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Additional Information

- 1 Modal Decomposition of the unsteady non-reactive flow field in a swirl-stabilized combustor operated by a Lean
- 2 **Premixed injection system**
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13 ABSTRACT

14 This work is focused on the numerical study of low-order coherent structures of a high-swirled laboratory-scaled 15 combustor operated by a Lean Premixed (LP) injection system in non-reacting conditions through different flow modal 16 decomposition techniques. This will provide valuable insight into the time-spatial modal structure detecting coherent 17 spatial patterns. Experiments suggest the appearance of a self-excited hydrodynamic instability characterized by a single 18 dominant frequency. On the one hand, the dominant pulsating energy components associated with the Precessing Vortex 19 Core (PVC) are identified through the application of a Proper Orthogonal Decomposition (POD) to the instantaneous 20 velocity field. On the other hand, Dynamic Mode Decomposition (DMD) is proven to effectively highlight the relation 21 between the frequency of the most dominant unsteady vortex structures and their spatial distribution within the combustor. 22 Since DMD analysis generates a global frequency spectrum in which each mode corresponds to a specific discrete 23 frequency, its application has been demonstrated to be more efficient than POD when dealing with temporally coherent 24 problems. In this way, the DMD technique has proved to be a robust and systematic method that can give accurate and consistent interpretations of the periodic physics underlying hydrodynamic instabilities in the combustor studied in the 25 26 present investigation.

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28 KEYWORDS

29 Swirling flow, LES, PVC, POD, DMD

30 LIST OF NOTATION

- 31 D_{ext} external diameter of the swirler exit
- 32 f frequency of a given structure
- 33 M number of scalar flow magnitudes used in POD
- 34 *N* number of temporal snapshots
- 35 R_{ext} outer radius of injection
- 36 r grid-scale factor
- 37 St Strouhal number
- $38 \quad S_W \quad \text{swirl number}$
- 39 U POD left-singular vectors
- 40 $U_{Swirler}$ bulk velocity from the swirler
- 41 V_1 flow field POD matrix
- 42 *V*₂ flow field DMD matrix
- 43 W POD right-singular vectors
- 44 y^+ non-dimensional boundary layer distance
- 45 GREEK SYMBOLS
- 46 λ DMD modal eigenvalue
- 47 $\boldsymbol{\Phi}$ DMD modal shape
- 48 ϕ swirl vane angle
- 49 Σ POD diagonal matrix
- 50 ψ_i POD spatial modes
- 51 Δt time step
- 52 τ reference timescale
- 53 τ_{PVC} precession period of the central vortex
- 54 τ_{rot} rotation time scale associated with the Vortex Breakdown Bubble
- 55 ABBREVIATIONS

56	AMR	Adaptive Mesh Refinement			
57	CFD	Computational Fluid Dynamics			
58	CRZ	Central Recirculation Zone			
59	DMD	Dynamic Mode Decomposition			
60	ICE	Internal Combustion Engine			
61	LDI	Lean Direct Injection			
62	LES	Large Eddy Simulation			
63	LP	Lean Premixed			
64	PIV	Particle Image Velocimetry			
65	POD	Proper Orthogonal Decomposition			
66	PSD	Power Spectral Density			
67	PVC	Precessing Vortex Core			
68	SVD	Singular Value Decomposition			
69	RMS	Root Mean Square			
70	VBB	Vortex Breakdown Bubble			

71

72 1. INTRODUCTION

Aeronautical gas turbine engines present the main challenge of increasing the efficiency of the cycle while keeping the pollutant emissions below stringent restrictions [1]. This has led to the design of new injection-combustion strategies working on relatively problematic operating points such as those close to the lean extinction limit. In this context, the Lean Direct Injection (LDI) concept has emerged as a promising technology to reduce oxides of nitrogen (NO_x) for nextgeneration aircraft gas turbine engines [2]. Swirling flows are commonly found in most practical applications such as gas turbine combustors, swirl burners, furnaces,

Swirling flows are commonly found in most practical applications such as gas turbine combustors, swirl burners, furnaces, spraying machines, whirlpools, cyclone separators and vortex shedding from aircraft wings [3]. The effect of the swirl intensity in swirling jets is well defined in the literature [3-5]. The swirl number (*S*), defined as the ratio of the axial flux of angular momentum to the product of the axial momentum flux and a characteristic radius [6], is usually employed to quantify the swirling features. Strong swirl (i.e., $S > S_{cr} \approx 0.6$) leads both to the Vortex Breakdown Bubble (VBB) and the formation of a Central Recirculation Zone (CRZ), which is especially efficient both in improving fuel-air mixing and

84 in stabilising flames. Nevertheless, this also induces undesired effects in practical applications since the system becomes 85 less receptive to external control, increasing pressure drops in non-reacting flows and combustion instabilities with an 86 eventual local flame quenching in reacting applications due to the appearance of a Precessing Vortex Core (PVC). The 87 PVC is characterised by the precession of the swirling jet around its axis and usually appears after the onset of the vortex 88 breakdown. Such phenomena are strongly unsteady and three-dimensional, being complex to study experimentally and 89 even numerically. In this context, advanced statistical data processing techniques based on linear-algebra tools such as 90 the Proper Orthogonal Decomposition (POD) [7] and the Dynamic Mode Decomposition (DMD) [8] have emerged in 91 the recent past with the aim of shedding some light on the flow diagnostics to characterise their structure and extract 92 complementary information.

93 These two powerful tools complement each other and have been applied to extract the low-order coherent structures acting 94 as precursors of the global self-sustained oscillations. On the one hand, the POD technique serves to identify the modes 95 that represent the highest energy content through spatial correlations of a given flow field variable. Even though the 96 statistical analysis of flow fields using POD has been established as a valuable tool for the characterisation of coherent 97 vortex structures, it is not well-considered for reacting flows since its decomposition technique does not account for 98 density variations. On the other hand, the DMD technique allows detecting in a more precise (less biased) way both the 99 frequencies and the stability eigenmodes of the flow field through the extraction of spatial modal (low-dimensional 100 coherent) structures and their corresponding growth/decay rates.

