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1 **Reconstruction of the 3D hydrodynamics in a baffled stirred tank using Proper Orthogonal**  
2 **Decomposition**

3  
4

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12 In this work, the unsteady turbulent flow in a four-baffled stirred tank equipped with a Rushton  
13 turbine is computed with ANSYS FLUENT<sup>®</sup> using the sliding mesh technique. The POD algorithm is  
14 applied first to each mesh zone (fixed and rotating) and, in a novel and original way, to the full 3D  
15 CFD data without distinguishing between the stationary and rotating zones. The resulting modes  
16 cannot be regarded as spatial modes revealing the underlying flow structure. The POD results  
17 showed that 99.9% of the system variance is recovered with the first three modes. The  
18 reconstruction of the velocity field from these modes reveals the trailing vortices plus the mean flow.  
19 The accuracy of the POD reconstructed flow fields is quantified. The present work is the first  
20 evidence of a POD reconstruction of the unsteady turbulent flow performed over the entire 3D  
21 domain in a baffled stirred tank.

22

23 Keywords:

24 Proper Orthogonal Decomposition; full 3D velocity reconstruction; Computational Fluid Dynamics;  
25 RANS turbulence model; baffled mixing tank; Rushton turbine.

26 Highlights:

- 27 • 3D POD global reconstruction of mean and organised components of a turbulent flow in a  
28 baffled stirred tank.
- 29 • 3D POD application on fixed and rotating reference frames.

- 30 • Implementation of 3D POD on a mesh with a stationary zone and a rotating zone without  
31 zone separation.
- 32 • Accuracy computation through instantaneous and localized error for 3D POD reconstruction.

## 33 1. Introduction

34 Stirred tank reactors are widely used in chemical and biochemical industrial applications. The  
35 hydrodynamics of such systems has been the subject of numerous experimental (Ng & Yianneskis,  
36 2000; Bugay et al., 2002; Baldi et al., 2004; Escudié & Liné, 2004; Ducci & M, 2007) and  
37 Computational Fluid Dynamic (CFD) studies that revealed its complexity (Hartmann et al., 2004;  
38 Delafosse et al., 2008, 2009). Besides the hydrodynamic aspects, additional models describing the  
39 chemical or biochemical reactions have to be implemented in the CFD software in order to couple  
40 mixing and reaction and perform predictive simulations. In some applications, it is important to  
41 consider the time varying flow field but the computational cost for solving simultaneously  
42 momentum and chemical equations is often prohibitive. In such situations, it is advantageous to find  
43 a way to access the spatio temporal variation for the velocity field without solving the Reynolds-  
44 Averaged Navier-Stokes equations throughout the process duration. Since the flow in a stirred tank is  
45 periodic and organized, the reduced order model approaches, such as Proper Orthogonal  
46 Decomposition (POD), can be used to achieve this objective.

47 Due to its elegance and practicality, this mathematical procedure has been used to identify, study  
48 and model the dynamics of large-scale average spatial structures of the fluctuating velocity field for  
49 turbulent flow (Sirovich, 1987a, 1987c, 1987b; Berkooz et al., 1993; Borée, 2003; Joshi et al., 2009;  
50 Tirunagari et al., 2012; Du et al., 2013; El-Adawy et al., 2018). In terms of average kinetic energy,  
51 these large structures (named coherent structures) dominate in the fluctuating flow, it follows that  
52 their identification is crucial in the study of fluid dynamics. This fact evidences the relevance and  
53 convenience of the POD to identify such organized structures.

54 Specifically, POD allows the most energetic structures or modes (on average) of an ensemble of  
55 functions or experimental or numerical data to be extracted. Each of these modes will have a spatial  
56 part or field (topos, eigenvectors) and a temporal part (chronos). In this way, it is possible to identify  
57 and study the spatial organization and temporal variations of each POD mode. Such a decomposition  
58 is very convenient because it allows understanding the role of each component individually or in  
59 combination with other modes. Indeed, a linear superposition of selected POD modes can be used to  
60 represent all the members of the ensemble. The selection of modes to be used depends on the  
61 temporal and spatial scale of interest. It can also be shown that such a reduced order method is  
62 optimal in terms of minimizing the mean-square error between the input data and its modal  
63 decomposition. This fact represents an extremely attractive numerical advantage (Holmes et al.,  
64 1996).

65 The POD methodology has also been shown to be effective for studying instabilities (Hasal, 2000;  
66 Hasal et al., 2004) and the transition to the turbulent regime in fluids (Knight & Sirovich, 1990;  
67 Holmes et al., 1996). In Arányi et al., (2013) the technique was also used to study complex flows. This  
68 technique has also proved to be very useful for the analysis of turbulent flow fields in mixing tanks  
69 (Raju et al., 2005; Gabelle et al., 2013; de Lamotte et al., 2018b; Janiga, 2019; Fernandes del Pozo et  
70 al., 2020; Mikhaylov et al., 2021). For example Raju et al., (2005) implemented the POD algorithm to  
71 study the structures associated to the fluctuations about the mean flow induced by the impeller in a  
72 stirred tank. In this work, experimental PIV (particle image velocimetry) data were used as input to  
73 the method for different diameters of a Rushton-type turbine, and Reynolds numbers between 4,000  
74 and 80,000. Moreover (Liné et al., 2013) used experimental PIV data from a mixing tank to study the  
75 presence of coherent structures and the turbulent phenomena associated. In addition, the kinetic  
76 energy and its viscous dissipation were successfully obtained from the POD methodology. Likewise  
77 (Gabelle et al., 2013, 2017; Fernandes del Pozo et al., 2020) used the decomposition method in 2D  
78 PIV data to reconstruct organized motion induced by impeller blades without performing angle-  
79 averaged sampling. The manner in which energy was transferred between the POD modes was also

