Understanding flow structures in urban areas is being widely recognized as a challenging concern due to its effect on urban development, air quality, and pollutant dispersion. In this study, state-of-the-art data-driven methods for modal analysis of urban flows are used to understand better the dominant flow processes that occur in this phenomenon. Higher-order dynamic mode decomposition (HODMD), a highly-efficient method to analyze turbulent flows, is used with traditional techniques such as proper orthogonal decomposition (POD) to analyze high-fidelity simulation data of a simplified urban environment. Furthermore, the spatio-temporal Koopman decomposition (STKD) will be applied to the temporal modes obtained with HODMD to perform spatial analysis. The flow interaction within the canopy influences the flow structures, particularly the arch vortex. The latter is a vortical structure generally found downstream wall-mounted obstacles that appears due to flow separation. Therefore, the main objective of the present study is to characterize the mechanisms that promote these dynamics in urban areas with different geometries. Remarkably, among all the vortical structures identified by the HODMD algorithm, low- and high-frequency modes are classified according to their relation with the arch vortex. They are referred to as vortex-generators and vortex-breakers, respectively. This classification implies that one of the processes driving the formation and destruction of major vortical structures in between the buildings is the interaction between low- and high-frequency structures. The high energy revealed by the POD-decomposition for the vortex-breaker modes points to this destruction process as the mechanism driving the flow dynamics. Furthermore, the results obtained with the STKD method show how the generating- and breaking-mechanisms are originated along with the streamwise and spanwise directions.

I. INTRODUCTION

The study of the flow around building-like obstacles has been extensively addressed in the literature due to its implications in urban-environment phenomena, i.e. pollutant dispersion, air quality, and heat propagation. The very high levels of air pollution to which the vast majority of the urban population is exposed are undoubtedly related to a myriad of health issues. The hunt is for predictive models capable of accurately reproducing the pollutant and thermal distributions within urban environments. Some of these models have already been introduced by the European Union (EU). However, their inability to provide the spatio-temporal accuracy required to model pollutant dispersion through urban environments forces researchers to improve those methods to ensure urban sustainability. As an example, to establish a proper action plan to alleviate the associated adverse consequences, several studies have focused their efforts on analyzing the spatio-temporal structures of the flow. The main point is to identify the three-dimensional flow regions responsible for the pollutant dispersion within a given urban geometry. Therefore, the objective of this study is to apply recently-developed tools from system dynamics, notably higher-order dynamic mode decomposition (HODMD), to turbulent flows within urban environments to understand how different city configurations influence the mechanisms leading the flow dynamics.

The large number of spatio-temporal features present in the high-dimensional nonlinear system of a turbulent flow complicates the analysis. Nonetheless, the fact that physical-flow features are shared across a wide variety of flows suggests that they may be used to describe the dynamics of such a flow. One of the first studies aiming at identifying the flow structures around a wall-mounted obstacle was performed by Hunt et al. Using flow-visualization techniques, they proved the absence of a closed surface, i.e. a separation bubble or cavity, in the wake of the obstacle, due to the interaction of four different vortical structures. They discovered two large vortices on both sides of the obstacle, as well as a roof vortex at the cube top. The well-known arc vortex is formed on the leeward side of the obstacle due to the separation region appearing downstream of the block, which causes the structures above to move closer. Together with the horseshoe vortex, these vortical structures are the consequence of the interaction of the outer flow with the urban-canopy layer. Understanding their underlying physics is essential for developing strategies to reduce pollution-dispersion and perform pedestrian-comfort assessments. Based on this idea, the arch vortex has been extensively analyzed in various configurations. For instance, Becker et al. experimentally studied the flow structures around three-dimensional rectangular blocks in a suburban boundary layer. They analyzed the arc-shaped vortices formed on the leeward side of the obstacle for different angle-of-incidence (AOI) values using laser-Doppler-anemometry (LDA) measurements together with oil-film visualizations. They reported the dislocation of one of the vortex legs until AOI = 60°, which causes the vortex leg to be displaced to the top of the obstacle. Furthermore, Zhu et al. used particle-image-velocimetry (PIV) measurements to analyze the three-dimensional wake patterns of the flow through a wall-mounted cylinder. They concentrated on the formation process of the arch and tip vortices and documented their apparition in both the time-averaged and the instantaneous fields. Therefore, the arch vortex is a prominent structure in flows through surface-mounted
obstacles responsible for the flow interaction on the leeward side of the block.

Vinuesa et al. [9] also aimed to investigate the influence of the inflow conditions on such coherent structures around a wall-mounted square cylinder using direct numerical simulation (DNS). While the sharp edges of the obstacle maintain the separation point regardless of inflow conditions, the resultant structures and topology of the wake downstream in both laminar- and turbulent- inflow scenarios varies considerably. The influence of the growing boundary layers on both sides of the obstacle, in particular, causes a difference in behavior in both wakes, since the turbulent one is slightly wider in the time-averaged field. In addition, Vinuesa et al. [9] noted that the horseshoe vortex was modified by streamwise variations in the turbulent-inflow simulation. This emphasizes the importance of having well-established inflow conditions in both experimental and numerical analyses to ensure flow consistency.

The apparent complexity of urban-based environments, on the other hand, leads to more intricate physics due to the interaction of flow structures around individual buildings. Oke [2] provided an analysis of the resultant flow regimes as a function of the geometrical parameters that define an urban model. Interestingly, the author discovered that the street width was the critical parameter in establishing the flow regimes [2]: in the case of narrow streets, the flow above the canopy can barely reach down to the street (skimming flow), and only one vortex can be seen between the obstacles; gradually broader streets lead to the wake-interference regime first and then to the isolated-roughness flow, which exhibits much more contact with the flow above the roofline. Meinders [10] further examined this classification by analyzing the interaction of flow patterns around wall-mounted rectangular obstacles with different spacing ratios in the streamwise direction. The separated shear layer from the first obstacle reattached on the windward side of the downstream obstacle for the lowest separation, resulting in an inter-obstacle area with an arc-shaped vortex confined by the side flow [10]. With larger separation ratios, flow reattachment occurs in the region between the obstacles, from which a second horseshoe vortex emerges on the windward side of the downstream obstacle. This results in similar flow patterns for both obstacles, but with lower intensity in the downstream block due to the flow disruption of the upstream block [10].

A wide range of criteria to identify these vortical structures has been developed. Monnier et al. [11] aimed at identifying the main flow patterns present in the wind-tunnel flow around the geometry of the Mock Urban Setting Test (MUST) experiment using different criteria. They started evaluating the vorticity components, namely the wall-normal and spanwise mean components, \( \omega_1 \) and \( \omega_2 \), respectively, to identify the location of the arch vortex. Using the modulus of the spatially-averaged vorticity vector allowed them to define a local threshold to properly characterize the influence of the AOI on this vortical structure, extracting similar conclusions to those of Becker et al. [6]. They also employed some popular methods for vortex identification, based on the second invariant of the velocity gradient tensor, i.e. the Q-criterion [12] and the \( \lambda_2 \) criterion [12]. However, they improved the identification of large-scale vortical structures using the normalized angular momentum technique \( \Gamma_1 \), introduced by Sousa [13] to locate the center of vortical structures downstream of a single cuboid obstacle. This method allowed the authors to describe the relationship between the arch vortex and high-turbulence areas. Monnier et al. [11] concluded that the arch vortex is located in between high-turbulence areas. They consist of two regions of significant streamwise velocity fluctuations on both sides of the obstacles due to the separation of the shear layer and a high spanwise velocity fluctuating region along the windward face of the downstream obstacle. This experimental study led to relevant conclusions in analyzing coherent structures in a more realistic urban model.