101 Lumley [9] was the first to use the Proper Orthogonal Decomposition (POD) technique to track the behaviour of coherent 102 structures in turbulent flows. From then on, POD has been extensively used to analyse many different complex flows. In 103 the reciprocating ICE field, POD has been applied to analyse issues such as acoustic impact and spark-ignition misfire both experimentally [10-16] and numerically [17, 18], and more recently to study pressure resonance phenomena [19] 104 105 through CFD simulations. Meanwhile, in aeronautical research, POD has demonstrated to be useful for multiple 106 applications such as the analysis of the aircraft engine noise [20-22], and the optimisation of compressors [23, 24] and 107 turbines [25], being also able to identify from external aerodynamic fluctuations [26] to wing aeroelastic responses [27]. 108 Specifically, aeroengine combustors have been experimentally investigated through POD decomposition techniques. 109 Based on the PIV measurements, the presence of the Vortex Breakdown and the precession of the vortex core have been 110 partially revealed and characterised in strongly swirling jets using modal decomposition analysis both in non reactive [28-111 34] and reactive [35-37] conditions. Nevertheless, as a consequence of experimental diagnosis shortcomings (e.g.,

sampling frequency of the Stereo PIV system can be sometimes much smaller than the PVC frequency [30]), temporaland spatial-detailed CFD simulations have emerged as a potential tool to successfully characterise the coherent structures within the combustor through pressure, vorticity and species signals decomposition rather than dealing just with velocity. In this way, the POD technique applied to numerical studies has characterised the Vortex Breakdown Bubble and the transition to helical breakdown modes in non-reacting conditions [38, 39], the combustion dynamics and flame interactions in reactive conditions [40-43], and the impact of variations of thermal load and global equivalence ratio on combustion acoustics noise levels [44].

119 On the other hand, the Dynamic Mode Decomposition technique [8] has been used in recent turbulent flow investigations [45, 46]. So far, this post-processing tool has been limitedly employed for simple modal flow decomposition in 120 121 reciprocating engines [18, 19]. In fact, even in gas turbine research, its application to the combustion problem is still scarce, focused on experimental PIV data analysis based on velocity and vorticity fields [47], Schlieren jet flow [48] and 122 123 shear layer flow [49] measurements. It has been only in the very recent years when DMD has been successfully applied 124 both to experimental aero-engine investigations, such as cavity flows [50], fan [51] and combustion [52-53] noise, and to 125 CFD studies to a lesser extent (e.g., radial [24] and centrifugal [54] compressors, and swirled-stabilised lean combustors 126 [55]), where DMD has allowed obtaining flame structures and dominant acoustic modes.

127 The present work reports on a detailed numerical study of the low-dimensional dynamics of the pressure and velocity 128 field evolution in a gaseous-fueled swirled-stabilised academical combustor in non-reacting conditions for which detailed 129 measurements are available [56]. The primary motivation of this study is to develop systematic advanced mathematical procedures for the analysis of complex data sets used for comparison, validation and identification of physical 130 131 mechanisms. Precisely, POD and DMD modal post-processing decomposition techniques are applied to a Dynamic 132 Smagorinsky Large Eddy Simulation CFD model of an academic combustor operated by a Lean Premixed (LP) injection 133 system. The predictive capability of the model has been previously validated to reveal the unsteady behaviour of flow 134 field features in the chamber and its complex interactions with the geometry. This work constitutes the first attempt to 135 apply and compare POD and DMD techniques to the studied non-reacting test case. The non-reacting flow is known to 136 be a crucial step in LDI combustor research since the success or failure of ignition (and re-ignition at high-altitude) is known to directly depend on local conditions just before ignition, especially on the mixture quality and the turbulence 137 138 level at the near-injection region. Aditionally, by first considering a non-reacting case, the objective is to isolate the flow-139 dynamics solely related to the injection, decoupling the resulting modes and features from those related to combustion.

In addition, the reduced complexity when compared to a reacting case is helpful to define and validate the implementationof the data-driven modal decomposition techniques.

The application of these decomposition methods allows extracting the most energetic 3D spatial modes and reveal how to promote particular modes that may be of interest for the mixing process or, in reverse, how to weaken or even eliminate modes that may be harmful (e.g., in case their main frequency as identified by the decomposition techniques is close to a resonance frequency of the chamber, the turbine blades downstream, etc.). In addition, identifying the frequencies of the different modes can allow geometric modifications that redistribute the acoustic energy to a more convenient frequency band, for instance one that is already masked by other noise sources such as the compressor or the jet mixing process.

The remainder of the paper is organised as follows. In **Section 2**, an overview of the mathematical models of POD and DMD techniques is presented. **Section 3** describes the model combustor, spatial discretisation of the computational domain, and imposed boundary conditions. Furthermore, the model validation of the LES simulation is here reported together with the data preparation for decomposition. **Section 4** discusses the simulation outcomes, first in terms of predicted flow topology features, and then the POD and DMD decomposition results. Finally, the conclusions of the study, including a summary of the comparisons between POD and DMD, are given in **Section 5**.

154

155 2. DATA ANALYSIS TECHNIQUES

The Proper Orthogonal Decomposition (POD) and Dynamic Mode Decomposition (DMD) methods of ensembles of the instantaneous pressure and velocity fields are employed to obtain a deeper insight into the time-spatial modal characteristics of the unsteady coherent flow structures. Both techniques transform the pressure and velocity fields in a finite series of products of spatial functions with time-dependant coefficients.

160 **2.1. Proper Orthogonal Decomposition**

The Proper Orthogonal Decomposition (POD) technique, also called Principal Component Analysis (PCA) consists in the flow decomposition into coupled spatial and temporal orthogonal modes. In this way, the spatial structures comprising most of the flow field energy are identified through the ordering of the contribution of each mode. Please note that the full flow field can be reconstructed through the superposition of all modes. The evolution of the flow field in CFD simulations is usually presented in a sequence of *N* temporal snapshots (v_i).

165 The evolution of the flow field in CFD simulations is usually presented in a sequence of N temporal snapshots (v_i), 166 gathered in a matrix V:

$$V_1^N = \{ v_{1,} v_{2,} \dots, v_{N_i} \}$$
(1)

167 These snapshots should be separated by a constant time step (Δt_{POD}) and usually contain a quantity M of scalar flow 168 magnitudes such as velocity and vorticity components, density, pressure, or species.