80 studied. Also it is reported in the literature the application of the POD on CFD data for the study of  
81 turbulent swirling flow in an axisymmetric sudden pipe expansion (Howard et al., 2017). The order  
82 reduction technique used proved to be quite robust in reducing the transient database, showing its  
83 potential to provide valuable insights into the flow structure. By using a large array of pressure and  
84 velocity data, POD was able to pick out several key flow features, including the movement of  
85 vortices, and the structure and period of the precessing flow. This was followed by the  
86 reconstruction of the flow field de Lamotte et al., 2018a, 2018b assessed the dynamics for a stirred  
87 tank by applying POD to a 2D domain using CFD and PIV data. As reported in this work, the reduced  
88 order method was able to decompose the fluid flow into different structures: mean flow, coherent  
89 structures, and turbulent flow. Also (Janiga, 2019) applied the POD algorithm for the analysis of  
90 coherent structures and macro-stability present in a 3D (3-dimensional), 3C (3-component velocity)  
91 LES (Large Eddy Simulation) simulation for an unbaffled stirred tank. In this numerical experiment the  
92 sliding meshing technique was implemented, thus the simulation domain was divided into a fixed  
93 part and a rotating part. A similar work was recently published by (Mikhaylov et al., 2021b). The data  
94 was created through a Direct Numerical Simulation (DNS) with a “frozen rotor” approach and  
95 Reynolds numbers of 500, 600 and 700. In this research, POD was useful to reconstruct the temporal  
96 evolution of large-scale organized vortical structures behind the blades of a Rushton impeller in a  
97 non-baffled stirred tank. It was found that the first two modes dominate the energy spectrum by  
98 carrying 90% of the total mean kinetic energy. It also is relevant to mention that some higher modes  
99 (3<sup>rd</sup>, 4<sup>th</sup> and 5<sup>th</sup>, 6<sup>th</sup>) came in pairs in the energy ranking.

100 These two latest remarkable works show the feasibility of the numerical recipe for model order  
101 reduction in very complex flow fields. However, some important points were not addressed. For  
102 example in (Janiga, 2019), the POD decomposition was applied to each part of the mesh separately  
103 but a reconstruction of the 3D, 3C velocity field for the bulk was not performed. In general, it is  
104 neither simple nor straightforward to determine the relationship and similarity between the POD  
105 method for separate parts of the domain and the POD method corresponding to taking the domain

106 as a whole. This is due to the essentially statistical nature of the method. Additionally an analysis of  
107 the efficiency of the POD method in terms of calculation time, global and localized error was not  
108 provided. (Mikhaylov et al., 2021b) performed the reconstruction of coherent structures just in the  
109 zone around the impeller blades at low Reynolds number through the POD treatment of the velocity  
110 field expressed in a rotating frame. Finally, in both investigations the presence of baffles in the  
111 simulated stirred tanks was not considered. The incorporation of these elements is of great  
112 importance due to their contribution to the mean flow (circulation loops) and their decisive role in  
113 mixing phenomena. To sum up, running time-resolved CFD (Large Eddy Simulation or U-RANS) and  
114 applying Reduced Order Modeling such as POD (Proper Orthogonal Decomposition or Karhunen-  
115 Loève decomposition) is appealing because it generates a time-varying velocity fields at a moderate  
116 expense while preserving the spatial resolution (Du et al., 2013; de Lamotte et al., 2018b). This opens  
117 the route to both refined and cost-effective description of the unsteady velocity fields. From this  
118 brief review of the existing literature on the subject, it appears that the POD analysis of the flow field  
119 in a baffled stirred tank, in the fully turbulent regime (at a Reynolds number  $> 10^4$ ), using CFD data  
120 computed with a sliding mesh approach has not been considered yet.

121 The main objective of the present work is to perform a numerical reconstruction of a three-  
122 dimensional velocity field in a four-baffled stirred tank, operated in a turbulent regime, making use of  
123 the Proper Orthogonal Decomposition. In that regime, DNS and LES are time consuming and POD  
124 post-processing relies on a huge set of instantaneous 3D velocity fields. In contrast, the unsteady  
125 RANS method addresses the calculation of the transient mean flow and, despite the filtering of  
126 turbulence scales; it was preferred here since our prior objective is to establish the methodology for  
127 the velocity field reconstruction in the entire domain. Whatever the approach used to produce CFD  
128 results, a major difficulty resides in the presence of a fixed and a rotating mesh zone. It is shown that  
129 the velocity field reconstruction using a per-zone treatment of the CFD data is complex and  
130 cumbersome whilst a global treatment of the entire volume offers significant advantages. Originally,  
131 it appears that the main flow features of the 3D velocity fields are correctly recovered with the global

132 treatment but the eigenvectors do not correspond to spatial modes, as is typically the case in POD  
133 treatment. In order to assess the relevancy of our reconstruction method in terms of efficiency and  
134 accuracy both the average error and the instantaneous and localized errors were calculated. Finally,  
135 an analysis of the numerical cost is presented. There is no record that such a scenario has been  
136 addressed before.

