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Mathematical multi-scale model of water purification

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In this work, we consider a mathematical model of the water treatment process and determine the effective characteristics of this model. At the microscopic length scale, we describe our model in terms of a lattice random walk in a high-contrast periodic medium with absorption. Applying then the upscaling procedure, we obtain the macroscopic model for total mass evolution. We discuss both the dynamic and the stationary regimes and show how the efficiency of the purification process depends on the characteristics of the macroscopic model.

KEYWORDS

absorption, correctors, high-contrast periodic media, random walk, upscaling

MSC CLASSIFICATION

35B27, 35B40, 47D07, 60J28

1 | INTRODUCTION

The problem of water purification has great practical importance and gives rise to many interesting mathematical questions. Mathematical modeling of water treatment has become increasingly popular in recent years; see, for example, previous studies [1–3]. In the present work, we deal with mathematical models for the treatment of wastewater in biofilm

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reactors and in filters filled with granules which are made of nano-porous super-hydrophilic materials. We use here a combination of a probabilistic approach and a homogenization technique for modeling the purification process.

To clarify the motivation of the model, we shortly describe one of the biofilters used in industrial water purification process. A biofilm reactor is a tank of cylindrical shape which is about 1 m high and of diameter about 20 cm. It is packed with parallelepipeds consisting of thin pressed polymer fibers. A typical volume of such a parallelepiped is 15–20 cm³, and the fibers are small rods whose length is about 1 cm. Each such a rod is covered with a thin biologically active biofilm, these biofilms being filled with bacteria for which impurities within water are a nutrition. Water is supplied to the upper cross section of the device and then trickles down drop by drop along the rods so that the biofilms covering the rods are getting wet. The material of biofilms is designed in such a way that its diffusion coefficient is much smaller than that in the surrounding fluid domain. The polluted water penetrates the biofilms and the impurities are consumed by the bacteria. The intensity of this process depends on the concentration of both the bacteria and the impurities at the biofilms boundary. The averaged speed of water also influences the said intensity. The biofilter is efficient if the said averaged speed is sufficiently small. Altogether, there are several millions of such rods in the device, they are called basic elements of the biofilter. We would like to construct an adequate model of the mentioned above consumption process for one rod and then to model the whole process of water purification. Our goal is to evaluate the drop in the water pollution level. Several models of this type have been considered in a number of works, in particular in Oliinyk and Airapetyan [4] and Bobyleva and Shamaev [5].

In Bobyleva and Shamaev [5], the consumption of impurities in one basic element is described by a system of differential equations including a diffusion equation in 3D cylindrical domain and a transport equation at the rod border. This problem does not have an analytic solution. So it is natural to simulate its solution numerically. To this end in Bobyleva and Shamaev [5], the whole cylindrical tank is divided into horizontal layers, and the drop of the impurity concentration at each layer is calculated numerically. Also, in Bobyleva and Shamaev [5], the asymptotic analysis of the system is performed provided a small thickness of the rods.

Let us move on to another model of water treatment. One of the most common pollutants of the wastewater is petrol and oils impurities, and the water purification from oil and petrol products refer to the highly important environmental problems. One of the modern methods of water purification is described in Kuligin et al. [6]. It is the filtering method using granules made of innovative nano-porous super-hydrophilic materials. For the practical implementation, a design of the classical pressure filter for granulated filter bed was chosen. The system is represented by a vertical cylindrical filter with a distribution system below and above. The filter is filled with granulated bed of the grade 0.7–1.7 mm, preliminary impregnated with water. The filter has a height of 1.5 m and an average pore diameter of 6.5 nm. The diffusion coefficient in the granules is much smaller than that in the surrounding solute.

In the present work, we suggest a mathematical model based on a probabilistic interpretation of the water purification process described in Kuligin et al. [6]. It is assumed that the movement of the impurities at the microscale is described in terms of a Markov process. Namely, the impurities can enter the porous granules with a positive probability and then either be absorbed there or leave.

Also, it is assumed that the basic purification elements are located periodically. We then divide each periodicity cell into a finite number of cubes, introduce the lattice formed by the centers of these cubes, and perform the corresponding discretization of the Markov process. For the obtained random walk, we define the transition probabilities between the sites of the same cell or neighboring cells. This yields the description of the model at the microscopic level.

Our goal is to provide the macroscopic description of this process based on upscaling procedure. It will be shown that the coefficients involved in the macroscopic model, that is, the effective characteristics of the water purification process, can be expressed through the characteristics of the model at the microscopic scale by means of solving a system of linear algebraic equations.

The main characteristics of the quality of a water filter is the rate of decay of impurities concentration depending on the distance to the upper cross section of the filter. In this work, we provide some examples of calculating this rate.

The advantage of the model proposed in this work is its flexibility, it can be easily adapted to any geometry of absorbing films. This model can be used for better understanding complex treatment systems and for optimizing the parameters of water purification devices in accordance with the restrictions on the device productivity and the purification quality.

Various phenomena in media with a high-contrast microstructure have been widely studied by the specialists in applied sciences, and then, since the 1990s, high-contrast homogenization problems have been attracting the attention of mathematicians. Homogenization problems for partial differential equations describing high-contrast periodic media have

been intensively investigated in the existing mathematical literature. In the pioneer work [7], a parabolic equation with high-contrast periodic coefficients has been considered. It was shown that the effective equation contains a nonlocal in time term which represents the memory effect. In the literature on porous media, these models are usually called double porosity models. Later on in Allaire [8], with the help of two-scale convergence techniques, it was proved that the solutions of the original parabolic equations two-scale converge to a function which depends both on slow and fast variables.

2 | MATHEMATICAL MODEL AND METHODS

In this section, we discuss mathematical models of water treatment process and the methods of studying these models. We assume in what follows that the diffusion of impurities is approximated by discrete processes in a high-contrast environment. The presence of high-contrast characteristics is natural in the considered models. Indeed, as was mentioned in Section 1, the diffusion in biofilms or hydrophilic granules is much smaller than that in the surrounding fluid domain. Also, the ratio between the size of the granules and the size of the whole filter is a small parameter, it is denoted by ε . We then assume that the ratio between diffusion coefficients in the granules and in the surrounding fluid is of order ε^2 . Since water trickles through a porous medium in the filter, its velocity is rather small. Our next assumption is that, at the microscopic length scale, this velocity is of order ε .

The asymptotic (large time) analysis of the corresponding difference equations is based on homogenization and approximation techniques of double porosity type discrete models. Notice that, after rescaling, at the macroscopic length scale, the velocity and the diffusion in the fluid domain are of the same order, and due to smallness of the diffusion in the granules, the time that a diffusive particle spends in a granule is comparable with the observation time.

We introduce a discrete time random walk $\hat{X}^{(\varepsilon)}(n)$ on \mathbb{Z}^d , $d \geq 1$ in a periodic high-contrast medium that models the discretized process of water purification at the microscopic length scale; see Section 3. This random walk approximates the diffusion of impurities in a filtering device and inherits appropriate parameters of the diffusion.

In the next section, the non-perturbed transition matrix in the fluid part is denoted by P^0 , it does not depend on ε . This matrix is then perturbed by a non-symmetric matrix εD which represents a small convection term. A small diffusion in the granules is represented by a matrix $\varepsilon^2 V$. We assume that D and V do not depend on ε and emphasize that for each $\varepsilon > 0$, the matrix $P^0 + \varepsilon D + \varepsilon^2 V$ is a transition matrix for the random walk $\hat{X}^{(\varepsilon)}(n)$.

The absorption process at the filter is modeled by partial absorption of a random walker at the so-called astral sites. To describe the absorption process, we modify the random walk by adding the absorbing state $\{\star\}$. Thus, our model at the microscopic level is the random walk with absorption.

Next, we study the large time behavior of this process by applying the *upsampling procedure*; see Section 4. Recalling that the transition probabilities of the random walk at the microscopic level depend on a small positive parameter ε , we make a proper diffusive scaling of the random walk that also includes absorption and study the limit behavior of the rescaled process $\mathcal{X}_\varepsilon(t)$, as $\varepsilon \rightarrow 0$. It turns out that there is a nice and useful description of the limit process as a two-component continuous time Markov process $\mathfrak{X}(t) = (\mathcal{X}(t), k(t))$. Its first component $\mathcal{X}(t)$ evolves in the space $\mathbb{R}^d \cup \{\star\}$, while the second component is a jump Markov process $k(t)$ with a finite number of states.

