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A MADELUNG-TYPE MULTIFRACTAL MODEL FOR ATMOSPHERIC POLLUTANT DYNAMICS

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Abstract: This manuscript proposes a Madelung-type multifractal model for atmospheric pollutant dynamics. The formulation preserves the conservative advection-diffusion-reaction-deposition structure used in classical air-quality modelling, while adding a weak, regularized curvature-sensitive correction intended to represent unresolved intermittency, plume focusing, concentration localization, and heterogeneity-driven accumulation. The model defines the atmospheric domain, pollutant concentration vector, atmospheric burden, effective transport velocity, anisotropic turbulent diffusivity, boundary-layer mixing, sectoral emissions, wet scavenging, dry deposition, gravitational settling, reduced chemical transformations, aerosol diagnostics, and observation operators for calibration and validation. A heterogeneity index is introduced to account for orographic confinement, surface roughness, land-use structure, boundary-layer stability, and humidity or heat-island effects. The multifractal contribution is formulated through a regularized concentration amplitude, a curvature-sensitive potential, a mobility-controlled drift, and a bounded diffusivity correction, so that the additional term modifies but does not replace the classical transport core. An illustrative synthetic simulation demonstrates numerical implementability, plume migration under imposed wind, localized accumulation near emission gradients, and exploratory scale-sensitive diagnostics. The proposed framework is therefore best interpreted as a physically constrained modelling extension that requires calibration and independent validation with meteorological, emissions, station, and remote-sensing data before operational use.

Keywords: *air-quality modelling, atmospheric pollutants, Madelung-type model, multifractal dynamics, pollutant dispersion*

INTRODUCTION

Classical atmospheric-pollution modelling is usually built around Eulerian conservation equations for advection, turbulent diffusion, emissions, chemical transformation, and removal. This structure is scientifically well established and underlies major regional air-quality systems such as CMAQ [1]. It remains indispensable because pollutant concentration is constrained by mass conservation, meteorological transport, boundary-layer mixing, emissions, chemistry, and deposition. However, classical dynamics becomes incomplete when it is used as a purely smooth, mean-field advection-diffusion-reaction description. In real atmospheric environments, pollutant fields are shaped by intermittent turbulence, urban roughness, topographic confinement, boundary-layer stability transitions, plume meandering, precipitation scavenging, and nonlinear chemistry. These mechanisms generate localized concentration hot spots, sharp gradients, non-Gaussian dispersion, and scale-dependent concentration patterns that are not fully represented by simple Fickian diffusion.

Online meteorology-chemistry models show that atmospheric composition and meteorology are strongly coupled, especially when boundary-layer physics, radiative forcing, clouds, aerosols, and transport are solved consistently [2, 3]. Lagrangian stochastic dispersion theory also demonstrates that unresolved turbulent fluctuations can strongly affect pollutant trajectories and concentration variance, even when the mean wind is known [4]. Near the surface, Monin-Obukhov similarity remains a central framework for turbulent exchange, but it also highlights that stability-dependent mixing is not constant and that weakly ventilated or stable boundary layers can favor pollutant trapping [5]. These considerations motivate a model that preserves the conservative chemical-transport core but allows additional scale-sensitive closures.

A further reason to go beyond purely classical dynamics is that turbulent atmospheric fields often exhibit intermittent cascade behavior. Multifractal descriptions of turbulent energy dissipation and anisotropic atmospheric cascade processes provide a mathematical basis for describing scale-dependent variability and concentration localization [6, 7]. Anomalous-diffusion theory shows that transport in heterogeneous or trapping-dominated media may deviate from ordinary Brownian/Fickian assumptions [8]. In pollutant dynamics, this does not mean that standard transport equations should be discarded; rather, it suggests that additional physically regularized terms can be introduced to represent unresolved focusing, filamentation, and intermittency.

Chemical and particulate pollutants add further complexity. Gas-phase VOC-NO_x-O_x-HO_x chemistry is nonlinear and can produce regime-dependent ozone and secondary aerosol responses [9, 10]. Dry deposition depends on aerodynamic, quasi-laminar, canopy/surface, and particle-size-dependent resistances [11, 12]. Satellite remote sensing and data assimilation provide additional constraints, but they require explicit observation operators and error-aware validation procedures [13, 14]. The objective of the present trimmed model is therefore to combine the minimum necessary classical transport-reaction-deposition framework with a controlled Madelung-type multifractal correction and an explicit observation-validation layer.

MATERIALS AND METHODS

Model domain, species vector, and atmospheric burden

Let the atmospheric modelling domain be

$$\Omega \subset \mathbb{R}^d, \quad d \in \{2, 3\}, \quad \mathbf{x} = (x, y, z), \quad t \in [0, T]. \quad (1)$$

Here, Ω is the horizontal-vertical atmospheric domain, d is the spatial dimension, $\mathbf{x}$ is the position vector with horizontal coordinates x, y and altitude z , t is time, and T is the final simulation time. Vectors are denoted by bold upright symbols; their individual coordinate components are scalar. Tensors and matrices are also shown in bold and are identified explicitly in the text.