## 137 2. Theoretical background

138 As indicated by (Kosambi, 1943; Loève, 1945; Karhunen, 1946; Berkooz et al., 1993; Holmes et al.,  
139 1996) the proper orthogonal decomposition (POD) or Kosambi-Karhunen–Loève decomposition  
140 consists of a practical procedure that extracts the most energetic components (on average) from an  
141 ensemble of functions (in the continuous case) or experimental (physical or numerical) data (in the  
142 discrete case). The key idea of the technique is to provide a vector space basis with the special  
143 condition that the average square projection of the data ensemble in this vector space is maximum.  
144 In this scenario it is possible to reduce a large number of interdependent variables to a much smaller  
145 set of uncorrelated variables while maintaining the spatial and temporal resolution of the original  
146 ensemble of variables (Liang et al., 2002; Kerschen et al., 2005). When applied to fluid flow analysis,  
147 the data ensemble can be obtained from a series of experimental or simulated velocity fields.

148 Once the spatial structure of the ensemble is extracted and represented by a set of orthogonal  
149 functions named eigenvectors (or modes), the members of the original ensemble can be represented  
150 as linear combination of these modes. The most striking property of the POD is that the  $p$ -modes  
151 reconstruction (finite truncations in the modal expansion) is optimal as it minimizes the mean square  
152 of error in comparison with any other possible orthogonal basis having the same dimension  $p$ . Should  
153 the data ensemble be made of a collection of instantaneous three-dimensional velocity fields, the  
154 original field  $\vec{U}(\mathbf{x}, t)$  is approximated as a linear combination of  $p$  modes,  $\vec{\phi}_k(\mathbf{x})$  weighted by time  
155 varying coefficients,  $a_k(t)$ .

$$\vec{U}_{POD}(\mathbf{x}, t, p) = \sum_{k=1}^p a_k(t) \vec{\phi}_k(\mathbf{x}) \quad (1)$$

156 The Direct and the Snapshots methods are the most popular POD approaches. The choice of the  
 157 method depends on the spatial and temporal resolution contained in the data ensemble. For  
 158 example, when the spatial resolution is very high compared with the time resolution, the Snapshots  
 159 Method is less demanding in terms of computational cost (Sirovich, 1987a, 1987b, 1987c; Smith et  
 160 al., 2005).

161 The POD equations

162 Let us consider  $N$  arbitrary 3D velocity fields,  $\vec{U}_n$ , sampled in  $L$  points at time  $t_n$  with  $n \in \{1, \dots, N\}$ .  
 163 Using the POD terminology, these instantaneous 3D velocity fields are named snapshots. Then, the  
 164 idea is to find the most “typical” or “characteristic” structures  $\vec{\phi}_k(\mathbf{x})$  in the set of  $\vec{U}_n$ .

165 The data ensemble is first arranged in a matrix  $\underline{M}_{3L \times N}$  of the form:

$$\underline{M} = \begin{pmatrix} u_1^{(1)} & \dots & u_1^{(N)} \\ \vdots & \dots & \vdots \\ u_L^{(1)} & \dots & u_L^{(N)} \\ v_1^{(1)} & \dots & v_1^{(N)} \\ \vdots & \dots & \vdots \\ v_L^{(1)} & \dots & v_L^{(N)} \\ w_1^{(1)} & \dots & w_1^{(N)} \\ \vdots & \dots & \vdots \\ w_L^{(1)} & \dots & w_L^{(N)} \end{pmatrix} = (\mathbf{U}^{(1)} \quad \dots \quad \mathbf{U}^{(N)}) \quad (2)$$

166 Such a matrix is known as the *snapshots matrix*  $\underline{M}$ . From (2) the covariance or correlation tensor  $\underline{R}$   
 167 can be constructed following the Direct or Snapshot method as follows:

$$\underline{R} = \begin{cases} \frac{1}{N} \underline{M} (\underline{M})^T & \text{Direct method} \\ \frac{1}{N} (\underline{M})^T \underline{M} & \text{Snapshot method} \end{cases} \quad (3)$$



168 The correlation tensor contains the degree to which and the manner in which, the velocities at  
 169 different points are correlated. Consider the velocity vector  $\mathbf{U}_1$  at a point 1 and the velocity  $\mathbf{U}_2$  at a  
 170 point 2 of the fluid domain. If the velocities  $\mathbf{U}_1$  and  $\mathbf{U}_2$  are statistically dependent their correlation will  
 171 be different from zero, otherwise such correlation will be zero. Using the Direct method, the  
 172 covariance tensor is represented by a  $3L \times 3L$  matrix, where  $L$  represents the number of data  
 173 points. This array represents a time-averaged two-point spatial correlation. Such a process makes the  
 174 computational cost immense when the number of points in the studied domain is large (the size of  
 175 the tensor  $\underline{R}$  is  $(3L)^2$ ).

176 Alternatively, it is possible to apply the Snapshot method proposed by (Sirovich, 1987a; Smith et al.,  
 177 2005) which is always valid when the ergodic hypothesis is fulfilled (all accessible microstates in the  
 178 phase space have the same probability to occur over a long period). In this case, the covariance  
 179 tensor is represented by a  $N \times N$  matrix and a correlation is sought between the different realizations  
 180 of the velocity. Such a process makes the computational cost less prohibitive compared with the  
 181 Direct method (the size of the tensor  $\underline{R}$  is only  $N^2$ ). Due to this advantage, the Snapshot method is  
 182 used in this work.

183 This Snapshot approach consists in solving an eigenvalue problem to find the eigenvalues  $\lambda_k$  and  
 184 eigenvectors  $\vec{Y}_k$  through a diagonalization of the correlation tensor  $\underline{R}$  (snapshot case from (3)):

$$\underline{R}\vec{Y}_k = \lambda_k\vec{Y}_k \quad (4)$$

185 The eigenvalues  $\lambda_k$  are the same for the Direct method and the Snapshot method because (3) is a  
 186 Hermitian matrix. However, the eigenvectors are different for both approaches.