The second coordinate $k(t)$ of the process specifies the position of the random walk in the period. The process $k(t)$ does not depend on $\mathcal{X}(t)$; the intensities $\lambda(k)$ and transition probabilities μ_{kj} , $k \neq j$, $k, j = 0, 1, \dots, M$, of its jumps are expressed in terms of the transition probabilities of the original random walk. When $k(t) = 0$, the first component $\mathcal{X}(t)$ evolves along the trajectories of a diffusion process in \mathbb{R}^d , but when $k(t) \neq 0$, then the first component remains still until the second component of the process takes again the value equal to 0. Thus, the trajectories of $\mathcal{X}(t)$ coincide with the trajectories of a diffusion process in \mathbb{R}^d on those time intervals where $k(t) = 0$. As long as $k(t) \neq 0$, then $\mathcal{X}(t)$ does not move, and only the second component of the process evolves, that is, figuratively speaking, the process lives during this period in the “astral” space $A = \{x_1, \dots, x_M\}$. It follows from the above description of the upsampling process that the memory effect appears if we take the projection of this process onto the zero component corresponding to $k(t) = 0$.

In Section 5, we provide an example of the macroscopic (effective) model, both in dynamic and stationary regimes. Appendix A deals with auxiliary periodic problems for the correctors. Here, we prove two key technical statements and derive the formulae for the effective characteristics of the macroscopic model. In Appendix B, we calculate the effective matrix and the effective drift for one example and show the relation between the models at the microscale and macroscale.

The mathematical background of the present work has been partly developed in Piatnitski and Zhizhina [9], where we studied a symmetric random walk in a high-contrast medium and constructed the limit process on the extended state

space. In the present work, we supplement the symmetric random walk with an additional drift and absorption, which leads to a significant modification of our previous scheme. A crucial step in our approach is constructing several periodic correctors which are introduced as solutions of auxiliary difference elliptic equations on the period.

3 | MICROSCALE DESCRIPTION: HIGH-CONTRAST DISCRETE MODELS

In this section, we provide a detailed description of the random walk that models the discrete approximation of the purification process on the microscopic length scale. Given a probability space $(\Omega, \mathcal{F}, \mathbf{P})$, we consider a family of random walks $\hat{X}^{(\varepsilon)}(n)$ in \mathbb{Z}^d , $d \geq 1$ with transition probabilities that depend on a small parameter ε , $0 < \varepsilon \leq \varepsilon_0$. We denote by $p^{(\varepsilon)}(x, y)$ the transition probabilities $p^{(\varepsilon)}(x, y) = \Pr^{(\varepsilon)}(x \rightarrow y)$, $(x, y) \in \mathbb{Z}^d \times \mathbb{Z}^d$ of the random walk $\hat{X}^{(\varepsilon)}(n)$:

$$\sum_{y \in \mathbb{Z}^d} p^{(\varepsilon)}(x, y) = 1 \quad \forall x \in \mathbb{Z}^d. \quad (1)$$

Denote the transition matrix of the random walk by $P^{(\varepsilon)} = \{p^{(\varepsilon)}(x, y), x, y \in \mathbb{Z}^d\}$. We assume that for each ε , the random walk satisfies the following properties:

- *Periodicity.* The functions $p^{(\varepsilon)}(x, x + \xi)$ are periodic in x with a period Y for all $\xi \in \mathbb{Z}^d$, and Y is being independent of ε . In what follows, we identify the period Y with the corresponding d -dimensional discrete torus \mathbb{T}^d .
- *Finite range of interactions.* There exists $c > 0$ that does not depend on ε such that

$$p^{(\varepsilon)}(x, x + \xi) = 0, \quad \text{if } |\xi| > c. \quad (2)$$

- *Irreducibility.* The random walk is irreducible in \mathbb{Z}^d .

We suppose that the transition matrix $P^{(\varepsilon)}$ is a small perturbation of a fixed transition matrix $P^0 = \{p_0(x, y)\}$ that corresponds to a symmetric random walk, that is,

$$p_0(x, y) = p_0(y, x), \quad (x, y) \in \mathbb{Z}^d \times \mathbb{Z}^d, \quad \sum_{y \in \mathbb{Z}^d} p_0(x, y) = 1 \quad \forall x \in \mathbb{Z}^d. \quad (3)$$

We say that $y \sim x$, $x, y \in \mathbb{Z}^d$, if $p_0(x, y) \neq 0$. Let Λ_x be a finite set of $\xi \in \mathbb{Z}^d$ such that $x + \xi \sim x$. In what follows, we use the notation

$$p_0(x, y) = p_0(x, x + \xi) = p_\xi(x) \quad (4)$$

for all $x, y \in \mathbb{Z}^d$ such that $x \sim y$ and $y = x + \xi$.

Thus, the normalization condition can be rewritten as

$$\sum_{\xi \in \Lambda_x} p_\xi(x) = 1.$$

The transition matrix $P^{(\varepsilon)}$ has the following form:

$$P^{(\varepsilon)} =: P^0 + \varepsilon D + \varepsilon^2 V. \quad (5)$$

The transition probabilities $p^{(\varepsilon)}(x, y)$ describe the so-called high-contrast periodic structure of the environment. As was explained in Section 2, the matrix P^0 characterizes the diffusive part of the impurities motion outside of granules, the matrix εD corresponds to the small convection in the motion outside of granules, and the matrix $\varepsilon^2 V$ describes the small diffusion inside the granules and the flux of impurities into and out of the granules.

In order to characterize the matrices P^0 , $D = \{d(x, y)\}$ and $V = \{v(x, y)\}$, we divide the periodicity cell into two sets

$$\mathbb{T}^d = A \cup B; \quad A, B \neq \emptyset, \quad A \cap B = \emptyset, \quad (6)$$

and assume that $B \subset \mathbb{T}^d$ is a connected set such that its periodic extension denoted $B^\#$ is unbounded and connected. Here, the connectedness is understood in terms of the transition matrix P^0 . Two points $x', x'' \in \mathbb{Z}^d$ are called connected if there

exists a path x^1, \dots, x^L in \mathbb{Z}^d such that $x^1 = x', x^L = x''$ and $p_0(x^j, x^{j+1}) > 0$ for all $j = 1, \dots, L - 1$. As a consequence, we get that

$$P^0 \text{ is irreducible on } B^\sharp. \tag{7}$$

We also denote by A^\sharp the periodic extension of A . Then, $\mathbb{Z}^d = A^\sharp \cup B^\sharp$.

In addition to the above-formulated conditions on $P^{(\epsilon)}$ and the general assumptions (3) and (7), the following conditions on the matrices P^0, D and V are imposed:

- $p_0(x, x) = 1$, if $x \in A^\sharp$;
- $p_0(x, y) = 0$, if $x, y \in A^\sharp, x \neq y$;
- $p_0(x, y) = 0$, if $x \in B^\sharp, y \in A^\sharp$;
- $d(x, y) = 0$, if at least one of x or $y \in A^\sharp$;
- $v(x, y) = 0$, if $x, y \in B^\sharp, x \neq y$;
- the elements of matrices D and V satisfy the relation

$$\sum_{y \in \mathbb{Z}^d} d(x, y) = 0, \quad \sum_{y \in \mathbb{Z}^d} v(x, y) = 0 \quad \forall x \in \mathbb{Z}^d. \tag{8}$$

- there exists a constant $c > 0$ such that

$$p_0(x, y) = d(x, y) = v(x, y) = 0, \quad \text{if } |x - y| \geq c.$$

It is worth noting that the relation (8) is a direct consequence of the fact that both $P^{(\epsilon)}$ and P^0 are the transition matrices of the corresponding random walks. From the periodicity of D and V it also follows that

$$d_{max} := \max_{x, y \in \mathbb{Z}^d} |d(x, y)| < \infty, \quad v_{max} := \max_{x, y \in \mathbb{Z}^d} |v(x, y)| < \infty.$$

Summarizing all above conditions, we conclude that the non-zero transition probabilities defined by (5) have the following structure:

- $p^{(\epsilon)}(x, y) = p_0(x, y) + O(\epsilon)$, when $x, y \in B^\sharp$ (rapid movement);
- $p^{(\epsilon)}(x, x) = 1 + O(\epsilon^2)$, when $x \in A^\sharp$ (slow movement);
- $p^{(\epsilon)}(x, y) \asymp \epsilon^2$, when $x, y \in A^\sharp, x \neq y$ (slow movement);
- $p^{(\epsilon)}(x, y) \asymp \epsilon^2$, when $x \in B^\sharp, y \in A^\sharp$ (rare exchange between A^\sharp and B^\sharp).

Here and later on, the symbol \asymp indicates that the ratio between the right- and left-hand sides admits positive lower and upper bounds. The above choice of the transition probabilities reflects a slow drift (of the order ϵ) given by matrix D in the fast component, and also a significant slowdown (of the order ϵ^2) of the random walk inside the slow component.

Further, we add to the above random walk an absorption process consistent with the structure of the periodic environment, assuming that the absorption occurs only inside the inclusions A^\sharp . For the description of the complete process, we will denote by $\mathbb{S} = \mathbb{Z}^d \cup \{\star\}$ the state space of the new process, where $\{\star\}$ is the absorption state. Then, the transition matrix of the complete process with absorption has the following form:

$$Q^{(\epsilon)} = P^{(\epsilon)} + \epsilon^2 W = (P^0 + \epsilon D + \epsilon^2 V) + \epsilon^2 W, \tag{9}$$

where $Q^{(\epsilon)}(\star, \star) = 1, W(x, \star) = m > 0$ and $W(x, x) = -m$ for all $x \in A^\sharp$, otherwise $W(x, y) = 0$.

