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Modelling of Tracer Fluxes in Complex Canopies by Means of Conformal Mapping and Multifractal Formalism

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Abstract

We present a simple physics based model of pollutant concentration and associated fluxes in a fractal canopy. model provides a closed system of equations for approximating mean-field concentration, and spatial flux distribution within the canopy. Our approach is based on methods of theoretical physics (conformal mapping and multifractal formalism), that have recently emerged [2] in application to the problem of modelling tracer dispersion. For a rough boundary with a given fractal spectrum, the model provides a method for predicting the mean concentration and the probability distribution of concentration fluxes, which influence tracer deposition. We also develop a simple, but scientifically rigorous, algorithm to generate realisations of flux distributions within complex canopies. The proposed framework can be used as a valuable performance check of more complicated CFD models, or as a part of an integrated framework for the simulation and mitigation of hazardous events for military clients and first responders. We hope that after further validation, the proposed framework could be used to improve model performance in situations when numerous "what-if" scenarios are to be run within a short timeframe.

Introduction

The dispersive motion of tracer particles near irregular interfaces plays a crucial role in various transport phenomena in nature and technical applications. It has been traditionally a topic of significant interest in ecology, meteorology and industrial hydrodynamics, and can be used to model effects related to pollutant transport, turbulent dispersion, chemical reactors and mixing devices. There is a vast amount of literature on this subject, [14, 17, 6]. Critically, in all of these systems, interfacial confinement strongly influences the dispersion of tracer particles. Comprehensive study of this phenomena is a challenging task, even for advanced CFD models. Whilst the latter are able to accurately calculate tracer concentration at the mesh points, analytical models can be used to gain valuable statistical insights into phenomena which are important for model validation, interpretation and possible generalisation.

This necessitates the development of analytically treatable, yet scientifically sound, models based on clear physics principles to describe the dispersion of tracer particles over irregular surfaces. In this work, the irregular boundaries of interest exhibit fractal properties, which can result in the surface being rough or intermittent. Such models are desirable in order to promptly estimate the effect of interface morphology on a particular scenario of tracer transport.

In this current paper we extend our previous results [16] and present a mathematical model of a tracer plume generated by a steady point source above a fractal canopy. For the sake of simplicity, we restrict our consideration to the case of twodimensional steady flow. Our approach is based on methods of theoretical physics, conformal mapping and multifractal formalism, that have recently been applied to the problem of tracer dispersion (see [4, 2, 5, 9] and references therein).

Mean-field model

In this section we present a simple mean-field model for passive tracers dispersed over a fractal canopy. The mean-field model implies that we are only interested in a coarse-grained description of the tracer field. In particular, the distribution of concentration and associated flux, averaged over a spatial scale that exceeds that of the canopy (height, correlation length).

A rigorous derivation of this model is outside the scope of this paper. Here we present a phenomenological approach leading to simple analytical expressions that capture the main effect of tracer dispersion in this case. This approach includes an explicit dependence of the vertical concentration profile on the fractal dimension of the canopy.

In two-dimensions tracer dispersion, subject to steady flow past a flat boundary, is described by the well-known advectiondiffusion equation (ADE) [14]

$$U(y)\frac{\partial}{\partial x}\theta + D(y)\frac{\partial^2}{\partial y^2}\theta = 0,$$
 (1)

where θ is the mean tracer concentration, *y* is the vertical height, *x* is the downstream distance. U(y), D(y) are functions which describe velocity and diffusivity respectively and can be modelled by power-law profiles:

$$U(y) = v_0 \left(\frac{y}{y_0}\right)^m, \ D(y) = D_0 \left(\frac{y}{y_0}\right)^n,$$
 (2)

Equation 1 can be reduced to an ODE with a self-similar solution [14, 1]. For a point source located at x = 0, y = H, where H is the elevation of the source, the solution of this equation can be described by a Green's function which is *stretch-exponential* asymptotic.

$$G(\xi,\xi_0) \propto \exp[-\sigma(\xi-\xi_0)^q], \quad \xi(y,x) = \left(\frac{y}{y_0}\right) \left(\frac{y_0}{x}\right)^{\frac{1}{q}}, \quad (3)$$

where

$$q = 2 + m - n, \tag{4}$$

In these equations, y_0 gives the vertical scale of the velocity gradient, σ is a constant derived from v_0 , D_0 and y_0 . Furthermore, $\xi_0 = \xi(H, x)$. By employing the method of reflections we can construct a solution for the absorbing boundary: $\theta = G(\xi, \xi_0) - G(\xi, -\xi_0)$, that is, $\theta = 0$ at the boundary y = 0. This implies that the in general case, for all values of $m \neq n$, the flux near the boundary can be non-smooth and scales as

$$\frac{\partial \theta}{\partial y} \propto y^{(q-2)} \propto y^{(m-n)}, \ \xi \gg \xi_0 \tag{5}$$

Our approach is to exploit the "non-smoothness" of the model at the boundary. The roughness induced by a fractal canopy can be compensated for by imposing additional constraints on the free parameters, m and n.