169 POD can then be performed by solving the associated eigensystem of the diagonalised time-averaged correlation matrix

170 $V^T V$ [8]. Nevertheless, since $V^T V$ resolution can be computationally expensive (N x N matrix) an alternative approach

based on the Singular Value Decomposition (SVD) of *V* [57] is generally preferred:

$$\boldsymbol{V} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{W}^T \tag{2}$$

Here, the columns of U ($M \times N$ matrix) correspond to the left-singular vectors known as POD spatial modes ψ_i , which form an orthonormal basis of V. Note that the validity of this alternate approach is proved since the spatial modes are also the eigenvectors of $V^T V$. Next, Σ is a diagonal matrix of dimensions $M \times N$ whose non-zero elements correspond to the squared eigenvalues of $V^T V$ (usually called singular values) and thus represents the contribution of each spatial mode ψ_i to the total energy of matrix V, defined by Nikiforov [58] as the sum of all singular values. Finally, W corresponds to the right-singular vectors of V, being the temporal evolution $a_i(t)$ of each spatial mode ψ_i described by the rows of ΣW^T . Therefore, the overall flow field can be understood as a linear superposition of spatial and temporal data:

$$\boldsymbol{V}(\boldsymbol{x},t) = \sum_{i=1}^{N} \boldsymbol{\psi}_{i}(\boldsymbol{x}) \, \boldsymbol{a}_{i}(t) \tag{3}$$

The main interest of the POD technique is the possibility of dimensionality reduction, crucial in CFD simulations where output data is arranged in big matrices. In this way, the total flow field can be reconstructed by applying Eq. 3 taking into account a reduced number of modes *L* and ensuring that the reconstructed flow field \tilde{V} is the closest to the original by the minimisation of the Frobenius norm.

183 2.2. Dynamic Mode Decomposition

The Dynamic Mode Decomposition (DMD) technique aims at grouping coherent spatial features into modes (eigenvectors) of a single temporal frequency, allowing the identification of coherent but weakly-energetic modes in highly transient regimes. Recalling the matrix V_1^N introduced in **Section 2.1**, containing *N* snapshots of the flow field, and assuming these to be linearly correlated through an unknown matrix *A*, which in turn remains almost constant during the time $N \cdot \Delta t_{DMD}$ spanned by Eq. (4):

$$\boldsymbol{v}_{i+1} = A \boldsymbol{v}_i \tag{4}$$

189 Then, the evolution and dynamic characteristics of the flow field can be characterised by the eigenvalues (i.e., DMD

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- 190 eigenvalues) and eigenvectors (i.e., DMD modes) of this matrix. It should be clear that even if the flow field is non-linear,
- 191 matrix A provides a linear approximation of the flow evolution. Eq. (1) and Eq. (4) can be combined in matrix form:

$$\boldsymbol{V}_2^N = \boldsymbol{A} \boldsymbol{V}_1^{N-1} \tag{5}$$

- The eigendecomposition of A is usually too computationally expensive to be performed directly. Thus, Singular Value 192
- Decomposition (SVD) can be used again as in Section 2.1 in order to obtain $V_1^{N-1} = U\Sigma W^T$, then reformulating Eq. 5 as: 193

$$\boldsymbol{V}_2^N = \boldsymbol{A} \boldsymbol{U} \boldsymbol{\Sigma} \boldsymbol{W}^T \tag{6}$$

- Now, a new matrix \tilde{S} can be built through the manipulation of terms that are already known. The matrix \tilde{S} is constructed 194 195

ensuring *matrix similarity* with A:

$$\tilde{\boldsymbol{S}} \triangleq \boldsymbol{U}^T \boldsymbol{V}_2^N \boldsymbol{W} \boldsymbol{\Sigma}^{-1} = \boldsymbol{U}^T \boldsymbol{A} \boldsymbol{U}$$
⁽⁷⁾

Because of this similarity, the eigenvalues λ_i of \tilde{S} match those of A, with the advantage that \tilde{S} is of reduced size and easier 196 197 to solve. Then, the DMD modes Φ_i can be computed by mapping the eigenvectors y_i (eigenvector matrix Y) of \tilde{S} into the non-reduced space through U (note that U is the POD basis of V_1^{N-1}): 198

$$\boldsymbol{\Phi} = \boldsymbol{U}\boldsymbol{Y} \tag{8}$$

Since the numerical routine implemented in the present investigation normalise the calculated eigenvectors, it is necessary 199 200 to recover the modal amplitudes α_i . This can be easily done by solving the reconstructed flow field multiplied by the 201 unknown amplitudes against any snapshot of the flow [59]:

$$V_1 = \boldsymbol{\Phi}\boldsymbol{\alpha} \Rightarrow \boldsymbol{\alpha} = \boldsymbol{\Phi}^{-1} V_1 = Y^{-1} \boldsymbol{U}^* \boldsymbol{V}_1 \tag{9}$$

202 Please note that U is unitary and thus its conjugate transpose U^* is also its inverse. Now the system can be solved inverting 203 Y rather than the higher-order $\boldsymbol{\Phi}$. In this way, the full dynamics of the flow field, represented by the snapshot matrix at 204 discrete time steps t_k , can be reconstructed by the linear superposition of the DMD modes:

$$\boldsymbol{V}(\boldsymbol{x},t_k) = \Re\left\{\sum_{i=1}^{N-1} \boldsymbol{\Phi}_i(\boldsymbol{x})\alpha_i\lambda_i^{k-1}\right\} = \Re\left\{\boldsymbol{\Phi}\boldsymbol{D}_{iag}(\boldsymbol{\alpha})\boldsymbol{V}_{and}(\boldsymbol{\lambda})\right\}$$
(10)

Where $D_{iag}(\alpha)$ is the diagonal matrix of modal amplitudes, and $V_{and}(\lambda)$ is the Vandermonde matrix of the eigenvalues. 205 206 Furthermore, the single frequency (f_i) associated to each DMD mode can be recovered considering the time step (Δt_{DMD}) 207 between snapshots:

$$f_i = \frac{\omega_i}{2\pi} = \frac{\Im\{\ln(\lambda_i)\}}{2\pi\Delta t_{DMD}}$$
(11)