For N gaseous or particulate pollutant species, we can define the concentration vector

$$\mathbf{C}(\mathbf{x}, t) = (C_1(\mathbf{x}, t), C_2(\mathbf{x}, t), \dots, C_N(\mathbf{x}, t))^T, \quad C_i(\mathbf{x}, t) \geq 0, \quad (2)$$

where $\mathbf{C}$ is the vector of pollutant concentrations, C_i is the concentration of species i , and $i = 1, \dots, N$. Depending on the species, C_i may be expressed in $\text{mol} \cdot \text{m}^{-3}$, $\text{kg} \cdot \text{m}^{-3}$, or $\mu\text{g} \cdot \text{m}^{-3}$.

The total atmospheric burden of species i in the computational domain is

$$M_i(t) = \int_{\Omega} C_i(\mathbf{x}, t) dV, \quad (3)$$

where $M_i(t)$ is the domain-integrated pollutant mass or mole amount of species i , and dV is the volume element.

Conservative transport-reaction-deposition core

The concentration balance for species i can be written as

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (C_i \mathbf{v}_i) = -\nabla \cdot \mathbf{J}_i + E_i + R_i^{\text{chem}} - \Lambda_i C_i - D_i^{\text{dry}} + S_i^{\text{bc}}. \quad (4)$$

Here, $\mathbf{v}_i$ is the effective transport velocity of species i , $\mathbf{J}_i$ is the nonadvective flux, E_i is the emission source, R_i^{chem} is the net chemical production-loss tendency, $\Lambda_i C_i$ is wet-scavenging loss, D_i^{dry} is dry-deposition loss when represented as a volume tendency, and S_i^{bc} represents boundary or inflow forcing.

The non-advective flux is decomposed as

$$\mathbf{J}_i = -\mathbf{K}_i^{\text{eff}} \nabla C_i + \mathbf{J}_i^{\text{mf}} + \mathbf{J}_i^{\text{sgs}}, \quad (5)$$

with $\mathbf{K}_i^{\text{eff}}$ the effective diffusivity tensor, $\mathbf{J}_i^{\text{mf}}$ the Madelung-type multifractal flux, and $\mathbf{J}_i^{\text{sgs}}$ an optional subgrid flux used when unresolved processes are parameterized separately.

The effective diffusivity tensor is

$$\mathbf{K}_i^{\text{eff}} = D_i^{\text{mol}} \mathbf{I} + \mathbf{K}^{\text{turb}} + \mathbf{K}_i^{\text{mf}}. \quad (6)$$

Here, D_i^{mol} is the molecular diffusivity of species i , $\mathbf{I}$ is the identity tensor, $\mathbf{K}^{\text{turb}}$ is the turbulent eddy-diffusivity tensor, and $\mathbf{K}_i^{\text{mf}}$ is the multifractal correction to dispersion.

The effective velocity is decomposed as

$$\mathbf{v}_i = \mathbf{u} + \mathbf{v}_i^{\text{rel}} - v_{s,i} \mathbf{e}_z + \mathbf{v}_i^{\text{mf}}, \quad (7)$$

where $\mathbf{u}$ is the resolved meteorological wind, $\mathbf{v}_i^{rel}$ is pollutant-relative drift induced by unresolved meteorological or surface constraints, $v_{s,i}$ is the nonnegative gravitational settling speed, $\mathbf{e}_z$ is the vertical unit vector taken positive upward, and $\mathbf{v}_i^{mf}$ is the curvature-induced multifractal drift. For gases, $v_{s,i} = 0$.

For compressible or anelastic meteorological input, air density satisfies the scalar continuity equation

$$\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}) = 0, \quad (8)$$

with ρ_a the air density and $\mathbf{u}$ the resolved meteorological wind field. When using mixing ratio $q_i = C_i/\rho_a$, Equation (4) can be converted into a density-weighted form. Equation (8) is scalar: the air-density time derivative and the divergence of the vector mass flux are both scalar quantities. The wind is a vector field, but taking the divergence yields a scalar mass-balance equation.

Boundary-layer mixing and turbulent diffusivity

The turbulent diffusivity tensor may be written in anisotropic diagonal form as

$$\mathbf{K}^{\text{turb}} = \begin{pmatrix} K_x & 0 & 0 \\ 0 & K_y & 0 \\ 0 & 0 & K_z \end{pmatrix}. \quad (9)$$

Here, K_x and K_y are horizontal eddy diffusivities, and K_z is the vertical eddy diffusivity. A compact surface-layer expression for vertical mixing [5] can be written as

$$K_z(z, t) = \kappa u_*(t) z' \phi_h^{-1} \left(\frac{z'}{L} \right), \quad z' = z - d_0, \quad (10)$$

where κ is the von Karman constant, u_* is friction velocity, z' is height above displacement height, d_0 is displacement height, ϕ_h is the nondimensional heat or scalar stability function, and L is the Monin-Obukhov length.

The Monin-Obukhov length can be expressed as

$$L = - \frac{\rho_a c_p u_*^3 \theta_v}{\kappa g H_s}. \quad (11)$$

Here, c_p is the specific heat capacity of air at constant pressure, θ_v is virtual potential temperature, g is gravitational acceleration, and H_s is surface sensible heat flux.

Emissions, wet removal, dry deposition, and settling

The total emission source of species i is represented as a sum of sectoral contributions:

$$E_i(\mathbf{x}, t) = \sum_{s=1}^{N_s} e_{i,s}(t) a_s(x, y) p_s(z) \chi_s(t), \quad (12)$$

where N_s is the number of emission sectors, $e_{i,s}(t)$ is the sectoral emission intensity, $a_s(x, y)$ is the horizontal spatial allocation function, $p_s(z)$ is the normalized vertical injection profile, and $\chi_s(t)$ is a dimensionless activity or control factor.

