sources of heterogeneity, q and μ , are independent of the space variable \mathbf{x} , the equation returns to the homogeneous kinetic equation.

There are two purposes in the paper. The first one is to introduce an anisotropic diffusion law for the total population density $u(\mathbf{x}, t) := \int_A p(\alpha, \mathbf{x}, t) d\alpha$,

$$(1.2) \quad u_t = \nabla \cdot \mu^{-1} (\nabla \cdot (\mu \mathbb{D} u) - (\mathbb{N} + \mathbb{L}) u),$$

under two hypotheses for the probability distribution $q(\alpha, \mathbf{x})$,

$$\int_A q(\alpha, \mathbf{x}) d\alpha = 1 \quad \text{and} \quad \mathbb{E} := \int_A q(\alpha, \mathbf{x}) \mathbf{v}_\alpha d\alpha = \mathbf{0}.$$

In this macroscopic scale diffusion law, the diffusion tensor \mathbb{D} is given by

$$\mathbb{D} = \frac{1}{\mu(\mathbf{x})} \mathbb{M}, \quad \mathbb{M} := \int_A (\mathbf{v}_\alpha \otimes \mathbf{v}_\alpha) q(\alpha, \mathbf{x}) d\alpha,$$

where $\mathbb{M} = \mu \mathbb{D}$ is a quantity independent of the turning frequency μ . There are two correction vectors in (1.2). The first correction vector \mathbb{N} is given by (4.3) which is obtained after taking $\epsilon \rightarrow 0$ limit of (1.1) in Section 4.2. The second correction vector

\mathbb{L} is given by (6.1) and is obtained after considering the curvature effect in Section 6. For an isotropic diffusion case, the above diffusion tensor \mathbb{D} becomes scalar-valued, the second correction vector \mathbb{L} becomes zero, and (1.2) becomes

$$(1.3) \quad u_t = \nabla \cdot \left(\sqrt{\mu^{-1}D} \nabla(\sqrt{\mu D} u) \right),$$

where D is the scalar diffusivity. Detailed discussions for the derivation of the heterogeneous diffusion law are given in Sections 4 and 6.

There have been a lot of discussions about what is the correct diffusion law when the diffusivity is not constant. Three diffusion laws are often considered, which are

$$(1.4) \quad u_t = \nabla \cdot (D \nabla u),$$

$$(1.5) \quad u_t = \nabla \cdot (\sqrt{D} (\nabla \sqrt{D} u)),$$

$$(1.6) \quad u_t = \Delta(Du).$$

We call them Fick's law [5], Wereide's law [9], and Chapman's law [1] in the order. Recently, Hillen and Painter [7] derived a heterogeneous anisotropic diffusion equation,

$$(1.7) \quad u_t = \nabla \nabla (\mathbb{D}u) \left(\equiv \sum_{i,j=1}^n \frac{\partial^2}{\partial x_i \partial x_j} (D_{ij}u) \right),$$

which is a generalization of the homogeneous case considered by Hillen and Othmer [6]. An underlying assumption supporting the four diffusion laws (1.4)–(1.7) is that diffusivity alone can decide the diffusion phenomenon even in a heterogeneous environment. In this context, the two diffusion laws, (1.2) and (1.3), are different from others and the diffusivity alone does not complete the diffusion laws. The key of the new diffusion law (1.2) is in the separation of μ^{-1} and $\mathbb{M} := \mu \mathbb{D}$, where the spatial heterogeneities in $q(\alpha, \mathbf{x})$ and $\mathbf{v}_\alpha(\mathbf{x})$ are involved in \mathbb{M} .

The second purpose of the paper is to ensure that the suggested diffusion laws (1.2) and (1.3) correctly model diffusion phenomena and others don't. For a homogeneous case, the previous diffusion laws are all identical with each other and there is no issue left. However, for a heterogeneous case, they are all different and it is not an easy task to show which diffusion law is the correct one. Of course, the ultimate arbiter of validating such a theory is the comparison with experiments. Indeed, Milligen [8] and many other experimental scientists compared diffusion laws experimentally. However, there is no decisive conclusion or convincing evidence pointing to the correct diffusion law. This is in part due to the probabilistic nature of diffusion, and more importantly, because these experiments only focus on diffusivity which is not sufficient to determine the phenomenon. Instead of a physical experiment, we introduce *thought experiment* to test the validity of the diffusion law in Section 3. It can be seen that only the new diffusion law (1.2) passes this thought experiment test.

The paper is organized as follows. In Section 2, we start with a heterogeneous kinetic equation in a classical form and derive an anisotropic diffusion equation given in (2.3). However, we see that this model fails the thought experiment test in Section 3. The first correction term \mathbb{N} is obtained in Section 4.2 by taking a singular limit of the revertible kinetic equation (1.1). This correction term improves the performance of the diffusion law considerably which is confirmed by numerical computations in Section 5. However, this model fails the thought experiment test, too. The second correction term \mathbb{L} is obtained in Section 6 by balancing out the curvature effect of

integral curves of vector fields \mathbf{v}_α 's, which completes the derivation of the diffusion law (1.1). Numerical computations and the analysis of radial solutions confirm that the final diffusion law passes the thought experiment test. Some concluding discussions are given in Section 7. The issue of the paper appears in many similar situation as long as the randomness in a heterogeneous environment is the driving force of a phenomenon. Such a discussion is given in Appendix A.

2. ANISOTROPIC DIFFUSION FROM CLASSICAL KE

Consider a spatially homogeneous kinetic equation (KE for brevity),

$$(2.1) \quad p_t + \frac{1}{\epsilon} \mathbf{v} \cdot \nabla p = \frac{\mu}{\epsilon^2} \int_V (q(\mathbf{v})p(\mathbf{v}', \mathbf{x}, t) - q(\mathbf{v}')p(\mathbf{v}, \mathbf{x}, t)) d\mathbf{v}',$$

where μ and q are independent of the space variable \mathbf{x} and the set $V = V(\mathbf{x}) \subset \mathbf{R}^n$ is a collection of velocities at \mathbf{x} . This is a special case of (1.1) when \mathbf{v}_α 's are constant vector fields. Notice that the reaction term of (2.1) is linear with respect to the particle density p . This means that the collision is not between the particles in the system, but with background particles, i.e., p is the density of Brownian particles colliding with background molecules.

Hillen and Othmer [6] derived the anisotropic diffusion equation (1.7) with a constant diffusion tensor \mathbb{D} . Hillen and Painter [7, Eq. (14)] extended it to a spatially heterogeneous case by considering space dependent probability $q(\mathbf{v}, \mathbf{x})$. However, another source of spatial heterogeneity is the turning frequency μ . If the turning frequency μ is also a function of \mathbf{x} , then (2.1) becomes

$$(2.2) \quad p_t + \frac{1}{\epsilon} \nabla \cdot (\mathbf{v}p) = \frac{\mu(\mathbf{x})}{\epsilon^2} \int_V (q(\mathbf{v}, \mathbf{x})p(\mathbf{v}', \mathbf{x}, t) - q(\mathbf{v}', \mathbf{x})p(\mathbf{v}, \mathbf{x}, t)) d\mathbf{v}'.$$

There are three basic hypotheses of kinetic theory included in the equation which are (i) a particle takes a new velocity $\frac{1}{\epsilon} \mathbf{v}$ after a collision at \mathbf{x} according to the probability distribution $q(\mathbf{v}, \mathbf{x})$, (ii) the rate of collision $\frac{1}{\epsilon^2} \mu(\mathbf{x})$ depends on space variable, and (iii) this velocity is not changed until the next collision. Since the heterogeneity is taken at the moment of starting point of a new random walk, we may call it Ito type (see Appendix A for a related discussion).