208 Finally, the calculated DMD modes need to be ranked in relevance. To do so, Kou & Zhang [60] have recently proposed

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a simple criterion that considers the evolution of each dynamic mode within the whole sampling space, and ranks them
 according to their contribution to all samples:

$$E_{i} = \sum_{j=1}^{N} |\alpha_{i} \lambda_{i}^{j-1}| \|\boldsymbol{\Phi}_{i}\|_{F}^{2} \Delta t_{DMD}$$
(12)

211

212 3. COMPUTATIONAL SETUP AND METHODOLOGY

213 **3.1. Computational domain**

The computational investigation has been carried out based on the experimental gaseous configuration of the CORIA academical combustor [56], whose 3D model is depicted in **Figure 1**. This burner configuration contains four major components: a plenum to tranquillize the flow before entering the swirler, a radial-swirl injection system, a square crosssection combustion chamber (100x100x260 mm) and a convergent exhaust to prevent air recirculation. The combustor employs a radial swirler, composed of 18 channels inclined at 45° with an external diameter of D = 20 mm. The swirler creates a swirling air flow in the combustion chamber, in which gaseous methane is injected through a tube (d = 4 mm) acting as fuel injector located in the centre of the swirler.



221 222

Figure 1. Global view of the CORIA single burner computational domain.

In this work, a premixed gaseous injection strategy has been simulated at ambient conditions (T = 298 K; p = 1 atm), for

which detailed measurements are available [56]. The operating condition corresponds to a global equivalence ratio of

225 0.75, where the swirler and the central jet are fed with 5.612 g/s and 0.236 g/s of a fully mixed air-methane mixture,

respectively. Meanwhile, an inlet flow velocity of 28.8 m/s gives rise to a Reynolds mean number of 35,000 based on the mean diameter of the convergent inlet.

228 **3.2. Numerical Setup**

229 The Large Eddy Simulation reported in this paper is performed with the commercial code CONVERGE[™] [61], which 230 allows using simple orthogonal grids and automates the mesh generation process. A second-order-accurate (upwind) 231 spatial discretization scheme is used for the governing conservation equations, while a second-order (upwind) implicit 232 formulation is set for time discretization. Meanwhile, the transport equations are solved using the PISO algorithm. A 233 variable time-stepping algorithm is used in the current investigation, where the time-step is automatically calculated each 234 computational cycle, ensuring that the maximum CFL-number does not exceed 0.8 anywhere in the computational domain 235 at any instant [61]. This results in time steps in the order of 1 to 2 µs. The Dynamic Smagorinsky LES sub-grid scale 236 model has been chosen for the treatment of turbulence to characterize the unsteady non-reacting flow field.

The meshing strategy here employed is selected from a previous work where the authors defined a methodology to derive a mesh as a compromise between spatial resolution and computational cost in order to work out this multi-scale problem [62]. In this regard, the three-dimensional domain is discretized in a structured grid of hexahedrons with a base cell size of 2 mm. To ensure an accurate prediction of the flow behavior, the cell size is reduced in areas where a finer resolution is critical to the accuracy of the solution (i.e., the flow behavior within the small passages of the swirler), by applying a grid-scale factor (r), according to:

$$L_{scaled} = \frac{L_{base}}{2^r} \tag{13}$$

Following the conclusions extracted in the mentioned mesh methodology, a scale factor of three is applied as fixed embedding to the swirler and combustion chamber entrance. Additionally, another scale factor of three is applied in the adaptive mesh refinement algorithm (AMR), both to increase the spatial resolution where velocity gradients are significant and to maintain the proper level of mesh near the wall (see **Figure 2**). In this way, y^+ values between 30 and 100 have been ensured, the Werner and Wengle wall model being then used to determine the tangential components of the stress tensor at the wall. The total number of cells depends on the simulation timing and varies among 15 and 17 million.

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Figure 2. Computational mesh illustrating the strategy considered, consisting in 3 levels of fixed embedding, 3 levels of AMR, and 2 layers with 2 levels of wall refinement.

252 A mesh scaling of twice the baseline mesh size was used to stabilize the flow field for a given time before automatically 253 scaling down to the base mesh size and starting the usage of fixed embedding and AMR tools. This time has been chosen 254 as 25 rotations of the large coherent structures generated within the combustor ($\tau = \tau_{PVC} \approx 2$ ms, see Section 4.1), i.e. $|t/\tau| = 25$ (50 ms of physical time). The simulation was run for an additional time of $|t/\tau| = 50$ (100 ms) to stabilize 255 256 the overall mass flow rate and the velocity fields with the final mesh strategy. From this point, hereinafter treated as the 257 origin of times $(t/\tau = 0)$ turbulent statistical averages and higher-order moments started being calculated $(t/\tau \ge 0)$. 258 Statistics were computed from $t/\tau = 0$ to $t/\tau = 50$ (i.e., for 100 ms). The overall computational cost of the simulation 259 (from $t/\tau = -75$ to $t/\tau = 50$) is about 35k CPU hours and 300 GB of RAM memory.

260 3.3. Model Validation

Before applying the modal decomposition techniques, the accuracy of the LES prediction was evaluated by comparing the mean and fluctuating velocity profiles to experimental data available for 5 radial stations (x = 0 corresponds to the centerline of the chamber) located downstream of the swirler exit. As an example, **Figure 3** shows the radial distributions of the mean axial and tangential velocity components and their root-mean-square (representing the turbulent velocity or fluctuations), at five axial locations (z = 5, 10, 20, 30 and 40 mm) within the CORIA burner.