187 In order to recover the eigen-vectors in the spatial space, eigen-vectors  $\vec{Y}_k$  are transformed into  
 188  $\vec{\phi}_k$  using equation (5):

$$\vec{\phi}_k(\mathbf{x}) = \underline{M}\vec{Y}_k \frac{1}{\lambda_k}, \quad k = 1, \dots, N \quad (5)$$

189

190 Since the eigenvectors constitute an orthonormal basis, they obey the following relationship.

$$(\vec{\phi}_i)^T \vec{\phi}_j = \delta_{ij}, i, j = 1, \dots, N, \delta_{ij}: \text{delta de Kronecker} \quad (6)$$

191 After the calculation of the eigenvector,  $\vec{\phi}_k(x)$  the modal components  $a_k(t)$  are obtained as:

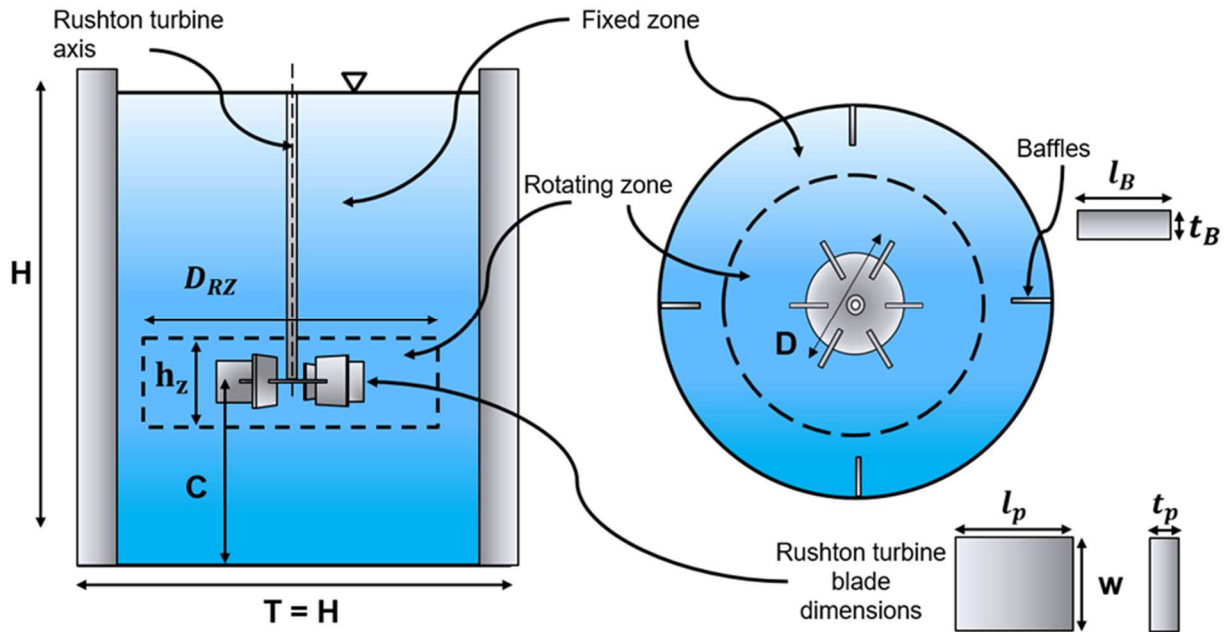
$$a_k(t) = \underline{M}^T \vec{\phi}_k, \quad k = 1, \dots, N \quad (7)$$

192 This completes all the elements necessary to reconstruct the velocity field according to (1).

### 193 3. Material and methods

#### 194 3.1 Stirred tank and simulation set up.

195 Unsteady RANS CFD simulation in a 70 L baffled stirred tank is performed to produce our numerical  
 196 data. The geometry of the flat-bottom stirred tank equipped with a Rushton turbine and four baffles  
 197 is presented in Figure 1. Likewise, Table 1 provides the dimensions of the simulated tank.



198  
 199 *Figure 1 Configuration of the simulated stirred tank.*

200 *Table 1 Dimensions (in meters) of the simulated stirred tank*

C	D	$D_{RZ}$	H	$h_z$	$l_B$	$t_B$	$l_p$	$t_p$	w
0.1500	0.1500	0.3000	0.4500	0.0600	0.0450	0.0050	0.0375	0.0020	0.0300

201

202 Water at room temperature and atmospheric pressure (density  $\rho = 998.2 \text{ kg. m}^{-3}$ , dynamic viscosity  
203  $\mu = 1.003 \times 10^{-3} \text{ kg. m}^{-1}. \text{s}^{-1}$ ) is used as working medium. The stirring speed is 150 RPM (revolutions  
204 per minute) what corresponds to an angular velocity  $\omega = 5\pi \text{ rad. s}^{-1}$  or a frequency  $f = 2.5 \text{ Hz}$ ,  
205 according to (8) the Reynolds number is 56250.