Using the kinetic equation (2.2), we can derive a diffusion law,

$$(2.3) \quad u_t = \nabla \cdot \left(\frac{1}{\mu} \nabla \cdot (\mathbb{M}u) \right) \left(\equiv \sum_{i,j=1}^n \left(\frac{\partial}{\partial x_i} \frac{1}{\mu} \frac{\partial}{\partial x_j} \right) (M_{ij}u) \right),$$

where

$$(2.4) \quad \mathbb{D} := \frac{1}{\mu} \mathbb{M} \quad \text{and} \quad \mathbb{M} := \int_V (\mathbf{v} \otimes \mathbf{v}) q(\mathbf{v}, \mathbf{x}) d\mathbf{v}.$$

A subtle change of a kinetic equation may end up with a completely different diffusion equation. The following derivation is standard and basically same as the one in Hillen and Painter [7] except the last step due to the heterogeneity in μ . First, take two hypotheses on $q(\mathbf{v}, \mathbf{x})$,

$$(2.5) \quad \int q(\mathbf{v}, \mathbf{x}) d\mathbf{v} = 1 \quad \text{and} \quad \mathbb{E} := \int q(\mathbf{v}, \mathbf{x}) \mathbf{v} d\mathbf{v} = 0.$$

Then the kinetic equation (2.2) is written as

$$(2.6) \quad p_t + \frac{1}{\epsilon} \nabla \cdot (\mathbf{v}p) = \frac{\mu}{\epsilon^2} (q(\mathbf{v}, \mathbf{x})u(\mathbf{x}, t) - p(\mathbf{v}, \mathbf{x}, t)).$$

If we integrate (2.6) over V , the right side becomes zero and we obtain

$$(2.7) \quad u_t = -\nabla \cdot \mathbf{J} \quad \text{with} \quad \mathbf{J}(\mathbf{x}, t) = \frac{1}{\epsilon} \int_V (\mathbf{v}p(\mathbf{v}, \mathbf{x}, t)) d\mathbf{v}.$$

Multiply $\epsilon \mathbf{v}$ to (2.6), integrate it over V , and obtain

$$\epsilon^2 \mathbf{J}_t + \int_V \mathbf{v} \nabla \cdot (\mathbf{v}p) d\mathbf{v} = \frac{\mu}{\epsilon} u \mathbb{E} - \mu \mathbf{J}.$$

If $\mathbb{E} \neq 0$, the advection term $\frac{\mu}{\epsilon} u \mathbb{E}$ blows up as $\epsilon \rightarrow 0$. In other words, taking the singular limit of (2.2) is valid only when $\mathbb{E} = 0$ as assumed in (2.5). Since $\epsilon^2 \mathbf{J}_t$ is the smallest term and the fractional population $p(\mathbf{v}, \mathbf{x}, t)$ is proportional to the probability distribution $q(\mathbf{v}, \mathbf{x})$ after enough number of collisions, we expect that

$$(2.8) \quad \epsilon^2 \mathbf{J}_t \rightarrow 0 \quad \text{and} \quad p \rightarrow qu \quad \text{as} \quad \epsilon \rightarrow 0.$$

These two are the ones needed for a rigorous convergence proof (see Remark 4.1). Then, after taking the singular limit as $\epsilon \rightarrow 0$, the flux \mathbf{J} becomes

$$\mathbf{J} = -\frac{1}{\mu} \int_V \mathbf{v} \nabla \cdot (\mathbf{v}q(\mathbf{v}, \mathbf{x})u) d\mathbf{v}.$$

Since the gradient operator ∇ is with respect to \mathbf{x} , we can take it out of the integration operator and obtain

$$\mathbf{J} = -\frac{1}{\mu} \nabla \cdot \left(\left(\int_V \mathbf{v} \otimes \mathbf{v} q(\mathbf{v}, \mathbf{x}) d\mathbf{v} \right) u(\mathbf{x}, t) \right) = -\frac{1}{\mu} \nabla \cdot (\mu \mathbb{D}u).$$

If μ is constant, $\frac{1}{\mu}$ enters inside the gradient and (2.7) gives (1.7) which is obtained by Hillen and Painter [7, Eq. (14)]. However, if μ is a function of \mathbf{x} , then $\frac{1}{\mu}$ cannot be placed inside the gradient and the final diffusion equation is (2.3) as we claimed.

Note that the spatial heterogeneity in $q(\mathbf{v}, \mathbf{x})$ is involved only at the moment of each collision and the velocity is not changed until the next collision. However, the spatial heterogeneity in the turning frequency $\mu(\mathbf{x})$ is involved in an accumulative way. For example, let $\mathbf{x}(t)$ be the position of a particle at time t and $t = t_n$, $n = 1, 2, \dots, N$, be the moments of collisions. Then, the expectation of $\int_{t_n}^{t_{n+1}} \mu(\mathbf{x}(t)) dt$ becomes 2. In other words, the heterogeneity in $\mu(\mathbf{x})$ is involved in an accumulative manner. This difference separates $\mu(\mathbf{x})$ and $q(\mathbf{v}, \mathbf{x})$ in the diffusion equation (2.3), where $q(\mathbf{v}, \mathbf{x})$ is included in \mathbb{M} . This is the first correction of classical diffusion laws. There are two more correction terms to come in later sections.

2.1. Restriction to isotropic diffusion. The anisotropic diffusion law (2.3) is reduced to an isotropic diffusion law when the probability q has no directional dependency, i.e., $q = q(\mathbf{x})$. Then, $\mathbb{M} = \frac{v^2}{n} I$, where v is the root mean square of particle speed and I is the identity matrix. The scalar diffusivity becomes $D = \frac{v^2}{n\mu}$ and the anisotropic diffusion equation is reduced to an isotropic one,

$$(2.9) \quad u_t = \nabla \cdot \left(\frac{1}{\mu} \nabla (\mu D u) \right).$$

If the turning frequency μ is constant, (2.9) returns to Chapman's law (1.6). The derivation by Chapman [1] is also based on the kinetic equation.

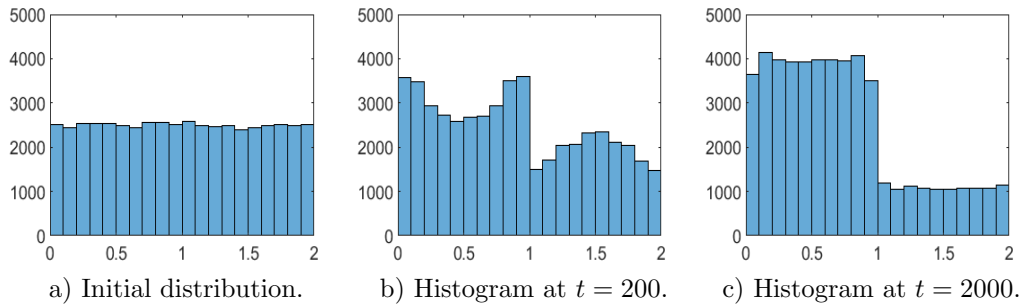


FIGURE 1. Histograms of a Monte-Carlo simulation of a velocity jump process. Parameters in (2.10)–(2.11) are used with $\epsilon = 0.01$.

