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The geometry of inertial particle mixing in urban flows, from deterministic and random displacement models

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We use Lagrangian measures, depicted by finite-time Lyapunov exponents, to characterize transport patterns of inertial pollutant particles formed in urban flows. Motivated by actual events we focus on flows in realistic urban geometry. Both deterministic and stochastic particle transport patterns have been identified, as inertial Lagrangian coherent structures. For the deterministic case, the organizing structures are well-defined and we extract them at different hours of a day to reveal the variability of coherent patterns. For the stochastic case, we use a random displacement model for fluid particles and derive the governing equation for inertial particles to examine the change in organizing structures due to “zeroth-order” random noise. We find that, (1) the Langevin equation for inertial particles can be reduced to a random displacement model; (2) using random noise based on inhomogeneous turbulence, whose diffusivity is derived from $k - \epsilon$ models, major coherent structures survive to organize local flow patterns and weaker structures are smoothed out due to random motion.

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I. INTRODUCTION

In recent decades, the fast growth of urban areas and heterogeneous use of land surfaces have generated great interests for scientists, engineers, and urban planners in understanding the physical processes associated with urban climates.1–4 In this problem, local physical processes are interconnected with synoptic and regional scale features (flow, terrain, etc.), providing neighborhood and street scales that are important for humans.2, 4 Fluid dynamical research focusing on urban environments provide valuable information in two directions. On the one hand, in the upscale direction, land use in urban and suburban areas creates inhomogeneity in the dynamical and thermal properties at the bottom boundary layer of the atmosphere, which in turn modifies regional and synoptic flows.5, 6 Additionally, land surface characterization provides valuable information on pollutant sources for their long-range dispersal.7 On the other hand, in the downscale direction, details of street architecture affects local wind and turbulence patterns driven by large, synoptic scale flows.8 Pollutants that affect human health, such as carbon monoxide, ozone, particulate matters (PM), and harmful materials, are highly variable within street-neighborhood scale flows.4 Characterizing transport patterns based on resolved urban flows is thus imperative for improvements on city planning and the quality of human lives. In this paper, we extract such patterns for both deterministic and stochastic flows in a real urban dispersion model.

In conventional studies of urban fluid dynamics, the focus is on the fluid motion and dispersion in idealized urban street canyons or for flow past isolated/regularly spaced buildings.9–12 While the studies on these models provide fundamental understandings of the phenomenology for urban flows, and are useful in a parameterization to represent land surface uses in regional-global scale models,

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they offer limited information on evaluating the effects of pollutant dispersion at human related scales. For operational use of urban climate forecast and warning issuances, an exact representation of the urban geometry should be considered. To emphasize our point, we note the Hermoso Park dispersion study (HPS) mandated by the state of Arizona to address policy-related questions on the well beings of residents in a legislative district in southeast Phoenix. It is claimed that the heightened respiratory illnesses in the area are related to high levels of pollutant concentrations. With real applications on air quality in mind, we focus our study on extracting pollutant patterns in the HP area, driven by wind and thermal forcing measured from a meteorological tower inside the area of interest.

Pollutant particles have finite-size and dynamically they behave differently than idealized fluid particles. In the case of rigid spheres, motions of finite-size particles are captured by the Maxey-Riley equations. Among atmospheric pollutants, the most common particles are particulate matters, characterized by their aerodynamic diameters. In particular, PM of diameter less than 10 μm (PM10, mainly combustion particles) and 2.5 μm (PM2.5, mainly organic compounds and sulfates) are of major concern due to their prevalence in the environment. For particles with small diameters (such as PM), simplifications to the Maxey-Riley equations can be made to approximate particle motions. Our study is based on the simplified set of equations, discussed in detail later.

As pointed out in Belcher, strong dispersion of contaminant parcels of air are induced by dividing streamlines that enhance topological dispersion. Clearly, identification of the topology of inertial particle flows will be a useful tool to locate regions of high dispersion, as well as regions of strong cumulation. In this vein, we use inertial Lagrangian coherent structures (ILCS), first described in Sapsis and Haller, to characterize inertial particle motion in the HP area. The ILCS are analogous to LCS for idealized fluid particles, sans the difference in the inertial effects on motions. We favor a Lagrangian approach, as they provide objective description of the flow topology. As a comparison, Eulerian criteria are based on instantaneous velocity fields or their gradient invariants, which are frame dependent. In the first half of our results, we use this methodology to examine the organizing patterns of PM with different diameters. Using output of street-scale wind models at different times of the day, we find the temporal variations of the organizing patterns in deterministic flows.

For previous works on ILCS, little is known on the effects of random noise on the coherent structures. The objective of obtaining stochastic ILCS is to find the most probable mixing patterns in a realistic environment. In the latter half of our results, we consider an inhomogeneous random displacement model (RDM) extension of the Maxey-Riley equations, whose randomness is based on parameterized diffusivity from resolved flow fields. We obtain stochastic ILCS for PM10 and PM2.5. Their relation with the deterministic ILCS will be discussed. We are only aware of two studies on stochastic LCS for idealized fluid flows, neither of which considered inhomogeneous noise for inertial particles.

The rest of the paper is organized as follows. In Sec. II, we discuss the simplified version of the Maxey-Riley equations and the corresponding random displacement extension. Using an approach in Rodean, we find that the stochastic term acts directly on the inertial equations. In Sec. III, we discuss the street-scale wind model from which we obtain background wind data and parameterized turbulence as inputs to our analyses. We also discuss numerical schemes for our analyses, as well as the computation of finite-time Lyapunov exponents (FTLE). In Sec. IV, we present results for both deterministic and stochastic ILCS associated with our flow. Lastly, in Sec. V we summarize our findings and discuss future directions.

II. MATHEMATICAL FORMULATION

A. The governing equations

To formulate the mathematical problem, we make the following physical assumptions. (1) Inertial particles are carried by background fluid particles, which conduct random position processes in inhomogeneous turbulence (i.e., the positions for fluid particles are governed by a RDM); (2) the random background fluid velocity affects inertial particle dynamics through viscous
drag; (3) the body force term experienced by an inertial particle is modeled by a deterministic force due to Lagrangian change in velocity of a fluid particle in its position plus random noise due to randomness in fluid velocity; (4) the random excitation of inertial particle velocity due to Brownian motion is negligible as compared to the randomness induced by background eddies.