Introduction of a fractal canopy requires modification of the flat boundary solution of equation (3), which is done by following the physics-based reasoning of Boffetta [4]. Very close to the boundary, tracer flux is purely diffusive because the advection term in (1) is negligible. Such a system will obey the scaling law for the diffusive transport near a fractal boundary [8].

$$\frac{\partial \theta}{\partial y} \propto y^{(2-d_f)},$$
 (6)

where d_f is the fractal dimension of the boundary.¹

If we assume that near the fractal boundary the general structure of *stretch-exponential* solution (3) still holds, we should be able to capture the "fractal-boundary" effect by the simple modification of exponent q (for non-fractal rough surfaces see [16]). In other words, we should be able to introduce variable exponent q(y) that matches limiting values of eqs. (3) and (6) (far away and close to the boundary) and reproduces the correct scaling properties of the flux. These limiting conditions for the function q(y) can be deduced from equations (4), (5) and (6).

$$q(y) \to q_0 = 4 - d_f, \ y \to 0, \tag{7}$$

$$q(y) \rightarrow q_{\infty} = 2 + m - n, \ y \rightarrow \infty.$$
 (8)

Based on these conditions we can propose the following parameterisation:

$$q(y) = q_{\infty} \frac{a + y/l_*}{1 + y/l_*}. \ a = \frac{q_0}{q_{\infty}},$$
 (9)

This representation provides smooth interpolation between two limiting values. The parameter l_* is the length scale at which diffusing behaviour of tracer dominates over advection. It can be estimated from power-law profiles (2), so $l_* \sim D(l_*)/U(l_*)$ and:

$$l_* \approx y_0 \left(\frac{1}{Pe}\right)^{\eta}, \ \eta = \frac{1}{1+m-n} \tag{10}$$

The parameter $Pe = v_0 H/D_0 \gg 1$ is the Peclet number of the flow and it is assumed to be large (hence $y_0 \gg l_*$).

Eqs.(3) and (9) provide closed analytical expressions for the mean-field theory of tracer particles dispersed by turbulent flow above the fractal canopy. It explicitly takes into account the velocity and diffusivity profiles of the turbulent flow (parameters m, n, v_0, D_0) as well as the fractal properties of the boundary (parameter d_f).

It is worth noting noting that the "variable exponent" approach (9) can also be used as the first approximation in any other stretch-exponential solution of ADE (1), for example, the reflecting canopy of [16]. It can also provide a simple, but still physically rigorous, parameterisation of the effect of the fractal canopy. Some examples of these solutions are presented in fig. 1. These profiles resemble recent experimental observations [16, 19].

It is worth noting that for the so-called conjugate profile $1/D(y) \propto dU(y)/dy$, so n = 1 - m, $q_{\infty} = 1 + 2m$ [14] and values q(0) and q_{∞} are rather close to one another (since $m \le 1$ and $d_f \approx 2$), hence $a \approx 1$ in (9).

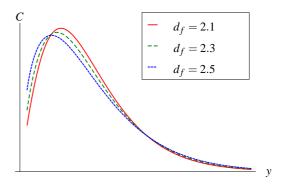


Figure 1: Vertical distribution of tracer concentration for three different fractal dimensions

A fine-grain model of tracer fluxes within a fractal canopy

Let us now establish an analytical framework for physics-based model of the tracer flux distribution within a complex canopy. This model provides a mechanism for calculation of tracer depositions, since the latter is an integral of fluxes. To model the intermediate tracer fluxes within the fractal canopy we need to resolve the tracer distribution on small scales, that is, smaller than the canopy scale. In order to enable analytical progress we employ ideas of conformal invariance and multifractal formalism of the advection diffusion equation [2, 5, 4]. The key element of our modelling framework recently explored in those works relates to the conformal invariance of ADE (1), provided that velocity U can be described by means of potential (i.e. $\mathbf{U} = \nabla \phi$). This implies that the powerful analytical methods of harmonic functions can be applied to the study of complex fluxes associated with ADE. In the current paper we demonstrate this approach for the simplest flow with a constant value of U.