2.2. Monte-Carlo simulation. We perform a Monte-Carlo simulation of a velocity jump process given by the kinetic equation. We will see that the simulation converges to a steady state of (2.9), not of any of (1.4)–(1.6). For simplicity, we do the simulation in the one space dimension. The simulation is based on a discrete kinetic equation scenario. We take a space domain $\Omega = [0, 2]$ with four possible choices of velocities,

$$(2.10) \quad v_{1\pm} = \pm\epsilon, \quad v_{2\pm} = \pm 2\epsilon, \quad x \in \Omega.$$

The probability to choose a velocity after a collision and the turning frequency are

$$(2.11) \quad q(v_{1\pm}, x) = \begin{cases} 0.5, \\ 0, \end{cases} \quad q(v_{2\pm}, x) = \begin{cases} 0, \\ 0.5, \end{cases} \quad \mu(x) = \begin{cases} 1, & 0 < x < 1, \\ 2, & 1 < x < 2, \end{cases}$$

where q satisfies the two conditions in (2.5). The two tensors $\mathbb{M} = \mu\mathbb{D}$ and \mathbb{D} in (2.4) are scalar-valued in the one space dimension, which are

$$D(x) = \begin{cases} \epsilon^2, & 0 < x < 1, \\ 2\epsilon^2, & 1 < x < 2, \end{cases} \quad M(x) = \begin{cases} \epsilon^2, & 0 < x < 1, \\ 4\epsilon^2, & 1 < x < 2. \end{cases}$$

In Figure 1, a Monte-Carlo simulation is given with the periodic boundary condition. The detail of the simulation is given in Appendix B. The initial position of each particle was chosen randomly and its histogram is given in Figure 1(a). We can observe that the particle density distribution converges to a non-constant steady state as $t \rightarrow \infty$. Figure 1(b) shows an intermediate stage before the particle distribution reaches a steady state. Figure 1(c) shows a final steady state. The particle density in the region $0 < x < 1$ is approximately four times bigger than the one in the region $1 < x < 2$ in the final stage. We find that the steady state is reversely proportional to μD . This is not a steady state of any of the three diffusion laws in (1.4)–(1.6), but of (2.9). However, we should not say yet that (2.9) is the correct diffusion equation and others not. We can only say that (2.9) is the correct diffusion law for the velocity jump process of the classical kinetic equation type. Then how can we say which diffusion law is correct? In the next section we develop a thought experiment to test anisotropic diffusion laws. We will see that the diffusion law (1.2) passes the test and others such as (1.7) and (2.3) fail.

3. THOUGHT EXPERIMENT

One of the reasons for the long-standing controversy over what is the correct heterogeneous diffusion law is that it is difficult to test by experiments. In this section

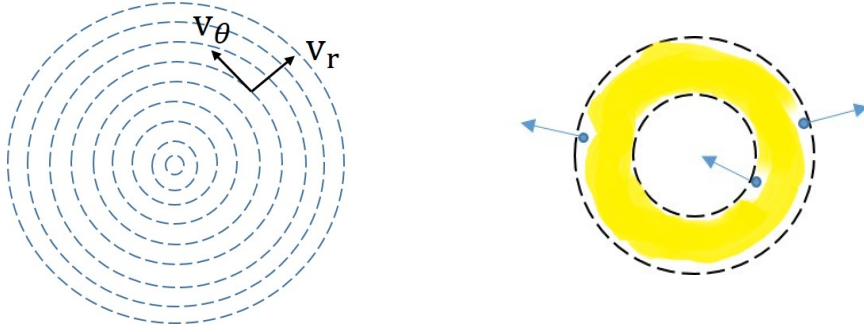


FIGURE 2. Anisotropic structure for the thought experiment in Section 3. Penetrable thin layers circled around the origin and filled with fresh water. We consider the dispersal of salty water along and across the channels.

we develop a thought experiment for an anisotropic dispersal in a radially symmetric system. Consider an anisotropic structure which consists of penetrable thin layers of microscopic scale level which are circled around the origin as demonstrated in Figure 2. Suppose that the structure is filled with fresh water and then salty water is added in a part of the system. We assume that the dispersal rate along circular channels is larger than the one across the layers. The salt particles will disperse along the circular channels and across them with different dispersal rates.

There are two checking points:

- (1) If the initial value is radial, the anisotropy will disappear and the solution dynamics should be identical to the one of the heat equation with the dispersal rate in the radial direction.
- (2) If the initial distribution of salt is concentrated at a single position, the density of the salt should be highest at the position all the time by the maximum principle.

These two are obvious without any experiment and the correct diffusion law should satisfy them. We call this test the thought experiment test.

Now we test if the anisotropic diffusion law (2.3) passes the thought experiment test. We first construct an example explicitly. Take the two dimensional space as the domain,

$$\Omega = \mathbf{R}^2,$$

and four unit vectors as a discrete set of possible velocities,

$$(3.1) \quad V(\mathbf{x}) = \{\pm \mathbf{v}_r(\mathbf{x}), \pm \mathbf{v}_\theta(\mathbf{x})\}, \quad \mathbf{v}_r(\mathbf{x}) = \frac{(x, y)}{|\mathbf{x}|}, \quad \mathbf{v}_\theta(\mathbf{x}) = \frac{(-y, x)}{|\mathbf{x}|}$$

(see Figure 2). The anisotropic structure of the system is included in the probability distribution of taking the four vectors which are

$$(3.2) \quad q(\pm \mathbf{v}_r, \mathbf{x}) = \frac{1}{2(1+k)}, \quad q(\pm \mathbf{v}_\theta, \mathbf{x}) = \frac{k}{2(1+k)}, \quad k \geq 1.$$

In this setting, the probability to move to the circumference direction $\pm \mathbf{v}_\theta$ is k times larger than the radial one. We take $k \geq 1$ and use it to control the anisotropy of the problem. Since

$$\mathbf{v}_r \otimes \mathbf{v}_r = \frac{1}{|\mathbf{x}|^2} \begin{pmatrix} x^2 & xy \\ xy & y^2 \end{pmatrix} \quad \text{and} \quad \mathbf{v}_\theta \otimes \mathbf{v}_\theta = \frac{1}{|\mathbf{x}|^2} \begin{pmatrix} y^2 & -xy \\ -xy & x^2 \end{pmatrix},$$

the matrix \mathbb{M} in (2.4) is given by

$$(3.3) \quad \mathbb{M} = \frac{1}{(1+k)|\mathbf{x}|^2} \begin{pmatrix} x^2 + ky^2 & (1-k)xy \\ (1-k)xy & kx^2 + y^2 \end{pmatrix}.$$

In the example, we take the turning frequency as $\mu = 1$ for simplicity. If $k = 1$, the anisotropy disappears and

$$\mathbb{D} = \frac{1}{\mu(1+1)|\mathbf{x}|^2} \begin{pmatrix} x^2 + y^2 & 0 \\ 0 & x^2 + y^2 \end{pmatrix} = \frac{1}{2}.$$

Therefore, we return to the heat equation, $u_t = \frac{1}{2}\Delta u$. If $k > 1$, we obtain an anisotropic diffusion.

3.1. Numerical computation and Monte-Carlo simulation. In Figure 3, a numerical solution of (2.3) is given. The initial distribution is the delta-distribution centered at the origin and the tensor \mathbb{M} in (3.3) is taken with $k = 25$. Two snap shots at $t = 7$ and $t = 20$ are given in Figure 3. In this computation, the diffusion equation (2.3) is solved on a domain $\Omega = [-10, 10] \times [-10, 10]$ with the zero Dirichlet boundary condition. The diffusion model (2.3) does not pass the thought experiment test. The salt was placed at the origin initially. However, the salt is moving away from the origin and the water at the origin becomes fresh. The support of the solution moves away in radial direction, which is not a correct diffusion phenomenon.

One might think the kinetic equation (2.2) is correct but the derivation for the diffusion equation (2.3) is incorrect. To test the property of the kinetic equation (2.2), a Monte-Carlo simulation is given in Figure 4. In the simulation, a particle walks in the radial or in the circumference direction randomly after taking one of the four directions in the set $V(\mathbf{x})$ given in (3.1). The probability to walk in the circumference direction is $k = 25$ times larger than the one in the radial direction in the simulation. The total of 10^5 particles started the origin. By comparing the two results, we can say that the diffusion model (2.3) explains this Monte-Carlo simulation correctly. The observed drifting phenomenon in the radial direction is the property of the velocity jump process and the diffusion equation (2.3) explains it correctly.

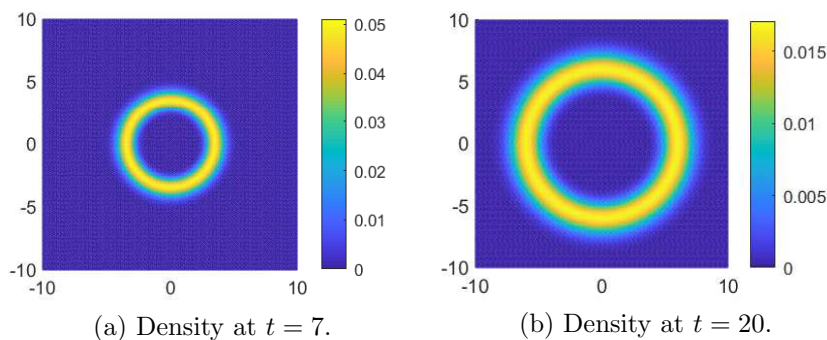


FIGURE 3. Numerical simulation of (2.3) with (3.3) and $k = 25$.