At the ground boundary $\partial\Omega_g$, dry deposition and surface emissions are imposed through the flux condition

$$\mathbf{n} \cdot \mathbf{J}_i = F_i^{\text{surf}} - v_{d,i} C_i \quad \text{on } \partial\Omega_g, \quad (13)$$

with $\mathbf{n}$ the outward unit normal, F_i^{surf} the surface emission flux, and $v_{d,i}$ the dry-deposition velocity of species i .

For gases, a resistance formulation [11] gives

$$v_{d,i} = (r_a + r_b + r_c)^{-1}. \quad (14)$$

Here, r_a is aerodynamic resistance, r_b is quasi-laminar boundary-layer resistance, and r_c is canopy or surface resistance.

For particles of diameter d_p , the Stokes-Cunningham settling speed [12] can be expressed as

$$v_s(d_p) = \frac{\rho_p d_p^2 g C_c(d_p)}{18\mu_a}, \quad (15)$$

with ρ_p particle density, d_p the particle diameter, $C_c(d_p)$ the Cunningham slip correction factor, and μ_a the dynamic viscosity of air. In Equation (7), settling acts downward through the term $-v_{s,i} \mathbf{e}_z$.

The wet-scavenging coefficient is written as

$$\Lambda_i(t, \mathbf{x}) = \lambda_{0,i} P^{\beta_i} + \lambda_{\text{in},i} f_c. \quad (16)$$

Here, $\lambda_{0,i}$ is the below-cloud scavenging prefactor, P is precipitation intensity, β_i is the precipitation-sensitivity exponent, $\lambda_{\text{in},i}$ is the in-cloud scavenging coefficient, and f_c is cloud fraction.

Heterogeneity, loading, and Madelung-type multifractal correction

The atmospheric heterogeneity index is defined as

$$H_i(\mathbf{x}, t) = w_o O + w_r R + w_l L_u + w_b B + w_h H_u, \quad (17)$$

where H_i is the heterogeneity index for species i , O is orographic confinement, R is aerodynamic roughness, L_u is land-use or urban-form class, B is boundary-layer stability or ventilation deficit, H_u is humidity or heat-island influence, and w_o, w_r, w_l, w_b, w_h are dimensionless weights.

The heterogeneity potential entering the drift closure can be defined as

$$V_i^{\text{het}}(\mathbf{x}, t) = \alpha_i \mathcal{N}[H_i(\mathbf{x}, t)], \quad (18)$$

where V_i^{het} is the heterogeneity potential, α_i is its amplitude, and $\mathcal{N}[\cdot]$ is a normalization operator that maps the heterogeneity index to a bounded interval. High positive gradients of V_i^{het} represent spatial constraints that can redirect pollutant drift.

A trimmed loading field is introduced as

$$\frac{\partial L_i}{\partial t} = G_i^{\text{met}} + \int_{\Omega} W_i(\mathbf{x}, \mathbf{x}', t) C_i(\mathbf{x}', t) dV' - v_i L_i + \eta_i. \quad (19)$$

Here, L_i is the pollutant accumulation loading field, G_i^{met} is meteorological loading due to stagnation or stable stratification, W_i is a nonlocal transfer kernel, v_i is a local ventilation or release coefficient, and η_i represents unresolved loading forcing.

The regularized concentration amplitude can be written as

$$A_i(\mathbf{x}, t) = \sqrt{C_i(\mathbf{x}, t) + \varepsilon_i}, \quad (20)$$

where A_i is the Madelung-type concentration amplitude and $\varepsilon_i > 0$ is a small concentration floor used to avoid singular behaviour in low-concentration regions.

The curvature-sensitive potential can be expressed as

$$U_i^{\text{mf}} = -\ell_i^2 \frac{\nabla \cdot (\mathbf{A}_i^{\text{aniso}} \nabla A_i)}{A_i}, \quad (21)$$

with U_i^{mf} the Madelung-type curvature potential, ℓ_i a characteristic multifractal length scale, and $\mathbf{A}_i^{\text{aniso}}$ a dimensionless anisotropy tensor controlling directional curvature sensitivity.

The curvature-induced drift is

$$\mathbf{v}_i^{\text{mf}} = -\mu_i \nabla U_i^{\text{mf}}. \quad (22)$$

Here, $\mathbf{v}_i^{\text{mf}}$ is the multifractal drift velocity and μ_i is a mobility coefficient. This term should be calibrated in a weak-curvature regime so that it corrects, rather than replaces, the classical transport core.

The associated multifractal flux and diffusivity correction can be written as

$$\mathbf{J}_i^{\text{mf}} = C_i \mathbf{v}_i^{\text{mf}}, \quad \mathbf{K}_i^{\text{mf}} = D_i^{\text{mf}} \left[1 + \gamma_i \left(\frac{|\nabla C_i|}{C_i + C_{0,i}} \right)^{p_i} \right] \mathbf{I}, \quad (23)$$

where D_i^{mf} is the baseline multifractal diffusivity, γ_i is the gradient-sensitivity coefficient, $C_{0,i}$ is a regularization concentration, p_i is a nonlinear exponent, and $\mathbf{I}$ is the identity tensor.