$$Re = \frac{\rho f D^2}{\mu} \quad (8)$$

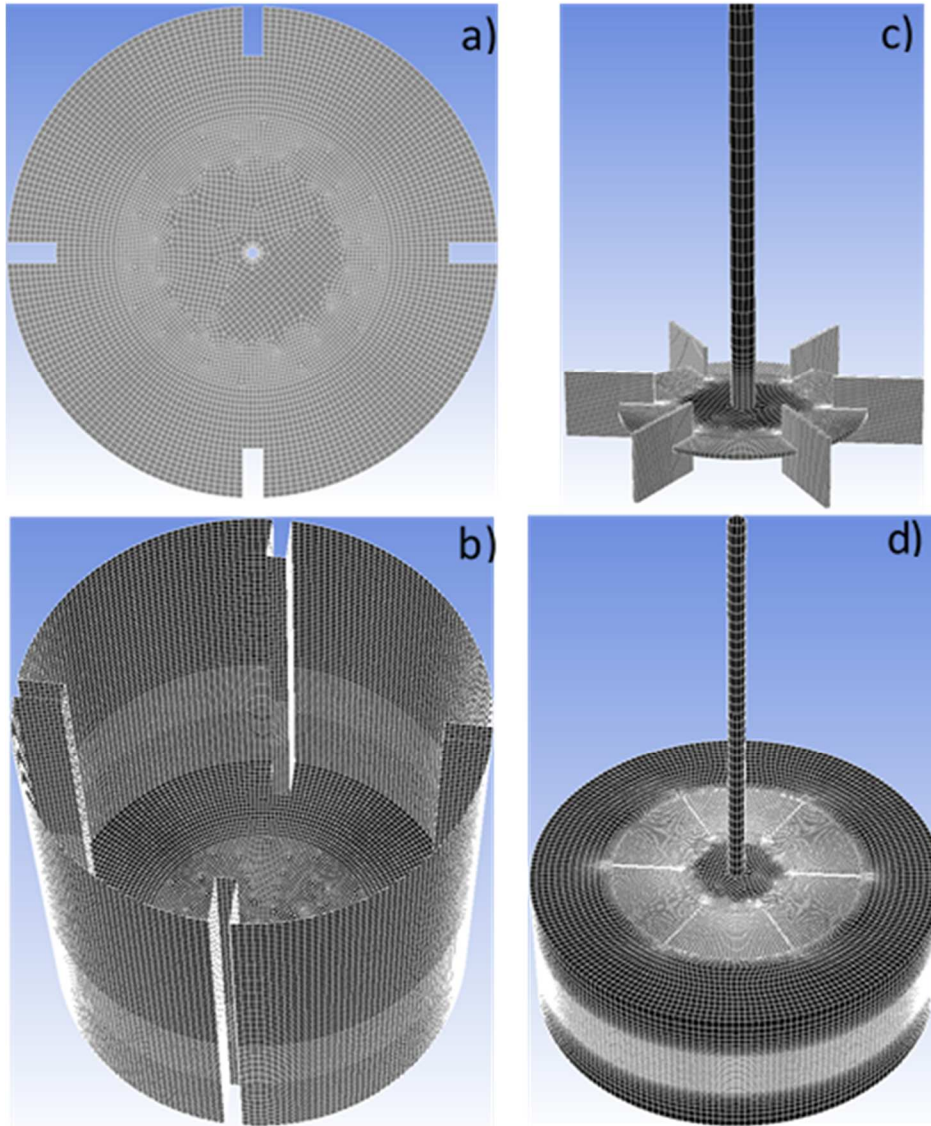
206 The power number  $N_p$  for the Rushton turbine is deduced from the torque on the impeller ( $P =$   
207  $C \omega = 6.5 \text{ Watts}$ ) according to equation (9)

$$N_p = \frac{P}{\rho f^3 D^5} \quad (9)$$

208 The calculated value  $N_p = 5.4$  allows determining the volume averaged viscous dissipation of kinetic  
209 energy  $\bar{\varepsilon}$  computed from equation (10), we obtain a value of  $0.090 \text{ m}^2. \text{s}^{-3}$  or  $90 \text{ W. m}^{-3}$ .

$$\bar{\varepsilon} = \frac{N_p f^3 D^5}{V} = \frac{4}{27 \pi} N_p f^3 D^2 \quad (10)$$

210 The mesh grid (1,129,140 cells and 1,184,282 nodes), models, settings and the numerical simulation  
211 procedure are identical to those used in a previous work (Delafosse et al., 2008). The standard  $k - \varepsilon$   
212 turbulence model is used with a standard wall function. A symmetry boundary condition is adopted  
213 on the free surface. The domain is divided into two zones: the fixed zone contains the walls, baffles,  
214 the major part of the shaft, and the volume outside the rotating zone, the latter is a cylindrical  
215 domain, which contains the impeller and a small portion of the shaft (see Figure 1). It must be  
216 noticed that a structured mesh made of hexahedrons was built in that zone (Figure 2). The starting  
217 point was a projection of all necessary edges on a horizontal plane followed by the creation of as  
218 many surfaces as needed to further build the impeller shape. Each face was meshed and the volume  
219 mesh obtained using the sweeping method. Owing to this strategy, the mesh is made of prismatic  
220 cells and it is almost invariant by rotation around the vertical axis.



221

222 *Figure 2. Mesh FLUENT views of the most important parts of the simulated tank: a) Top surface of the tank, b) External walls*  
 223 *of the tank, c) Shaft and Rushton turbine, d) Shaft and rotating zone of the simulation domain.*