Following Rodean,\textsuperscript{30} the fluid velocity standard deviation terms due to body force and buoyancy, and two random terms due to stochastic drag and body force.\textsuperscript{31} Following randomness in fluid velocity; (4) the random excitation of inertial particle velocity due to Brownian motion is negligible as compared to the randomness induced by background eddies.

\[
\dot{u} = 3 \frac{a}{R} \left[ \frac{D(u + u_{dr})}{Dt} + \eta W_b \right] = -\frac{1}{\epsilon} (v - u_f) + \left( 1 - \frac{3R}{2} \right) g. \tag{2}
\]

where \( u_f \) is the random fluid particle velocity, \( u \) a deterministic fluid velocity resolved by models or measurements, \( u_{dr} = \partial K(x) / \partial x \) a deterministic drift velocity due to turbulence inhomogeneity, and \( \sigma W_a \), a vector Wiener process with standard deviation \( \sigma(x, t) = \sqrt{2K} \), dependent on local diffusivity \( K(x, t) \). As discussed in detail in Rodean,\textsuperscript{30} the drift term \( u_{dr} \) is derived exactly from a consistency condition based on the Fokker-Planck equation to enforce a well-mixed condition when random noise is inhomogeneous (see also Thomson\textsuperscript{31} and it is independent from the random noise term \( \sigma W_a \). We explain the validity of RDM for background fluid in later texts.

Consider typical urban flow length scales of order 1–10 meters, the size of PM is very small, where we can safely neglect the Faxéen correction term.\textsuperscript{32} We also follow prior studies to neglect the Basset history force term.\textsuperscript{15, 19, 20} Justifications for removal of the history force term for small particles have been provided in Sapsis et al.\textsuperscript{33} In this asymptotic limit, the model for the motion of a single spherical particle is the following:

\[
\dot{x} = v, \quad \dot{v} = \frac{3}{2} \left[ \frac{D(u + u_{dr})}{Dt} + \eta W_b \right] = -\frac{1}{\epsilon} (v - u_f) + \left( 1 - \frac{3R}{2} \right) g. \tag{2}
\]

where \( g \) is the vector of gravity, \( u, u_{dr}, \) and \( u_f \) are from the ambient fluid velocity Eq. (1), \( \eta W_b \) is another vector Wiener process with standard deviation \( \eta \) and independent from \( \sigma W_a \), and

\[
R \equiv \frac{2 \rho_f}{\rho_f + 2 \rho_p}, \quad S_t \equiv \frac{2}{9} \left( \frac{a}{L} \right)^2 R e_f, \quad \epsilon \equiv \frac{S_t}{R}. \tag{3}
\]

Here, \( \rho_f \) and \( \rho_p \) are the densities of the fluid and of the particle, respectively; \( R \) is the density ratio distinguishing neutrally buoyant particles \( (R = 2/3) \) from aerosols \( (0 < R < 2/3) \) and bubbles \( (2/3 < R < 2) \); \( a \) is the radius of the spherical particle; \( L \) is a characteristic length scale of the flow; the fluid Reynolds number is \( R e_f \equiv U L / \nu \), with typical large-scale fluid velocity \( U \) and fluid viscosity \( \nu \); time is non-dimensionalized with the characteristic time scale \( L / U \). The first term in the square bracket of Eq. (2) is the body force experienced by a fluid particle due to deterministic background fluid particle motion, and in the second term the standard deviation \( \eta \) characterizes fluid velocity variance (hence the entire square bracket describes stochastic body force experienced by a fluid particle in position of the inertial particle). These two terms, together with the factor \( 3R/2 \), gives the body force experienced by an inertial particle. The first term on the right-hand side of this equation is the viscous drag term, where \( u_f \) is random. The second term on the right-hand side is a buoyancy term. Note that, we do not use \( Du_f / Dt \) for the body force term since \( \sigma W_a \) is not differentiable.

In the deterministic case where \( \sigma = \eta = 0 \) and \( u_{dr} = 0 \), provided that the velocity deformation is not too strong with respect to the parameter \( \epsilon \),\textsuperscript{34, 35} there exists a slow manifold \( M_s \) that attracts dynamics in the phase space.\textsuperscript{20} The inertial equations resolve a problem on backward-tracking of trajectories due to a reverse-time numerical instability, the deterministic ILCS is then extracted based on the slow dynamics.\textsuperscript{21}

For the stochastic case, we rearrange the equation for \( v \) and write in terms of velocity fluctuation \( v_f = v - u - u_{dr} \) as

\[
dv_f = -\frac{v_f}{\epsilon} dt + \left( \frac{3R}{2} - 1 \right) \left[ D(u + u_{dr}) - g dt \right] + \frac{\sigma}{\epsilon} dW_a + \frac{3R}{2} \eta dW_b. \tag{4}
\]

Notice that Eq. (4) is also a Langevin equation, with the Lagrangian decorrelation time scale \( \epsilon \), drift terms due to body force and buoyancy, and two random terms due to stochastic drag and body force. Based on the 3D results in Rodean,\textsuperscript{30} the fluid velocity standard deviation \( \eta = b_i u^* \) and the position standard deviation \( \sigma_i = 2 b_i^2 u^* / (C_{0e})^{1/2} \), both are order one quantities as far as the size parameter \( \epsilon \) is concerned. Here, \( C_0 = 5.7 \) is a semianalytical constant, \( b_i \) an empirical constant in the \( i \)th direction,
\[ i = 1, 2, 3, \varepsilon = u^3/kl \] the local energy dissipation rate estimated by the crude first-order closure, \( u^* \) the dimensionless friction velocity, \( k = 0.4 \) the von Karman constant, and \( l \) a local dimensionless length scale. We further simplify this expression by arguing that the first stochastic term is dominant in the regime of interest (small-size aerosols, \( St \ll 1 \), hence \( 1/\varepsilon \equiv R/St \gg R \)), thus we drop the last term in Eq. (4). We discuss choices of \( b_i, u^* \), and \( l \) in Sec. III.