Reduced chemistry and aerosol diagnostics

For a chemical reaction m , the reaction rate is [9, 10]

$$r_m = k_m(T, I_\lambda, RH) \prod_{j=1}^N C_j^{v_{jm}}. \quad (24)$$

Here, r_m is the rate of reaction m , k_m is the rate coefficient, T is temperature, I_λ is actinic or solar radiation intensity, RH is relative humidity, and v_{jm} is the reactant stoichiometric coefficient of species j in reaction m .

The net chemical tendency of species i can be defined as

$$R_i^{\text{chem}} = \sum_{m=1}^{N_r} (v'_{im} - v_{im}) r_m, \quad (25)$$

where N_r is the number of chemical reactions, while v'_{im} and v_{im} are product and reactant stoichiometric coefficients for species i in reaction m .

For aerosol diagnostics, modal and moment-based descriptions can be retained without solving a full aerosol dynamic equation [15, 16]:

$$M_k = \int_0^\infty d_p^k n(d_p) dd_p, \quad C_{\text{PM}_{2.5}} = \frac{\pi \rho_p}{6} \int_0^{2.5 \mu\text{m}} d_p^3 n(d_p) dd_p. \quad (26)$$

Here, M_k is the k -th moment of the particle diameter distribution, $n(d_p)$ is the number distribution with respect to particle diameter, and $C_{PM2.5}$ is the mass concentration of particles with aerodynamic diameter below 2.5 μm .

Observation operators, calibration, and validation

A generic observation equation [13] is

$$\mathbf{y}(t_k) = \mathcal{H}_k[\mathbf{C}(t_k), \mathbf{m}(t_k), \mathbf{s}(t_k)] + \boldsymbol{\epsilon}_k. \quad (27)$$

Here, $\mathbf{y}(t_k)$ is the observation vector at time t_k , $\mathcal{H}_k$ is the observation operator, $\mathbf{m}$ denotes the vector of meteorological auxiliary variables, $\mathbf{s}$ denotes the vector of surface or land-use auxiliary variables, and $\boldsymbol{\epsilon}_k$ is the observation-error vector.

For aerosol optical depth, an approximate column operator can be written as

$$\tau_{AOD}(x, y, t) = \int_0^{z_{\text{top}}} \sum_{a=1}^{N_a} \xi_a(z, t) C_a(x, y, z, t) dz, \quad (28)$$

where τ_{AOD} is aerosol optical depth, z_{top} is the upper limit of the atmospheric column, N_a is the number of aerosol modes or components, ξ_a is mass-extinction efficiency, and C_a is aerosol mass concentration.

A strong-constraint variational cost function for calibration or data assimilation [14] can be expressed as

$$J = \frac{1}{2}(\mathbf{C}_0 - \mathbf{C}_b)^T \mathbf{B}^{-1}(\mathbf{C}_0 - \mathbf{C}_b) + \frac{1}{2} \sum_k (\mathcal{H}_k[\mathbf{C}(t_k)] - \mathbf{y}_k)^T \mathbf{R}_k^{-1}(\mathcal{H}_k[\mathbf{C}(t_k)] - \mathbf{y}_k), \quad (29)$$

where J is the cost function, $\mathbf{C}_0$ is the initial concentration state, $\mathbf{C}_b$ is the background initial state, $\mathbf{B}$ is the background-error covariance matrix, $\mathbf{y}_k$ is the observation vector at time t_k , and $\mathbf{R}_k$ is the observation-error covariance matrix.

Model validation should include at least the following metrics:

$$\begin{aligned} \text{RMSE}_i &= \sqrt{\frac{1}{N_o} \sum_{k=1}^{N_o} (C_{i,k}^{\text{mod}} - C_{i,k}^{\text{obs}})^2}, \quad r_i \\ &= \frac{\sum_k (C_{i,k}^{\text{mod}} - \overline{C_i^{\text{mod}}}) (C_{i,k}^{\text{obs}} - \overline{C_i^{\text{obs}}})}{\sqrt{\sum_k (C_{i,k}^{\text{mod}} - \overline{C_i^{\text{mod}}})^2 \sum_k (C_{i,k}^{\text{obs}} - \overline{C_i^{\text{obs}}})^2}} \end{aligned} \quad (30)$$

Here, RMSE_i is the root-mean-square error, r_i is the Pearson correlation coefficient, N_o is the number of observations, $C_{i,k}^{\text{mod}}$ is the modelled concentration, $C_{i,k}^{\text{obs}}$ is the observed concentration, and overbars denote sample means.

Baseline-relative predictive skill can be defined as

$$\text{Skill}_i = 1 - \frac{\text{RMSE}_{i,\text{model}}}{\text{RMSE}_{i,\text{baseline}}}, \quad (31)$$

where Skill_i measures improvement relative to a chosen baseline, such as persistence, climatology, or a standard chemistry-transport model without the multifractal term. Positive values indicate improvement relative to the baseline.

RESULTS AND DISCUSSION

To demonstrate how the trimmed model can be explored computationally, an illustrative two-dimensional simulation was generated using synthetic data. The purpose of this simulation is not validation and not operational forecasting. It is a controlled numerical experiment showing how the conservative transport core and the weak Madelung-type correction can produce plume migration, localized accumulation, and scale-sensitive concentration structure under idealized conditions.