The example of the section tells us that, even if a diffusion equation correctly models a given velocity jump process, the model equation may fail to explain the diffusion phenomenon. It is clear that the classical kinetic equation does not give the correct heterogeneous diffusion phenomenon. This motivates us to develop a better

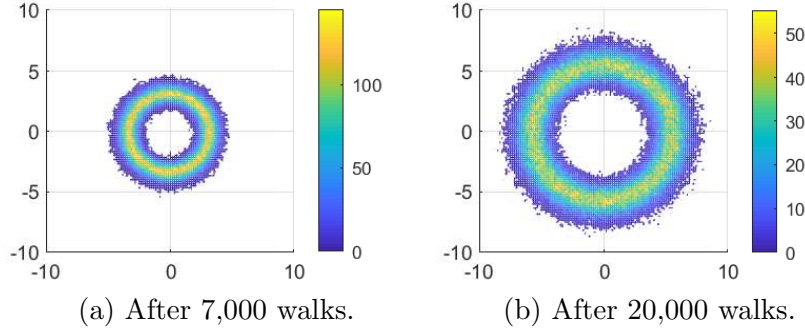


FIGURE 4. Monte-Carlo simulation for the velocity jump process (2.2) with 10^5 particles. One thousand walks correspond to $t = 1$.

velocity jump process that may give a correct diffusion phenomenon. In Section 4, we introduce a revertible kinetic equation and derive a diffusion law based on it.

3.2. Radial solutions. Since the anisotropic structure of the thought experiment is radially symmetric, the solution is radial if the initial value is. Using this fact, we may test the validity of diffusion laws analytically by comparing equations for radial solutions. Take polar coordinates (r, θ) which give $x = r \cos \theta$ and $y = r \sin \theta$. After changing variables, we obtain

$$u_t = \nabla \cdot (\nabla \cdot (\mathbb{M}u)) = \frac{1}{1+k} \left(u_{rr} + \frac{k}{r^2} u_{\theta\theta} + \frac{2-k}{r} u_r \right).$$

If the solution u is a radial function, we have $u_{\theta\theta} = 0$ and obtain a simplified system,

$$(3.4) \quad \begin{cases} u_t = \frac{1}{1+k} (u_{rr} + \frac{2-k}{r} u_r), & r, t > 0, \\ u(r, 0) = u_0(r), & r > 0, \\ u_r(0, t) = 0, & t > 0. \end{cases}$$

The first order term $\frac{2-k}{r} u_r$ gives large drift phenomenon in the radial direction for k large, which explains the nonphysical phenomenon of drifting salty water. If $k = 1$, this term becomes the one for the radial solution of the heat equation. In conclusion, the model pass the thought experiment test only when there is no anisotropy, i.e., only when $k = 1$.

Numerical solutions of (3.4) are given in Figure 5 for three cases of $k = 1, 9$, and 25 . We can see that the support of the solution moves away from the origin if $k = 9$ or $k = 25$. This is the same phenomenon observed in Figures 3 and 4.

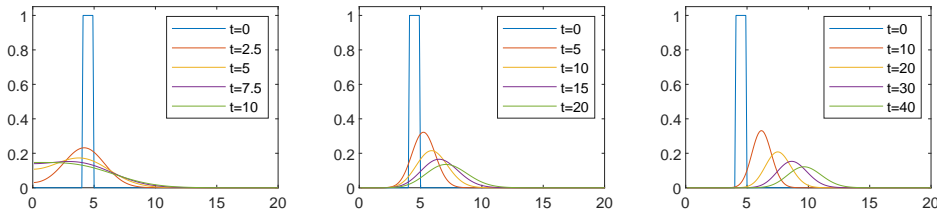


FIGURE 5. Numerical solutions of (3.4) with $k = 1, 9, 25$ from the left.

4. ANISOTROPIC DIFFUSION LAW AND A REVERTIBLE KE

We return to the revertible kinetic equation (1.1) in this section and take its singular limit to obtain an anisotropic diffusion equation,

$$(4.1) \quad u_t = \nabla \cdot \left(\mu^{-1} (\nabla \cdot (\mu \mathbb{D}u) - \mathbb{N}u) \right),$$

where

$$(4.2) \quad \mathbb{D} = \mathbb{D}(\mathbf{x}) = \frac{1}{\mu(\mathbf{x})} \int_A (\mathbf{v}_\alpha \otimes \mathbf{v}_\alpha) q(\alpha, \mathbf{x}) d\alpha,$$

$$(4.3) \quad \mathbb{N} = \mathbb{N}(\mathbf{x}) = \int_A (D\mathbf{v}_\alpha) \mathbf{v}_\alpha q(\alpha, \mathbf{x}) d\alpha.$$

Here, $D\mathbf{v}_\alpha$ denotes the derivative matrix of the vector field \mathbf{v}_α . We first introduce the notion of revertibility and then set the coefficients to make (1.1) a revertible kinetic equation.

4.1. Revertible kinetic equation. The main contribution of the paper is in introducing a revertible kinetic equation and developing a diffusion theory based on it. Let X_n be the position of a particle after n steps of random walks. If the random walk is spatially homogeneous, the expectation of the random variable X_n is same as the initial position, i.e., $E(X_n) = X_0$. However, if the process is spatially heterogeneous, then $E(X_n) \neq X_0$ in general. However, if

$$E(X_2) = X_0$$

whenever the second walk is in the opposite direction of the first one, we call the random walk system **revertible**. In other words, the particle can return to the previous position by taking the opposite direction. The discrete system given in (3.1) is not revertible. If the first walk is in the \mathbf{v}_θ direction, the particle cannot return to the starting position even if the second walk is in the $-\mathbf{v}_\theta$ direction. The particle will be placed at a layer farther from the origin.

The velocity jump process corresponding to a homogeneous kinetic equation is revertible, but a heterogeneous one is not because of the following reason. The hypothesis that a particle keeps its velocity until the next collision is flawless. However, together with other components of the system such as the turning frequency μ depending only on \mathbf{x} , the revertibility is lost in a heterogeneous case. For example, if the mean speed at X_1 is faster than at X_0 , the particle goes further than the starting position at the second step, i.e., $E(X_2) \neq X_0$, even if it takes exactly the opposite direction in the second step.

The revertible kinetic equation of this paper,

$$p_t + \frac{1}{\epsilon} \nabla \cdot (\mathbf{v}_\alpha p) = \frac{\mu(\mathbf{x})}{\epsilon^2} \int_A \left(q(\alpha, \mathbf{x}) p(\alpha', \mathbf{x}, t) - q(\alpha', \mathbf{x}) p(\alpha, \mathbf{x}, t) \right) d\alpha', \quad (1.1)$$

is designed to obtain the revertibility. In this system, the main hypothesis is that a particle moves along a velocity vector field chosen at the moment of collision. The particle changes its direction along an integral curve and also changes its speed. In this way a particle returns to the previous position by taking the vector field of the opposite direction. Note that this hypothesis breaks the fundamental assumption of the kinetic theory that a particle maintains its velocity until the next collision. We take two hypotheses on the velocity vector fields which make the discussion valid:

$$(4.4) \quad \mathbf{v}_{-\alpha} (:= -\mathbf{v}_\alpha) \in V \quad \text{if} \quad \mathbf{v}_\alpha \in V,$$

and

$$(4.5) \quad q(-\alpha, \mathbf{x}) = q(\alpha, \mathbf{x}).$$

Under these two hypotheses, a particle may return back to the previous position by taking a velocity vector field $\mathbf{v}_{-\alpha}$ if \mathbf{v}_α is the previous one.