Our Eq. (1) differs from typical Lagrangian stochastic models (LSM) (Ref. 30 and 36) that consider Langevin equations for fluid velocities. The problem we consider is inhomogeneous, which in the LSM approach would require many terms to deal with correlated random noise. The simplicity in \( u_f \) allows us to focus on the Langevin equation for \( v_f \). In general, LSM is more appropriate than RDM. RDM is applicable in the “far field” regime, when the time scale is much greater than the Lagrangian decorrelation scale of fluid velocity and when the random noise is Gaussian.\(^30\) We are not particularly interested in reproducing a dispersion cloud for specialized release events. Instead, we explore answers to the following questions: (1) What is the most likely trajectory that an inertial particle would take in a stochastic environment? (2) What organizing structure can we obtain from these most tenable trajectories, so we obtain an overview of regions that are more vulnerable to pollutant dispersions? We also assume Gaussian statistics for the random noise. Under these conditions we are in a regime where RDM Eq. (1) is valid. In this vein, we also study simplified version for Eq. (2). In the long-time limit, this equation should reduce to the diffusion limit, governed by a RDM (Thomson,\(^31\) Rodean\(^30\)), to be derived later.

We also consider stochastic back trajectories for structure extraction, with reasons given later in the section. Following earlier work on backward-time LSM,\(^37\) we find that the consistency condition merely requires the reflection of the velocity \( u + u_{dr} \). It is noted that (Thomson,\(^31\) Flesch \textit{et al.}\(^35\)) for turbulence in an incompressible flow, the probability density for forward-time models and backward-time models are identical, Smith’s\(^38\) reciprocal theorem also applies. This implies that we can simply run the backward-time RDM model to obtain the statistics on the composition of particles observed at a point \( x \) at a time \( t \).

### B. Reduction of Langevin equation to random displacement model

We reparameterize Eq. (4) in time such that \( \varepsilon = \alpha T \), where \( \alpha \to 0 \) and \( T \) is order one, a time scale felt for the long-term stochastic trajectories. Applying the methodology discussed in Rodean,\(^30\) we integrate Eq. (4) in time to obtain

\[
\varepsilon \int_0^t \frac{v_f}{T} dt = \int_0^t \alpha \left( \frac{3R}{2} - 1 \right) \left[ D(u + u_{dr}) - g dt \right] + \frac{\sigma}{T} dW_a.
\] (5)

In the \( \alpha \to 0 \) limit, the leading order balance in the above equation is between the first and third term on the right-hand side. If we further assume that on average the velocity fluctuation jump \( [v_f]_0^t \) as well as the two drift forces in the integrand are order one, over time the second term on the right-hand side supersedes the left-hand side and can be considered as a first-order correction, thus

\[
\int_0^t \frac{v_f}{T} dt = \int_0^t \alpha \left( \frac{3R}{2} - 1 \right) \left[ D(u + u_{dr}) - g dt \right] + \frac{\sigma}{T} dW_a.
\] (6)

Noting that \( v_f = dx_f/dt \), where \( x_f \) is the position process for the fluctuations, the left-hand side can be expressed as

\[
\int_{x_0}^{x_f} \frac{dx_f}{T} = \int_0^t \alpha \left( \frac{3R}{2} - 1 \right) \left[ D(u + u_{dr}) - g dt \right] + \frac{\sigma}{T} dW_a.
\] (7)

Differentiating with respect to \( t \) and multiplying by \( T \) and converting \( v_f \) back to \( v \) we obtain the RDM for the inertial particle displacement,

\[
\frac{dx}{dt} = u + u_{dr} + \varepsilon \left( \frac{3R}{2} - 1 \right) \left[ \frac{D(u + u_{dr})}{Dt} - g \right] + \sigma W_a.
\] (8)
This expression converges towards an inertial equation for the slow dynamics

\[
\frac{dx}{dt} = u + \epsilon \left( \frac{3R}{2} - 1 \right) \left[ \frac{Du}{Dt} - g \right]
\]

in the deterministic limit, first derived in Haller and Sapsis\textsuperscript{20} using singular expansion. The random position process consists of the slow manifold velocity, a deterministic drift term due to inhomogeneous turbulence and a random walk term from the RDM for background fluid particles. Note that we cannot directly use the singular perturbation approach here since \( \dot{W}_a \) is not differentiable.

C. Inertial Lagrangian coherent structures

LCS are distinguished material lines/surfaces that attract/repel local trajectories at the maximal rates.\textsuperscript{39, 40} Recently, it has become popular that FTLE be used to extract LCS. Basing on local dynamics of trajectories, FTLE offers an objective description of how nearby trajectories stretch with the background flow. As a result, local material lines that repel nearby trajectories the most is identified. Reciprocally, attractors are found as local maximizers of FTLE when trajectories are integrated in backward-time. In the first development of the theory, FTLE fields do not distinguish large stretching from shear.\textsuperscript{22} This difficulty has been resolved in a recent development based on a variational theory.\textsuperscript{41}

The LCS methodology was first extended to study inertial particle mixing in Sapsis and Haller,\textsuperscript{21} where they studied the mixing topology for inertial particles inside hurricane Isabelle. Using the singular perturbation,\textsuperscript{20} the authors overcome the numerical instability of source inversion for finite-size particles. As a result, both forward-time and backward-time trajectories are computed based on the slow manifold dynamics, and coherent structures are extracted. ILCS has also been used to identify prey dynamics in jellyfish feeding,\textsuperscript{42} where the authors locate regions near a jellyfish that prey cannot escape predation.