Here, we focus on Oke’s classification [2] to extract through data-driven procedures the key dominant patterns present in the three-dimensional instantaneous fields of the flow through urban environments with different separation ratios. In this regard, the objective is to characterize the main flow processes responsible for the formation and destruction of such vortical structures, thus gaining further understanding of the dynamical processes governing urban flows. To this end, we employ different techniques related to modal decompositions. First, we use proper-orthogonal decomposition (POD) [14] to identify those spatial modes energetically more relevant to the system as well as their associated time coefficients. We compare them with the results obtained using a recently-developed higher-order variant of dynamic-mode decomposition (DMD) [15], named HODMD [16]. Via this novel nonlinear dynamic mode decomposition approach, we can analyze the dynamics of a highly complex turbulent flow [16–20], cleaning noisy artifacts and small amplitude modes from data. Recently, Amor et al. [21] showed the potential of HODMD to understand the complicated physics of the wake in a wall-mounted square cylinder [16]. Like DMD, HODMD decomposes spatio-temporal data into a group of modes oscillating in time and space, representing the leading flow dynamics.

Following the introduction to urban flows, the present work provides a general overview of the performed numerical simulations in § II. A summary of the mathematical concepts behind the modal-decomposition techniques used to characterize the flow structures over the numerical simulation data is addressed during § III. The mechanisms driving the flow dynamics within urban environments, which are the result of the application of different data-driven tools, are further investigated in § IV. Finally, a summary of the main conclusions of the project is provided in § VI and the justification of the selected modes is performed in Appendix A through the calibration process of the methods.

A review of the formation and destruction mechanisms of arch vortices in urban flows has already been addressed in a companion paper [22]. Here, a detailed analysis of the modal-decomposition techniques, which shed light on the mechanisms driving the flow dynamics, will be addressed with an overview of the high-order numerical simulations carried out to perform the present analysis.
II. NUMERICAL SIMULATIONS

The high-order spectral-element code Nek5000 [23] was used to solve the incompressible Navier–Stokes equations governing the flow in the cases under consideration. Based on the spectral-element method (SEM) of Patera [24], Nek5000 exhibits both geometrical flexibility and the accuracy of the high-order spectral methods [9, 25–30]. Due to the flow complexity in urban environments, high-order methods need to be used to resolve all the relevant flow structures properly. In this database, we use a well-resolved large-eddy simulation (LES), the resolution of which is close to that of a direct numerical simulation (DNS) [27]. This code has been extensively used for high-fidelity simulations of complex turbulent flows, see Refs. [28,30]. Additional details on the numerical scheme and employed resolution can be found in Ref. [31].

The geometrical domain is composed of two wall-mounted obstacles, as depicted in Fig. 1. The size of the computational box dimension varies according to the separation of the obstacles. While the wall-normal and spanwise directions remain the same for the three cases, the streamwise length changes proportionally to the separation $\ell$, which modifies the computational cost of the numerical simulation associated with each case. The obstacles are then defined by the height $h$, length $w_b$ and width $b$. All dimensions are normalized with the height of the obstacle $h$. The velocity field is given by $v(x,y,z,t)$, where $x$, $y$, and $z$ are the streamwise, wall-normal, and spanwise directions, respectively, and $t$ is time. Every velocity is normalized with the free stream velocity. The components of the velocity are $v = (u,v,w)$, which denote the streamwise, wall-normal, and spanwise components, respectively. Using Reynolds decomposition, $v$ is defined as $v = V + \tilde{v}$, where $V = \overline{v}$ is the average in time and $\tilde{v}$ is the turbulent fluctuation. Primes are reserved for intensities $v' = \overline{v^2}^{1/2}$.

As inflow condition, a numerically-tripped [32,33] laminar Blasius profile allows the flow for undergoing a rapid transition to turbulence without needing to accelerate the flow before reaching the obstacles [34]. This numerical tripping consists of a weak wall-normal volume that is randomly added in the forcing terms of the incompressible Navier–Stokes equations to create flow disturbances, thus inducing turbulence. The inflow is located at $x/h = -10$, the tripping force is applied at $x/h = -9$, allowing the boundary layer for developing in the region upstream the obstacles, i.e. $-8 \leq x/h \leq -1$. In this region, both $z$-averaged friction and momentum-thickness Reynolds numbers, i.e. $Re_\tau$ and $Re_\theta$ respectively, increase in the streamwise direction, reaching turbulent conditions for $x/h \geq -2$. The adverse pressure gradient induced by the obstacles leads to an increase of the Rota-Clause pressure-gradient parameter and a decrease in the skin-friction coefficient. The stabilized outflow condition developed by Dong et al. [35] is used as an outflow condition. At the upper part of the domain, a combination of outflow and Dirichlet conditions is used to simulate an open-air urban environment: a zero-stress condition is applied in the wall-normal direction, and a Dirichlet condition in the other two directions [23]. Finally, periodicity is applied in the spanwise direction. Wall condition is applied to the bottom plane of the domain and the surfaces of the obstacles.

![Fig. 1: Schematic representation of the numerical domain, where $L_y = 3h$ and $L_z = 4h$. The flow is from left to right. (Top) and (bottom) show side and top views, respectively.](image-url)
TABLE I: Temporal parameters of the datasets of the numerical simulations carried out for the three flow regimes identified by Oke [2]. The parameter $\ell/h$ refers to the separation-to-height ratio between the obstacles in the streamwise direction, $T_i$ and $T_f$ are the initial and final times of the database and $\Delta T$ is the total database timespan. Furthermore, $\Delta t$ represents the time interval between snapshots and $N_f$ is the number of fields.

| Flow regime            | $\ell/h$ | $T_i$   | $T_f$   | $\Delta T$ | $\Delta t$ | $N_f$ | Color code |
|------------------------|----------|---------|---------|-------------|-------------|-------|------------|
| Skimming flow (SF)     | 1        | 38.65   | 117.38  | 78.73       | 0.35        | 225   |            |
| Wake interference (WI) | 2        | 80.40   | 144.60  | 64.20       | 0.3         | 215   |            |
| Isolated roughness (IR)| 4        | 83.30   | 145.60  | 62.30       | 0.7         | 90    |            |

We consider a spectral-element mesh with an eight-point Gauss–Lobatto–Legendre (GLL) quadrature in each element. The mesh is refined in the near-obstacle area in order to increase resolution, which has a direct impact on flow statistics. Following the criteria of Negi et al. [27], the mesh here employed satisfies all the resolution criteria to be considered a well-resolved LES.

The analyzed database has the temporal parameters gathered in Table I. Note that this information is critical for the analysis of the spatio-temporal structures of the flow since they define the system’s dynamical behavior, which is closely related to the time span and time step of the snapshots to be analyzed. All the introduced parameters are expressed in convective time units, i.e. a ratio between a characteristic length and a velocity. In the present case, time is obtained from the freestream velocity $U_\infty$ and the height of the obstacle, $h$.