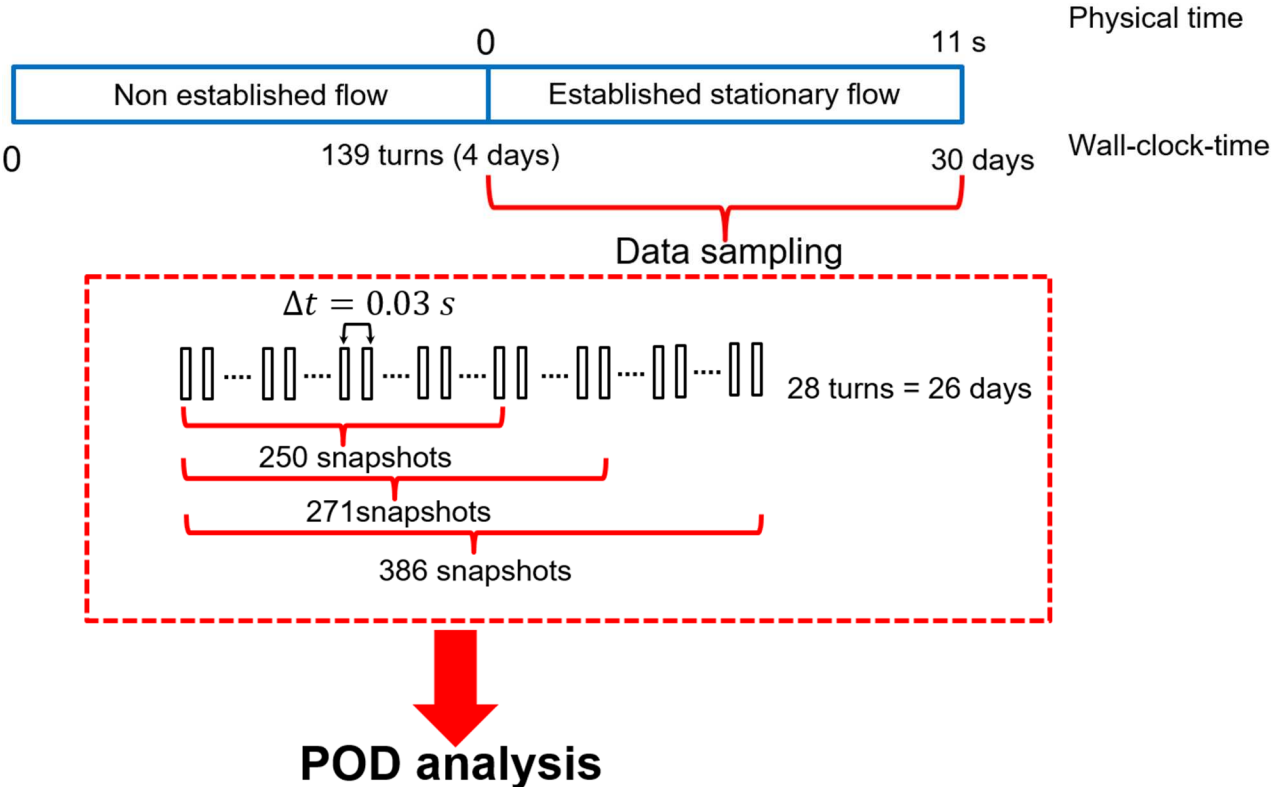
224 The CFD calculations and data treatment were performed with ANSYS-FLUENT R20 on a parallel  
 225 computer equipped with 40 processors Intel Xeon(R) E5-2660, 2.60 GHz. The time step used in the  
 226 simulation is  $\Delta t_{CFD} \approx 5 \cdot 10^{-4} s$  corresponding to an angular rotation of 0.5 degrees per time step  
 227 and a Courant number less than 1 in the whole domain to ensure numerical stability. Third order  
 228 discretization scheme are used. Within each time step, 30 iterations of the non-linear solver were  
 229 necessary to reach a plateau at  $10^{-4}$  for the velocity and continuity residuals.

230 The convergence toward a stationary flow was assessed using two criteria: the equality between the  
 231 torque on the turbine and the torque on the external walls of the tank, and the equality between the

232 volume integral of the turbulent dissipation rate and the power input. Regarding the first criterion, it  
 233 is found that the torque on the turbine and the turbine shaft is practically identical to the torque  
 234 generated on the external walls of the tank. Regarding the second criterion, the ratio of energy  
 235 dissipation to the power input is 98%. The stationary flow field was established after 139 turbine  
 236 revolutions (4 days of simulation) (see “Physical convergence of the numerical results” in  
 237 Supplementary Information)

238 3.2 Sampling and data processing

239 The sampling of CFD data consists of a set of 3D velocity fields or snapshots collected in the entire  
 240 simulated domain (1,129,140 cells). A total physical time of 11 s, representing 28 complete rounds of  
 241 the turbine and requiring 26 days of computations, was spanned. During this time lapse, 386  
 242 snapshots were taken every 53 computational time steps. The time interval between two samples is  
 243  $\Delta t_{st} = 0.03 \text{ s}$  ( $\Delta t_{st} = 53 \Delta t_{CFD}$ ). A sensitivity of the results to the number of snapshots is presented  
 244 in the result section. Figure 3 provides an overview of the sampling data chosen in the present study.



245 **POD analysis**

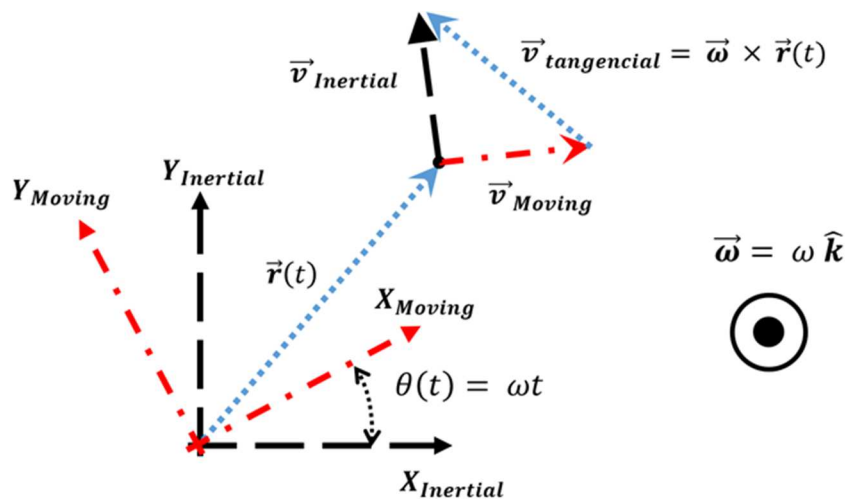
246 *Figure 3. Sampling data sets collected for apply POD. Each rectangle represents a snapshot of registered velocity.*