Let $l_0^\infty(\mathbb{Z}^d)$ be the Banach space of bounded functions on \mathbb{Z}^d vanishing at infinity with the norm $\|f\| = \sup_{x \in \mathbb{Z}^d} |f(x)|$. Similarly, we consider the Banach space of bounded functions on \mathbb{S} : $l_0^\infty(\mathbb{S}) = l_0^\infty(\mathbb{Z}^d) \oplus \mathbb{R}$.

We note that random walks with symmetric transition probabilities of the form

$$P^{(\epsilon)} = P^0 + \epsilon^2 V \tag{10}$$

have been studied in Piatnitski and Zhizhina [9]. In the present work, we supplement the model with drift and absorption. Our goal is to derive the effective evolution equation under the diffusive scaling.

4 | UPSCALING

4.1 | Rescaled process

In what follows, we study the scaling limit of the random walk on \mathbb{S} with transition matrix $Q^{(\varepsilon)}$ and use ε as the scaling factor. Denote $\varepsilon\mathbb{Z}^d = \{z : \frac{z}{\varepsilon} \in \mathbb{Z}^d\}$, then $\varepsilon\mathbb{Z}^d = \varepsilon A^\# \cup \varepsilon B^\#$, and let $\varepsilon\mathbb{S} = \varepsilon\mathbb{Z}^d \cup \{\star\}$. In what follows, the symbols x and y are used for the variables on \mathbb{Z}^d (fast variables), while the symbols z and w for the variables on $\varepsilon\mathbb{Z}^d$ (slow variables). Notice that the state $\{\star\}$ does not change under the scaling.

We introduce now the rescaled process. Denote by T_ε the transition operator associated with the transition matrix (9):

$$T_\varepsilon f(z) = \sum_{w \in \varepsilon\mathbb{S}} q_\varepsilon(z, w) f(w) = \sum_{w \in \varepsilon\mathbb{Z}^d} q_\varepsilon(z, w) f(w) + q_\varepsilon(z, \star) f(\star), \quad f \in l_0^\infty(\varepsilon\mathbb{S}), \quad z \in \varepsilon\mathbb{S}, \quad (11)$$

where

$$q_\varepsilon(z, w) = Q^{(\varepsilon)}\left(\frac{z}{\varepsilon}, \frac{w}{\varepsilon}\right), \quad \frac{z}{\varepsilon}, \frac{w}{\varepsilon} \in \mathbb{S},$$

and $Q^{(\varepsilon)}(\cdot, \cdot)$ are elements of the matrix $Q^{(\varepsilon)}$; see (9). Namely,

$$q_\varepsilon(z, w) = p^{(\varepsilon)}\left(\frac{z}{\varepsilon}, \frac{w}{\varepsilon}\right) - \varepsilon^2 m \mathbf{1}_{\{z=w\}} \mathbf{1}_{\{z \in \varepsilon A^\#\}}, \quad \text{if } z, w \in \varepsilon\mathbb{Z}^d,$$

where the elements of the matrix $P^{(\varepsilon)}$ were defined in (9); $q_\varepsilon(z, \star) = \varepsilon^2 m$, if $z \in \varepsilon A^\#$; $q_\varepsilon(z, \star) = 0$, if $z \in \varepsilon B^\#$; $q_\varepsilon(\star, z) = 0$ for all $z \in \varepsilon\mathbb{Z}^d$, and $q_\varepsilon(\star, \star) = 1$. Then, the operator

$$L_\varepsilon = \frac{1}{\varepsilon^2} (T_\varepsilon - I) \quad (12)$$

is the difference generator of the rescaled process $\mathcal{X}_\varepsilon(t)$ on $\varepsilon\mathbb{S} = \varepsilon\mathbb{Z}^d \cup \{\star\}$ with transition operator T_ε . The rescaled process has two components:

$$\mathcal{X}_\varepsilon(t) = \{\hat{X}_\varepsilon(t), \hat{s}(t)\}, \quad (13)$$

where $\hat{X}_\varepsilon(t) = \varepsilon \hat{X}^{(\varepsilon)}\left(\left[\frac{t}{\varepsilon^2}\right]\right)$ is the rescaled random walk on $\varepsilon\mathbb{Z}^d$ and the latter component $\hat{s}(t)$ lives on $\{\star\}$.

The goal of the paper is to describe the limit behavior of the rescaled process $\mathcal{X}_\varepsilon(t)$, as $\varepsilon \rightarrow 0$, to construct the limit process, and to find the explicit expressions for all effective characteristics of the limit process.

4.2 | Extended random walk

Homogenization of non-stationary processes in high-contrast environments often results in the effective equations with nonlocal in time terms representing the memory effect. As was shown in Piatnitski and Zhizhina [9], the limit process for a random walk in a high-contrast environment remains Markov if we equip the original random walk with additional component(s) and consider the obtained random walk in the extended state space.

In this subsection, we describe the constructions of an extended random walk introduced in Piatnitski and Zhizhina [9]. We equip the random walk $\hat{X}_\varepsilon(t)$ (the first component in 13) with an additional component(s) in the same way as it has been done in Piatnitski and Zhizhina [9]. Assume that the set A defined in (6) contains $M \in \mathbb{N}$ sites of \mathbb{T}^d : $A = \{x_1, \dots, x_M\}$. For each $k = 1, \dots, M$ we denote by $\{x_k\}^\#$ the periodic extension of the point $x_k \in A$, then

$$\varepsilon\mathbb{Z}^d = \varepsilon B^\# \cup \varepsilon A^\# = \varepsilon B^\# \cup \varepsilon \{x_1\}^\# \cup \dots \cup \varepsilon \{x_M\}^\#. \quad (14)$$

We assign to each $z \in \varepsilon\mathbb{Z}^d$ the index $k(z) \in \{0, 1, \dots, M\}$ depending on the component in decomposition (14) to which z belongs:

$$k(z) = \begin{cases} 0, & \text{if } z \in \varepsilon B^\#; \\ j, & \text{if } z \in \varepsilon \{x_j\}^\#, \quad j = 1, \dots, M. \end{cases} \quad (15)$$

With this construction in hand, we introduce the metric space

$$E_\varepsilon = \{(z, k(z)), z \in \varepsilon\mathbb{Z}^d, k(z) \in \{0, 1, \dots, M\}\}, \quad E_\varepsilon \subset \varepsilon\mathbb{Z}^d \times \{0, 1, \dots, M\}, \quad (16)$$

with a metric that coincides with the metric in $\varepsilon\mathbb{Z}^d$ for the first component of $(z, k(z)) \in E_\varepsilon$.

The index $k(\star) = \star$ is assigned to the state $z = \{\star\}$. Thus, the extended version of the absorption state is $\{\star, \star\}$, but for simplicity, we will keep the notation $\{\star\}$. Denote $\mathbb{S}_{E_\varepsilon} = E_\varepsilon \cup \{\star\}$, and in what follows instead of $\mathcal{X}_\varepsilon(t)$, we consider the extended process

$$\mathfrak{X}_\varepsilon(t) = \{\mathcal{X}_\varepsilon(t), k(t)\}, \quad k(t) \in \{0, 1, \dots, M, \star\}.$$

We denote the space of bounded functions on $\mathbb{S}_{E_\varepsilon}$ by $\mathcal{B}(\mathbb{S}_{E_\varepsilon})$ and construct the transition operator T_ε of the process $\mathfrak{X}_\varepsilon(t)$ on $\mathbb{S}_{E_\varepsilon}$ using the same transition probabilities as in operator (11):

$$\begin{aligned} (T_\varepsilon f)(z, k(z)) &= \sum_{w \in \varepsilon\mathbb{S}} q_\varepsilon(z, w) f(w, k(w)) \\ &= \sum_{w \in \varepsilon\mathbb{Z}^d} q_\varepsilon(z, w) f(w, k(w)) + q_\varepsilon(z, \star) f(\star), \end{aligned} \quad (17)$$

$$(T_\varepsilon f)(\star) = f(\star), \quad f \in \mathcal{B}(\mathbb{S}_{E_\varepsilon}).$$

Then, T_ε is a contraction on $\mathcal{B}(\mathbb{S}_{E_\varepsilon})$:

$$\|T_\varepsilon f\|_{\mathcal{B}(\mathbb{S}_{E_\varepsilon})} \leq \sup_{(z, k(z)) \in \mathbb{S}_{E_\varepsilon}} |f(z, k(z))|, \quad f \in \mathcal{B}(\mathbb{S}_{E_\varepsilon}).$$

Remark 1. Since the point $(z, k(z)) \in E_\varepsilon$ is uniquely defined by its first coordinate $z \in \varepsilon\mathbb{Z}^d$, then we can use $z \in \varepsilon\mathbb{Z}^d$ as a coordinate in E_ε (considering E_ε as a graph of the mapping $k : \varepsilon\mathbb{Z}^d \rightarrow \{0, 1, \dots, M\}$). In particular, for the transition probabilities of the random walk on E_ε , we keep the same notations $q_\varepsilon(z, w)$ as in (11).