III. METHODOLOGY FOR MODAL DECOMPOSITION

A. Proper-orthogonal decomposition (POD)

The proper orthogonal decomposition (POD) is a modal-decomposition technique, introduced in the field of fluid mechanics by Lumley [14], which aims at extracting coherent patterns from a given flow field. Thus, the objective of the POD algorithm is to decompose a set of data of a given field variable into a minimal number of modes (basis functions) that capture as much energy as possible. This process implies that POD modes are optimal in minimizing the mean-square error between the signal and its reconstructed representation. For instance, if the field variable to be examined is the velocity, the modes representing such variable are optimal to capture the kinetic energy of the flow field. This low-dimensional latent space provided by the POD modes is attractive for interpreting the most energetic and dominant patterns within a given flow field. Let us consider a vector field $q(\xi, t)$, which may represent e.g. the velocity or the vorticity field depending on a spatial vector $\xi$ and time. In fluid-flow applications, subtracting the temporal mean $\bar{q}(\xi)$ allows for the analysis of the unsteady component of the field variable:

$$x(t) = q(\xi, t) - \bar{q}(\xi), \quad t = t_1, t_2, \ldots, t_k$$  \hspace{1cm} (1)

where $x(t)$ represents the fluctuating component of the vector data with its temporal mean removed. This representation emphasizes the idea that the data vector $x(t)$ is being considered as a collection of snapshots at different time instants $t_k$. If the $m$ snapshots are then stacked into a matrix from, we obtain the so-called snapshot matrix $X$:

$$X = [x(t_1), x(t_2), \ldots, x(t_m)] \in \mathbb{R}^{J \times K},$$  \hspace{1cm} (2)

where $J$ represents the number of points in $x$, $y$ and $z$. The objective of the POD analysis is to find the optimal basis to represent the given set of data $x(t)$. This can be solved finding the eigenvectors $\Phi_j$ and the eigenvalues $\lambda_j$ from:

$$C \Phi_j = \lambda_j \Phi_j, \quad \Phi_j \in \mathbb{R}^J, \quad \lambda_1 \geq \cdots \geq \lambda_N \geq 0,$$  \hspace{1cm} (3)

where $C$ states for the covariance matrix of the input data, defined as

$$C = \sum_{i=1}^{K} x(t_i) x^T(t_i) = X X^T \in \mathbb{R}^{J \times J}.$$  \hspace{1cm} (4)

The size of this matrix depends on the spatial degrees of freedom of the problem. In the case of fluid flows, this value is usually large since it equals the number of grid points times the variables to be considered. The POD modes are derived from the eigenvectors of Eq. (3), with the eigenvalues reflecting how well each eigenvector $\Phi_j$ represents the original data in the $\ell_2$-sense. This enables a hierarchy of modes in terms of captured energy, which improves understanding of the most prominent patterns, e.g. in a specific flow field.
Another method for computing the POD algorithm is based on the singular-value decomposition (SVD) [36], which can be applied directly on the snapshot matrix \( X \) to obtain the left \( \Phi \) and right \( \Psi \) singular vectors as

\[
X = \Phi \Sigma \Psi^T, \tag{5}
\]

where \( \Phi \in \mathbb{R}^{J \times J} \), \( \Psi \in \mathbb{R}^{K \times K} \) and \( \Sigma \in \mathbb{R}^{J \times K} \). The matrix \( \Sigma \) contains the singular values \( \{\sigma_1, \sigma_2, \ldots, \sigma_N\} \) along its diagonal, which relates to the eigenvalues as \( \sigma_j^2 = \lambda_j \). Moreover, the left and right singular vectors correspond to the eigenvectors of matrices \( XX^T \) and \( X^T X \), respectively. Therefore, the SVD can be seen as a rectangular-matrix decomposition technique capable of computing the POD modes.

### B. Higher order dynamic mode decomposition (HODMD)

Aiming at identifying the spatio-temporal coherent patterns present in high-dimensional flow data, Schmid [15] developed a data-driven tool which retrieved the spatially-correlated structures with similar behavior in time. This methodology, known as dynamic-mode decomposition (DMD), provides not only a reduction in dimension concerning a reduced set of modes which best reproduce the input flow-field, but also a model for the interaction of those modes in time.

The method decomposes the vector field data \( \mathbf{v}(\mathbf{x}, t) \) as an expansion of \( M \) Fourier-type modes:

\[
\mathbf{v}(\mathbf{x}, t) \approx \sum_{m=1}^{M} a_m \mathbf{u}_m(\mathbf{x}) e^{(\delta_m + i\omega_m)t},
\]

for \( k = 1, \ldots, K \), where \( \mathbf{u}_m \) represents the DMD modes weighted by an amplitude \( a_m, \omega_m, \) their associated frequencies and \( \delta_m \), their associated growth rates, which symbolize the temporal growth or decay of the \( \mathbf{u}_m \) modes in time.

The standard DMD algorithm assumes a linear relationship of two consecutive snapshot matrices using the linear Koopman operator \( \mathbf{R} \). To this end, a general snapshot matrix \( \mathbf{V}_{k_2} \) can be defined for \( k_1 < k_2 \) so that its columns represent the snapshots varying equidistantly between \( k_1 \) and \( k_2 \), namely:

\[
\mathbf{V}_{k_2} = [\mathbf{v}_{k_1}, \mathbf{v}_{k_1+1}, \ldots, \mathbf{v}_{k_2}]. \tag{7}
\]

Therefore, using the previous nomenclature, the standard DMD can be defined based on the Koopman operator as

\[
\mathbf{V}_2^K \approx \mathbf{R} \mathbf{V}_1^{K-1} \tag{8}
\]

where \( \mathbf{V}_2^K \) and \( \mathbf{V}_1^{K-1} \) represent the second to last snapshots and the first to the second last snapshots of the data matrix, respectively. Recalling Eq. (6), this equation might be seen as the simplest equation exhibiting such behavior [37]. The Koopman matrix \( \mathbf{R} \), which is independent of \( k \), contains the dynamical information of the system. Recently, Le Clainche & Vega [37] extended the DMD method for the analysis of various types of flows, e.g. turbulent, multi-scale or transitional flows and noisy experimental data. Based on Takens’ delayed-embedded theorem [37], the higher order dynamic mode decomposition (HODMD) relates \( d \) time-delayed snapshots using higher-order Koopman assumption defined as

\[
\mathbf{V}_d^{K} \approx \mathbf{R}_1 \mathbf{V}_1^{K-d} + \mathbf{R}_2 \mathbf{V}_2^{K-(d-1)} + \ldots + \mathbf{R}_d \mathbf{V}_d^{K-1}, \tag{9}
\]

which relates each flow field with the \( d \) subsequent fields. The HODMD algorithm can be encompassed into three main steps.

1. **Step 1: Dimension reduction**

First of all, the SVD technique is employed to reduce spatial redundancy and filter out noise caused by numerical or experimental errors. The truncated SVD allows for the reduction of the original snapshot data into a series of linearly independent vectors of dimension \( N \) (where \( N < J \) is the spatial complexity), based on a certain tolerance \( \varepsilon_{\text{SVD}} \):

\[
\mathbf{V}_1^K \approx \mathbf{W} \Sigma \mathbf{T}^T, \tag{10}
\]

where \( \Sigma \) includes the singular values \( \sigma_1, \ldots, \sigma_N \) and \( \mathbf{W}^T \mathbf{W} = \mathbf{T}^T \mathbf{T} = \mathbf{I} \) are \( N \times N \) unitary matrices. Note that the parameter \( \varepsilon_{\text{SVD}} \) is tunable based on previous information of the simulation or experimental data, e.g. if the noise level of the snapshots is known in advance, then \( \varepsilon_{\text{SVD}} \) may be set to be comparable to that level (see details in Ref. [19]). Above all, this parameter determines the number \( N \) of SVD retained modes as

\[
\frac{\sigma_{N+1}}{\sigma_1} \leq \varepsilon_{\text{SVD}}. \tag{11}
\]
Following the definition in Eq. (10), the reduced snapshot matrix $\tilde{\mathbf{V}}$ can be defined as
\[ \mathbf{V}_1^K \approx \mathbf{W} \Sigma \mathbf{V}^T \equiv \mathbf{W} \mathbf{T}_1^K. \] (12)

The dimension of this reduced snapshot matrix is $N \times K$.