4.2. Diffusion equation with a correction term. Now we consider the singular limit of (1.1) and derive (4.1) formally. The first part of the derivation is parallel to the classical kinetic equation case in Section 2. Since $\int_A q(\alpha, \mathbf{x}) d\alpha = 1$ and $u(\mathbf{x}, t) = \int_A p(\alpha, \mathbf{x}, t) d\alpha$, we may rewrite (1.1) as

$$(4.6) \quad p_t + \frac{1}{\epsilon} \nabla \cdot (\mathbf{v}_\alpha p) = \frac{1}{\epsilon^2} \mu(\mathbf{x}) (q(\alpha, \mathbf{x}) u(\mathbf{x}, t) - p(\alpha, \mathbf{x}, t)).$$

Integrate (4.6) over A and obtain a conservation law,

$$(4.7) \quad u_t = -\nabla \cdot \mathbf{J},$$

where the flux \mathbf{J} is given by

$$\mathbf{J}(\mathbf{x}, t) = \frac{1}{\epsilon} \int_A (\mathbf{v}_\alpha p(\alpha, \mathbf{x}, t)) d\alpha.$$

Multiply $\epsilon \mathbf{v}_\alpha$ to (4.6), integrate the result over A , and obtain

$$(4.8) \quad \epsilon^2 \mathbf{J}_t + \int_A \mathbf{v}_\alpha \nabla \cdot (\mathbf{v}_\alpha p) d\alpha = \frac{\mu(\mathbf{x})}{\epsilon} u \mathbb{E} - \mu(\mathbf{x}) \mathbf{J}.$$

Under the two hypotheses (4.4) and (4.5), we obtain

$$\mathbb{E} = \frac{1}{2} \int_A (q(\alpha, \mathbf{x}) \mathbf{v}_\alpha + q(-\alpha, \mathbf{x}) \mathbf{v}_{-\alpha}) d\alpha = \frac{1}{2} \int_A q(\alpha, \mathbf{x}) (\mathbf{v}_\alpha - \mathbf{v}_\alpha) d\alpha = 0.$$

Since $\epsilon^2 \mathbf{J}_t$ is the smallest term and the fractional population $p(\mathbf{v}, \mathbf{x}, t)$ is proportional to the probability distribution $q(\alpha, \mathbf{x})$ after an enough number of collisions, we expect that

$$(4.9) \quad \epsilon^2 \mathbf{J}_t \rightarrow 0 \quad \text{and} \quad p(\alpha, \mathbf{x}, t) \rightarrow q(\alpha, \mathbf{x}) u(\mathbf{x}, t) \quad \text{as} \quad \epsilon \rightarrow 0.$$

This is the part needed to make the derivation rigorous (see Remark 4.1). Then, after taking $\epsilon \rightarrow 0$ limit, the flux \mathbf{J} in (4.8) becomes

$$(4.10) \quad \mathbf{J} = -\frac{1}{\mu(\mathbf{x})} \int_A \mathbf{v}_\alpha \nabla \cdot (\mathbf{v}_\alpha q(\alpha, \mathbf{x}) u) d\alpha.$$

The steps to derive the flux in (4.10) are parallel to ones for the classical kinetic equation case in Section 2. The difference comes now. Since the vector fields \mathbf{v}_α 's depend on the space variable \mathbf{x} , we use the product rule,

$$\nabla \cdot (\mathbf{v}_\alpha \otimes \mathbf{v}_\alpha q(\alpha, \mathbf{x}) u(\mathbf{x}, t)) = \mathbf{v}_\alpha \nabla \cdot (\mathbf{v}_\alpha q(\alpha, \mathbf{x}) u) + (D\mathbf{v}_\alpha) \mathbf{v}_\alpha q(\alpha, \mathbf{x}) u.$$

Then, the flux is rewritten as

$$\mathbf{J} = -\frac{1}{\mu(\mathbf{x})} \int_A \mathbf{v}_\alpha \nabla \cdot (\mathbf{v}_\alpha q(\alpha, \mathbf{x}) u) d\alpha = -\frac{1}{\mu(\mathbf{x})} \left(\nabla \cdot (\mu \mathbb{D}u) - \mathbb{N}u \right),$$

where \mathbb{D} and \mathbb{N} are given by (4.2) and (4.3), respectively. After substituting the flux to the conservation law (4.7), we obtain the diffusion law (4.1). In Section 5, we will observe that this correction term fixes the nonphysical phenomenon considerably. However, it still requires an extra correction.

Remark 4.1. *The rigorous convergence proof required in (2.8) and (4.9) has been obtained for some special cases only (see [2, 3]) and remains open for general cases. In the system constructed for the thought experiment, the solution of (1.1) blows up at the origin. It is related to the curvature of integral curves which diverges from the origin. Hence, the convergence can be obtained only under suitable conditions on the vector fields.*

4.3. Restriction to isotropic diffusion. The anisotropic diffusion law (4.1) is reduced to an isotropic diffusion law when the matrix \mathbb{M} is the identity matrix multiplied by a constant. For example, if the system has no directional dependency, we obtain

$$\mathbb{M} = \frac{v^2}{n} \quad \text{and} \quad \mathbb{N} = \frac{v}{n} \nabla v,$$

where $v = v(\mathbf{x})$ is the root mean square of possible speeds at \mathbf{x} . Then, the diffusion law (4.1) becomes

$$u_t = \nabla \cdot \frac{1}{n\mu} \nabla (v^2 u) - \nabla \cdot \frac{1}{n\mu} v u \nabla v = \nabla \cdot \left(\frac{v}{n\mu} \nabla (v u) \right).$$

The diffusivity is given by $D = \frac{v^2}{n\mu}$ in n space dimensions and we may rewrite the equation as

$$(4.11) \quad u_t = \nabla \cdot \left(\sqrt{\mu^{-1} D} \nabla (\sqrt{\mu D} u) \right),$$

which is the diffusion law (1.3). If μ is constant, this diffusion law becomes Wereide's diffusion law (1.5). For the isotropic diffusion case, (4.11) is the final diffusion law introduced in the paper. However, for the anisotropic diffusion, we need another correction term which is introduced in Section 6.

5. THOUGHT EXPERIMENT WITH THE FIRST CORRECTION TERM \mathbb{N}

In this section we do the thought experiment test for the diffusion law (4.1). We take the same vectors in (3.1). The difference is that we take them as vector fields and each particle moves along an integral curve before the next collision. We use the same matrix \mathbb{M} in (3.3). The derivative matrixes are

$$D\mathbf{v}_r = \frac{1}{|\mathbf{x}|^3} \begin{pmatrix} y^2 & -xy \\ -xy & x^2 \end{pmatrix}, \quad D\mathbf{v}_\theta = \frac{1}{|\mathbf{x}|^3} \begin{pmatrix} xy & -x^2 \\ y^2 & -xy \end{pmatrix},$$

and

$$(D\mathbf{v}_r)\mathbf{v}_r = \frac{1}{|\mathbf{x}|^4} \begin{pmatrix} xy^2 - xy^2 \\ -x^2y + x^2y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad (D\mathbf{v}_\theta)\mathbf{v}_\theta = \frac{1}{|\mathbf{x}|^4} \begin{pmatrix} -x(y^2 + x^2) \\ -y(y^2 + x^2) \end{pmatrix}.$$

Therefore, the first correction vector \mathbb{N} in (4.3) is

$$(5.1) \quad \mathbb{N} = -\frac{k}{(1+k)|\mathbf{x}|^2} \mathbf{x}.$$

5.1. Numerical computation and Monte-Carlo simulation. In Figure 6, a numerical solution of (4.1) is given when $k = 25$. The initial value is taken from Figure 3(a) for comparison. The diffusion equation (4.1) is solved on the domain $\Omega = [-10, 10] \times [-10, 10]$ with the zero Dirichlet boundary condition. In Figure 6(b), a snap shot for the solution is given when $t = 13$. We can see that the support of the solution expands inward and outward almost equally. We can clearly see the difference between the two diffusion laws (2.3) and (4.1). The correction term

$-\nabla \cdot (\mathbb{N}u)$ in (4.1) pushes back the solution toward the origin and corrects the drift phenomenon in radial direction.