4.3 | Limit process

In this subsection, we construct a limit process, which is a Markov process completely determined by its generator. We denote $E = \mathbb{R}^d \times \{0, 1, \dots, M\}$, and $C_0(E)$ stands for the Banach space of continuous functions vanishing at infinity. Together with E , we consider $\mathbb{S}_E = E \cup \{\star\}$ and denote $C_0(\mathbb{S}_E) = C_0(E) \oplus \mathbb{R}$. Then, $F \in C_0(\mathbb{S}_E)$ can be represented as $F = (F(z, k), F(\star))$, where

$$F(z, k) = \{f_k(z) \in C_0(\mathbb{R}^d), \quad k = 0, 1, \dots, M\}, \quad F(\star) \in \mathbb{R},$$

and the norm in $C_0(\mathbb{S}_E)$ is equal to

$$\|F\|_{C_0(\mathbb{S}_E)} = \max \{ \|F(z, k)\|_{C_0(E)}, |F(\star)| \},$$

where

$$\|F\|_{C_0(E)} = \max_{k=0,1,\dots,M} \|f_k\|_{C_0(\mathbb{R}^d)}.$$

Consider the operator

$$LF(z, k) = (\Theta \cdot \nabla \nabla f_0(z) + b \cdot \nabla f_0(z)) \mathbf{1}_{\{k=0\}} + L_A F(z, k), \quad LF(\star) = 0, \quad (18)$$

where $\mathbf{1}_{\{k=0\}}$ is the indicator function, Θ is a positive definite matrix defined in (A16), b is a vector of the effective drift defined also below by (A15), and the symbol \cdot stands for the inner product in \mathbb{R}^d or, in the case of matrices, in \mathbb{R}^{d^2} ; in particular, $\Theta \cdot \nabla \nabla f_0 = \text{Tr}(\Theta \nabla \nabla f_0)$. Both Θ and b are the effective characteristics of the limiting process. The operator L_A is a generator of a Markov jump process

$$L_A F(z, k) = \sum_{\substack{j=0 \\ j \neq k}}^M \alpha_{kj} (f_j(z) - f_k(z)) + m (F(\star) - f_k(z)) \mathbf{1}_{\{k \neq 0\}}, \quad (19)$$

with

$$\begin{aligned} \alpha_{0j} &= \frac{1}{|B|} \sum_{x \in B} \sum_{y \in \{x_j\}^\#} v(x, y), \quad \alpha_{j0} = \sum_{x \in B^\#} v(x_j, x), \quad j = 1, \dots, M, \\ \alpha_{kj} &= \sum_{y \in \{x_j\}^\#} v(x_k, y), \quad j, k = 1, \dots, M, \quad j \neq k. \end{aligned} \quad (20)$$

Notice that the parameters α_{jk} , $j, k = 0, 1, \dots, M$, are non-negative and define intensities of the limit Markov jump process on the period Y .

The operator L is defined on the core

$$\mathfrak{D} = \mathfrak{D}_E \oplus \mathbb{R} \subset C_0(\mathbb{S}_E), \tag{21}$$

where

$$\mathfrak{D}_E = \{(f_0, f_1, \dots, f_M), f_0 \in C_0^\infty(\mathbb{R}^d), f_j \in C_0(\mathbb{R}^d), j = 1, \dots, M\} \tag{22}$$

is a dense set in $C_0(E)$. One can check that the operator L on $C_0(\mathbb{S}_E)$ satisfies the positive maximum principle, that is, if $F \in \mathfrak{D}$ and $\max_{E \cup \{\star\}} F(z, k) = F(z_0, k_0)$, then $LF(z_0, k_0) \leq 0$. Since L_A is a bounded operator in $C_0(\mathbb{S}_E)$, the operator $\lambda - L$ is invertible for sufficiently large λ . Then, by the Hille–Yosida theorem, the closure of L is a generator of a strongly continuous, positive, contraction semigroup $T(t)$ on $C_0(\mathbb{S}_E)$.

Let us describe the limit process $\mathfrak{X}(t)$ generated by the operator L . It is a two-component continuous time Markov process $\mathfrak{X}(t) = \{\mathcal{X}(t), k(t)\}$, where the first component $\mathcal{X}(t)$ lives in $\mathbb{R}^d \cup \{\star\}$, the second component is a continuous time jump Markov process $k(t)$ on the state space $K = \{0, 1, 2, \dots, M, \star\}$. The process $k(t)$ does not depend on the other components; its transition rates α_{ij} are expressed in terms of the transition probabilities of the original random walk; see (20). The probability of jump between any two states $i, j \in \{0, 1, 2, \dots, M\}$, $i \neq j$, is equal to α_{ij} . The absorbing state $\{\star\}$ is reachable only from the “astral” states $\{1, 2, \dots, M\}$ with the same intensity m . Thus, the matrix corresponding to the generator L_A has the following form:

$$\begin{pmatrix} -\sum_{j=1}^M \alpha_{0j} & \alpha_{01} & \dots & \alpha_{0M} & 0 \\ \alpha_{10} & -\sum_{j=0, j \neq 1}^M \alpha_{1j} - m & \dots & \alpha_{1M} & m \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \alpha_{M0} & \alpha_{M1} & \dots & -\sum_{j=0}^{M-1} \alpha_{Mj} - m & m \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix}. \tag{23}$$

When $k(t) = 0$, the first component $\mathcal{X}(t)$ evolves along the trajectories of a diffusion process in \mathbb{R}^d with the corresponding effective characteristics, while when $k(t) \neq 0$, the first component $\mathcal{X}(t)$ remains still until $k(t)$ takes again the value 0. Thus, the trajectories of $\mathcal{X}(t)$ coincide with the trajectories of a diffusion process in \mathbb{R}^d on those time intervals where $k(t) = 0$. As long as $k(t) \neq 0$, the first component $\mathcal{X}(t)$ does not move, and only the second component $k(t)$ of the process evolves. Additionally, the process $k(t)$ can jump from the astral states $\{1, \dots, M\}$ to the absorbing state $\{\star\}$ with intensity m , and upon reaching this state, the process never leaves it.

4.4 | Main result: The convergence of semigroups

In this subsection, we formulate the main result of this work on convergence (upscaling) to the limit process constructed in the previous subsection.

Let $l_0^\infty(E_\epsilon)$ be a Banach space of functions on E_ϵ vanishing as $|z| \rightarrow \infty$ with the norm

$$\|f\|_{l_0^\infty(E_\epsilon)} = \sup_{(z, k(z)) \in E_\epsilon} |f(z, k(z))| = \sup_{z \in \mathbb{Z}^d} |f(z, k(z))|, \tag{24}$$

and denote $l_0^\infty(\mathbb{S}_{E_\epsilon}) = l_0^\infty(E_\epsilon) \oplus \mathbb{R}$. For every $F \in C_0(\mathbb{S}_E)$, we define the function $\pi_\epsilon F \in l_0^\infty(\mathbb{S}_{E_\epsilon})$ as follows:

$$(\pi_\epsilon F)(z, k(z)) = \begin{cases} f_0(z), & \text{if } z \in \epsilon B^\sharp, k(z) = 0; \\ f_1(z), & \text{if } z \in \epsilon \{z_1\}^\sharp, k(z) = 1; \\ \dots & \\ f_M(z), & \text{if } z \in \epsilon \{z_M\}^\sharp, k(z) = M, \end{cases} \tag{25}$$

and $\pi_\epsilon F(\star) = F(\star)$. Then, π_ϵ defines a bounded linear transformation $\pi_\epsilon : C_0(\mathbb{S}_E) \rightarrow l_0^\infty(\mathbb{S}_{E_\epsilon})$.

Theorem 1. *Let $T(t)$ be a strongly continuous, positive, contraction semigroup on $C_0(\mathbb{S}_E)$ with generator L defined by (18)–(19) and T_ϵ be the linear operator on $l_0^\infty(\mathbb{S}_{E_\epsilon})$ defined by (17).*

Then, for every $F \in C_0(\mathbb{S}_E)$,

$$\|T_\epsilon^{\lfloor \frac{t}{\epsilon^2} \rfloor} \pi_\epsilon F - \pi_\epsilon T(t)F\|_{l_0^\infty(\mathbb{S}_{E_\epsilon})} \rightarrow 0 \text{ for all } t \geq 0, \tag{26}$$

as $\epsilon \rightarrow 0$.

Proof. The proof of (26) relies on the approximation techniques from Ethier and Kurtz [10] used for the proof of convergence of semigroups. According to results of Ethier and Kurtz [10, Theorem 6.5, Ch.1], the semigroup convergence stated in (26) is equivalent to the statement which is the subject of the next lemma.