2. Step 2: The DMD-$d$ algorithm

The higher-order Koopman assumption, defined in Eq. (9), is now applied to the reduced snapshot matrix as
\[ \mathbf{V}_d^{K} \approx \tilde{\mathbf{R}}_1 \mathbf{V}_1^{K-d} + \tilde{\mathbf{R}}_2 \mathbf{V}_1^{K-(d-1)} + \ldots + \tilde{\mathbf{R}}_d \mathbf{V}_d^{K-1}, \] (13)
where $\tilde{\mathbf{R}}_k = \mathbf{W}^T \mathbf{R}_k \mathbf{W}$ is used for $k = 1, \ldots, d$. The above equation may be cast in a more generic form by incorporating the modified snapshot matrix $\mathbf{V}_1^{k-d+1}$ and the modified Koopman matrix $\tilde{\mathbf{R}}$ as
\[ \mathbf{V}_2^{K-d+1} = \tilde{\mathbf{R}} \mathbf{V}_1^{K-d}, \] (14)
where the many Koopman operators $\tilde{\mathbf{R}}_1, \ldots, \tilde{\mathbf{R}}_K$ are then combined into a single matrix after some computations, from which the eigenvalue problem can be solved to obtain the DMD modes, frequencies and growth rates defining the DMD expansion of Eq. (6). Sorted in decreasing order of the mode amplitudes, this expansion is further reduced by removing the modes such that:
\[ a_m/a_1 < \epsilon_{\text{DMD}}, \] (15)
for $m = 1, \ldots, M$, where $\epsilon_{\text{DMD}}$ represents a parameter tunable by the user. The number of retained modes, $M$, represents the spectral complexity of the analysis. This complexity, together with the spatial one, determines the performance of the HODMD algorithm, which reduces to the standard DMD when $d = 1$. In complex fluid flows, the spatial complexity is usually smaller than the spectral one, $N < M$, where the standard DMD fails, thus requiring the use of the DMD-$d$ algorithm. Furthermore, using the tunable parameters $\epsilon_{\text{SVD}}$ and $\epsilon_{\text{DMD}}$, enables for retaining only the large scales of the input data, which is particularly interesting for complex turbulent flows involving a large number of scales.

C. Spatio-temporal Koopman decomposition (STKD)

Spatio-temporal Koopman decomposition (STKD) is an extension of HODMD introduced to identify spatio-temporal structures as an expansion of traveling and standing waves driving the flow dynamics both in the streamwise and spanwise directions. For the streamwise direction, the spatio-temporal modes $u_{mn1}$, and growth rates $\nu_{mn2}$ are defined in the following modal expansion, which reconstruct the original flow field analyzed as
\[ \mathbf{v}(x_j, y, z, t_k) \approx \sum_{m, n_1=1}^{M, N_1} a_{mn1} \tilde{\mathbf{u}}_{mn1}(y, z) e^{i((\delta_m + i\omega_m)t_k + (\nu_{mn1} + i\alpha_{mn1})x_j)}, \] (16)
for $k = 1, \ldots, K$ and $j = 1, \ldots, J$. It must be emphasized that the spatio-temporal expansion is useful when the data exhibit exponential/oscillatory behavior in both the $x$ coordinate and time. In this case, it is interesting to compare the expansion (16) with the purely temporal expansion (6). This expansion can be easily obtained by simply applying HODMD to the DMD modes in Eq. (6), resulting in the following DMD expansion:
\[ \mathbf{u}_m(x_j, y, z) \approx \sum_{n_1=1}^{N_1} a_{n_1} \tilde{\mathbf{u}}_{mn1}(y, z) e^{i((\nu_{mn1} + i\alpha_{mn1})x_j)}, \] (17)
for $j = 1, \ldots, J$. Eq. (16) is obtained by combining this solution with Eq. (6), where the spatio-temporal amplitudes are defined as $a_{mn1} = a_m a_{n_1}$. In a similar way, it is possible to obtain spatio-temporal expansions defined along the spanwise direction as
\[ \mathbf{v}(x, y, z_r, t_k) \approx \sum_{m, n_1=1}^{M, N_1} a_{mn1} \tilde{\mathbf{u}}_{mn1}(x, y) e^{i((\delta_m + i\omega_m)t_k + (\lambda_{mn1} + i\beta_{mn1})z_r)}, \] (18)
for $k = 1, \ldots, K$ and $r = 1, \ldots, R$, where $\lambda_{mn1}$ and $\beta_{mn1}$ are the growth rates and wavenumbers related with the spanwise direction. Using this expansion it is also possible to describe the analyzed data as a group of traveling waves, the phase velocity of which is defined as $c_{mn1} = \omega_m / \beta_{mn1}$. A more detailed description of the method can be found in Refs. [20, 38].
IV. MEAN-FLOW STRUCTURES

A large number of studies have focused on the flow around a square wall-mounted cylinder of different aspect ratios, which is interesting due to the myriad of physical phenomena occurring at the same time: a recirculation bubble formed on the windward side of the cylinder induces an adverse pressure gradient that thickens the incoming boundary layer, which then produces a shear layer around the obstacle. Simultaneously, a horseshoe vortex progressively gets wider around the two sides of the cylinder, which accelerates the flow close to the obstacle due to the favorable pressure gradient induced by the geometry. A separated wake is then formed downstream the obstacle with a self-sustained oscillation process and a downward motion from the top of the obstacle, which is responsible for the widening of the wake [9]. This configuration has been extensively analyzed both experimentally [39, 40] and numerically [41, 42]. In such a fashion, a two-dimensional approach allows for studying the turbulent features in the von Kármán vortex street occurring in the wake in a more organized fashion than in a finite-length wall-mounted cylinder [43, 44].

However, the more complex flow encountered in wall-mounted cylinders is characteristic of important technological applications such as pollutant dispersion in urban environments and impact on pedestrian comfort [2]. The flow around a wall-mounted square cylinder of finite length is highly three-dimensional. The topology of the flow consists of free-end downwash flow, spanwise shear flow and upwash flow from the wall, which relate to the tip, base and spanwise vortices. Due to the interaction between these three components, the near wake is then characterized by an arch-shaped structure downstream the obstacle [45]. The formation of the arch vortex, which consists of two spanwise vortical legs, one on each side of the cylinder, and their connection or bridge near the free end, is closely related to the symmetric shedding modes, which induce an arch-type structure even on the instantaneous field [7]. This section aims at providing an overview of the main vortical structures present in the flow around two wall-mounted obstacles using the mean-flow streamlines, which are obtained from the database discussed in § II.

Hunt et al. [1] performed an experimental analysis in order to examine the general pattern of the streamlines of the flow around a single surface-mounted bluff obstacle. They concluded that a closed mean streamline surface did not exist in the wake of the obstacle due to the interaction of 4 different vortical structures: the horseshoe vortex formed around the obstacle, the roof vortex and the vortices of the obstacles sides, both having a strong interaction with the wake, which yield to the so-called arch vortex downstream the obstacle. Therefore, the characterization of these vortices allows the hypothesis of no-closed surface in the wake to be established. The interaction between these structures emerges from the trailing vortex pattern that starts at the upper corners of the cube. This pair of counter-rotating vortices are known to extend farther downstream the obstacle, forming a dipole or a quadrupole structure depending on the obstacle aspect ratio. Wang and Zhou [45] found that above a critical falling in between \( h/b = 3 \) and 5 (\( h \) and \( b \) being the height and width, respectively) the streamwise vorticity distribution was of a quadrupole type and below this critical value, the distribution was of a dipole type. Burgeois et al. [46] reviewed the salient flow features using the experimental results from an open-test-section suction wind-tunnel. They identified the vortex cores by means of the \( \lambda_2 \)-criterion [12] and they confirmed the existence of a single pair of streamwise vortices in the wake (for \( h/b \) below the critical value).