In our context, we extract ILCS that organize pollutant particle dynamics. We use the inertial equation approach, since in forward-time we only deal with three-dimensional physical space instead of the full six-dimensional phase space, and in backward-time this is the only way to obtain back-trajectories correctly. We obtain the entire inertial particle mixing geometry for both deterministic and stochastic environments. The deterministic case is a direct extension from our previous work,\textsuperscript{35} yet the stochastic case has not been considered before. The more general LSM formulations for inertial particles involves extra modeling, such as a modified Lagrangian decorrelation time, which is not a direct result from the Maxey-Riley equations.\textsuperscript{43, 44} Using Maxey-Riley equation directly in backward-time, as demonstrated in Haller and Sapsis,\textsuperscript{20} results in numerical instability even for deterministic trajectories.

We address the stochastic ILCS in the following approach. With the use of the RDM, we estimate the probability that a trajectory evolves in an environment with turbulent eddies. In forward-time, the concept is straightforward: we find the most likely trajectory that an inertial particle starting from \( x_0, t_0 \) would end up, after some integration time \( T \) (expectation of \( x \)). The most likely repelling structures is thus ILCS based on the mean trajectories. In backward-time, we find stochastic trajectories, again starting from \( x_0, t_0 \). Expectation of the random trajectories show the most likely starting point for the particle occupying \( x_0 \) at time \( t_0 \). As mentioned earlier, this interpretation of probability is valid because of the forward–backward probability equivalence and the validity of reciprocal theorem with RDM. Attracting ILCS are then obtained again from the mean trajectories.

III. NUMERICAL DETAILS

A. Urban wind model

We use the quick urban and industrial complex (QUIC) model developed at the Los Alamos National Laboratory to resolve street-scale urban flows at HP. The numerical model consists of a wind model, QUIC-URB, and an inhomogeneous LSM dispersion model, QUIC-PLUME. For
reasons mentioned in Sec. II, since we study the inertial dynamics based on RDM and the slow manifold, we did not use QUIC-PLUME. QUIC-URB is based on the Röckle approach, in which a mass-consistent diagnostic wind model computes the 3D flow fields around buildings. An initial wind field is prescribed based on an incident flow, and superimposed on this are various time-averaged flow effects of buildings. The QUIC-URB utilizes empirical algorithms for determining initial wind fields on the rooftop, in upstream recirculation zones, in the downwind cavity and wake of a single building, and in street canyons between buildings. A mass-consistent wind field is produced similar to traditional diagnostic wind models, but special treatment of boundary conditions is needed at the building walls.

The QUIC simulations were initiated from data collected during the HP study campaign conducted in early 2009. A 10 m meteorological tower inside the study area was instrumented with two sonic anemometers for flow, turbulence, and flux measurements and radiometers for incoming, outgoing, and net solar radiation. For more details of the field measurements and the model domain, the readers are referred to discussions and Fig. 13 in Fernando et al.

Based on the data input, the simulations were performed on two domains: an outer domain that covered the entire HP area and an inner domain around the meteorological tower. The computation area was $4900 \times 4220 \times 280 \text{ m}^3$, with 20 m horizontal and 4 m vertical resolution for the outer domain, and a $1200 \times 1050 \times 140 \text{ m}^3$ area with 5 m horizontal and 2 m vertical resolution for the inner domain. Trees and vehicles were excluded and the terrain was considered flat, which is a good approximation.

B. Details of deterministic and random displacement model

The QUIC-URB outputs are dimensional variables. We use a typical length scale of a building inside the HP area, $L = 45 \text{ m}$, and an appropriate velocity scale at the particular time, say, $U = 1(3) \text{ m/s}$ for 6 a.m. (6 p.m.), to non-dimensionalize our problem. The Lagrangian integration time is 40 time units. Henceforth, the dimensional integration time is 30 (10) min for the two cases. We examine dynamics for both PM$_{10}$ and PM$_{2.5}$. Since the fluid velocity scale varies, the parameter $\epsilon$ changes at different times. For example, consider PM density to be 1000 times of air, then at 6 a.m., $\epsilon_{2.5} = 7.7199 \times 10^{-7}$, $\epsilon_{10} = 1.2352 \times 10^{-5}$ and at 6 p.m., $\epsilon_{2.5} = 2.316 \times 10^{-6}$, $\epsilon_{10} = 3.706 \times 10^{-5}$.

We have two different datasets from QUIC-URB. On January 16, 2009, one-hour averages of observational measurements were available at every hour of the day, hence allowing the study of variability of structures over time. We used velocity interpolation between two frames of data to extract the ILCS based on this slowly varying unsteady flow. On February 15, 2009, one-minute averages of observational measurements were available in the morning, hence the background flow reflects better reality. We study stochastic ILCS with this dataset.

For the deterministic case, we focus on two representative hours from the data: 6 a.m., and 6 p.m. The 6 a.m. and 6 p.m. cases represent flows during the rush hours, where emission from the streets are likely to be high and they may quickly align with ILCS. In order to obtain high resolution results on ILCS, we use a grid size of 0.25 m over the entire inner domain to generate deterministic trajectories. The Lagrangian integration code is parallelized and ran on a 14 node cluster with 224 central processing units to achieve such a high resolution. Trajectories are computed using the fourth order Runge-Kutta methods from the inertial equation. Repelling (attracting) ILCS are computed from the forward-time (backward-time) integrations.

For the stochastic case, we need to compute $K$. We only consider a diagonal diffusion tensor, where dimensionless $K_i = 2b_i^b ku^1/C_i$. We use parameters implemented in QUIC-PLUME, where in the horizontal direction, $b_1 = b_2 = 2$ and in the vertical direction, $b_3 = 1.3$. This anisotropy reflects a vertical density stratification. The friction velocity $u^* = (k \Delta z / U) \partial \bar{u}/\partial z$ is based on vertical wind shear, and $\Delta z$ is the smallest distance of the particle to a wall/ground/roof. $l$ is a local length scale, taken to be the smaller of $z + \zeta_0$ or $l_{eddy}$, where $z$ is the height from the ground/roof, $\zeta_0$ is the roughness length taken to be 1 m in dimensional units, and $l_{eddy} = ku/|\partial u/\partial z|$.