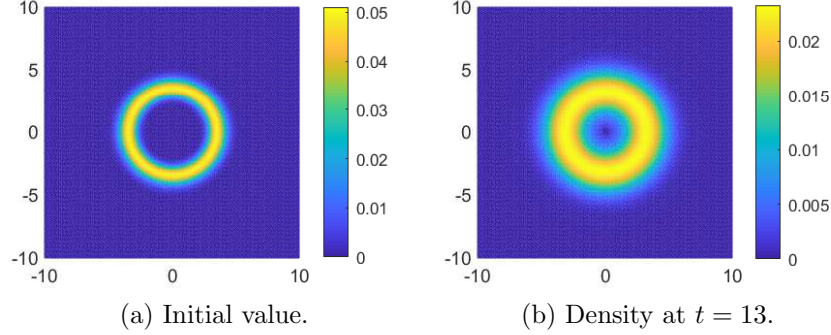


FIGURE 6. Numerical simulation of (4.1) with (3.3), (5.1), and $k = 25$.

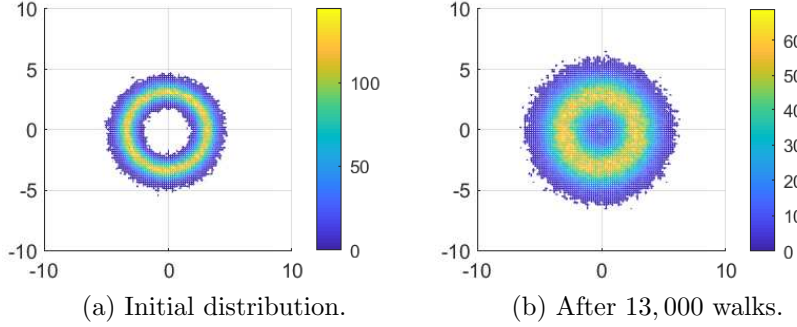


FIGURE 7. Monte-Carlo simulation for the velocity jump process (1.1) with 10^5 particles. One thousand walks correspond to $t = 1$.

In Figure 7, the result of a Monte-Carlo simulation is given for the revertible velocity jump process. In the simulation a particle walks in radial or in circumference direction randomly. The difference is that when a particle moves in the circumferential direction, it stays in the same circle around the origin, which is the integral curve of \mathbf{v}_θ . The chance to walk in the circumference direction is $k = 25$ times larger than the one in the radial direction. We took the total of 10^5 particles distributed initially as in Figure 4(a). We can see that the diffusion law (4.1) explains this Monte-Carlo simulation correctly. The drifting phenomenon in the radial direction has been corrected by introducing a revertible velocity jump process. However, the equation for radial solution in the next section shows that (4.1) still requires another correction.

5.2. Radial solutions. Next, we consider the equation for radial solutions. In terms of polar coordinates, the correction vector \mathbb{N} and the advection term are written as

$$\mathbb{N} = -\frac{k}{(1+k)r} \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix}, \quad \nabla \cdot (\mathbb{N}u) = -\frac{1}{1+k} \frac{k}{r} u_r.$$

Then, the diffusion equation (4.1) becomes

$$u_t = \nabla \cdot \nabla \cdot (\mathbb{M}u) - \nabla \cdot (\mathbb{N}u) = \frac{1}{1+k} \left(u_{rr} + \frac{k}{r^2} u_{\theta\theta} + \frac{2}{r} u_r \right).$$

If u is a radial function, we obtain a simplified equation,

$$(5.2) \quad \begin{cases} u_t = \frac{1}{1+k}(u_{rr} + \frac{2}{r}u_r), & r, t > 0, \\ u(r, 0) = u_0(r), & r > 0, \\ u_r(0, t) = 0, & t > 0. \end{cases}$$

The advection term in (3.4) consists of two part, $\frac{2}{r}u_r$ and $\frac{-k}{r}u_r$, where $\frac{2}{r}u_r$ pushes the particle toward origin and $\frac{-k}{r}u_r$ away from the origin. The second term is cancelled out by the correction term $-\nabla \cdot (\mathbb{N}u)$. Note that the remaining advection term is $\frac{2}{r}u_r$. However, for the case of the radial solutions of the heat equation in two space dimensions, the corresponding advection term is $\frac{1}{r}u_r$. In conclusion, even if the diffusion equation (4.1) improves the solution behavior considerably as observed in Figure 6(b), it does not satisfy the thought experiment yet. We need another correction process.

A numerical solution of (5.2) is given in Figure 8(4.1). The solution behavior for small $t > 0$ is reasonable. However, as t increases, the solution develops a singularity at the origin. For example, the numerical solution profile at $t = 20$ has a local maximum at $r = 0$. The singularity grows as time increases. This is because the number of particle in each circular channel converges to constant and the channel size shrinks to zero at the origin. Hence, the solution blows up at the origin instantly.

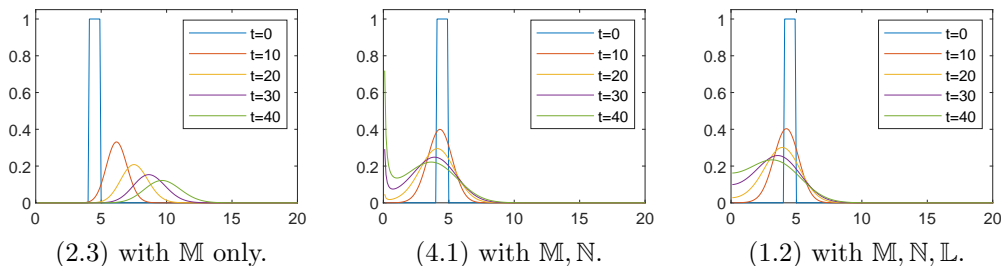


FIGURE 8. Snap shots of radial solutions (x -axis: radial direction, $k = 25$).

6. CURVATURE CORRECTION

In this section we introduce the second correction term that counts the curvature of integral curves of vector fields \mathbf{v}_α . This correction term is useful only for an anisotropic diffusion case. If the diffusion is isotropic, the resulting correction term becomes zero. Note that the probability to choose a velocity fields $\pm\mathbf{v}_r$ was set to be identical in (3.2) for convenience. However, the probability for a particle to disperse inward bound should be larger than the one of outward bound since the boundary of inside layer is smaller than the outside one (see the right side of Figure 2).

Let N_α be the curvature vector of integral curves of a vector field \mathbf{v}_α . In other words, the norm $\|N_\alpha\|$ is the scalar curvature and N_α takes the direction of the principal normal vector. Therefore, the correcting advection term should be in the opposite direction of the principal normal vector. We conjecture that the ratio of the two probabilities for a particle move to the inward layer and outward one is identical to the ratio of the two boundary perimeters. To equalize the two ratios, we

introduce the second correction vector,

$$(6.1) \quad \mathbb{L} := -\frac{1}{2} \sum_{\alpha \in A} \mathbb{M} N_{\alpha},$$

which becomes zero if the integral curves are straight lines. This correction vector completes our final anisotropic diffusion equation (1.2). The curvature correction term \mathbb{L} in (6.1) is not a driven one. It is not obtained in a homogenization process neither. We have simply computed it using the fact that the probability should be balanced with the circumference length of layers.

6.1. Numerical computation. We return to the example in Section 3 to check if the final diffusion model (1.2) resolves the remaining issue. The principle normal vectors of the four vector fields are

$$N_r = N_{-r} = 0, \quad N_{\theta} = N_{-\theta} = -\frac{\mathbf{v}_r}{|\mathbf{x}|}.$$

Therefore,

$$(6.2) \quad \mathbb{L} = -\frac{1}{2}(\mathbb{M} N_{\theta} + \mathbb{M} N_{-\theta}) = \mathbb{M} \frac{\mathbf{v}_r}{|\mathbf{x}|} = \frac{1}{2|\mathbf{x}|^2} \mathbf{x}.$$

In Figure 9, the numerical solution of (1.2) is given when the initial value is taken from Figure 3(a). The solutions of the three models are given together for comparison. The solution of (2.3) moves away from the origin. The correction term \mathbb{N} in (4.1) pushes the solution back to origin. However, the correction term \mathbb{N} pushes particles too much. Finally, the curvature correction term \mathbb{L} pushes the solution to the radial direction and gives a better result.