Meinders [10, 47] extended the work on flow structures around wall-mounted cubes by analyzing the interaction between the obstacles when more than one cuboid was introduced. Using oil-film visualizations, Meinders experimentally analyzed the influence of the separation distance between the obstacles, i.e. \( \ell \), on the flow around an in-line tandem disposition of two cubes. It was proved that the separation variance only led to a substantial modification of the mean flow patterns. In Fig. 2, the streamline time-averaged flow patterns for the three flow regimes are depicted. These flow regimes are the skimming flow (SF), the wake interference (WI) and the isolated roughness (IR) [2]. The main conclusions here addressed are in good agreement with the experimental results of Meinders [10]. For the lowest separation \( \ell/h = 1 \), i.e. the skimming-flow regime, the separated shear

![Image 1](image1.png)

(a) Skimming flow  
(b) Wake interference  
(c) Isolated roughness

FIG. 2: Main vortical structures formed around two wall-mounted obstacles with different separation ratios: (a) \( h/\ell = 1 \), (b) 0.5 and (c) 0.25, visualized by means of streamlines. Note the arch on the leeward side of the obstacles. The arrow indicates flow direction.
layer reattaches on the downstream side edge of the downstream obstacle, which leads to an inter-obstacle region characterized by an arc-shaped vortex, confined by the flow on the sides and the separated shear layer. In addition to this, a horseshoe vortex emerges upstream of the windward face of the leading cube and it is deflected downstream along the sides due to the presence of the downstream obstacle. The wake-interference regime, with a separation ratio \( \ell/h = 2 \), exhibits similar flow patterns to those of the skimming flow. However, in this case, the intermediate arch vortex does not span the whole region in between the obstacles; the separation is large enough for the flow on the sides to interact slightly with the inter-obstacle region. For the isolated-roughness regime, i.e. \( \ell/h = 4 \), the flow eventually reattaches within the inter-obstacle region; the shear layer detaches from the sides and top edges of the upstream obstacle and breaches the inter-obstacle spacing before reattaching on the lower wall. Because of that flow reattachment, a second horseshoe vortex emerges in front of the downstream cube. In the three flow regimes, a second arch vortex is formed on the leeward side of the downstream obstacle, albeit with a lower intensity. This is mainly due to the flow disruption of the upstream obstacle, which induces a different turbulent-intensity level upstream of the second one [2, 9, 47].

V. SPATIO-TEMPORAL STRUCTURES: UNDERSTANDING URBAN FLOWS

Data-driven modal decompositions are powerful techniques to extract the energetically-important features from a given flowfield. Having identified the main flow structures present in the time-averaged fields in § IV, the analysis over the instantaneous fields will allow for the characterization of the main mechanisms driving the flow dynamics. In this section, we first analyze the results obtained using POD for modal decomposition of the urban database discussed in § II. In Fig. 3 we show the singular-value distribution normalized with its maximum value \( \sigma_m / \sigma_1 \), where \( m \) represents the mode number, and the cumulative energy for the POD modes corresponding to the three reference cases. The objective is to identify energy gaps that make some modes energetically more relevant than others. However, this distribution is highly dependent on the input data, where the number of fields varies from case to case, see § II. Despite this, an energy gap between the second and third modes for all regimes reveals that the first two modes contain the more relevant information of the flow. The energy of the most dominant POD mode for the wall-normal component, in particular, represents roughly 45% of the maximum energy value of the other velocity components. This means that the influence of the wall-normal velocity fluctuations is lower than that of the other velocity components. This is consistent with the findings of Monnier et al. [11], who discovered that for a zero-incidence angle, the streamwise and spanwise fluctuating components are more significant than the wall-normal component. On the basis of the above, the wall-normal component will be omitted from the analysis and only the streamwise and spanwise components will be further studied for the three flow regimes.

Starting with the streamwise velocity field, Fig. 4 depicts the orthogonal POD basis for the modes corresponding to the three flow regimes. First of all, regarding the first two modes, it could be noted their apparent similarity, dominated by fluctuating regions on both sides of the blocks, mainly due to the interaction of the wake region with the shear layer on both sides. These regions match with the high-turbulent-kinetic-energy (TKE) regions of the streamwise component identified by Monnier et al. [11] for an array of building-like blocks. However, the main differences among regimes depend on the position of the

![FIG. 3: Left: Singular-value distribution normalized with its maximum value \( \sigma_1 \) of the POD modes corresponding to the complete set of velocity components (streamwise, wall-normal and spanwise) of the (red) skimming-flow, (blue) wake-interference and (black) isolated-roughness regime. Right: Cumulative singular-value spectrum normalized with the cumulative sum of the eigenvalues \( \sum_{i=1}^{M} \sigma_m \), where \( m \) indicates the number of modes. Note that the number of retained modes coincides with the number of columns of the snapshot matrix, i.e. 225, 215 and 90, respectively.](image-url)
secondary structures, which are associated with the downstream block. For instance, while these fluctuating regions span the zone in between the obstacles for the skimming flow and the wake interference cases, in the isolated roughness, they are only located on the immediate leeward side of the upstream block. In such a fashion, increasing the separation of the obstacles does not yield more fluctuating regions, at least for the more energetic modes, as it occurs in a vortex-shedding case. The structures observed in the first two modes are remarkably similar to those associated with the high-frequency vortex-breaker modes. Higher modes are more focused on the wake as well as the creation of these vortical structures. Particularly, for all cases, the third and fourth modes are clearly impacted by certain major fluctuating areas on the wake. This pattern is quite similar to that of the time-averaged field, therefore these results suggest that these modes can be associated with the formation process of such structures.

After these first modes, the similarity among the many cases begins to diverge, each with its own set of properties. In the isolated-roughness regime, modes 5, 6, 7 and 10 exhibit flow structures around the downstream obstacle independently, a fact that suggests that the flow behaves independently around both obstacles. This is the only regime providing such isolated structures. The difference between the skimming-flow and the wake-interference regimes, on the other hand, is based on the intersection of the fluctuating areas in the wake-interference regime owing to the increasing spacing between the obstacles, as shown in modes 4 and 6.

In terms of the spanwise component, Fig. 5 depicts the set of POD orthogonal modes for all flow regimes. On the basis of the singular-value distribution of Fig. 3, the first two modes will be firstly analyzed. Unlike the streamwise-component scenario, increasing the distance between the obstacles increases the number of high-intensity flow structures of spanwise fluctuating regions, although the width of these structures decreases. These results could be connected to the interplay of lateral flow within the canopy, which suggests that the arch vortex formed on the leeward side of the upstream obstacle is shattered. Moving on to the modes that are related to the creation of such vortical structures, it is worth noting that modes 6 and 7 are not as uniform
as the previous ones; the two separated and symmetric areas may suggest that these areas are connected to the formation of each of the legs of the arch vortex. The spanwise-velocity component, like the streamwise one, reveals some isolated features exclusively for the downstream obstacle of the isolated-roughness regime. As a result of the loss of energy in the flow after the first obstacle, the method identifies two types of flow structures, placed upstream and downstream of the obstacles.

Each of these POD modes are associated with temporal coefficients, and a quantitative analysis can be performed on them with the aim of characterizing their dominant frequencies. The fast-Fourier-transform (FFT) technique will be used to generate, from the temporal data, the power spectrum revealing the most prominent frequencies of each mode.

Fig. 6 depicts the power spectrum for the first ten POD modes of all flow regimes. Low- and high-frequency modes within the frequency range $[0, 2]$ are distinguished for the three flow regimes. Frequency values are found to match in all cases, with the isolated-roughness case yielding clearer results due to a higher power-spectral density in the peak frequency. The first two modes are dominated by a peak frequency in the range $\omega_m = [1 - 1.2]$. Modes 3 - 6 are seen to be of low frequency, which suggests that they could be connected with the creation of significant vortical structures such as the arch vortex. Higher modes present flow structures which might result from the combination of the previous modes and if even higher modes ($m > 10$) were studied, certain high-frequency phenomena would be captured due to the smaller turbulent-flow scales associated with them.