266

Figure 3. Mean and RMS Axial (a) and Tangential (b) velocity profiles obtained from LES at five axial locations. 267 268 At a first glance, the global flow topology and the amplitude of the mean and RMS velocity profiles are well reproduced. 269 The mean velocity profiles (left side of Figures 3(a) and 3(b)) obtained from the CFD code show that the computed 270 velocity field is, qualitatively, in good agreement with experiments throughout the five stations and the LES seems to 271 accurately capture the jet opening angle, denoted by the peaks of the mean velocity components around x = 10 mm. 272 Moreover, the high mean tangential velocity values observed on the left side of Figure 3(b) confirm the strong swirl 273 number of the injection system at the injection plane, reaching values as high as those obtained for the axial component. 274 This leads to the formation Vortex Breakdown Bubble (VBB) and thus to the generation of a Central Recirculation Zone 275 (CRZ). On the other hand, the turbulent velocity, given by the root mean square value (i.e., the RMS depicted on the right 276 side of the figures), is slightly over-predicted. This could be partly attributed to the fact that the PIV resolution used for 277 measurements is 1 mm [56], which is larger than the LES filter size in the near-injection zone, resulting in smaller 278 measured RMS values due to averaging effect within the probe. For a complete model validation and LES quality 279 assessment, please refer to a previous work by the authors [62].

280 3.4. Data preparation for decomposition

281 In order to apply the modal decomposition procedures presented in Section 2, the instantaneous pressure field is exported

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to text files containing the cell centroid coordinates [**x y z**] and its corresponding static pressures **p**. For this analysis, a total of 200 snapshots are gathered during a simulated physical time of 20 τ (from $t/\tau = 30$ to $t/\tau = 50$), which implies a spectral resolution of 33.3 Hz. Data are then exported every 0.1 ms (±1 µs due to the variable time-stepping algorithm), corresponding to 50-100 simulation time steps. This implies obtaining a sampling frequency of 10 kHz, which is enough to apply the Nyquist criterion in order to isolate the relevant information. This allows optimizing both the processing computational cost and storage space.

However, since the adaptive mesh refinement algorithm is continuously modifying the number of cells, the spatial coordinates of each exported snapshot do not remain constant. Therefore, the raw data require some preliminary treatment as the decomposition techniques require constant spatial coordinates. In this previous step, a subset of 1 million random cells (preventing any user-induced biasing) is selected from the first snapshot and taken as spatial reference. A sensitivity study performed by the authors suggested the size of the subset provides an adequate compromise between computational cost and spatial resolution.

294 The procedure to relate the coordinates of the cell centroids of subsequent snapshots (which will have changed due to the 295 AMR, as stated) is to identify the nearest neighbour of each of the reference coordinates. To do so, a k-d tree data structure 296 [63] is generated in order to organize the raw coordinates from each new snapshot. Then, a searcher algorithm [64] 297 computes both the indices of the new snapshot cells that best match the reference coordinates and the Euclidean d_i between 298 them. A validation is performed to discard cells whose computed distance d_i to their corresponding reference is greater 299 than 1mm, thus ensuring spatial consistency. Hence, only the pressure and velocity values of the suitable cells of a given 300 snapshot are stored in the corresponding vector v_i defined in Section 2. Finally, once the snapshot matrix V is assembled, 301 rows with "NaN" values (from cells that failed the validation) are discarded, thus obtaining a suitable matrix of consistent 302 and continuous pressure and velocity values at nearly constant spatial locations.

303

304 4. RESULTS AND DISCUSSION

305 4.1. Flow Morphology

A preliminary analysis of the raw pressure and velocity fields is carried out to characterize the swirling flow dynamics and to assess the presence of time-evolving structures within the combustor. The generation of unsteady coherent structures depends mainly on the swirl intensity, defined by the swirl number S_W , which can be expressed according to Eq. (13) [65]:

$$S_w = \frac{1}{R_{ext}} \frac{\int_0^{R_{ext}} \rho u_z u_\theta r^2 dr}{\int_0^{R_{ext}} \rho u_z^2 r dr}$$
(13)

When S_W exceeds a critical value in the swirler outlet region (typically 0.6 in such flows [42]), a phenomenon known as Vortex Breakdown Bubble (VBB) occurs, leading to the formation of a Central Recirculation Zone (CRZ) encompassed by the inner mixing shear layer. In the present work, the swirl number evaluated in the injection plane of the combustion chamber is 0.76 [56], implying that the formation of a VBB is expected. The VBB can be described as the formation of a free stagnation point and a recirculation zone with a surrounding 3D spiral flow in the core.



Figure 4. Contours of instantaneous (a) and time-averaged (b) axial velocity at $t/\tau = 27$ in a central cut of the CORIA burner.

318 Figure 4(a) shows the contour of the instantaneous axial velocity field at $t/\tau = 27$, whereas Figure 4(b) depicts the 319 time-averaged axial velocity field. Even though the recirculation zones shown in Figure 4(b) may appear to be confined 320 regions with well-defined boundaries (zero-axial velocity regions are highlighted in black) the instantaneous flow field is 321 much more dynamic and complex. The time-averaged axial velocity field hides the highly unsteady local assymetry, 322 turbulent mixing, and interactions that take place in this region. The boundary of the CTRZ is barely seen in the 323 instantaneous field, which shows smaller and isolated recirculation zones with a high degree of unsteadiness. Furthermore, 324 the contours show that the LES grid can resolve a large extent of small-scale turbulent structures. 325 When the central vortex core starts precessing around the combustor axis of symmetry at a given frequency (f_{PVC}), it

326 produces hydrodynamic instabilities. The frequency of precession is a function of the combustor design and the swirl

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intensity at the inlet. This unstable mode, typically related to the VBB, can be defined as the Precessing Vortex Core 327

328 (PVC), and it is usually located along the outer boundary of the CRZ. Further downstream of the injection position,

329 turbulence breaks this large vortical structure into small scale ones, no coherent PVC being detected.

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Figure 5. Instantaneous visualization of the Precessing Vortex Core identified through a pressure iso-surface of the 333 instantaneous pressure $\bar{p} = 101.1$ kPa at $t/\tau = 25$.

334 The structure of the PVC generated within the combustor is well captured by LES and visualized in Figure 5 through an 335 iso-surface of the unsteady pressure field. The PVC presents an asymmetric shape around the central axis and tends to 336 align with it near the inlet. However, when it reaches the stagnation point, it forms a spiral pattern further downstream in 337 the axial direction. The image exhibits two rotating helicoidal branches ejected from inside the swirler entering the chamber and being reoriented by the mean rotating flow. The swirling motion induces a centrifugal force that drives the 338 339 large and coherent vortical structures away from the central axis. These coherent structures are the primary source of 340 unsteadiness in the swirler outlet region and have a substantial impact on flame propagation. In fact, the flame front can 341 be affected by the highly turbulent aerodynamic stretching caused by the PVC, thus leading to local quenching or 342 extinction.