The intermittent structure of fluxes induced by the fractal canopy can be understood by considering similar results for the Laplacian transport [4, 9, 5, 3, 18]. The latter can be easily deduced from the solution of the Laplace equation in polar coordinates, and can be interpreted in terms of the *winding angle* of the boundary (the angle tangential to the boundary profile) [4, 9, 5]. Effectively, local changes in winding angle result in a local "flux anomaly" that can be estimated as $\delta J \sim \varepsilon^r$, $r = 1 - \delta \phi / \pi$ where ε is the linear size of the area of the deformation and $\delta \phi$ is the change of the winding angle caused by this deformation (which can be either positive or negative). As $\varepsilon \to 0$ any sharp changes in the winding angle reasoning provides a valuable intuitive method for finding critical locations of the tracer distribution in complex canopies.

We now provide a more rigorous framework to describe tracer flux distribution by means of conformal mapping. The confor-

¹We assume the boundary to be a monofractal, so we need only one parameter to characterize its fractal dimension. For multifractal canopies we need to average final expressions over multifractal spectrum

mal invariance of the ADE implies that its solutions (concentration and associated fluxes) in any complex planar domain can be constructed from a solution in a simpler domain. We make use of a formal substitution $\theta(z) \rightarrow \theta(w)$, where z = x + iy and w = F(z) is a conformal mapping to the new domain. For a long time this method has been applied to harmonic functions and bi-harmonic functions [18], but results [2, 5, 3] extend it to the domain of ADE.

According to [2], [5], under a conformal transformation concentration fluxes along and across the boundary are transformed as

$$J_z = |F'|J_w, \tag{11}$$

where F' = dF(z)/dz, J_z and J_w are fluxes calculated in the original and the transformed domain, $\Re(J), \Im(J)$ are normal and tangential components of those fluxes.

Relation (11) allows an important conclusion to be drawn regarding the spatial structure of fluxes within the complex canopy. Let us assume that in the simple (non transformed) domain, the flux J_w has no singularities. This means that any singularities of flux in the transformed domain can be introduced only by the derivative of the mapping function F. Given that F is fully determined by the geometry of the boundary of the transformed domain, it is possible to produce general solutions that can be used for any values of the dynamic parameters, including mean velocity and diffusivity.

To illustrate this point it is instructive to consider a general model of a piece-wise boundary (see Fig 2). This model can be considered as a first approximation for any shape of the canopy, with accuracy that can be refined as necessary. The conformal mapping of this boundary to the half space is given by the well-known Schwarz-Christoffel transformation [13, 15].

$$F(z) = A \int_0^z \prod_{1}^n (x - a_i)^{\mu_i} dx + B$$
(12)

for which F' is given by

$$F'(z) = A \prod_{1}^{n} (x - a_i)^{\mu_i}, \qquad (13)$$

where *A* and *B* are constants, a_i corresponds to the pre-image locations of the vertices in the *z* domain, and $\mu_i = \phi_i/\pi$, such that ϕ_i is the exterior angle measured between adjacent vertices in the transformed domain. In particular note that $-1 \le \mu \le 1$.

Eqs. (11), (13) express the above mentioned property that intermittent structure of the concentration flux in rough (piece-wise) canopies can be presented as a spatial distribution of "anomalies" (zeros for $\mu \ge 0$ and singularities for $\mu \le 0$). It is important to stress that because of the constraint $-1 \le \mu \le 1$ these singularities are integrable, so the flux integral (or averaged flux per unit of boundaries) never diverges. This is a manifestation of the fact that the total flux is preserved by conformal transformation [2, 5], which is known as the Makarov theorem [9, 8]).

In order to have all terms in (11) defined we need to have an analytical solution for the flux distribution in the non-transformed domain. The examples considered in the literature are flux between two concentric circles with axial flow when one circle is "tracer-absorbing" ($\theta = 0$) and another one is "traceremitting"($\theta = \theta_0 = const$), see [11], [5]. The tracer flux between two parallel plates with constant flow is a particular case of the above configuration. Another partially relevant case (which still enables some analytical progress) is the solution for the point-source above the flat boundary in the constant flow (i.e. m = n = 0 in (2)). This solution can be written in the form (see details in [5])

$$G(z, z_0) = K_0(\kappa | z - z_0|) \exp(\kappa x), \qquad (14)$$

where K_0 is a modified Bessel function of the second kind and $\kappa = U_0/D_0$. For the absorbing boundaries (G = 0), the required solution again can be written by employing the method of images, so we arrive at

$$\theta(z, z_0) = G_0(z, z_0) - G_0(z, z_0^*), \tag{15}$$

where $z_0^* = (x - x_0, y + y_0)$ is the position of imaginary source. From here we can calculate flux $J = \partial \theta / \partial z$ and plug it in (11).