The scalar pollutant field was simulated on a 20 km x 20 km horizontal domain with a 101 x 101 finite-difference grid and a 10 s time step over 2 h. The resolved wind was fixed at $u = 2.0 \text{ m}\cdot\text{s}^{-1}$ eastward and $v = 0.25 \text{ m}\cdot\text{s}^{-1}$ northward. The baseline eddy diffusivity was $K_0 = 80 \text{ m}^2\cdot\text{s}^{-1}$, locally reduced in a synthetic urban-stability/valley heterogeneity field. The source term combined one localized point source and one road-like line source. Chemical transformation, dry deposition, and wet removal were represented by a first-order loss coefficient. The multifractal correction was intentionally weak, with $l_{mf} = 450 \text{ m}$ and mobility $\mu_{mf} = 0.020$, so that it sharpened curvature-sensitive plume structure without overwhelming classical advection and eddy diffusion.

The simulated heterogeneity and emission fields are shown in Figure 1 and Figure 2. The heterogeneity field mimics urban roughness, topographic confinement, and weak-ventilation zones; the emission field mimics a strong industrial source and a weaker traffic corridor.

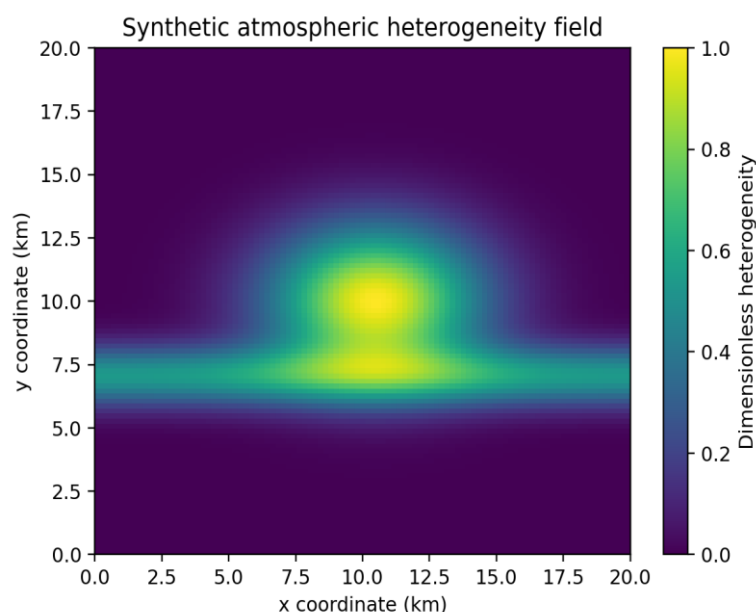


Figure 1. Synthetic atmospheric heterogeneity field used to reduce turbulent mixing and introduce accumulation-favoring spatial structure

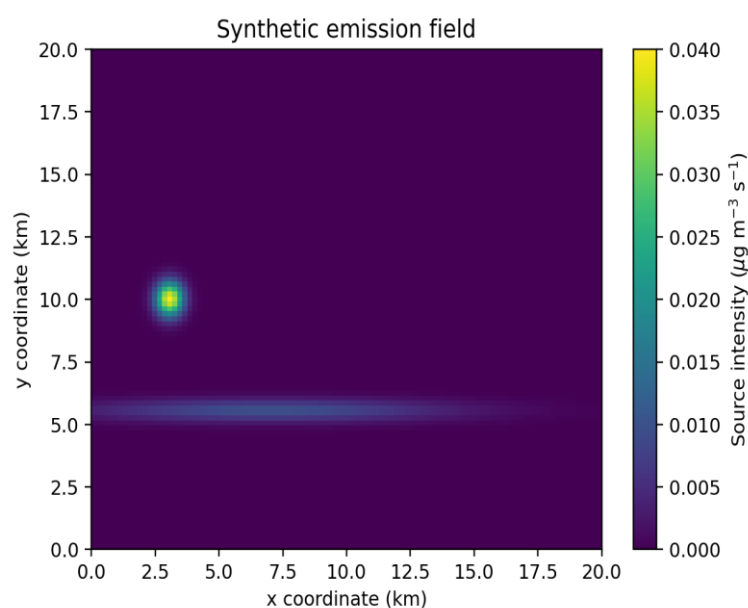


Figure 2. Synthetic emission field containing a localized point source and a road-like line source

The resulting concentration fields after 30, 60, and 120 minutes are shown in Figures 3-5. The plume is advected eastward and slightly northward by the imposed wind. As expected, the point-source plume remains the dominant feature, while the road-like line source produces a weaker elongated contribution. The heterogeneity-dependent diffusivity and weak curvature-sensitive drift favor localized accumulation and produce a sharper, more structured plume than would be obtained from purely homogeneous diffusion.