343 The presence of instantaneous negative axial and tangential velocities in the region near the centerline of the combustion 344 chamber can be directly attributed to the existence of the PVC. Meanwhile, a rotation time scale associated to the PVC 345 can be defined to identify some unsteady flow structures, as shown in Eq. (14):

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$$\tau_{rot} = \frac{2\pi R_i}{u_{\theta,i}} \tag{14}$$

346 where R_i is the mean radius of the convergent inlet and u_{θ} is the mean tangential velocity component in the inlet plane of 347 the combustion chamber (see Section 3.1 for geometric details). For the combustor here investigated, the rotation time 348 scale evaluated though Eq. (8) at the combustion chamber inlet is around 2 ms.





³⁴⁹ 350 Figure 6. Time evolution of the PVC in one cycle of the precession motion. PVC is identified using an iso-surface of the 351 instantaneous pressure $\bar{p} = 101.1$ kPa.

³⁵² Figure 6 presents four different snapshots to show the development of the so-called branches of the PVC within one cycle 353 of the precession obtained from the LES. As can be noticed, the number of branches can vary with the course of time 354 since just one helicoidal finger-like structure is now visualized. The turnover (or one complete rotation) time of this vortex 355 structure is estimated at $\tau_{PVC} = 2.0$ ms, close to the rotation time scale defined by Eq. (14), and corresponding to a precessing frequency of about $f_{PVC} = 500$ Hz. The structure at $t/\tau_{PVC} = 32$ (considering an arbitrary absolute time after 356 357 the flow stabilization as the start of a given rotation) is aligned to the central axis, but at $t/\tau_{PVC} = 32.25$ it is taken away 358 from the core and turns in a spiral shape along the axial direction. The vortex spiral evolves from the shear layer due to 359 Kelvin-Helmholtz instabilities in both the axial and azimuthal directions. Once the vortical structure has completed one

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360 cycle, it is again driven towards the central axis and spreads outward rapidly breaking up into small-scale structures.
361 These helical filaments present counterclockwise winding in space and clockwise rotation in time. Moreover, velocity
362 vectors around the PVC showed clockwise rotation all along the filament. Indeed, the outer edge was observed to have
363 positive axial velocity, while the inner regions had reverse flow. This PVC motion afffects the flow evolution in the
364 combustion chamber and improves turbulence intensity and mixing levels. However, at given conditions a probable
365 resonant coupling with low-frequency acoustic oscillation in the chamber can exist. The behavior and incidence of the
366 PVC is more complex in reactive cases, not studied in the present work.

367

368 **4.2. POD decomposition**

369 A spectral analysis of the 3D flow field pattern is performed to capture the dominant coherent structures and confirm the occurrence of PVC in the swirler outlet region. Proper Orthogonal Decomposition is applied as described in Section 2 to 370 371 obtain the orthonormal spatial modes ψ_i (with their principal values σ_i) and their corresponding temporal evolution 372 coefficients a_i . The relevance of each mode is characterized by measuring their overall energy contribution (through the 373 principal values) to the total energy of the snapshot matrix. As the mean pressure of the chamber is not substracted, the 374 first POD mode ψ_l is homogeneously distributed through the chamber, resulting in a singular value σ_l that represents a 375 high percentage of the matrix energy (please note that the mean pressure is around 100 kPa, and the acoustic fluctuations 376 are small when compared to the mean component).

Since the main interest of this study lies on extracting the unsteady structures within the combustor, the first mode related to the mean homogeneous pressure can be ignored. In this way, the remaining pulsating energy distribution among the subsequent modes is shown in the Pareto chart of **Figure 7**. It can be seen that POD modes ψ_2 to ψ_{17} gather approximately 40% of the remaining energy, with 20% being gathered just by modes ψ_2 to ψ_6 . Meanwhile, modes ψ_2 to ψ_{100} represent 80% of the remaining energy, with the rest of the modes ($\psi_{101-208}$) representing just 20% of the remaining energy.

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FOD Mode $[\Psi_i]$ Figure 7. Pareto chart showing the singular values associated with POD modes ψ_2 to ψ_{208} and accumulated contribution to the remaining energy after discarding the first mode related to the mean homogeneous pressure.

385 Besides the energy contribution of each mode, the analysis of its evolution in the frequency domain is carried out using the information contained within the time coefficients $a_i = \sigma_i W_i^T$. In this regard, Figure 8 shows the amplitude of the 386 POD modes in the frequency domain based on normalized periodograms of right-singular vectors W_i^T . The strength of 387 the energy of each spatial mode is shown through the Power Spectral Density (PSD) function of the time coefficient 388 389 associated with its corresponding mode. The high energy content exhibited by modes ψ_2 to ψ_6 in Figure 7 is here 390 confirmed, and the spectral content of the higher-order modes (i.e., ψ_7 to ψ_{17}) appears nearly flat in comparison. It can 391 also be seen how each of the most energetic POD modes (ψ_2 to ψ_6) only feature a well-defined frequency of interest, 392 making it possible to attribute a specific phenomenon of known frequency to each mode when combined with the analysis 393 of the spatial distribution of the modal energy. Nevertheless, higher-order modes (ψ_7 to ψ_{17}) present some kind of spectral 394 mixing with several dominant frequencies ascribed to them. Furthermore, it is interesting to note how the two dominant 395 frequency peaks (i.e., 526 Hz and 1053 Hz) seem to have two different POD modes with the same spectrum associated. 396 This fact is consistent with the experimental measurements. (i.e., 507 Hz and 999 Hz, respectively) reported in the 397 literature [66].