We would like to emphasize again that intermittent distribution of the flux is the result of the geometrical properties of the boundary (the first term in (11)) and will emerge for any initial distribution of flux (the second term in (11)). Employing any complex initial distribution of flux results in unnecessary analytical and numerical complications, while the main structure of flux anomalies remain unchanged. In order to capture the main effect of spatial intermittency of concentration fluxes it is reasonable to start with a very simple initial model for flux distribution (for instance taking J_z to be a constant), but with a more realistic model of canopy.

As an example of application of the proposed framework we considered the effect of a complex boundary based on the Sierpinski arrowhead fractal (see Fig 2). We employ the Schwarz-Christoffel Toolbox for MATLAB [7] to perform the necessary calculations. Critically, note the correlation between the geometric shape of the boundary and the flux anomalies that are introduced.

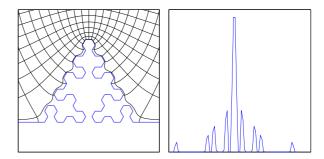


Figure 2: Geometric flow characteristics near a fractal surface. Left: the streamlines and equipotential lines; Right: the flux, J, introduced by the conformal mapping on the surface.

Extending the proposed framework to take random boundaries into consideration is straightforward. This can be done by simply averaging the final expressions over given statistical distributions (PDF) $p(a_i)$ and $p(\mu_i)$ in (13). This amounts to the "ensemble average" function $\langle F' \rangle$ in (11). Sometimes properties of this distribution can be deduced from the physics-based considerations. One example of this constraint, already mentioned, is total flux conservation (since flux is preserved by conformal mapping). The total flux conservation implies that ensembleaveraged mean function $\langle F'(z) \rangle$ should provide the same mean value for the total flux. Another example is $\langle \mu_i \rangle = 0$ in the case of a perfectly flat canopy, or $\langle \mu_i \rangle = \phi_0/\pi = const$ for a canopy with a constant slope. The important point is that functions $p(a_i)$ and $p(\mu_i)$ can be deduced only from the canopy properties, but are not inter-related to the advection-diffusion problem.

For given PDFs p(a) and $p(\mu)$ we can use (13) to generate realisations of the associated flux distribution. The ability to generate high fidelity distributions of tracer fluxes is a valuable capability of the proposed framework, with applications in the field of hazard simulation. Applications of this concept are particularly important for validation of data fusion algorithms (source backtracking, optimal sensor placement and harmful exposure prediction) [10], which are often built on numerous realizations of intermittent concentration fields. A more comprehensive study of this topic will be presented in a separate paper.

As we have discussed above there is an intimate connection between the statistics of spatial flux distribution within the complex canopy and the statistics of the winding angle within the same canopy. This connection is especially useful in the case of multifractal canopies for which the PDF of the winding angle can be derived from a multifractal spectrum $f(\alpha)$ by means of well-known formalism [4, 9, 12]. This leads to the following PDF for the flux distribution (for details see [4]).

$$p(J) = \frac{C}{J} \delta^{f(\alpha)}, \ \alpha(J) = (\log \delta)^{-1} \log \left(\frac{J}{\overline{J}}\right), \ \delta = \frac{H}{x},$$
 (16)

where *C* is a normalization factor, *x* is the downstream distance, \overline{J} is the averaged flux calculated from the mean-field approximation (3), (9).

In can be shown that for a simple approximation of shape of function $f(\alpha)$ (i.e. linear or parabolic), PDF p(J) can be reduced to a distribution with the power-law tails that are very sensitive to the parameters of $f(\alpha)$ (maximum, mean, width etc). These results will be presented elsewhere. Examples of this PDF are depicted in fig 3.

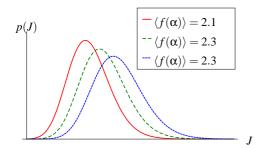


Figure 3: Example of PDF for cross-boundary flux for three different fractal spectra

Conclusions

We have presented a simple physics based model of the concentration and associated fluxes in the fractal canopy. The model provides a closed system of equations for the mean-field approximation as well as for the spatial flux distribution within the canopy. The proposed framework explicitly relates properties of the tracer transport (mean turbulent velocity and diffusivity) to the morphology of the underlying fractal surface (fractal spectrum). It can be used as a valuable performance check of more complicated CFD models, or as a part of an integrated framework for the simulation and mitigation of hazardous events for military clients and first responders. We hope that after further validation, the proposed framework can provide a valuable trade-off between the model performance and its scientific rigour in situations where numerous "what-if" scenarios are to be run within a short timeframe.

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