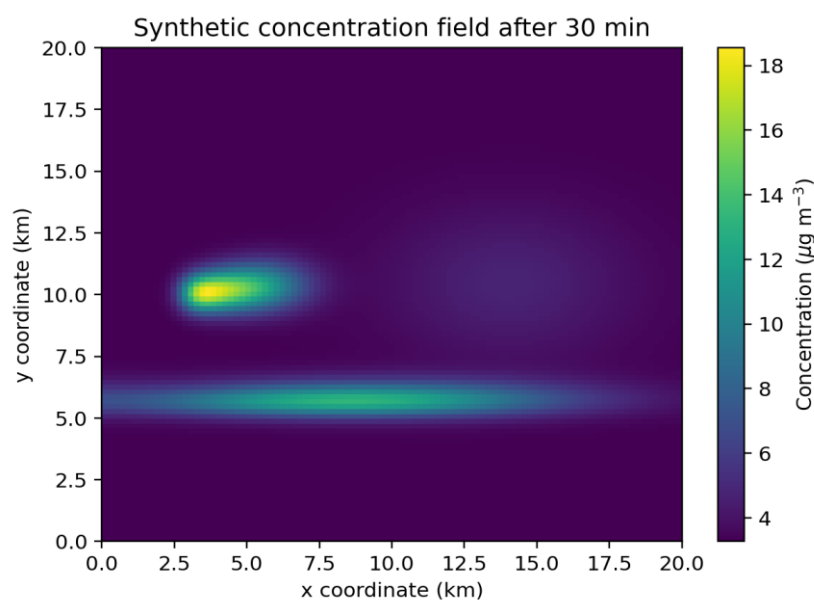


Figure 3. Synthetic concentration field after 30 minutes

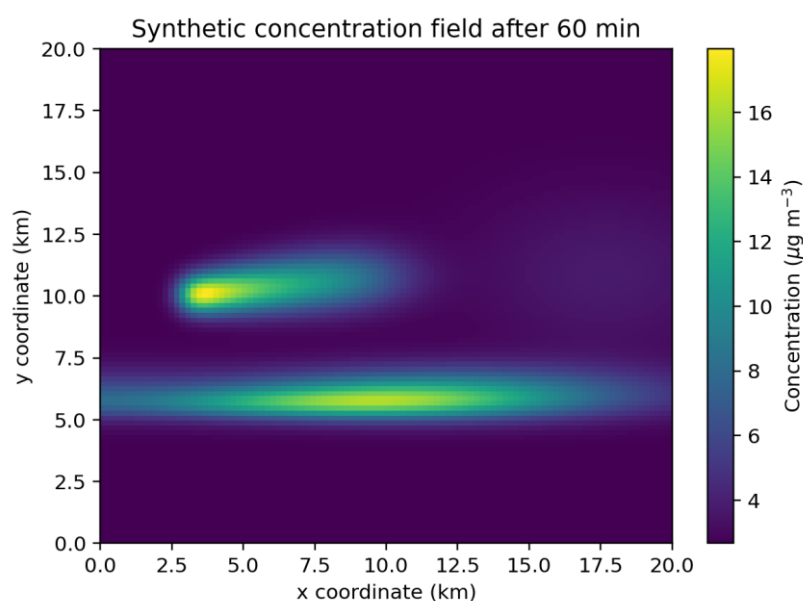


Figure 4. Synthetic concentration field after 60 minutes

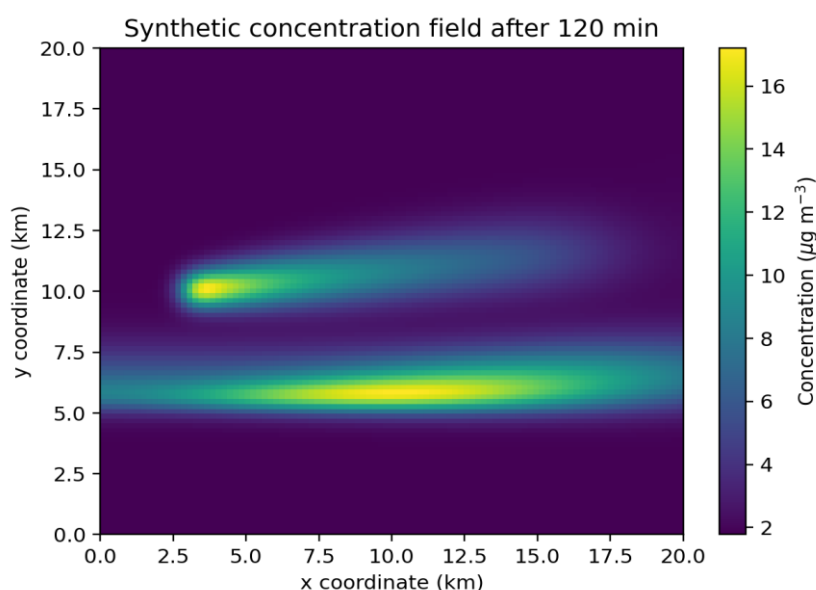


Figure 5. Synthetic concentration field after 120 minutes

Figures 6-8 summarize the time evolution of the simulation. The peak concentration rises rapidly to an early maximum and then gradually decreases; Table 1 reports values of 18.55, 17.97, and 17.21 $\mu\text{g}\cdot\text{m}^{-3}$ at 30, 60, and 120 minutes, respectively. The mean concentration decreases from 4.18 to 3.51 $\mu\text{g}\cdot\text{m}^{-3}$ over the two-hour experiment, consistent with the decreasing total burden shown in Figure 7. The centroid initially shifts westward and subsequently eastward, while its north-south coordinate decreases from 10.00 to 8.90 km. This concentration-weighted centroid reflects the evolving distribution of the whole field under transport, spatially distributed emissions, and removal; it should not be interpreted as the trajectory of a passively advected particle.