Lemma 1. *For every $F \in \mathfrak{D}$, where \mathfrak{D} was defined by (21), there exists $F_\epsilon \in l_0^\infty(\mathbb{S}_{E_\epsilon})$ such that*

$$\|F_\epsilon - \pi_\epsilon F\|_{l_0^\infty(\mathbb{S}_{E_\epsilon})} \rightarrow 0, \tag{27}$$

and

$$\|L_\epsilon F_\epsilon - \pi_\epsilon LF\|_{l_0^\infty(\mathbb{S}_{E_\epsilon})} \rightarrow 0 \text{ as } \epsilon \rightarrow 0. \tag{28}$$

Proof. For every $F = ((f_0, f_1, \dots, f_M), F(\star)) \in \mathfrak{D}$ with $(f_0, f_1, \dots, f_M) \in \mathfrak{D}_E$, we should construct a function F_ϵ for which the convergence in (27)–(28) holds. To this end, we denote

$$\hat{f}_0^\epsilon(z) = f_0(z) + \epsilon \nabla f_0(z) \cdot h\left(\frac{z}{\epsilon}\right) + \epsilon^2 \nabla \nabla f_0(z) \cdot g\left(\frac{z}{\epsilon}\right) + \epsilon^2 \sum_{j=1}^M q_j\left(\frac{z}{\epsilon}\right) (f_0(z) - f_j(z))$$

and take $F_\epsilon \in l_0^\infty(\mathbb{S}_{E_\epsilon})$ of the following form:

$$F_\epsilon(z, k(z)) = \begin{cases} \hat{f}_0^\epsilon(z), & \text{if } z \in \epsilon B^\sharp, k(z) = 0, \\ f_1(z), & \text{if } z \in \epsilon \{x_1\}^\sharp, k(z) = 1, \\ \dots & \dots \\ f_M(z), & \text{if } z \in \epsilon \{x_M\}^\sharp, k(z) = M, \end{cases} \tag{29}$$

and $F_\epsilon(\star) = F(\star)$. Here, $h(y), g(y), q_j(y), j = 1, \dots, M$, are periodic bounded functions that will be defined below. The boundedness together with (29) immediately imply that

$$\|F_\epsilon - \pi_\epsilon F\|_{l_0^\infty(\mathbb{S}_{E_\epsilon})} = \sup_{z \in \epsilon \mathbb{Z}^d} |F_\epsilon(z, k(z)) - \pi_\epsilon F(z, k(z))| \rightarrow 0,$$

as $\epsilon \rightarrow 0$. Thus, convergence (27) holds.

Next, we prove the second convergence stated in (28). Since $(L_\epsilon F_\epsilon)(\star) = (LF)(\star) = 0$, it suffices to show that

$$\|L_\epsilon F_\epsilon - \pi_\epsilon LF\|_{l_0^\infty(\mathbb{S}_{E_\epsilon})} = \sup_{z \in \epsilon \mathbb{Z}^d} |L_\epsilon F_\epsilon(z, k(z)) - \pi_\epsilon LF(z, k(z))| \rightarrow 0. \tag{30}$$

In the proof of (30), we use the same arguments as in the paper [9]. According to (17) and (9), the operator L_ϵ can be written as

$$L_\epsilon = \frac{1}{\epsilon^2} (P_\epsilon^0 + \epsilon D_\epsilon + \epsilon^2 V_\epsilon + \epsilon^2 W_\epsilon - I) = L_\epsilon^0 + V_\epsilon + W_\epsilon,$$

with

$$L_\epsilon^0 = \frac{1}{\epsilon^2} (P_\epsilon^0 + \epsilon D_\epsilon - I), \tag{31}$$

where for $z \in \epsilon \mathbb{Z}^d$,

$$P_\epsilon^0 F(z, k(z)) = \sum_{w \in \epsilon \mathbb{Z}^d} p_0\left(\frac{z}{\epsilon}, \frac{w}{\epsilon}\right) F(w, k(w)), \quad D_\epsilon F(z, k(z)) = \sum_{w \in \epsilon \mathbb{Z}^d} d\left(\frac{z}{\epsilon}, \frac{w}{\epsilon}\right) F(w, k(w)),$$

and

$$V_\epsilon F(z, k(z)) = \sum_{w \in \epsilon \mathbb{Z}^d} v\left(\frac{z}{\epsilon}, \frac{w}{\epsilon}\right) F(w, k(w)), \quad W_\epsilon F(z, k(z)) = w\left(\frac{z}{\epsilon}, \frac{z}{\epsilon}\right) F(z, k(z)) + w\left(\frac{z}{\epsilon}, \star\right) F(\star).$$

We consider next separately the cases when $z \in \epsilon B^\sharp$, and $z \in \epsilon A^\sharp$. Since the second component in E_ϵ is a function of the first one, in the remaining part of the proof for brevity, write $F_\epsilon(z)$ instead of $F_\epsilon(z, k(z))$.

Let $z \in \varepsilon B^\sharp$. The first component ($k(z) = 0$) of F_ε in (29) can be written as a sum

$$F_\varepsilon(z) = F_\varepsilon^P(z) + F_\varepsilon^Q(z), \quad z \in \varepsilon B^\sharp, \quad (32)$$

where

$$F_\varepsilon^P(z) = f_0(z) + \varepsilon \nabla f_0(z) \cdot h\left(\frac{z}{\varepsilon}\right) + \varepsilon^2 \nabla \nabla f_0(z) \cdot g\left(\frac{z}{\varepsilon}\right), \quad (33)$$

$$F_\varepsilon^Q(z) = \varepsilon^2 \sum_{j=1}^M q_j\left(\frac{z}{\varepsilon}\right) (f_0(z) - f_j(z)). \quad (34)$$

Since $W_\varepsilon F_\varepsilon(z) = 0$, if $z \in \varepsilon B^\sharp$, then

$$L_\varepsilon F_\varepsilon = (L_\varepsilon^0 + V_\varepsilon) F_\varepsilon = L_\varepsilon^0 (F_\varepsilon^P + F_\varepsilon^Q) + V_\varepsilon F_\varepsilon = L_\varepsilon^0 F_\varepsilon^P + L_\varepsilon^0 F_\varepsilon^Q + V_\varepsilon F_\varepsilon. \quad (35)$$

In order to estimate

$$\sup_{z \in \varepsilon B^\sharp} |L_\varepsilon F_\varepsilon(z) - \pi_\varepsilon L F(z)| = \sup_{z \in \varepsilon B^\sharp} |L_\varepsilon^0 F_\varepsilon^P(z) + L_\varepsilon^0 F_\varepsilon^Q(z) + V_\varepsilon F_\varepsilon(z) - \pi_\varepsilon L F(z)|, \quad (36)$$

we use the following two propositions.

Proposition 1. *There exist bounded periodic functions $h(y) = \{h_i(y)\}_{i=1}^d$ and $g(y) = \{g_{im}(y)\}_{i,m=1}^d$ (correctors), and a positive definite matrix $\Theta > 0$, and a vector b such that $L_\varepsilon^0 F_\varepsilon^P \rightarrow \Theta \cdot \nabla \nabla f_0 + b \cdot \nabla f_0$, that is,*

$$\sup_{z \in \varepsilon B^\sharp} |L_\varepsilon^0 F_\varepsilon^P(z) - \Theta \cdot \nabla \nabla f_0(z) - b \cdot \nabla f_0(z)| \rightarrow 0, \quad \text{as } \varepsilon \rightarrow 0, \quad (37)$$

where F_ε^P is defined in (33).

The proof of this proposition is based on the corrector techniques, it is given in Appendix A.

Proposition 2. *There exist bounded periodic functions $q_j(x)$, $j = 1, \dots, M$, on B^\sharp such that*

$$\sup_{z \in \varepsilon B^\sharp} \left| (L_\varepsilon^0 F_\varepsilon^Q + V_\varepsilon F_\varepsilon)(z) - \sum_{j=1}^M \alpha_{0j} (f_j(z) - f_0(z)) \right| \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0, \quad (38)$$

where $\alpha_{0j} > 0$ are constants defined in (20) and F_ε^Q is introduced in (34).

The proof of Proposition 2 is the same as that in Piatnitski and Zhizhina [9]. We provide it in Appendix A for presentation completeness.