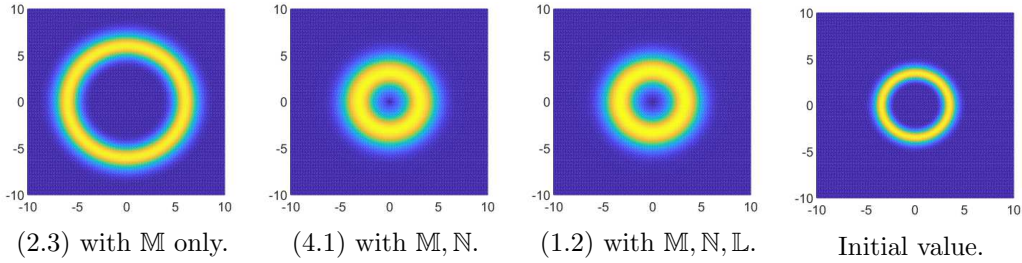


FIGURE 9. Solution snapshots and initial value ($t = 13$ and $k = 25$).

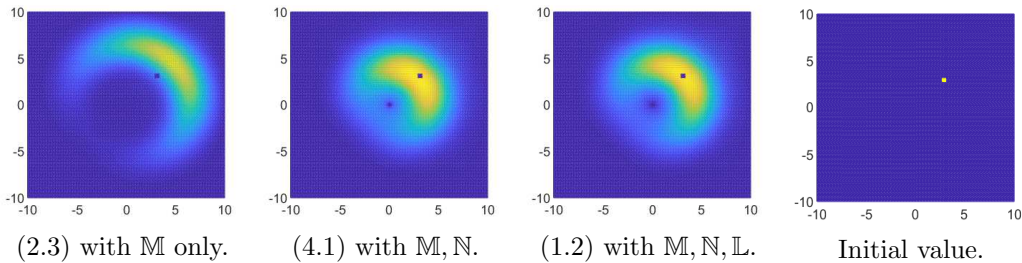


FIGURE 10. Solution snapshots. The deposition position is marked dark ($t = 15, k = 9$).

6.2. Radial solutions. Using the polar coordinates, the diffusion equation (1.2) is written as

$$u_t = \nabla \cdot \frac{1}{\mu} (\nabla \cdot (\mathbb{M}u) - (\mathbb{N} + \mathbb{L})u) = \frac{1}{1+k} \left(u_{rr} + \frac{k}{r^2} u_{\theta\theta} + \frac{1}{r} u_r \right).$$

If u is a radial solution, it satisfies

$$(6.3) \quad \begin{cases} u_t = \frac{1}{1+k} (u_{rr} + \frac{1}{r} u_r), & r, t > 0, \\ u(r, 0) = u_0(r), & r > 0, \\ u_r(0, t) = 0, & t > 0. \end{cases}$$

Finally, we have obtained the heat equation for radial solutions. The coefficient $\frac{1}{1+k}$ appears since only the dispersal in the radial direction is counted for radial solutions. The advection term $\frac{1}{r} u_r$ is identical to the heat equation case in two space dimensions. In other words, the diffusion model (1.2) satisfies the criteria in Section 3 that the anisotropy disappears for radial solutions and the heat equation is satisfied. Numerical solutions of (6.3) are given in Figure 8(1.2) which is simply the solution of the heat equation.

6.3. Simulation for a non-radial solution. So far, only radial solutions have been considered. To compare the real capability of diffusion laws, we have compared the non-radial solutions of the diffusion laws in Figure 10. The initial value is a characteristic function that is 1 in a small square centered at the point $(3, 3)$ as marked in the figures. You can see how the particles diffuse in the anisotropic structure of the example. The solution of (2.3) obtained from the classical kinetic equation shows an unrealistic phenomenon in which chemical particles move away from the initial deposition site. Obviously it fails the second criterion of our thought experiment. Great improvement can be found in the simulation of (4.1), which is based on the revertible kinetic equation. The correction term pushes back the chemical particles. However, the maximum density shifts slightly towards the origin. Finally, in the third case, even if the solution distribution is not significantly different from the case of (1.2), the maximum density is placed exactly at the initial deposition site. In other words, (1.2) passes the second criterion of the thought experiment.

6.4. Magic of Fick's law. Fick's law (1.4) is one of the most widely used diffusion laws. It was obtained by mimicking Fourier's law of heat conduction and was very successful. Einstein [4] took this diffusion theory and found a way to show the existence of atoms. In general, Fick's law is successful when particles have constant speed or, equivalently, the temperature is constant. The example in section 2.2, Figure 1, is when the average speed is not constant. As we have already saw, Fick's law failed in the case.

How about the thought experiment? Note that the setup of the thought experiment in Section 3 is a case when the particle speed is constant. Hence, we find that the situation is similar to an anisotropic heat conduction case. Hence, one might think that Fick's law would give a good result. In fact, it is more than that. For the specific case that \mathbb{M}, \mathbb{N} and \mathbb{L} are given by (3.3), (5.1), and (6.2), respectively, we may do some computation to obtain

$$\nabla \cdot (\mathbb{M}u) - (\mathbb{N} + \mathbb{L})u = \mathbb{M}\nabla u.$$

Therefore, our main diffusion equation (1.2) turns into

$$u_t = \nabla \cdot \left(\frac{1}{\mu} \mathbb{M} \nabla u \right) = \nabla \cdot (\mathbb{D} \nabla u),$$

which is exactly Fick's law. Temperature is another name of the root mean square of molecular speed. It seems that, if the temperature is homogeneous, the new diffusion law (1.2) returns to Fick's diffusion law. However, it is just a conjecture.

7. CONCLUSION

The main conclusion of this paper is that the classical heterogeneous kinetic equation (2.2) does not give the correct diffusion phenomenon. Four diffusion laws in (1.4)–(1.7) do not give the correct diffusion phenomenon, neither. To derive a realistic anisotropic diffusion law, we introduced a revertible kinetic equation (1.1). Then, we have obtained an anisotropic diffusion law,

$$u_t = \nabla \cdot \mu^{-1} (\nabla \cdot (\mu \mathbb{D} u) - (\mathbb{N} + \mathbb{L}) u), \quad (1.2)$$

where \mathbb{D} is the usual diffusion tensor. The two correction terms, \mathbb{N} and \mathbb{L} , can fix non-physical dispersal phenomenon of classical diffusion laws. In particular, the second term \mathbb{L} is a curvature correction term of the revertible kinetic equation.

Thermophoresis, which is also known as thermomigration, thermodiffusion, the Soret effect, or the Ludwig–Soret effect, is a dispersal phenomenon that converges to a nonconstant steady state under temperature gradient. It is known as the last mass transport phenomenon without atomic level explanation. The classical diffusion laws do not explain the phenomenon. We claim that the reason of the failure is in the underlying assumption that the diffusivity alone decides the diffusion phenomenon. It is true for a homogeneous diffusion, but not for a heterogeneous one. For an isotropic diffusion phenomenon, the anisotropic diffusion law (1.2) is written as

$$u_t = \nabla \cdot \left(\sqrt{\mu^{-1} D} \nabla (\sqrt{\mu D} u) \right). \quad (4.11)$$

Let $T = T(\mathbf{x})$ be the temperature which varies in space. Since the diffusivity D and the turning frequency μ are functions of temperature, we may write $\mu = \mu(T)$ and $D = D(T)$. Then, (4.11) is written as

$$u_t = \nabla \cdot \left(D \nabla u + \frac{1}{2\mu} \frac{\partial(\mu D)}{\partial T} u \nabla T \right).$$

This is our molecular level explanation of the thermophoresis phenomenon obtained using the new diffusion law (4.11). The thermal coefficient is given by the temperature sensitivity of μD .