We use 1000 realizations for each initial condition $x_0$. To accommodate the size of stochastic simulations, we reduce the resolution of initial conditions to $5 \times 5 \times 2 \text{ m}$, and only focus on...
smaller regions of interest. The inertial equations are computed based on explicit Euler methods with Gaussian white noise. For comparison, we also examine for a sample initial condition, the full Maxey-Riley equations and the inertial equations. We use implicit Euler for the deterministic parts of the full Maxey-Riley equations, explicit random noise is added in the end of the time step.

In our formulations, no-slip boundary conditions are considered. This is because when particles approach the boundary, their background velocity approaches zero. As a result, particles fall to the ground due to the gravity term if the boundary condition is set to be reflective. Since there is no reason that a pollutant particle cannot stick to rough building surfaces, and the no-slip boundary condition preserves vertical structure when particles hit the wall, we prefer using the no-slip boundary condition.

One concern of the no-slip boundary condition is that the setup makes the random term near the wall not really Gaussian. In our RDM formulation, eddy diffusivity is based on the nearest ground or wall, hence diffusion is very limited for trajectories near buildings, and this near-wall non-Gaussianity does not affect major dynamics in the interior of the domain. A further concern is that, for an initial condition near the wall, if there is equal probability for the particle to stick to the wall or disperse away from the wall, the expectation can be nowhere near any of the high probability regions. However, consider two nearby particles, the realizations for one of them completely hit the wall, and the realizations for the other completely disperse away, the separation measured between the averaged trajectories for these particles are still large and the ILCS should still be highlighted, so we should be safe as far as the ILCS are concerned.

For RDM formulation, Wilson and Yee\textsuperscript{49} pointed out that a constraint on the time stepping size is needed. Following their paper, for our inhomogeneous eddy parameterization in 3D, we require a constraint on the time stepping of the RDM

\begin{equation}
\sqrt{\frac{2K}{\Delta t}} \frac{1}{K} \left| \frac{\partial K_i}{\partial x_i} \right| \ll 1,
\end{equation}

where \(\cdot\) denotes the norm of the argument vector.

Finally, we use a linear extrapolation technique developed in Tang \textit{et al.}\textsuperscript{50} to deal with trajectories leaving the outer domain. The extrapolation is done in 2D horizontal surfaces. This is because with a no-slip boundary condition at \(Z = 0\) and incompressibility, 3D extrapolation would leave the external flow motionless. Since the resolved flow on the outer domain is almost two-dimensional and unidirectional\textsuperscript{8} due to the small size of buildings in nearby districts, it is not unreasonable to implement just the 2D extrapolation at every height. Between the inner and outer, and outer and extrapolated domains, we use a filter to smoothly transition the velocity data, to avoid development of spurious structures.

Note that in Fernando \textit{et al.},\textsuperscript{4} density for pollutant particles is reported for two different times of the day. Their result is specific to a particular emission characteristics, which is not the main goal of our study. We focus on obtaining the flow topology, which is an overall evaluation of the patterns inside the domain of interest. High pollutant densities are expected to accumulate along attracting structures and high dispersion to associate with repelling structures, as a result of ILCS extraction.

\section*{C. Computation of FTLE and extraction of ILCS}

The computation of FTLE is relatively well-known now, henceforth we briefly outline the methodology. We compute the particle displacements starting from initial condition \((x_0, t_0)\) using the inertial Eq. (9) in the deterministic case, and Eq. (8) in the stochastic case. For the stochastic case, we compute the ensemble of realizations to obtain the mean trajectory \(\mathbb{E}(x)\). Denoting the trajectory \(x(t; x_0, t_0)\), we define the Cauchy-Green strain tensor field as

\begin{equation*}
M_{ij}(x_0) \equiv \begin{bmatrix} \frac{\partial x(t; x_0, t_0)}{\partial x_0} \end{bmatrix}^T \begin{bmatrix} \frac{\partial x(t; x_0, t_0)}{\partial x_0} \end{bmatrix},
\end{equation*}

where
where \( [\partial x/\partial x_0]^T \) denotes the transpose of the deformation gradient tensor \( \partial x/\partial x_0 \). The FTLE field, \( FTLE(t_0(x_0)) \), is then defined as the scalar field that associates with each initial position \( x_0 \) the maximal rate of stretching along \( x(t; x_0, t_0) \),

\[
FTLE(t_0(x_0)) = \frac{1}{2 |t - t_0|} \ln \lambda_{\text{max}}(M),
\]

with \( \lambda_{\text{max}}(M) \) denoting the maximum eigenvalue of \( M \).

Traditionally, ILCS boundaries are identified as the highlighters of the FTLE field. It is known that highlighters of the FTLE field alone would indicate both shear and hyperbolic structures. As we notice, the employment of the structure identification criteria to separate these two types of structures based on Haller\textsuperscript{41} for three-dimensional flows is still under development (Haller, private communications). In our current study, we only consider such highlighters in backward FTLE as major attractors, with acceptance that there might be false positives due to shear structures. We leave such decomposition processes to later studies.

IV. RESULTS

A. Deterministic transport

We first discuss results from the deterministic model as our baseline geometry. Fig. 1 reveals the full three-dimensional view of backward-time ILCS at 6 a.m. on January 16, 2009 for PM\textsubscript{2.5} and PM\textsubscript{10}, respectively. The region is viewed from the south. Since backward-time structures highlight attracting motion, the ILCS in Fig. 1 show patterns where deterministic particles cluster. Major structures can be identified in the wake of several big buildings in the northeast corner of the figure (e.g., building A). When particle size is small, trajectories behave more like fluid particle trajectories. As such, recirculating bubbles at the roof top can be seen in most buildings in Fig. 1(a). The tails trailing these tall buildings indicate material surfaces which attract nearby trajectories. They highlight the converging flow structures coming from the north and south of the buildings. Also, at the foot of these buildings, shielding structures can be located where trajectories from the outside and inside of building wakes collapse. These shields are the boundaries of wakes near the buildings.