Since

$$\pi_\varepsilon L F(z) = (\Theta \cdot \nabla \nabla f_0(z) + b \cdot \nabla f_0(z)) \mathbf{1}_{\{k=0\}} + (L_A F)(z, 0), \quad z \in \varepsilon B^\sharp, \quad (39)$$

where

$$(L_A F)(z, 0) = \sum_{j=1}^M \alpha_{0j} (f_j(z) - f_0(z)),$$

then Propositions 1 and 2 together with (36) and (39) yield

$$\sup_{z \in \varepsilon B^\sharp} |L_\varepsilon F_\varepsilon(z) - \pi_\varepsilon L F(z)| \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0. \quad (40)$$

Next, we consider the case when $z \in \varepsilon A^\sharp$ and prove that

$$\sup_{z \in \varepsilon A^\sharp} |L_\varepsilon F_\varepsilon(z) - \pi_\varepsilon L F(z)| \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0. \quad (41)$$

Let $z \in \varepsilon \{x_k\}^\# \subset \varepsilon A^\#$. From (29), (31), and continuity of the functions f_k , it follows that

$$\begin{aligned} (L_\varepsilon F_\varepsilon)(z) &= (L_\varepsilon^0 + V_\varepsilon + W_\varepsilon)F_\varepsilon(z) = V_\varepsilon F_\varepsilon(z) + W_\varepsilon F_\varepsilon(z) = \\ &= \sum_{\substack{j=1 \\ j \neq k}}^M \sum_{y \in \{x_j\}^\#} v(x_k, y)(f_j(z) - f_k(z)) \\ &+ \sum_{x \in B^\#} v(x_k, x)(f_0(z) - f_k(z)) + m(F(*) - f_k(z)) + o(1), \end{aligned} \tag{42}$$

as $\varepsilon \rightarrow 0$. Here, we have used the fact that $f_k(z') = f_k(z) + o(1)$ as $|z - z'| \rightarrow 0$. Recall that $x, y \in Y$ are variables on the periodicity cell, and $v(x_k, x_j)$ are the elements of the matrix V . On the other hand, according (19) and (25) $\pi_\varepsilon LF(z)$ for $z \in \varepsilon \{x_k\}^\#$ has the following form:

$$\pi_\varepsilon LF(z) = \sum_{\substack{j=0 \\ j \neq k}}^M \alpha_{kj}(f_j(z) - f_k(z)) + m(F(*) - f_k(z)), \quad k = 1, \dots, M, \tag{43}$$

where the constants α_{k0}, α_{kj} are given by (20). Thus, relations (42) and (43) imply (41).

Finally, (30) is a consequence of (40) and (41), and Lemma 1 is proved. □

It remains to recall that (26) is a straightforward consequence of the above approximation theorem. This completes the proof of Theorem 1. □

5 | DYNAMICS OF POLLUTION: STATIONARY REGIME

In this section, we consider an example of the limit dynamics in the case when the astral set A contains one point. We also derive an equation on the first component $\rho_0(x, t)$ describing a visible dynamics of the pollution density.

Denote by

$$\rho(x, t) = (\rho_0(x, t), \rho_1(x, t), \rho_2(t))$$

the three-component density of pollution, where $\rho_0(x, t)$ is the density outside of micro-granules, $\rho_1(x, t)$ is the density inside of micro-granules, and $\rho_2(t)$ is the density of pollution accumulated (or absorbed) as a result of cleaning by time t . The conservation principle reads

$$\int (\rho_0(x, t) + \rho_1(x, t))dx + \rho_2(t) \equiv \text{const} \quad \forall t.$$

The corresponding model at microscopic scale is a one-point astral model with absorption. Then, for the limit dynamics, we obtain the following evolution equations for $\rho(x, t)$:

$$\partial_t \rho = L^* \rho,$$

or

$$\begin{cases} \partial_t \rho_0 = \Theta \cdot \nabla \nabla \rho_0 - b \cdot \nabla \rho_0 - \lambda_0 \rho_0 + \lambda_1 \rho_1, \\ \partial_t \rho_1 = -(\lambda_1 + m) \rho_1 + \lambda_0 \rho_0, \\ \partial_t \rho_2 = m \int \rho_1(x, t) dx, \end{cases} \tag{44}$$

with initial data $\rho(x, 0) = (\pi_0(x), \pi_1(x), \pi_2)$. Here, Θ, b are the effective diffusion matrix and the effective drift depending on the geometry of the microscale model, and $\lambda_0 > 0, \lambda_1 > 0$ are the rates of exchanging between inside and outside regions: λ_0 is the intensity of the water flows into cleaning inclusions, while λ_1 is the intensity of flows from inclusions. Since the set A consists of only one point, we have $\lambda_0 = \alpha_{01}$ and $\lambda_1 = \alpha_{10}$. All the coefficients in (44) are the parameters of the limit model. In Appendices A and B, we will show how the effective parameters Θ and b can be found from the microscale model.

The solution of the second equation in (44) has the form

$$\rho_1(x, t) = e^{-\lambda_1 t} \pi_1(x) + \lambda_0 \int_0^t e^{-\lambda_1(t-s)} \rho_0(x, s) ds,$$

$$\lambda_m = \lambda_1 + m = \alpha_{10} + m.$$

After substitution of $\rho_1(x, t)$ into the first equation in (44), we obtain the following evolution equation on ρ_0 :

$$\partial_t \rho_0 = \Theta \cdot \nabla \nabla \rho_0 - b \cdot \nabla \rho_0 - \lambda_0 \rho_0 + \lambda_0 \lambda_1 \int_0^t e^{-\lambda_m(t-s)} \rho_0(x, s) ds + \lambda_1 e^{-\lambda_m t} \pi_1(x), \quad (45)$$

with $\rho_0(x, 0) = \pi_0(x)$.

Let us consider the stationary problem $L^* \rho = 0$ for the macroscopic model in $\Pi = \mathbb{T}^{d-1} \times \mathbb{R}_+$. The equation on $\rho_0(x)$ takes the form

$$\begin{aligned} \Theta \cdot \nabla \nabla \rho_0(x) - b \cdot \nabla \rho_0(x) - \lambda_0 \rho_0(x) + \frac{\lambda_0 \lambda_1}{\lambda_1 + m} \rho_0(x) &= \\ = \Theta \cdot \nabla \nabla \rho_0(x) - b \cdot \nabla \rho_0(x) - \lambda_0 \frac{m}{\lambda_1 + m} \rho_0(x) &= 0, \end{aligned} \quad (46)$$

with a boundary conditions

$$\rho_0(x|_{x_d=0}) = \varphi(x), \quad \rho_0(x|_{x_d=\infty}) = 0, \quad (47)$$

where x_d is the direction of the drift. Here, $\varphi(x) \geq 0$ is the profile of the initial concentration on the upper cross section.

Assuming that the initial profile φ is a constant function, one can reduce the dimension in problem (46)–(47) and obtain a one-dimensional stationary problem that reads

$$\begin{cases} \theta \rho_0'' - b \rho_0' - \kappa \rho_0 = 0, & \kappa = \lambda_0 \frac{m}{\lambda_1 + m}, \\ \rho_0(0) = 1, \quad \rho_0(+\infty) = 0. \end{cases} \quad (48)$$

Thus, the rate of the purification process is equal to $R_{pur} = \frac{1}{2\theta} \left(\sqrt{b^2 + 4\theta\kappa} - b \right)$, and for sufficiently small θ , we get $R_{pur} \approx \frac{\kappa}{b}$.

Remark 2. If the astral set A contains more than one point, that is, $|A| = M > 1$, then the kernel $K(t - s)$ in (45) is a linear combination of exponents $e^{-\kappa_j(t-s)}$ with $\kappa_j > 0$, $j = 1, \dots, M$.

6 | CONCLUSIONS

The present work deals with mathematical models of wastewater purification process in nano-porous filters. We propose a multi-scale model of a water treatment device whose basic purification elements are located periodically. Assuming that the discretization procedure applies at the microscopic length scale, we describe the diffusion of impurities as a lattice random walk in a high-contrast periodic medium with absorption. We define this random walk in terms of the transition probabilities.

The main goal of our study is to obtain the effective characteristics of the water purification process, that is, the coefficients of the corresponding macroscopic model. To this end, we use the upscaling procedure and show that the effective characteristics can be expressed in terms of the microscopic characteristics of the model and several auxiliary functions being solutions of auxiliary systems of linear algebraic equations. These functions are the so-called correctors, and the size of these systems only depends on the number of points in the period.

Since the diffusion of impurities differs essentially inside and outside of the micro-granules, we investigate the limit dynamics of a three-component random walk, the last component represents the absorbed impurities. We then show how the memory term appears in the evolution equation for the first component of this system and derive the corresponding effective parameters.

The methods of investigation of the proposed mathematical model rely on a combination of probabilistic approaches with homogenization and approximation techniques.

We also consider the stationary regime and show how the efficiency of the purification process depends on the characteristics of the macroscopic model. The main parameter of the quality of water purification is the exponent that specifies the rate of decay of impurities concentration as the distance to the upper cross section of the filter grows. We provide some examples of calculating such an exponent.

The advantage of the proposed model is a possibility to adapt it to more complex geometries of absorbing films. The model considered in this work can be used for better understanding complex treatment systems and for optimizing the parameters of water purification devices in accordance with the restrictions on the device productivity and the purification quality.

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CONFLICT OF INTEREST STATEMENT

This work does not have any conflicts of interest.