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Figure 8. Power Spectral Density of the time coefficient associated with POD modes $\psi_{2.17}$ in the frequency domain. Finally, the spatial distribution of the POD modes can be visualized in **Figure 9** by plotting the values of the left-singular vectors ψ_i contained in the columns of U associated with each of the reference coordinates that were selected when building the snapshot matrix V. The POD modes are represented through an iso-surface of the 5% (blue) and 95% (red) percentiles of the distribution of the real values of the mode $\Re{\{\psi_i\}}$. In this way, the red and blue surfaces correspond to the opposite, most extreme values of the instantaneous pressure fluctuation, when reconstructed by multiplying the mode spatial amplitude ψ_i by the time evolution $a_i(t)$.

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409 Inspecting the shapes of modes ψ_2 and ψ_3 in Figure 9, it is clearly seen how the higher amplitudes are oscillating in 410 opposite sides at the periphery of the CRZ. This single helical instability, born inside the swirler and reoriented by the 411 mean rotating flow when entering the chamber, corresponds to the structure of the PVC defined in Section 4.1. In fact, 412 the computed frequency of 526 Hz associated to these POD modes completely matches the precession frequency of the 413 PVC, as estimated by Eq. (14) and represented in the time evolution of the PVC (see Figure 6). Please note that red and 414 blue iso-surfaces correspond to a single structure where instantaneous pressure assumes strong positive and strong 415 negative values separated by an angular distance of about π . Furthermore, these modes ψ_2 and ψ_3 resemble one another 416 and are shifted in phase by $\pi/2$ (see Figure 10). As already observed by Oberleithnner et al. in a swirling jet facility

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- 417 composed by four tangential slots [29], this first pair of modes describes a travelling azimuthal wave with wavenumber
- 418 /m/=1 having a $\pi/2$ phase shift.

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Figure 10. Frontal view of the spatial distribution of the first four POD modes ψ_{2-5} . Both mode pairs describe rotating structures with the same frequency with azimuthal wavenumber /m/=1 for modes ψ_2 and ψ_3 and with /m/=2 for modes ψ_4 and ψ_5 .

424 The next two modes (ψ_4 and ψ_5) in **Figure 9** are interesting since their amplitudes are again predominantly gathered in 425 the CRZ, but featuring a PVC with double spiral pattern structures and twice its rotating frequency (f = 1053 Hz). These 426 modes show a similar pattern to ψ_2 and ψ_3 but, in this case, characterized by the appearance of two vortices separated by 427 an angular distance of about $\pi/2$. In such a case, the two modes seem rotated about $\pi/4$ with respect to each other, so that 428 a travelling azimuthal wave with wavenumber m/m = 2 can be associated to them. The occurrence of this other coherent 429 structure explains what was hinted in Figures 5 and 6, namely the intermittent emergence and disappearance of the 430 branch-like structures of the PVC during the simulation. They describe coherent structures that are first growing and then 431 decaying in the streamwise direction. Since the angles of the two pair of modes (ψ_2 - ψ_3 and ψ_4 - ψ_5) are in a ratio of about 432 2:1 and being the azimuthal periods of the waves |m| = 1 and |m| = 2 in the same ratio, it can be established that the two 433 pairs of modes rotate at the same frequency and that the double helix (POD modes ψ_4 and ψ_5) is a harmonic of the single 434 helix (POD modes ψ_2 and ψ_3).

In contrast with previous modes, the maximum amplitudes of ψ_6 are contained in a more uniform shape (see Figure 9). Moreover, the frequency content of this particular mode, peaking around 190 Hz (see Figure 8), is quite lower than the previous PVC modes. This spatial mode can be attributed to the generation of a well-defined CRZ since its period of around 5 ms is really close to the minimum amount of simulated time that the instantaneous axial velocity component needs to be time-averaged in order to identify the CRZ in the mean axial velocity field. Therefore, this axisymmetric fluctuation of the sixth mode of the flow is related to the axial displacement of the vortex breakdown location and is not correlated with the identified harmonic structures.

Subsequent POD modes ($\psi_7 - \psi_{13}$) in **Figure 9** present a pattern of low-frequency and low-energy coupled effects. Since the flow is not entirely axisymmetric after passing through the 18 radial channels and emerging from the swirler, a high number of POD modes with similar but distorted shapes is expected as a consequence of the strong interaction among the unsteady PVC, the high turbulent CRZ and the strong shear layers. Finally, higher-order POD modes (ψ_{50} , ψ_{100} , ψ_{150} and ψ_{200}) are represented to demonstrate the smaller size of these low-energetic structures and how, even so, they remain connected in a dominant spiral pattern, which might suggest potential acoustics coupling.

448 **4.3. DMD decomposition**

449 As previously introduced in Section 2, Dynamic Mode Decomposition is a well-suited tool for an in-depth frequency analysis since each mode is forced to contain a single frequency. Following the procedure outlined in the theoretical 450 451 background, the relevance E_i of each mode is computed considering the totality of the snapshots and then normalized with $E_{i}/max(E)$ to evaluate the relevance of the resulting DMD modes Φ_{i} . In this way, Figure 11 shows a chart where 452 453 DMD modes have been ordered according to their associated frequency and ranked using a normalized Kou & Zhangs's 454 criterion [60], highlighting the eight most coherent modes at the frequencies of interest. Furthermore, the spatial 455 distribution of the highly energetic flow regions pulsating at these different six mode frequencies can be visualized in 456 Figure 12, following the same procedure used in the POD analysis.



457 **Frequency** [kHz] 458 Figure 11. Normalized relevance $E_i/max(E)$ of the spectrum of DMD modes, highlighting the six most coherent modes at 459 the frequencies of interest.

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featuring oscillation frequencies of 197, 527 and 978 Hz, respectively. These frequencies are consistent with the dominant and sub-dominant frequency given by POD analysis. In fact, the spatial distributions and the modal relevance information of the dominant DMD modes (i.e., $\boldsymbol{\Phi}_8$, $\boldsymbol{\Phi}_{20}$, $\boldsymbol{\Phi}_{48}$) represented in **Figure 12** confirm and validate the correlations between frequency content and spatial morphology of the associated structures suggested by the POD energy ranking. Furthermore, these energetic modes seem to be located in a more compacted/confined region than the higher frequency ones, which seem to penetrate further downstream the combustion chamber and get more disordered.