247 Finally, because the POD is a statistical method it is necessary to check that the number of snapshots  
248 as well as the time window of data acquisition are sufficient to capture the structures carrying the  
249 highest variance in the flow. The total simulation time must be long enough to record sufficient  
250 information of the rotational motion while the sampling frequency must be high enough to prevent  
251 the filtering of small-scale fluid motion. In addition, attention must be paid regarding the sampling  
252 frequency to avoid the collection of snapshots “in phase” with the impeller rotation (see “Impeller  
253 rotation and data sampling” in Supplementary Information).

254 A typical POD decomposition requires that velocity vectors and cell location be expressed in the  
255 same frame. This is the case when POD is performed on experimental PIV data, since velocities are  
256 generally measured in a fixed plane (Liné et al., 2013; Rodriguez et al., 2013). Some particular  
257 attention must be paid when dealing with CFD data. In a previous work, Mikhaylov and co-workers  
258 used CFD to compute the velocity field in an unbaffled stirred tank. The problem was solved in a  
259 rotating reference frame using a single mesh domain (Mikhaylov et al., 2021a). Here also, velocities  
260 are expressed in the rotating frame and calculated at some fixed position in that frame. In the  
261 present work dealing with a stirred tank, the presence of baffles necessitates to split the fluid domain  
262 into two mesh zones, a fixed one and a rotating one. In order to satisfy the above-mentioned  
263 condition for a typical POD decomposition, velocities must be expressed in the inertial frame for the  
264 fixed zone and in the rotating frame for the moving zone. The export of data, in FLUENT, extracts  
265 velocities expressed in the inertial frame. Thus, prior to the POD treatment, the data collected in the  
266 rotating zone have to be converted into velocities in the moving frame (see Figure 4). Then, the POD  
267 treatment was performed separately for each set of velocities. This “per zone approach” corresponds  
268 to the procedure adopted by Janiga when two mesh zones are present in the CFD model (Janiga,  
269 2019).

270 Alternatively, a global POD treatment considering the two zones altogether (with the entire velocity  
271 field expressed in the inertial frame) is attempted with a view of performing the 3D reconstruction of

272 the flow field in the entire fluid domain. This global approach has not been yet proposed in the  
 273 literature for baffled stirred tanks and its feasibility remains to be demonstrated. We will show that  
 274 the global treatment is feasible bearing in mind that its essential purpose is not to perform a  
 275 hydrodynamic study of the fluid flow structure but a reconstruction of the velocity field by means of  
 276 a linear combination of POD modes. Evidence of that will be provided in the section of 5.3. Assessing  
 277 the accuracy of the flow field reconstruction.



279 *Figure 4. 2D schematic representation for the velocity vector expressed in the inertial and moving frames. The inertial frame*  
 280 *is equivalent to the laboratory frame of reference. The moving and rotating frame share the same origin. The rotating frame*  
 281 *rotates around the Z-axis with angular velocity  $\omega$ . In that frame, the coordinates of the rotating cells are time independent.*

282 Before going into the details, it is of utmost importance to observe that the data extracted from the  
 283 CFD code are the components of the velocity vectors expressed in the inertial frame (laboratory  
 284 reference frame). In addition, this information is referenced with respect to a cell index. Thus, each  
 285 3D snapshot results in an array containing the cell index in the first column followed by the three  
 286 components of the velocity vector in the inertial reference frame ( $\vec{U}_F(CI)$ ). The first step of the POD  
 287 treatment consists in rewriting the three components of the velocity in a column vector  
 288 corresponding to one snapshot. The rows of the matrix  $\underline{M}$  represent the grid cells and the columns  
 289 represent the time instants at which the data were registered. When moving along a row, the time  
 290 changes but a given line always corresponds to the same cell index  $CI$  as illustrated in Figure 5.

As time passes the position of each cell changes due to mesh rotation.  
The velocity is always recorded in the same cell over time.

Cell index	$\vec{r}(t = t_0)$	$\vec{r}(t = t_1)$	.....	$\vec{r}(t = t_N)$
1	$\vec{U}_{Cell 1}$	$\vec{U}_{Cell 1}$	.....	$\vec{U}_{Cell 1}$
2	$\vec{U}_{Cell 2}$	$\vec{U}_{Cell 2}$	.....	$\vec{U}_{Cell 2}$
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
$k^{th}$	$\vec{U}_{Cell k}$	$\vec{U}_{Cell k}$	.....	$\vec{U}_{Cell K}$

291

292 Figure 5. Schematic representation of the data recording used to build the snapshot matrix  $\underline{M}$  for  $N$  snapshots and  $k$  cells.  
293 The velocity is always registered for a given cell although, for those cells belonging to the rotating zone, the spatial  
294 coordinates change over time due to the mesh rotation.