Because of the large number of frequencies and spatio-temporal structures present in turbulent flows, identifying flow patterns is challenging, and therefore it is critical to test the robustness of the results. To that end, the previous results will be compared to those obtained with a highly efficient tool for the analysis of complex flows, i.e. the higher-order DMD. The modified Koopman operator employed in the HODMD algorithm yields a solution fulfilled by all sub-groups of data (snapshots) simultaneously evaluated and capable of capturing large-scale and large-amplitude features from the highly-varied frequencies seen in the flow \[48\]. Therefore, the HODMD algorithm (also known as DMD-d) is used for this purpose with varied tolerances and values

FIG. 5: POD orthogonal basis of the spanwise velocity fields at $y/h = 0.25$ for the different flow regimes. For each regime, from the upper left to the lower right, first to tenth modes are sequentially presented. Contours of the velocity of the modes are normalized with the $L_\infty$-norm and vary between $-1$ (blue) and $+1$ (red).
FIG. 6: Power spectrum of FFT scaled with the Strouhal number $St$ and applied to the temporal coefficients of the POD modes: (red) skimming-flow, (blue) wake-interference and (black) isolated-roughness regimes. As in Figures 4 and 5, modes from 1 to 10 are shown from top-left to bottom-right.

In Appendix A we provide a detailed overview of the calibration process of the identification method of the modes. In particular, Fig. 7 shows the frequency versus amplitude of the different modes computed using DMD-d for the three flow regimes. Although this technique can be used to analyze datasets with snapshots that are not equally spaced in time, the intricacy of the flow described here would make modeling much more challenging. As a result, the DMD-d analysis can be conducted considerably more efficiently if the data specifications in Table I are used. The very large number of modes calculated with each variation requires the use of well-established criteria to identify the most robust modes that best characterize the entire system [48]. The dominant mode, i.e. the one with the highest amplitude, is located between the frequencies $\omega_m = 1$ and $\omega_m = 1.2$, while the rest of the modes are subharmonics and harmonics of it. This mode will be referred to as mode A. In addition, another relevant mode is the one with the lowest frequency ($\omega_m = 0.1$), called as mode B, since it is the first mode to appear in the spectrum and the periodicity of the main physics is led by its frequency. Hence, studying in detail the two modes selected, will provide a general idea of the main dynamics driving the flow. Details about the remaining modes are presented below in § V C. It is worth noting that for the SF case, the method identifies two large-amplitude modes with similar frequency values, a fact that does not occur for the other two flow regimes. However, we have selected the higher amplitude mode as mode B in this case. The lower-frequency mode, mode A, has been selected comparing the three different test cases satisfying the criterion $|f_{m1} - f_{m3}| < \epsilon$, where $f_{m1}$ and $f_{m3}$ represent the frequency value in two different test cases and $\epsilon$ is a tolerance set by the user. Besides, the modal-assurance criterion [49, 50] has been used to conclude that the mode selected in the three cases as modes A and B represent the same flow physics. Note as well that the relative error made in the calculations remains fenced in the set of tolerances used. The goal of this study, however, is to identify the largest-amplitude modes in order to provide a broad description of the fundamental patterns driving the flow, rather than to build any accurate reduced-order models based on the

FIG. 7: DMD-d modes. Amplitude scaled with its maximum value ($\hat{a}_m = a_m/a_0$) versus frequency $\omega_m$ computed for (red) skimming flow, (blue) wake interference and (black) isolated roughness. The modes here represented are the result of a calibration process of the user parameters, from where $\epsilon_{\text{SVD}} = \epsilon_{\text{DMD}} = 10^{-3}$, $d = 20$ for SF ($K = 225$ snapshots) and WI ($K = 215$ snapshots) and $d = 10$ for IR ($K = 90$ snapshots) have been selected as reference.
physical knowledge of the flow. As a result, the relative error will not be examined further in this study.

Fig. 8 shows a three-dimensional view of the main DMD modes presented in Fig. 7 as a function of the separation ratio between the obstacles, aiming at providing a general overview of the main flow structures related to each mode. Fig. 8 (left) corresponds to the vortex-generator low-frequency mode, mode A, whereas the vortex-breaker high-frequency mode, mode B, is depicted in Fig. 8 (right). Indeed, their structures are linked to the first two highest-in-energy POD modes. These results are further discussed in the following sections.

A. Generation process of the main vortices

In the first case, the vortex-generator mode presents some characteristic three-dimensional structures which relate to the formation of the arch and horseshoe vortices in a low-frequency fashion. First, with regard to the streamwise velocity component, a dome-like structure prevails in the intermediate section of the obstacles. Increasing the distance between the obstacles does not result in a reallocation of such a flow pattern, which remains in the same place throughout all flow regimes. This indicates that when the flow reaches this region in the WI and IR cases, it interacts with the canopy, which does not happen in the SF regime, where the flow in between the obstacles remains trapped, i.e. the spherical structure covers the same region as the separated zone between the obstacles. Note as well that the dome feature in the IR case is complemented by a structure on the wake which extends through both lateral sides up to the leeward side of the downstream obstacle. These conclusions were already extracted from the analysis of the time-averaged fields in the streamwise direction at the symmetry plane \( z/h = 0 \), where the increased separation between the buildings yielded a higher interaction of the flow within this zone. On the other hand, although not presenting relevant flow structures in the constant-\( y \) planes analyzed in Fig. 9, the wall-normal velocity component of mode A exhibits a three-dimensional pattern on the upper windward side of the upstream obstacle, which is shared among all the flow regimes. At this location, the flow experiences a high-velocity region due to the impact of the flow over the edge and the shear layer on the upper part of the obstacle. This region is then followed by another fluctuating part in the wall-normal direction in between the obstacles. Albeit to a lesser extent, the downstream obstacle in the IR case also exhibits a similar flow structure. Finally, similar to the wall-normal component, the flow encounters a high-spanwise velocity gradient over this zone owing to the effect of the flow over the edges of the first obstacle, which tends to deviate the flow towards the outside regions of the domain.
(a) Skimming flow

(b) Wake interference

(c) Isolated roughness

FIG. 9: DMD modes of the streamwise and spanwise velocity fields with selected frequencies, represented at $y/h = 0.25$ for the different flow regimes. Contours of the velocity of the modes are normalized with the $L_\infty$-norm and vary between $-1$ (blue) and $+1$ (red). The bold-face frequencies represent the vortex-generator and the vortex-breaker modes, modes A and B, respectively. The rest of the modes are the result of the interaction between the above-described modes and are known as harmonic modes.

Furthermore, the second obstacle has comparable structures on its windward lateral edges as a result of the flow reattachment that occurs in the IR case. On the other hand, due to the slight interaction of the flow in the spanwise direction within this region, several fluctuating zones develop in between the obstacles. This characteristic distinguishes this generating mode from the breaker modes, which exhibit substantial spanwise variations between the obstacles. This result suggests that these structures could be connected with the destruction of the vortical structures in this region. To conclude, it can be state that the flow features that dominate in the vortex-generator mode are located close to the first obstacle rather than on the wake, emphasizing the idea of being a formation-type mode.

B. Breaking process of the main vortices

The three-dimensional structures of the vortex-breaker mode are illustrated in Fig. 8 (right). This mode is closely connected with the wake as opposed to what was observed in the previous case. For all of the flow regimes investigated here, the spanwise-fluctuating areas are shown to occupy the whole intermediate zone between the obstacles. As a result, increasing the distance between the obstacles leads to a greater number of fluctuation areas in the spanwise direction: in the IR case, up to three alternating structures may be seen, whereas only one can be seen in the SF regime. Conversely, the streamwise component of the
FIG. 10: Main flow patterns of the vortex-generator and vortex-breaker modes shown in Fig. 7 visualized by means of streamlines for the three flow regimes. The arrows indicate the direction of the flow in each panel. Note the arch-shaped structure on the leeward side of the upstream obstacle and the helicoidal flow structures in between the obstacles.

present mode does not exhibit the same behavior; the structures on the leeward side of the upstream obstacle remain unchanged for all three flow regimes. However, another oscillating zone arises connected to the downstream obstacle, the position of which is modified among the various regimes. Finally, in terms of velocity in the wall-normal direction, as the separation increases, the flow interacts inside the canopy with considerably more significance, resulting in larger flow structures for both the WI and IR cases.