468 $\Phi_{140}(1735 \text{ Hz})$ $\Phi_{205}(2010 \text{ Hz})$ $\Phi_{94}(3077 \text{ Hz})$ $\Phi_{198}(4310 \text{ Hz})$ 469 Figure 12. Spatial distribution of the eight more coherent DMD modes within the combustor. Each mode is represented 470 by iso-surfaces indicating the 2% (blue) and 98% (red) percentiles of the spatial energy distribution of the real values of 471 each mode $\Re{\{\Phi_i\}}$.

473 As stated before, the benefit of DMD is that modes are organized in terms of a single frequency, unlike POD for which 474 multiple frequencies are forced to be grouped together making the individual impact of a single frequency more difficult 475 to discern. Hence, in addition to the main hydrodynamic PVC modes reported both in the POD analysis (Section 4.2) and 476 in the literature [29, 38, 52, 66], DMD here applied also allows detecting modal structures at higher frequencies, multiples 477 of the natural frequency -527 Hz- of the PVC (e.g., 1735 Hz, 2610 Hz, 3877 Hz and 4318 Hz), that do not respond to any 478 previous knowledge. These higher modes show more spatial variation in the azimuthal direction (see the cross-sectional 479 view in Figure 13), and a concomitant reduction in the scale of vortices when increasing frequency similar to the VBB 480 harmonics modes reported in [67]. This seems to indicate a source flow phenomenon related to each individual channel 481 of the swirler. Vortices appear to emanate from the swirler outlet region with decreasing vorticity towards the axial 482 direction. In this way, spiral structures with harmonically oscillating vorticity in the streamwise direction can be identified 483 presenting a given number of branches equal to the number of times the natural frequency of the corresponding mode.

484 This can be attributed to continued formation of shear layers vortices due to the higher shear strength of the structures 485 emanating from each of the swirler channels and its interactions with the turbulence present in the recirculation zone.



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To close the discussion, the Strouhal numbers based on the main frequency peaks detected through POD and DMD are
calculated. The Strouhal number of a given perturbation can be evaluated through Eq. (15):

$$St = \frac{D_{ext} f}{U_{Swirler}}$$
(15)

491 with f the frequency of the identified structure, D_{ext} the external diameter of the swirler exit and $U_{Swirler}$ the bulk velocity

492 entering the combustion chamber from the swirler. The two peak Strouhal number are summarized in **Table 1**.

	PVC (1 st harmonic)			PVC (2 nd harmonic)			VBB (CRZ generation)		
	POD	DMD	EXP	POD	DMD	EXP	POD	DMD	EXP
Frequency [Hz]	526	527	507	1053	978	999	191	197	165
St [-]	0.47	0.47	0.45	0.95	0.88	0.89	-	-	-

⁴⁹³ 494

Table 1. Strouhal numbers for the main frequencies identified using POD and DMD techniques

Regarding the Strouhal numbers found in the literature [68], a PVC is usually found for a Strouhal number higher than 0.8. The frequency around 1000 Hz corresponding to the intermittent emergence and presence of the double-helical instability (and closely related to the single-helical instability structure detected at 500 Hz) is then identified as the main frequency of the PVC and the primary source of unsteadiness despite not having the highest amount of unsteady energy computed by POD, as shown in **Figure 8**. Therefore, the limitation of POD when attributing any physical significance to a particular frequency present in the flowfield is noted here again since some of that unsteady energy is distributed between the remaining modes instead of being grouped in a single frequency.

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503 5. CONCLUSIONS

504 In this paper, different modal decomposition techniques have been applied to the pressure data generated by a Large Eddy 505 Simulation to investigate the characteristics of the most powerful coherent structures of strongly swirled jets in a Lean Premixed combustor undergoing vortex breakdown. The numerical data have been post-processed through Proper 506 507 Orthogonal Decomposition (POD) and Dynamic Mode Decomposition (DMD) routines to retrieve information about the 508 flow dynamics, providing a systematic approach to identify the main mechanisms that sustain instabilities in the 509 combustor. By considering the pressure information of the entire computational domain at once, including complex 510 geometries such as the radial swirler, the overall amplitude for each frequency is adequately identified according to the 511 overall unsteady energy available in the flow.

Both the POD and DMD analyses extracted similar flow dynamics results associated to a global self-excited oscillatory 512 513 mode, namely the Precessing Vortex Core (PVC), having a single dominant frequency. This hydrodynamic instability 514 mode results in double-helical vortices and leads to a counter-rotating co-winding helical structure located between the 515 inner and the outer shear layer, enveloping the recirculation bubble. In this way, both decomposition techniques allowed 516 detecting two distinct eigenfunctions corresponding to azimuthal wavenumbers |m| = 1 and |m| = 2, which have been 517 found to yield a helical or double-helical breakdown mode, respectively, that dominate dynamics of the whole flow. Thus, 518 the flow oscillations are coherent with the dominant frequency of the global mode and, taking into account the phase shift 519 between the decomposition results, the precession of the vortex core can be attributed to the same frequency.

In addition, the DMD method implemented also allowed identifying some complex pulsating, intermittent and cyclical spatial patterns related to the harmonic helical branches of the PVC, not detected in previous investigations. In this way, spiral structures with harmonically oscillating vorticity in the streamwise direction have been identified presenting a given number of branches equal to the number of times the natural frequency of the corresponding mode. This can be attributed to the continued formation of shear layers vortices due to the higher shear strength of the structures emanating from each of the swirler channels and opens the door to specific design modifications.

In the view of the results, both the POD and the DMD have successfully extracted the flow dynamics associated with the dominant global instability mode, corresponding to a double-helical precessing vortex structure. In this way, DMD can be preferred to POD when the identification of low-energy and short-lived modes is sought. Since DMD generates a global frequency spectrum in which each mode correspond to a specific discrete frequency, its application has been demonstrated to be more efficient than POD when dealing with temporally coherent problems. Nevertheless, the price to pay is to require a more diffuse metric than in POD, raising DMD as a less appropriate option for performing Reduced-

532 Order-Models (ROMs) in some circumstances. Notwithstanding, DMD technique has proved to be a robust and 533 systematic method that can give more accurate and consistent interpretations of the periodic physics underlying 534 hydrodynamic instabilities in the Lean Premixed combustor studied in the present investigation.

535

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