Another interesting feature in the 3D structures is located at the southeast corner of the domain, between several parallel buildings (e.g., next to building B in Fig. 1(a)). Vortices can be located inside the street canyons and they tend to fill up the entire width of the canyons. In general, vortices are typical elliptic structures that are not highlighted by FTLE. However, high values can be obtained on the edge of a vortex, where particle trajectories from different regions of the flow get entrained into
FIG. 2. Attracting ILCS for deterministic dynamics evaluated at 6 a.m. on January 16, 2009. The two panels show structures associated with different particle sizes at \( Z = 1 \text{ m} \). (a) PM\(_{2.5}\). (b) PM\(_{10}\).

The vortex. It is indeed the case here as we examine local particle trajectories (not shown). Above the vortices in the street canyon we observe structures highlighting skimming flows. Separation between the skimming flows and recirculation vortices can be seen near the roof top of the parallel buildings as a streamwise sheet structure laying on top of the spanwise rolls. In this region, three of the four street canyons have smaller width which lead to the recirculating vortex, whereas one of the street canyon (on the west) has a wider gap, resulting in no noticeable circulating structure in between the buildings.

As a comparison, in Fig. 1(b), due to the bigger size of PM\(_{10}\) particles, they fall to the roof top/ground faster, hence no roof top circulation is found. The ILCS boundaries at the foot of the buildings appear to be much weaker than those in Fig. 1(a). Also, in the street canyon region the recirculating vortices seem to be less intense as compared to those structures based on PM\(_{2.5}\), indicating less attraction of trajectories originating in different parts of the domain.

To understand the organizing structures at a height important to human activities, we show slices of ILCS at 1 m height, for particles of different sizes and at different times of the day. In Fig. 2, the ILCS are obtained for PM\(_{2.5}\) and PM\(_{10}\). The tall building A seen in Fig. 1 can be found around \( X = 3100 \text{ m}, Y = 2200 \text{ m} \). The ILCS boundary upwind of A is very pronounced for both PM\(_{2.5}\) and PM\(_{10}\), but regions of strong attraction (highlighting mid-grey, red) appears to be wider for PM\(_{2.5}\). This structure corresponds to the convergence of flows at the leading edge of the tall building when trajectories from the upwind direction collapse into trajectories from the front of the building. These trajectories then move along the structure, around the sides of the building, with trajectories on the outside of the wake boundary moving downstream. Some of the trajectories are trapped inside the wake structure downwind of the building, as they get attracted to the backward-time FTLE in the trailing edge. As the PM size becomes larger, the ILCS boundaries (at \( Z = 1 \text{ m} \)) become smaller and weaker, indicating less contraction of trajectories. This is because for larger particle sizes, trajectories initiated at this height fall to the ground too quickly, leaving little chance for attractors to form (cf. trajectory comparison initiated at \( Z = 3 \) in Fig. 4 for different particle sizes).

Inside the street canyons next to building B, around \( X = 2800–3100 \text{ m} \) and \( Y = 1400–1800 \text{ m} \), we find signatures of recirculating vortices. Clearly seen in Fig. 2(b), the cells of the recirculating vortices fill up the width of the canyon. These cells are almost indistinguishable in Fig. 2(a), probably because the vortices are reaching a vertical boundary at \( Z = 1 \text{ m} \).
In order to show the geometry for repellers (or separating streamlines), so as to locate regions where high dispersion will occur, we plot the forward-time ILCS in Fig. 3. Again, particle sizes of PM2.5 and PM10 have been shown. At this height, major structures are located downwind of the tall buildings and inside the street canyons, when particle size is small. The structures inside the street canyon indicate the repelling geometry of the recirculating vortex. It is not too surprising that at this height, as particle size gets larger, the structures are less complex. This is because in forward-time, most particles fall to the ground and stick to the bottom, leaving less repelling ILCS to form. As a comparison, backward-time trajectories ascend higher as time progresses (in backward-time) and separate farther, resulting in the attracting ILCS being more distinguished.

We discuss structures formed around buildings A and B again for forward-time ILCS. First, in the street canyon region near building B, recirculating vortex cells are visible for both PM2.5 and PM10, corroborating with our findings from backward-time FTLE. On the other hand, the structure downwind of building A is indicative of separation among inertial particles going downstream and those trapped in the wake eddy. As particle size increases, this structure fades out, due to particle settling to the ground and so less separation is observed. Upstream of this building, there is a thin strip of low FTLE value, marked by an ellipse. High values of forward-time FTLE are expected if the incoming flow is predominantly two-dimensional and separate around the building. However, due to the low height and finite width of the building front, trajectories either fall to the ground, stick to the building facade, or entrain into an eddy at the downwind edge of the building. Thus the separatrix is not well distinguished here. However, we do notice a quick change in FTLE value as one traverse across this structure, indicating entrance of a region where particles are advected far downstream. As particle size increases, this region of low separation expands, indicating more particles settling upstream of the tall building A, and similarly near other buildings.

To further support our interpretation of the weak structure upwind of building A, we show several trajectories released at the upwind side, associated with forward-time FTLE, for different particle sizes in Fig. 4. We have compared three particle sizes: PM0 (idealized fluid), PM2.5, and PM10. A common feature of the ILCS for these sizes is two highly distinguishable separatrices at $Z = 20$ m. At $Z = 3$ m, however, PM0 and PM2.5 show local FTLE maximum on the upwind side of the building, whereas PM10 shows a local FTLE minimum. We show trajectories initiated near the structures at $Z = 20$ m in black, and those initiated near the structures at $Z = 3$ m in mid-grey (green). For the black trajectories, it is clear that the two trajectories outside of the upwind
structure separate around the building and advect far downstream. Trajectories initiated between the two FTLE maxima lines remain inside the building wake (although they may end up in different regions inside the wake). The separatrices at \( Z = 20 \text{ m} \) thus highlight trajectory separation around the building and entrainment in the wake. For the mid-grey (green) trajectories, they are initiated on the two sides of the separatrix at the upwind side of the building. Were they not falling to the ground (Figs. 4(a) and 4(b)), the trajectories would have moved around the building and thus a repelling topology could be found. For PM10, in Figs. 4(a) and 4(b), the two mid-grey (green) trajectories fall to the ground too soon, leaving no chance of strong separation in this region, hence we observe the FTLE minima.