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APPENDIX A: PROOFS OF THE PROPOSITIONS

Proof of Proposition 2. Taking into account the continuity of functions f_j and the fact that $|w - z| \leq c\varepsilon$ due to the finite range of interaction, we have

$$\begin{aligned} (L_\varepsilon^0 F_\varepsilon^Q + V_\varepsilon F_\varepsilon)(z) &= \sum_{j=1}^M \left((P_\varepsilon^0 - I) q_j \left(\frac{z}{\varepsilon} \right) \right) (f_0(z) - f_j(z)) \\ &+ \sum_{j=1}^M \sum_{w \in \varepsilon \{x_j\}^\#} v_\varepsilon(z, w) (f_j(z) - f_0(z)) + o(1), \end{aligned} \tag{A1}$$

where $o(1)$ tends to 0 as $\varepsilon \rightarrow 0$. From (38) and (A1), we deduce that the functions $q_j\left(\frac{z}{\varepsilon}\right)$, $z \in \varepsilon B^\sharp$, and constants α_{0j} should satisfy the following system of equations:

$$\begin{aligned} & \left((P_\varepsilon^0 - I)q_j\left(\frac{z}{\varepsilon}\right) \right) (f_0(z) - f_j(z)) + \sum_{w \in \varepsilon\{x_j\}^\sharp} v_\varepsilon(z, w)(f_j(z) - f_0(z)) \\ & = \alpha_{0j}(f_j(z) - f_0(z)), \quad j = 1, \dots, M. \end{aligned}$$

Then, for every $j = 1, \dots, M$, the function $q_j\left(\frac{z}{\varepsilon}\right)$ is a solution of the equation

$$(P_\varepsilon^0 - I)q_j\left(\frac{z}{\varepsilon}\right) = \sum_{w \in \varepsilon\{x_j\}^\sharp} v_\varepsilon(z, w) - \alpha_{0j}\mathbf{1}_{\varepsilon B}, \quad z \in \varepsilon B^\sharp, \quad (\text{A2})$$

which is equivalent to the following equation:

$$(P^0 - I)q_j(x) = \sum_{y \in \{x_j\}^\sharp} v(x, y) - \alpha_{0j}\mathbf{1}_B, \quad x \in B^\sharp, \quad (\text{A3})$$

where $\mathbf{1}_{\varepsilon B}$ and $\mathbf{1}_B$ are the characteristic functions of the sets εB^\sharp and B^\sharp , respectively, and $q_j(x)$ is Y -periodic. According to the Fredholm alternative equation (A3) has a unique up to an additive constant solution if

$$\left(\sum_{y \in \{x_j\}^\sharp} v(x, y) - \alpha_{0j}\mathbf{1}_B \right) \perp \text{Ker}(P^0 - I)^* \quad \text{with} \quad \text{Ker}(P^0 - I)^* = \mathbf{1}_B;$$

the last relation here follows from the irreducibility of P^0 on B^\sharp . Therefore, there are uniquely defined constants α_{0j} given by formula (20), such that Equation (A3) has a unique up to an additive constant bounded periodic solution $q_j(x)$, $x \in B^\sharp$. Proposition 2 is proved.

Proof of Proposition 1. Using (33), we get for all $z \in \varepsilon B^\sharp$:

$$\begin{aligned} L_\varepsilon^0 F_\varepsilon^P(z) &= \frac{1}{\varepsilon^2} (T_\varepsilon^0 - I) \left(f_0(z) + \varepsilon \nabla f_0(z) \cdot h\left(\frac{z}{\varepsilon}\right) \right) \\ &+ (T_\varepsilon^0 - I) \left(\nabla \nabla f_0(z) \cdot g\left(\frac{z}{\varepsilon}\right) \right) + \frac{1}{\varepsilon} D_\varepsilon \left(f_0(z) + \varepsilon \nabla f_0(z) \cdot h\left(\frac{z}{\varepsilon}\right) \right) + O(\varepsilon). \end{aligned} \quad (\text{A4})$$

Then, the vector function $h\left(\frac{z}{\varepsilon}\right)$ can be found from the relation

$$\frac{1}{\varepsilon^2} (T_\varepsilon^0 - I) \left(f_0(z) + \varepsilon \nabla f_0(z) \cdot h\left(\frac{z}{\varepsilon}\right) \right) = O(1). \quad (\text{A5})$$

Letting

$$p_\xi(x) = p_0(x, x + \xi), \quad d_\xi(x) = d(x, x + \xi), \quad x, x + \xi \in B^\sharp, \quad (\text{A6})$$

we represent $T_\varepsilon^0 f(z)$ as follows:

$$(T_\varepsilon^0 f)(z) = \sum_{\xi} p_\xi\left(\frac{z}{\varepsilon}\right) f(z + \varepsilon \xi), \quad z \in \varepsilon B^\sharp. \quad (\text{A7})$$

Due to (A7) and condition (2), the left-hand side of (A5) is well-defined and takes the form:

$$\begin{aligned}
 & \frac{1}{\varepsilon^2} \sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) (f_0(z + \varepsilon\xi) - f_0(z)) \\
 & + \frac{1}{\varepsilon} \sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) \left(\nabla f_0(z + \varepsilon\xi) \cdot h \left(\frac{z}{\varepsilon} + \xi \right) - \nabla f_0(z) \cdot h \left(\frac{z}{\varepsilon} \right) \right) \\
 & = \frac{1}{\varepsilon} \sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) \nabla f_0(z) \cdot \xi + \frac{1}{\varepsilon} \sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) \nabla f_0(z) \cdot \left(h \left(\frac{z}{\varepsilon} + \xi \right) - h \left(\frac{z}{\varepsilon} \right) \right) + O(1) \\
 & = \frac{1}{\varepsilon} \nabla f_0(z) \cdot \left(\sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) \left(\xi + \left(h \left(\frac{z}{\varepsilon} + \xi \right) - h \left(\frac{z}{\varepsilon} \right) \right) \right) \right) + O(1).
 \end{aligned} \tag{A8}$$

Thus, the periodic vector function $h(x)$ should satisfy the equation

$$(P^0 - I)(l(x) + h(x)) = 0, \quad x \in B^{\sharp}, \tag{A9}$$

where $l(x) = x$ is the linear function. The solvability condition for Equation (A9) reads

$$((P^0 - I)l, \text{Ker}(P^0 - I)^*) = ((P^0 - I)l, \mathbf{1}_B) = \sum_{x \in B} \sum_{\xi} p_{\xi}(x)\xi = 0.$$

Since $p_{\xi}(x) = p_{-\xi}(x + \xi)$, this condition is fulfilled, which implies the existence of the unique, up to an additive constant, periodic solution $h(x)$ of Equation (A9).

We follow the similar reasoning in order to derive an equation for the periodic matrix function $g(x)$, $x \in B^{\sharp}$. We will also obtain below the expressions for the effective matrix Θ and the drift b .

Collecting in (A4) the terms of the order $O(1)$, using relation (A9) on the function $h(x)$ and relation (8) on the matrix D , we obtain:

$$\begin{aligned}
 & \frac{1}{\varepsilon^2} \sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) (f_0(z + \varepsilon\xi) - f_0(z)) \\
 & + \frac{1}{\varepsilon} \sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) \left(\nabla f_0(z + \varepsilon\xi) \cdot h \left(\frac{z}{\varepsilon} + \xi \right) - \nabla f_0(z) \cdot h \left(\frac{z}{\varepsilon} \right) \right) \\
 & + \sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) \left(\nabla \nabla f_0(z + \varepsilon\xi) \cdot g \left(\frac{z}{\varepsilon} + \xi \right) - \nabla \nabla f_0(z) \cdot g \left(\frac{z}{\varepsilon} \right) \right) \\
 & + \frac{1}{\varepsilon} \sum_{\xi} d_{\xi} \left(\frac{z}{\varepsilon} \right) f_0(z + \varepsilon\xi) + \sum_{\xi} d_{\xi} \left(\frac{z}{\varepsilon} \right) \nabla f_0(z + \varepsilon\xi) \cdot h \left(\frac{z}{\varepsilon} + \xi \right) \\
 & = \frac{1}{\varepsilon} \nabla f_0(z) \cdot \left(\sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) \left(\xi + \left(h \left(\frac{z}{\varepsilon} + \xi \right) - h \left(\frac{z}{\varepsilon} \right) \right) \right) \right) \\
 & + \nabla \nabla f_0(z) \cdot \left(\sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) \left(\frac{1}{2} \xi \otimes \xi + \xi \otimes h \left(\frac{z}{\varepsilon} + \xi \right) + \left(g \left(\frac{z}{\varepsilon} + \xi \right) - g \left(\frac{z}{\varepsilon} \right) \right) \right) \right) \\
 & + \nabla f_0(z) \cdot \left(\sum_{\xi} d_{\xi} \left(\frac{z}{\varepsilon} \right) \left(\xi + h \left(\frac{z}{\varepsilon} + \xi \right) \right) \right) + O(\varepsilon)
 \end{aligned} \tag{A10}$$

$$\begin{aligned}
 & = \nabla \nabla f_0(z) \cdot \left(\sum_{\xi} p_{\xi} \left(\frac{z}{\varepsilon} \right) \left(\frac{1}{2} \xi \otimes \xi + \xi \otimes h \left(\frac{z}{\varepsilon} + \xi \right) \right) + (P^0 - I)g \left(\frac{z}{\varepsilon} \right) \right) \\
 & + \nabla f_0(z) \cdot \left(\sum_{\xi} d_{\xi} \left(\frac{z}{\varepsilon} \right) \left(\xi + h \left(\frac{z}{\varepsilon} + \xi \right) \right) \right) + O(\varepsilon).
 \end{aligned} \tag{A10}$$

Here, $\xi \otimes \eta$ is a matrix with elements $\xi_i \eta_j$, $i, j = 1, \dots, d$.