Apart from being quite similar to those of the first two POD modes, these structures are consistent with the results of Monnier et al. [11], with strong streamwise fluctuations on both lateral sides and a high turbulent spanwise region near to the windward side of the downstream obstacle. The arch vortex is known to exist between these regions, and these structures will be related to the process of breaking rather than creation, owing to its location on the wake.

C. Interaction of vortex-generator and vortex-breaker modes

Finally, the three-dimensional structures of the most significant DMD modes can be compared to those of the various modes identified by the algorithm. Specifically, the following lines will be dedicated to the classification of the modes in vortex-generator or breaking-vortex modes based on resemblance with the prior patterns. This allows for selecting the more robust modes identified by HODMD using a varied set of parameters. To complement the previous results related to modes A and B, Fig. 9 shows a contour representation of the DMD modes presented in Fig. 7. By general inspection, one could see the structures previously discussed for the main HODMD modes, which are highlighted in bold. From these structures, a limit frequency can be established such that greater frequency values result in flow patterns more focused on the wake and thus being of breaking-type.

For the SF case, the mode $\omega_m = 0.37$ still exhibits some flow trapped in between the obstacles and high spanwise fluctuations on the lateral edges of the first obstacle. Even though the flow in this region appears to be modified by the slight interaction with the surrounding flow, this mode can be thought of as a vortex-production mode with a different production mechanism. Higher-frequency modes ($\omega_m > 0.85$) are characterized as breaker modes since both the streamwise and spanwise components share the same flow features as the main one ($\omega_m = 1.22$). Note as well that higher-frequency modes exhibit smaller turbulent scales. This highlights the association of low-frequency modes with large flow scales (dominant patterns) and high-frequency modes with smaller turbulent structures. A similar conclusion can be extracted for the IR regime, where the threshold value is set for the mode with frequency $\omega_m = 0.57$, which shows some flow structures around the upstream obstacle combined with particular features on the wake. Hence, this mode may be regarded as a transitory mode between the vortex-generator and vortex-breaker modes. Finally, regarding the WI case, apart from the vortex-generator mode ($\omega_m = 0.13$), the lowest-frequency mode ($\omega_m = 0.45$) exhibits a flow pattern similar to that of the vortex-breaker mode. Therefore, in this situation, the threshold value should be set lower than this frequency, resulting in all modes fulfilling $\omega_m > 0.45$ becoming of breaking-type.
FIG. 11: Spectra of the STKD modes for the (left) streamwise and (right) spanwise directions. Amplitude scaled with the maximum value ($\tilde{a}_m = a_m/a_0$) versus wavenumber, $\alpha_m$ for the $x$-analysis and $\beta_m$ for the $z$-analysis, computed for (red) skimming flow, (blue) wake interference and (black) isolated roughness. The filled points represent the spatial modes obtained from the generator temporal modes while the empty markers represent the ones obtained from the breakers. The modes here represented are the result of a calibration process of the user parameters, from where $\epsilon_{\text{SVD}} = \epsilon_{\text{DMD}} = 10^{-4}$, $d = 5$ for every case.

The dominant flow structures of the above-described modes can be elucidated by means of streamlines. To that end, using this visualization technique, it is possible to relate the previous three-dimensional structures with the vortex-generating and vortex-breaking processes. Fig. 10 depicts the streamlines flow patterns of the vortex-generator and vortex-breaker modes for the three flow regimes. While the first mode resembles the arch-vortex structure, the second presents a helicoidal tunnel-shaped flow pattern in the region in between the obstacles, owing to the increased correlation in the spanwise direction. The location of these structures perfectly matches the gaps in between the velocity-fluctuating regions in the streamwise and spanwise directions. Therefore, since these regions define the location of such patterns, the number of structures is modified from case to case: up to three structures are observed in between the buildings for the IR regime. Consequently, the interaction of the flow within this region results in a mixing procedure, leading to the breaking process of the vortical structures.

Knowledge of the mechanisms of generation and destruction of relevant vortical structures within urban flows provides sufficient information to be able to perform studies of pollutant dispersion within urban environments, so that ground-level concentrations significantly higher than those occurring in the absence of the building can be avoided. Regions of strong recirculation have been demonstrated in the literature to increase the concentration of scalars [7]. In this sense, for pollutants emitted at street level, the vortex-breaker mode could provide, at a high frequency, a higher interaction with the surrounding clean air, while for the arc-generating mode, the flow between buildings could be hardly influenced by the flow outside. Therefore, B-type modes could be connected to the promotion of the pollutant dispersion within cities, whereas the generation of A-type modes should be minimized owing to their low interaction with the surrounding atmosphere. Another important aspect closely related with the pollutant-dispersion aspect is the direction of the fluctuations. Regarding vortex-breaker modes, the tunnel-shaped structures, mainly influenced by the arrow-shaped spanwise fluctuations, would disperse rapidly those pollutant emitted at the street level towards the atmosphere. However, the streamwise fluctuations, which are known to appear close to the building sides, produce an increased concentration of pollutants within the city.

After discussing the different generation and breaking mechanisms of the main vortical structures associated with the temporal modes obtained by HODMD, the STKD algorithm is applied to these modes in order to obtain the spatio-temporal modes, with the aim of understanding the mentioned mechanisms and how they link with the physics of the problem. As already shown in § III C, mode expansion can be applied to different spatial directions. In this work, we analyze both the streamwise and spanwise directions. Once the STKD is applied to the temporal HODMD modes, we obtain a spectrum of the spatio-temporal modes as can be seen in the Fig. 11 for both directions, where the modes obtained for the $x$-direction will be called X modes and the ones obtained in the $z$-direction will be the Z modes. As it is shown in this figure, the dominant wavenumber is $\alpha_m = 0.6$ for the X modes, and $\beta_m = 2.2$ for the Z modes. In general, the spatial modes obtained from the A modes have lower amplitude than the ones obtained from the B modes. After studying the results obtained from the spatio-temporal modes, it can be observed that the X modes are connected to the mechanisms of the breaking process and the Z modes showed the results of these mechanisms.

Fig. 12 shows the different structures appearing in the STKD analysis when applied to generator modes. The interaction zone for all the displayed modes is near and between the buildings, hence, the shedding of the arch vortex still have not started. This fact is also backed by the fact that the mean flow, represented by white-transparent structures, appears enveloping the structures.
of the dominant mode for each case preventing it from breaking. Many interesting phenomena can be extracted from these modes. Also, a phase shift appears in the streaks formed in the streamwise component of the Z mode between the real and imaginary part (the imaginary part is not shown for the sake of brevity), suggesting that these structures are traveling waves along the spanwise direction. It can also be seen that this structures move along the streamwise direction. For the Z modes, the streaks that appear in the streamwise component of the velocity envelope both buildings for the SF and WI regimes while these streaks are divided, creating a new structure in the second building. This phenomenon occurs since the IR regime has enough distance between the buildings for the turbulent flow to adapt. Something similar happens for the wall-normal component, where the cap-like structure starts to appear again in the second building.