We study the temporal variation of the structures by extracting ILCS for data from two different hours, for PM2.5. These ILCS at \( Z = 1 \text{ m} \) are shown in Figs. 5 and 6. At both times, the ambient wind appears to be predominantly from the east, thus the ILCS at both times are similar. However, the strength of the backward-time ILCS at 6 p.m. is larger than that at 6 a.m., probably due to the different incoming wind speeds. The forward-time ILCS at both times have similar strengths, probably due to the fact that they hit the ground very soon. Extraction at other times (not shown) indicate the variation of coherent structures throughout the day. Combining the three-dimensional versions of Figs. 5 and 6, one obtains the full description of the topology for deterministic inertial particle transport in the HP area.

FIG. 4. Particle trajectories initiated near forward-time ILCS upwind of building A. Black: released at \( Z = 20 \text{ m} \). Mid-grey (green): release at \( Z = 3 \text{ m} \). (a) Idealized fluid tracer. (b) PM2.5. (c) PM10.

FIG. 5. Comparisons of backward-time FTLE for PM2.5 at two different times on January 16, 2009, at \( Z = 1 \text{ m} \). (a) 6 a.m. (b) 6 p.m.
FIG. 6. Comparisons of forward-time FTLE for PM$_{2.5}$ at two different times on January 16, 2009, at $Z = 1$ m. (a) 6 a.m. (b) 6 p.m.

B. Stochastic transport

The actual urban environment is indeed stochastic, with uncertainties in the unresolved scales possibly changing our deterministic evaluations. In this subsection, we examine random inertial particle trajectories and ILCS based on realistic random noise from turbulent eddies.

We consider the most probable trajectory for an inertial particle embedded in the stochastic environment. The random displacement model described in Sec. II has been used. Coherent structures are based on the mean trajectories, with the interpretation that the stochastic ILCS is the most probable structure observed based on where inertial particles most likely go. In order to compare deterministic and stochastic models, we show in Fig. 7, for a single initial condition (next to a building complex so flow has a wake structure), trajectories from both formulations in forward and backward-time. The mid-grey (red) curves in Fig. 7(a) show stochastic mean trajectories, with the dashed line in forward-time and solid line in backward-time, based on the full Maxey-Riley equations. The dark-grey (blue) curves in the same panel show stochastic mean trajectories based on the inertial equations, and

the black curves show deterministic trajectories. The line styles are the same as the mid-grey (red) curves for forward and backward-time evolution. First, we find that the mean trajectories based on slow manifold equation and full equations are almost identical in forward-time. As a comparison, the differences between stochastic and deterministic trajectories are quite pronounced. Second, we find that the backward-time stochastic trajectory based on the full equations becomes unstable very quickly in backward time. This is to be expected since Eq. (4) is strongly unstable in backward-time due to the first term on the right-hand side. For comparison between the stochastic full equations and inertial equations, we show the clustering of random realizations by particles in different colors. The mid-grey (red) particles show forward-time trajectories based on the full equations and the dark-grey (blue) particles are from inertial equations. Clearly, the patterns are comparable, leading to similar statistics for single trajectories. On the other hand, the light-grey (cyan) particles are those from inertial equations in backward-time (no realizations from the full equations in backward-time survive the instability). Motivated by the fact that the two stochastic formulations result in identical mean trajectories in forward-time, the inertial equations has only half the degree of freedom and the full equations blow up in backward-time, we use inertial equations as the governing equations in our computation.

Due to the computational cost for random dynamics, we only focus on regions near the tall building A in our stochastic cases. The stochastic ILCS is in terms of FTLE fields computed from the mean of the random trajectories. In Fig. 8 we show forward-time stochastic ILCS for the tall building at $Z = 2$ m, for PM$_{2.5}$. This case is based on data from February 15, 2009 at 6 a.m. when the flow is predominantly from the south. In Fig. 8(a), the deterministic ILCS is shown, as a baseline case. The wake structure is very pronounced downwind of building A. We also plot the case with eddy diffusivity, determined from our previous discussion of the models, in Fig. 8(d). This is our upper bound on stochasticity because it is valid for realistic flows. In between, in Figs. 8(b) and 8(c), we consider 1/4 and 1/2 of the value of the eddy diffusivity, as a proxy to understand the variation of ILCS due to strength of randomness. As seen, when randomness is progressively increased towards the full value of eddy diffusivity, the major wake structure remains quite distinguishable.

![Figure 8](image_url)

**FIG. 8.** Forward-time stochastic ILCS near the tall building at $Z = 2$ m for PM$_{2.5}$ on February 15, 2009. (a) Deterministic. (b) 0.25 of the full eddy diffusivity. (c) 0.5 of the full eddy diffusivity. (d) Full eddy diffusivity.
FIG. 9. Backward-time stochastic ILCS near the tall building at $Z = 2$ m for PM$_{2.5}$ on February 15, 2009. (a) Deterministic. (b) 0.25 of the full eddy diffusivity. (c) 0.5 of the full eddy diffusivity. (d) Full eddy diffusivity.

As a comparison, we also show in Fig. 9 the backward-time stochastic ILCS in the same region. In the deterministic case, the mushroom-like wake structure trailing building A is clearly seen. At the southeast corner, due to the annex to building A, some closed structure is also seen as attractors. As we progressively increase stochasticity, the mushroom-like wake is still visible but fading, whereas the smaller structure disappears even with 1/4 of the full stochasticity. Finally, at the full strength, only the counter-rotating vortex cell survives random perturbations.

In Table I, we compute the correlation between the stochastic and deterministic FTLE fields to measure the variability of the ILCS by different levels of stochasticity. The correlation is computed as

$$C_{DS} = \frac{FTLE(D) \ast FTLE(S)}{Std[FTLE(D)] \ast Std[FTLE(S)]},$$

where $FTLE(D)$ and $FTLE(S)$ are the scalar FTLE fields in the deterministic and stochastic cases, respectively. $Std[FTLE]$ denotes the standard deviation of the scalar fields. As stochasticity increases, the correlation decreases, but even with full stochasticity, correlation of the structures is still above 70%. This indicates the robustness of major ILCS.