Denote by Φ and \mathfrak{b} the following periodic matrix and vector functions:

$$\Phi(y) = \frac{1}{2} \sum_{\xi \in \Lambda_y} p_\xi(y) \xi \otimes \xi + \sum_{\xi \in \Lambda_y} p_\xi(y) \xi \otimes h(y + \xi), \tag{A11}$$

$$\mathfrak{b}(y) = \sum_{\xi \in \Lambda_y} d_\xi(y)(\xi + h(y + \xi)) = \sum_{\xi \in \Lambda_y} d(y, y + \xi)(\xi + h(y + \xi)), \quad y \in B. \tag{A12}$$

Clearly, both the functions Φ and \mathfrak{b} depend on h . In order to ensure the convergence in (37), we should find a constant matrix Θ , a periodic matrix function $g(y)$ and a constant vector b such that

$$(\mathfrak{b}(y) - b, \mathbf{1}_B) = \sum_{y \in B} \sum_{\xi} d(y, y + \xi)(\xi + h(y + \xi)) - b|B| = 0. \tag{A13}$$

and, for any $k, m, 1 \leq k, m \leq d$,

$$\Phi_{km}(y) + (P^0 - I)g_{km}(y) = \Theta_{km}. \tag{A14}$$

The former equation yields

$$b = \frac{1}{|B|} \sum_{y \in B} \sum_{\xi} d(y, y + \xi)(\xi + h(y + \xi)). \tag{A15}$$

The solvability condition for (A14) reads

$$(-\Phi_{km} + \Theta_{km}, \text{Ker}(P^0 - I)^*) = (-\Phi_{km} + \Theta_{km}, \mathbf{1}_B) = 0.$$

Thus, Θ is uniquely defined as follows:

$$\Theta_{km} = \frac{1}{|B|} \sum_{y \in B} \Phi_{km}(y), \quad \text{where } \Phi(y) = \sum_{\xi} p_\xi(y) \xi \otimes \left(\frac{1}{2} \xi + h(y + \xi) \right), \tag{A16}$$

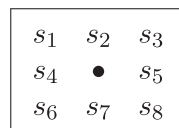
and $g(y)$ is a solution of Equation (A14) which is uniquely defined, up to a constant matrix. As was proved in Piatnitski and Zhizhina [9], the symmetric part of the matrix Θ defined by (A16) is positive definite, that is, $\Theta \eta \cdot \eta > 0$ for all $\eta \neq 0$.

This completes the proof of Proposition 1.

APPENDIX B: ONE EXAMPLE WITH CALCULATION OF EFFECTIVE PARAMETERS

In this section, we consider an example of a high-contrast discrete problem for which we calculate the effective characteristics Θ and b . These characteristics are then used in order to write down the upscaled equations and to describe the stationary regime; see Equations (46) and (48).

Let the periodicity cell Y be a square 3×3 of the two-dimensional lattice \mathbb{Z}^2 , and assume that A is the one-point subset of Y located at the center of Y , $B = Y \setminus A$. Let us enumerate the elements of B in accordance with their position on the cell Y :



We define the symmetric matrix $P_0|_{B^\#} = \{p_0(x, y), x, y \in B^\#\}$ describing the flow outside of cleaning elements as follows:

- $p_0(x, x \pm e_1) = p_0(x, x \pm e_2) = \frac{1}{4}$, if $x \in \{s_1, s_3, s_6, s_8\}$;
- $p_0(x, x \pm e_1) = \frac{1}{4}$, $p_0(x, x + e_2) = \frac{1}{2}$, if $x = \{s_2\}$;
- $p_0(x, x \pm e_2) = \frac{1}{4}$, $p_0(x, x - e_1) = \frac{1}{2}$, if $x = \{s_4\}$;
- $p_0(x, x \pm e_2) = \frac{1}{4}$, $p_0(x, x + e_1) = \frac{1}{2}$, if $x = \{s_5\}$;
- $p_0(x, x \pm e_1) = \frac{1}{4}$, $p_0(x, x - e_2) = \frac{1}{2}$, if $x = \{s_7\}$.

Other elements of the matrix $P_0|_{B^\#}$ are equal to 0.

Next, we introduce the matrix D , which determines a small (of the order ε) drift. The elements of this matrix $D = \{d(x, y)\}$, $x, y \in B^\#$ are defined by

$$d(x, x \pm e_2) = \mp K, \text{ if } x \in \{s_1, s_3, s_4, s_5, s_6, s_8\}, \text{ and } d(x, y) = 0, \text{ otherwise.} \quad (\text{B1})$$

Observe that relation (8) for D is fulfilled. These two matrices completely define our model at the microscopic length scale on the component $B^\#$.

In order to compute the matrix Θ and the vector b , we apply formulae (A16) and (A15), respectively. Since both Θ and b depend on h , it only remains to find the vector function $h(x) = \{h(x), x \in B\}$. This function is called the corrector, it is defined by Equation (A9). Recall that $h(x)$ is a periodic vector function that is fully defined by its values on the set B :

$$h = \{h(s_1) \in \mathbb{Z}^2, h(s_2) \in \mathbb{Z}^2, \dots, h(s_8) \in \mathbb{Z}^2\}, B = \{s_1, \dots, s_8\}. \quad (\text{B2})$$

We explain now how to find this vector function $(h_1(x), h_2(x))$. It is worth noticing that (A9) is a system of uncoupled equations, and we can solve it for each coordinate h_1 and h_2 separately. In order to determine the function $h_1 = \{h_1(s_1), h_1(s_2), \dots, h_1(s_8)\}$ being the first coordinate of the vector function h on B , we substitute $(x_1, 0)$ for $l_1(x)$ in (A9) and rewrite (A9) in the following way:

$$(P^0 - I)h_1(x) = -(P^0 - I)l_1(x) = -\sum_{\xi} p_{\xi}(x)\xi_1 =: \psi_1(x), x \in B^\#, \quad (\text{B3})$$

where $\xi = (\xi_1, \xi_2)$. Observe that $\psi_1(x)$ is periodic on \mathbb{Z}^2 . It can be represented as follows:

$$\begin{array}{|c|c|c|} \hline 0 & 0 & 0 \\ \hline \frac{1}{2} & \bullet & -\frac{1}{2} \\ \hline 0 & 0 & 0 \\ \hline \end{array}$$

Thus, $h_1 = (P^0 - I)^{-1}\psi_1$, and solving this system of linear equation, we obtain the following representation for $h_1(x)$:

$$\begin{array}{|c|c|c|} \hline -\frac{1}{11} & 0 & \frac{1}{11} \\ \hline -\frac{4}{11} & \bullet & \frac{4}{11} \\ \hline -\frac{1}{11} & 0 & \frac{1}{11} \\ \hline \end{array} \quad (\text{B4})$$

Similarly, letting $l_2(x) = (0, x_2)$, we deduce that the function $h_2(x)$ is a solution to the equation

$$h_2 = (P^0 - I)^{-1}\psi_2, \quad \text{where } \psi_2(x) = -(P^0 - I)l_2(x) = -\sum_{\xi} p_{\xi}(x)\xi_2,$$

with ψ_2 given by

$$\begin{array}{|c|c|c|} \hline 0 & -\frac{1}{2} & 0 \\ \hline 0 & \bullet & 0 \\ \hline 0 & \frac{1}{2} & 0 \\ \hline \end{array}$$

This yields the following representation for $h_2(x)$:

$$\begin{array}{|c|c|c|} \hline \frac{1}{11} & \frac{4}{11} & \frac{1}{11} \\ \hline 0 & \bullet & 0 \\ \hline -\frac{1}{11} & -\frac{4}{11} & -\frac{1}{11} \\ \hline \end{array} \quad (\text{B5})$$

Combining formula (A15) with (B1) and (B4)–(B5), one recovers the components of the vector b :

$$b = \frac{1}{|B|} \sum_{x \in B} \sum_{\xi = \pm e_2} d(x, x + \xi)(\xi + h(x + \xi)) = \frac{1}{8}(0, -12K) = \left(0, -\frac{3}{2}K\right),$$

where K is introduced in (B1).

Finally, the 2×2 matrix Θ can be calculated by the formula in (A16). Exploiting this formula and taking into account (B4)–(B5), we have $\Theta = \frac{9}{44} \mathbf{I}$, where \mathbf{I} is the unit 2×2 matrix.