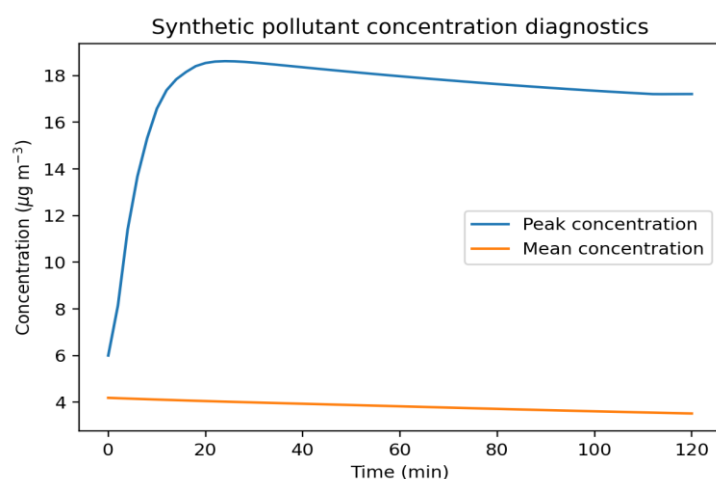


Figure 6. Peak and mean concentration diagnostics for the synthetic simulation

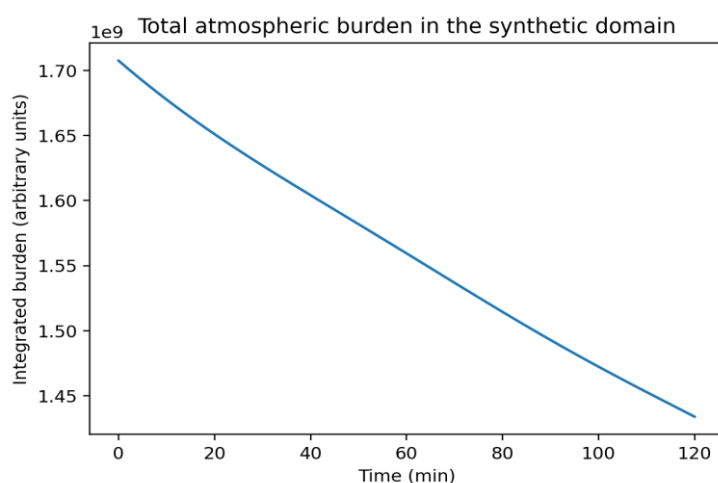


Figure 7. Total atmospheric burden in the synthetic computational domain

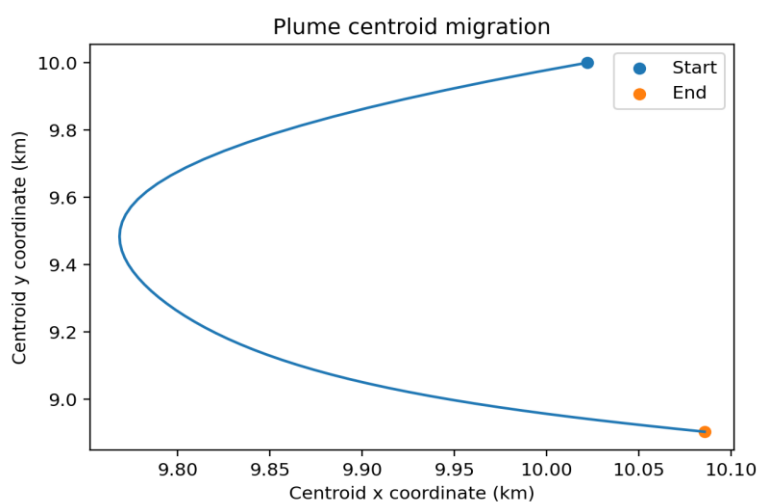


Figure 8. Plume centroid migration under the imposed eastward-northward wind field

A scale-sensitive diagnostic was also calculated from the concentration field. The curvature-focusing index measures concentration-weighted curvature activity, while the estimated D_2 index provides a simple box-counting-style indicator of concentration localization. These quantities should be interpreted only as exploratory diagnostics in this synthetic test; in real applications they would need sensitivity analysis, grid-refinement testing, and comparison against monitoring data.

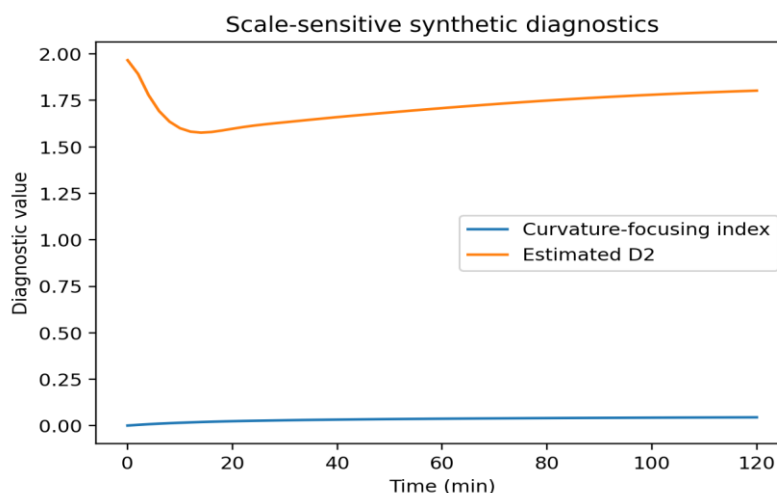


Figure 9. Exploratory multifractal-style diagnostics extracted from the synthetic concentration field

Table 1 gives representative diagnostic values extracted from the synthetic run.