Acknowledgments. Authors would like to thank Professors Thomas Hillen and Laurent Desvillettes for helpful discussions. They also thank two anonymous referees of the journal. Their comments gave authors insights to develop the diffusion model in this paper and to improve the presentation. This research was supported in part by National Research Foundation of Korea (NRF-2017R1A2B2010398 and NRF-2017R1E1A1A03070692).

APPENDIX A. IT IS A MATTER OF HOW TO DEAL WITH RANDOMNESS.

Diffusion is a phenomenon in which particles, population, information, etc. spread out by randomness. Since the randomness is the driving force of so many phenomena, the same theory repeats in many different fields with different terminologies. Volatility (or variance) refers to the degree to which a certain quantity changes rapidly. Note that volatility is not randomness. For example, we may say that the result of tossing a coin is random and the bet amount is the volatility. The speed and the turning frequency decide the volatility in the kinetic equation we considered in the paper. If volatility is constant, the phenomenon can be called homogeneous; if not, it can be called heterogeneous. The essence of heterogeneous diffusion theory is in how to deal with heterogeneous volatility. We considered two ways of dealing with it, the classical KE (2.2) and the revertible KE (1.1). It turned out that the revertible one provides a correct way to handle the heterogeneity.

We encounter the same situation in the stochastic calculus. Let B be a Wiener process and X be a right-continuous random process. Let $\pi := \{t_n : n = 0, \dots, N\}$ be a partition of $[0, 1]$ and denote the values of the random variables at $t = t_n$ as B_n and X_n . Roughly speaking, *Ito integral* of X with respect to B is a random variable defined in term of the limit,

$$\int_0^1 X dB = \lim_{\|\pi\| \rightarrow 0} \sum_{n=0}^{N-1} X_n (B_{n+1} - B_n), \quad (\text{Ito integral})$$

where the left end limit of each sub-interval $[t_n, t_{n+1}]$ is used for the integration. On the other hand, the Stratonovich integral is defined as

$$\int_0^1 X dB = \lim_{N \rightarrow \infty} \sum_{n=0}^{N-1} \frac{X_n + X_{n+1}}{2} (B_{n+1} - B_n), \quad (\text{Stratonovich integral})$$

where the mid-point of each sub-interval $[t_n, t_{n+1}]$ is used for the integration. These two different ways of dealing randomness (or volatility) give different properties of stochastic calculus. Since only the current information is used to compute the next step, the Ito integral gives a tool to handle the randomness more easily. The Stratonovich integral, on the other hand, provides a natural way to deal with the calculus itself. This is because Stratonovich's way of dealing with randomness is revertible as we will see below.

Consider X_n as a random walk system which denotes the value (or position) of the random variable X at the n -th time step. For a homogeneous case, the walk length $\Delta X|_n := |X_{n+1} - X_n|$ and the waiting time length $\Delta T|_n := t_{n+1} - t_n$ at n -th step are constant (or follow a given probability distribution at each step). If the walk length $\Delta X|_n$ is heterogeneous, we encounter the same situation as the heterogeneous kinetic equation case. Suppose that the walk length is given by a function $f(X)$ that depends on the value of the random variable X . If the walk length is taken using the information before departure, i.e., $\Delta X|_n = f(X_n)$, we may call it Ito type. Suppose that $X_0 = 0$ and the first and the second walks are in the opposite directions each other. Then, in general,

$$|X_2| = |f(X_0) - f(X_1)| \neq 0.$$

Therefore, an Ito type random walk system is not revertible. We call the classical kinetic equation (2.2) a Ito type since only the information at the moment of jump

is taken. If the walk length is chosen from the mid-point, i.e., $\Delta X|_n = f\left(\frac{X_n + X_{n+1}}{2}\right)$, it is called Stratonovich type. Then,

$$|X_2| = |f((X_0 + X_1)/2) - f((X_1 + X_2)/2)| = 0$$

if $X_2 = 0$. Therefore, the Stratonovich type random walk system is revertible. We call the revertible kinetic equation (1.1) a Stratonovich type because it is revertible, not because of the use of the mid-point.

APPENDIX B. MONTE-CARLO SIMULATION IN SECTION 2.2

The Monte-Carlo simulations in Section 2.2 clearly show that the spatial heterogeneities in $\mu(\mathbf{x})$ and $q(\mathbf{v}, \mathbf{x})$ should be separated as modeled in (2.3). Since the separation of μ and \mathbb{M} in the diffusion law is one of key issues and the simulation of the example is subtle, we discuss about it in detail in this section. This is the only example in the paper with nonconstant turning frequency which shows the importance of understanding the difference between $\mu(\mathbf{x})$ and $q(\mathbf{v}, \mathbf{x})$ when they are spatially heterogeneous. We took $\mu = 1$ in other examples to concentrate other issues. The Matlab code used for the simulation is given below and followed by a detailed explanation.

```
%% parameters
L=2;           % domain is [0,L]
eps=0.01;
M=5*10^4;     % total number of particles
T=200;       % final computation time
%% variables
dx=2*eps;    % walking distance is 2 times epsilon
u=rand(1,M)*L; % random initial positions
%% simulation
for i=1:M
    t=T;
    while t>0
        direction=(randi(2)*2-3); % +1 or -1
        if(u(i)<1)
            t=t-2;
            if(u(i)<dx&&direction<0)
                u(i)=2-(dx-u(i))/2;
            elseif(u(i)>1-dx&&direction>0)
                u(i)=1+(u(i)-1+dx)/2;
            else
                u(i)=u(i)+direction*dx;
            end
        else
            t=t-1;
            if(u(i)<1+dx&&direction<0)
                u(i)=1-2*(1+dx-u(i));
            elseif(2-dx<u(i)&&direction>0)
                u(i)=2*(u(i)-2+dx);
            else

```

```

        u(i)=u(i)+direction*dx;
    end
end
end
end
%% display
histogram(u,20);axis([0 L 0 2*M/20]);

```

If the turning frequency μ is constant, the velocity jump process is equivalent to the position jump process with a jumping (or waiting) time $\Delta t = \frac{2}{\mu}$ and a walking distance $\Delta x = |v|\Delta t$. Since the parameters in (2.10) and (2.11) are piecewise constant, the velocity jump process is equivalent to a position jump process with

$$(B.1) \quad \Delta x = 2\epsilon, \quad \Delta t = \begin{cases} 2, & 0 < x < 1, \\ 1, & 1 < x < 2, \end{cases}$$

as long as a particle stays in the same region after a jump. In the code, a particle jumps the same distance of $\Delta x = 2\epsilon$ in both regions, but the jumping time Δt depends on the region of the particle as given in (B.1). Notice lines of $t = t - 2$ and $t = t - 1$ in the code which reflect this dependence. Since the coefficients are piecewise constant, it is the behavior at the boundary of the two regions that makes the heterogeneous diffusion phenomenon. In a velocity jump process, the turning frequency is changed immediately after a particle enters a different region. However, the velocity is not changed until the next collision. Hence, a particle moves further if it jumps into a lower turning frequency region and moves shorter otherwise.¹ This makes a key difference. To compute the correct walking distance, we should compute Δt precisely. The formula is

$$\int_0^{\Delta t} \mu(x(t)) dt = 2,$$

where $x(t)$ is the position of the particle at time t . We get $\Delta t = 2$ if the particle stays in the region $0 < x < 1$, $\Delta t = 1$ if the particle stays in the other region $1 < x < 2$, and $1 < \Delta t < 2$ if the particle crosses the boundary. Therefore, if a particle moves into a different region, the walking distance should be recalculated since the speed is not changed yet until the next collision. The main for loop of the code is divided into six cases to do such calculations. Each of the $M (= 5 \times 10^4)$ particles walks until the final time $T (= 200)$.

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