We further study the variation of stochastic ILCS with respect to particle size in Fig. 10. In this figure, we compare the deterministic and fully stochastic cases directly. In the top panels, the forward-time (Fig. 10(a)) and backward-time (Fig. 10(b)) ILCS for PM$_{10}$ are shown. Compared to the deterministic cases of PM$_{2.5}$, these ILCS are slightly less well-pronounced, but still quite well defined. For the stochastic cases, again, the major structures survive random perturbations and act as the organizing centers for nearby inertial particle trajectories.

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<th>TABLE I. Correlation of stochastic and deterministic FTLE.</th>
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FIG. 10. Comparison between deterministic and stochastic ILCS near the tall building at \( Z = 2 \) m for PM10.
(a) Deterministic, forward-time. (b) Deterministic, backward-time. (c) Full eddy diffusivity, forward-time. (d) Full eddy diffusivity, backward-time.

V. DISCUSSIONS AND CONCLUSIONS

We have studied the mixing geometry for inertial particles in a realistic street-scale urban flow model. The model is focused in the Hermoso Park region in a district in Phoenix, Arizona. The interest is on how these geometry may relate to higher particulate matter density allegedly causing respiratory problems for local residents. We focus on the flow topology than specialized case studies because with such a geometry, we can estimate mixing patterns of pollutants from isolated release events anywhere inside the domain of interest. It also aids identification of patterns from continuous release events.

In order to objectively extract the mixing geometry, we used inertial Lagrangian coherent structures, because they offer objective description of transport patterns. For the deterministic case, the methodology is a direct application of results in Sapsis and Haller\(^2\) and Tang et al.\(^3\) We find the ILCS for different particle sizes and at different hours on January 16, 2009, with data initiated from measurements and flow simulated with QUIC-URB. The size effects on the structures have been discussed in detail. In particular, in the deterministic regime, as particle size becomes larger, attracting structures in the leading edge of large/individual buildings become weaker. In addition, particle size also affects the dynamics in street canyons, in that trajectories are less likely to converge strongly, hence less mixing of the inertial particles are observed. These results provide the baseline cases for our discussions on stochastic ILCS.

For the stochastic case, we choose random displacement model, as it is simpler to analyze than Lagrangian stochastic models. The stochastic ILCS is understood in terms of the most likely trajectory an inertial particle will take as it evolve inside the urban flow with inhomogeneous random noise due to spatially dependent eddy diffusivity. The ILCS is then obtained from the mean motion. With this concept, backward-time random walk models are also meaningful, as an estimate of where
a trajectory is most likely coming from in the past, so to estimate the tendency of attraction for each individual material particle. Evaluating the stochastic ILCS, we find that using eddy diffusivity based on $k-\varepsilon$ model, major structures still survive to serve as the organizing centers for stochastic inertial particle transport. As we vary the strength of eddy diffusivity, a correlation with the deterministic geometry is also obtained.

Here, with the more homogenized FTLE field due to eddy diffusion, the extrema curves/surfaces (serving as ILCS boundaries) are less distinguished as their deterministic counterparts. However, bearing in mind that ILCS are regions in the flow where trajectories exhibit similar types of Lagrangian motion, we can readily identify regions in the FTLE field with similar data values as the stochastic ILCS. Hence, hyperbolic regions are highlighting patches in the FTLE field where stochastic mean trajectories are expected to separate the most, whereas elliptic regions are low-value patches where stochastic mean trajectories stay together. In terms of automated extraction of the boundaries of such structures, one would have to rely on the identification of material lines on the steepest slopes in the FTLE field, as they mark the transition regions between most likely hyperbolic (plateaus in FTLE) and most likely elliptic (basins in FTLE) motion.

Note that the stochastic ILCS obtained with full eddy diffusivity are most robust and survive realistic disturbances, hence they are most likely to be found in a natural environment. Maps of stochastic ILCS such as those shown in Figs. 8–10 can thus aid easy identification of strong elliptic or hyperbolic structures important for material transport. Subsequently, regions in the real urban environment which are most susceptible to pollutant accumulation or dispersal can be found for decision makers to take any air quality counter measures.

There are several aspects that could help improve our understanding of stochastic ILCS in a realistic urban environment. First, we have only used a RDM for the stochasticity. In general, a LSM based on the Langevin equations is more suitable to account for the random nature of fluid trajectories. Conventional treatments of inertial effects are not directly using the governing Maxey-Riley equations, but an estimate of the finite synchronization time scale of inertial particles, which relates to an assumption that inertial particles travel at their settling velocities. A new formulation of the inertial dynamics based on Maxey-Riley equations with LSM (instead of RDM) on just the fluid trajectories may shed new light on stochastic inertial particle dynamics. Bearing the nicety of deterministic part of the inertial particle forces, we may use the approach outlined in this paper again for stochastic backward models. In this way, stochastic ILCS will be based on a more general formalism, and suited to more realistic environments.

Second, some careful treatments may also be needed for the boundary condition, since we are using a simple no-slip boundary condition and the results affect the Gaussian assumption. An improved formulation may better estimate the statistics for inertial particle trajectories and bear a higher confidence in evaluating the stochastic ILCS.

Third, with the presence of coherent structures, the diffusion process inside the domain may not be Gaussian, and thus we need to consider other choices of random noises to better reflect reality. Some of these non-Gaussianity has been incorporated in QUIC-PLUME for idealized fluid tracers, and we will need to formulate carefully in the case of inertial particles.

Overall, since particle density is a linear superposition of release events, the precise knowledge of geometry will aid fast estimates on the source and fate of dispersion for pollutants, chemical spills or malicious toxin releases. The use of mixing topology will aid environmental protection, mitigation, and homeland security applications. How to efficiently use ILCS in such applications will be explored in future studies.

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