Table 1. Representative diagnostics from the theoretical simulation*

t [min]	Mean C	Peak C	x_c [km]	y_c [km]	W [km]	CFI
0	4.18	6	10.02	10	8.1	0.001
30	3.99	18.55	9.78	9.62	7.87	0.029
60	3.82	17.97	9.79	9.3	7.59	0.038
120	3.51	17.21	10.09	8.9	7.14	0.045

*C is concentration in $\mu\text{g} \cdot \text{m}^{-3}$, x_c and y_c are centroid coordinates, W is localization width, and CFI is the curvature-focusing index

This illustrative simulation supports three methodological conclusions. First, the trimmed model is numerically implementable as a conservative advection-diffusion-reaction-deposition system with a regularized curvature correction. Second, even weak heterogeneity and curvature terms can influence plume localization and intermittency, especially near strong emission gradients. Third, no predictive claim can be made from theoretical data alone: the same workflow must be repeated with observed meteorology, station concentrations, emissions, and independent validation metrics before the multifractal correction can be considered empirically useful.

The proposed formulation should be interpreted as an extension of standard chemistry-transport modelling rather than as a replacement for it. Its main advantage is that it keeps the conservative transport-reaction-deposition balance as the governing backbone, while introducing a controlled scale-sensitive closure for heterogeneous, intermittent, and curvature-dominated concentration structures. This is relevant for urban canopies,

topographically confined basins, stable boundary layers, and complex source regions, where pollutant fields can exhibit sharp gradients, local trapping, plume filamentation, and non-Gaussian dispersion that are difficult to describe using homogeneous Fickian diffusion alone.

Directly relevant atmospheric studies include the investigation of multifractal cross-correlation surfaces of Hurst exponents for atmospheric pollutants by Stan *et al.* [17] and the multifractal cross-correlation analysis of aerosols and meteorological data by Marin *et al.* [18]. These studies provide a methodological context for examining scale-dependent relationships in atmospheric observations. Their statistical analyses complement the present transport formulation: cross-correlation diagnostics characterize relationships in measured time series, whereas the proposed Madelung-type closure modifies the evolution of a spatial concentration field. Such diagnostics could inform future comparisons between simulated and observed variability, but they do not establish the validity of the specific curvature-induced drift proposed here.

Comparable multifractal and nonlinear frameworks have already been used in several domains, supporting the methodological transferability of scale-sensitive modelling. Fractal approaches have been applied to acute thrombotic occlusion [19], while multifractal analysis has been used to investigate metformin hydrochloride delivery from MCM-48 mesoporous silica [20]. Related nonlinear and geometric frameworks have also been used to describe particle interactions [21], Kepler-type dynamics and skyrmionic structures [22], and surface-gauging contributions to extended interactions and spin [23]. These examples do not validate the atmospheric model directly, but they justify treating multifractal and nonlinear mathematical formalisms as transferable tools that must be adapted to the conservation laws, observables, and calibration procedures of each physical system.

From a broader theoretical perspective, the present model is also compatible with developments in the multifractal theory of motion that describe complex-system dynamics through holographic-type correspondences, scale-dependent constitutive relations, and symmetry-governed transformations [24 – 26]. Such approaches emphasize that macroscopic observables may arise from interactions distributed across multiple resolution scales and that equivalent dynamical descriptions can be formulated in hydrodynamic, geometric, or symmetry-based terms. Applied to atmospheric pollution, this viewpoint supports interpreting the Madelung-type contribution as an effective multiscale closure through which unresolved turbulent, topographic, and source-related heterogeneity modifies the observable concentration field. This connection remains conceptual rather than evidentiary, however, and its atmospheric relevance must be established through parameter calibration, identifiability analysis, and validation against independent monitoring data.

The Madelung-type correction is deliberately regularized through a concentration floor, bounded heterogeneity functions, finite multifractal length scales, and weak mobility coefficients. These restrictions are essential for physical consistency: the correction must remain secondary to mass conservation, meteorological advection, turbulent diffusion, emissions, chemistry, deposition, and scavenging. In practical applications, the multifractal parameters should be estimated using independent concentration measurements, meteorological fields, emission inventories, land-use descriptors, and satellite-derived products, and their added value should be quantified relative to a classical baseline model.

The synthetic simulation confirms that the reduced model can be implemented numerically and can generate interpretable diagnostics such as peak concentration, mean concentration, burden, plume centroid displacement, localization width, and curvature-focusing activity. However, the simulation remains illustrative because all inputs are theoretical. Consequently, the present results do not demonstrate predictive superiority; they only define a reproducible workflow that can be transferred to real datasets for sensitivity testing, parameter calibration, grid-refinement analysis, and independent validation.

CONCLUSIONS

A compact mathematical framework was developed for atmospheric pollutant dynamics by combining a conservative advection-diffusion-reaction-deposition model with a weak Madelung-type multifractal correction. The model incorporates boundary-layer mixing, emissions, removal processes, reduced chemistry, aerosol diagnostics, heterogeneity-driven loading, observation operators, calibration terms, and validation metrics. The theoretical simulation illustrates that the approach is computationally feasible and can reproduce plume transport together with localized, scale-sensitive structure. The next necessary step is validation against real monitoring and meteorological datasets to determine whether the multifractal correction provides statistically significant improvement over classical formulations.

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