Regarding Fig. 13, where the vortex-breaker modes are shown, the structures of the Z modes continue appearing between the buildings rather than on the sides of the buildings, which is what was expected. The reason behind this phenomena lies in the strong streamwise influence present in the flow, making the breaking mechanisms to appear near the arch vortex. Still, there is a big difference in the interaction of the dominant mode with the mean flow, since in the generator case it wraps the structures while in the breakers it cuts them. As explained previously, the Z modes show the results of the breaking mechanisms shown on the X modes. The X modes display large streamwise structures on the sides of the buildings (except in the IR case) that indicate the destruction of the main vortices and generating the turbulent wake. The results of this mechanism are shown in the Z modes, where a large cluster appears between the buildings after the arch vortex, suggesting an association with the shedding of the arch vortex.
FIG. 13: Three-dimensional iso-surfaces of the different spatio-temporal modes obtained from the breaker modes. (Top), (middle) and (bottom) show the SF, WI and IR cases respectively, while each column represents a different mode: the first column shows the streamwise velocity of the temporal generator mode, the second and third columns display the streamwise and wall-normal velocity of the dominant Z mode with a wavenumber of $\beta_m = 2.2$, and the last column represents the streamwise velocity of the dominant X mode with a wavenumber of $\alpha_m = 0.6$. Red and blue denote positive and negative velocities respectively, and the white-transparent structures represent the mean-flow of the spatio-temporal modes with zero wavenumber.

VI. SUMMARY AND CONCLUSIONS

A simplified urban environment model consisting of an array of two buildings with variable spacing ratios was examined using high-fidelity simulations. These simulations were carried out to provide a complete physical description of the fundamental mechanisms controlling the dynamics in different urban streets. The aim was to provide an insightful analysis of the physics of the flow within environments that simulate different types of urban areas. The growing expansion of cities boosts the search for physical models capable of reproducing the pollutant and thermal distributions within cities. Here, the three-dimensional flow patterns responsible for pollutant dispersion have been characterized. Isosurfaces and contour slices were used to demonstrate the complicated flow behavior of the modes identified by the POD and HODMD algorithms. The results show that the flow behavior can be split into low- and high-frequency phenomena, each with significant consequences related to the formation and destruction of vortical structures such as the arch or horseshoe vortices. The low- and high-frequency modes are named vortex-generator modes since their associated structures have been related to the mechanism triggering the formation of the arch vortex formed on the leeward side of both buildings. These structures are particularly noticeable on the windward side of the upstream obstacle for the wall-normal and spanwise velocity components and the leeward side for the streamwise one, which defines the location and shape of the arch vortex. Furthermore, this location is kept constant among the different flow regimes, which highlights the idea that the process of formation of the arch vortex does not strongly depend on the separation between the obstacles. HODMD, on the other hand, identifies a high-frequency mode that correlates with the largest-amplitude mode in all cases. Because of the streamline flow patterns in the intermediate section of the obstacles, they are referred to as vortex-breaker modes. The large amplitude of these modes emphasizes their importance in this sort of urban flow. Indeed, their structures are linked to the first two highest-in-energy POD modes. Furthermore, as the separation increases, the flow becomes more correlated in the spanwise direction, owing to the more significant interaction of the flow with the wake layer inside the canopy. This effect yields to fluctuating velocity regions occupying the whole section between the obstacles, thus being associated with the destruction of the vortical structures rather than their formation. Besides, the vortex-breaker modes will be
responsible for the emergence of high-TKE regions on both sides of the obstacles and on the windward side of the downstream obstacle. Interestingly, these results are consistent with the wind-tunnel results of Monnier et al. [11], performed on a scaled and slightly more complex urban environment. Therefore, the conclusions of the present work can be extrapolated to more realistic urban environments by considering that turbulence levels from one street to another are expected to decrease significantly. It is also interesting to note that the results provided by both POD and HODMD show that the wall-normal velocity component does not significantly influence the more prominent structures as the streamwise and the spanwise components do. Regarding the results obtained from the STKD analysis, the Z modes display the results of the mechanisms obtained in the X modes about the generation and destruction of the coherent structures. When analyzing the temporal generator modes, the X and Z modes show a phase shift between the real and imaginary parts. Consequently, traveling waves appear in each direction. In addition, the symmetry is conserved, and the influence area shows that the structures are still unbroken. On the other hand, when the STKD analysis is applied to the temporal breaker modes, the X modes show the main structures are broken, and the structures causing this destruction are shaped as large streaks in the streamwise direction. Meanwhile, the Z modes show the result of these mechanisms. To conclude, from an environmental point of view, urban areas with highly-separated buildings, namely the isolated-roughness regime, would exhibit much more interaction with clean air sources, thus enabling the rapid propagation of those pollutants emitted at the street level. However, power plants, commonly located close to urban centers, are also responsible for pollution issues within cities. In those cases, owing to the low interaction of the flow above the urban canopy with the streets, it would be convenient to decrease the separation between buildings, i.e. the skimming-flow regime. In such a fashion, the air at street level would also be in contact with clean sources of air through the arch-vortex legs.

Appendix A: Calibration process of the HODMD algorithm

The large number of phenomena associated with complex turbulent flows motivates the use of highly-efficient methods to properly identify the behavior of such dynamical structures. This Appendix aims at providing a brief summary of the calibration process concerning the HODMD algorithm. A well-established criteria must be used in order to identify the most robust modes that best characterize the system from the very large number of modes calculated with each variation. Fig. 14 shows the frequency versus amplitude of the different modes computed using HODMD with a variety of parameters for the three flow regimes. The largest-amplitude and lowest-frequency modes are selected since they possess the more relevant information about

![Fig. 14: DMD-d calibration. Amplitude scaled with its maximum value ($\hat{a}_m = a_m/a_0$) versus frequency $\omega_m$ computed with different tolerances for (top) skimming flow, (middle) wake interference and (bottom) isolated roughness. Squares represent $\epsilon_{\text{SVD}} = \epsilon_{\text{DMD}} = 10^{-3}$ and triangles, $10^{-4}$. Red, blue and black correspond to $d = 10, 20, 30$ for SF ($K = 225$ snapshots) and WI ($K = 215$ snapshots) and $d = 5, 10$ for IR ($K = 90$ snapshots).](image)
the system and the classification will be made based on this distinction. As highlighted in Fig. 14, these modes are known to form clusters throughout the spectrum. The amplitude and frequency of the selected modes will be, therefore, the average value of the collection of modes. The number of preserved modes is also a function of the tolerances employed, which were $\epsilon = 10^{-3}$ and $10^{-4}$ in this study. Similarly, the other user-controlled parameter, $d$, changes depending on the number of snapshots to be analyzed. The skimming-flow and wake-interference regimes, with $K = 225$ and 215 snapshots, respectively, were studied with $d = 10, 20$ and 50, whilst the 90 snapshots of the isolated roughness case were studied with $d = 5, 10$ and 15. Note that, as mentioned during the theoretical derivation of the Koopman operator (see § III B), when the number of snapshots is reduced, the value of $d$, which represents the characteristic sliding window process, must also decrease in the same proportion [48].

Furthermore, the relative error obtained in the calculations remains fenced in the set of tolerances used. The goal of this study, however, is to identify the largest-amplitude modes in order to provide a broad description of the fundamental patterns driving the flow, rather than to build any accurate reduced-order models based on the physical knowledge of the flow. As a result, the relative error has not be examined further in this study. Refer to Martínez-Sánchez [51] for a more detailed explanation of the calibration process and the influence of the error in the solution.

It is worth noting that when the distance between the obstacles increases, the flow complexity decreases, allowing a smaller number of snapshots to be used to estimate the same flow behavior. Note as well that, despite the fact that the number of snapshots in the isolated-roughness regime is smaller, the time span covered is of the same order of magnitude, as the time step between snapshots has been increased. This is particularly important when dealing with computationally expensive data, but one should bear in mind that in order to accurately represent smaller turbulent scales, a larger number of snapshots with a shorter time step should be utilized instead. However, in general, the HODMD provides a fair balance of computational cost and accuracy.

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