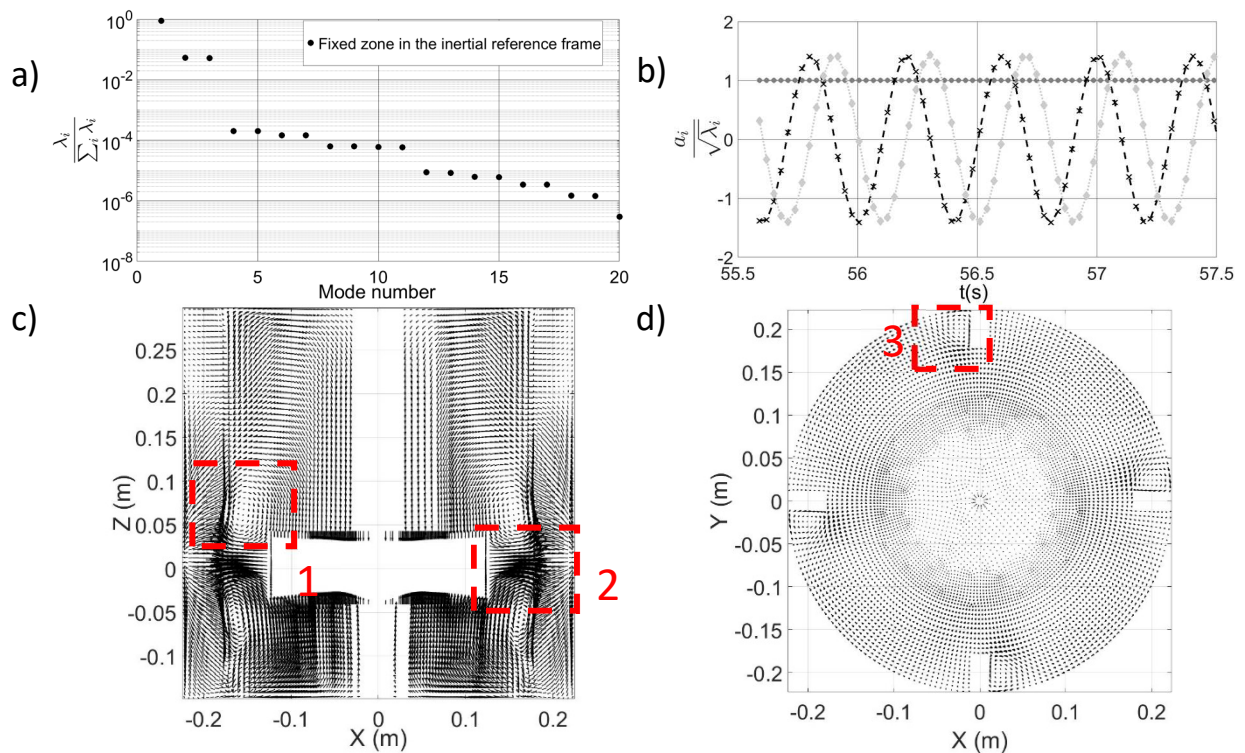
## 295 4. POD modal analysis

### 296 4.1 POD analysis in the fixed zone

297 First, the POD analysis is performed using 386 snapshots containing the velocity vector belonging to  
298 the fixed zone of the mesh,  $\vec{U}_{IF} = (U_x, U_y, U_z)_{IF}$ . Velocity components are here expressed in the  
299 inertial frame (IF). In that case, the relationship between the cell index and the cell location in the  
300 inertial reference frame is time independent. The mode spectrum is presented in Figure 6a, as well as  
301 the corresponding modal component and the vector field associated to the first mode. As expected,  
302 this first mode accounts for 90% of the total variance, its modal component is positive, almost time  
303 independent (Figure 6a,b) and thus this first mode reveals the structure of the mean flow. It is also  
304 remarkable the presence of two additional modes which carry about 10% of the total variance. These  
305 modes reveal a periodic fluid motion in the region outside the rotating zone of the grid, induced by  
306 the impeller rotation. As shown in Figure 6b, the corresponding modal components oscillate around  
307 zero with a period of 0.4 s corresponding to the impeller frequency of 2.5 Hz. The possibility of



308 identifying these oscillatory modes is an outstanding advantage that justifies the use of the POD  
 309 methodology. In addition, Figure 6c and Figure 6d, provide different views of the spatial  
 310 configuration contained in the first mode. Note that in Figure 6c an angular sector of 3.5 degrees is  
 311 visualized in a vertical XZ-plane. Well-known organized structures are present: jet flow, recirculation  
 312 loops, and vortices behind the baffles. Additionally, a predominantly axial fluid flow can be observed  
 313 near the shaft and in the regions above and below the rotating zone.



314

315 *Figure 6. POD analysis of the flow in the fixed zone of the mesh: a) mode spectrum, b) mode component associated with the*  
 316 *top three ranking modes, circles: first mode, x's second mode and rhomboids third mode (each data set is normalized by the*  
 317 *variance corresponding to each mode.), c) First eigenvector visualized in a vertical XZ plane, d) Top view of the first eigen-*  
 318 *vector. The main feature of the mean flow, i.e. radial jet flow, recirculation loops and coherent vortices behind the baffles*  
 319 *are clearly visible (red boxes 1, 2 and 3).*

320 The seemingly absence of velocity vectors in the central zone around the shaft (Figure 6c) is an  
 321 artefact due to the small number of grid points used to describe the shaft surface itself. Since there is  
 322 only one grid point every  $30^\circ$  around the shaft, the probability to find a grid node within the angular  
 323 sector of only  $3.5^\circ$  decreases as one approaches the shaft. Thus, the side view of the velocity field in  
 324 the sector may not contain enough information close to the shaft resulting in an apparent absence of

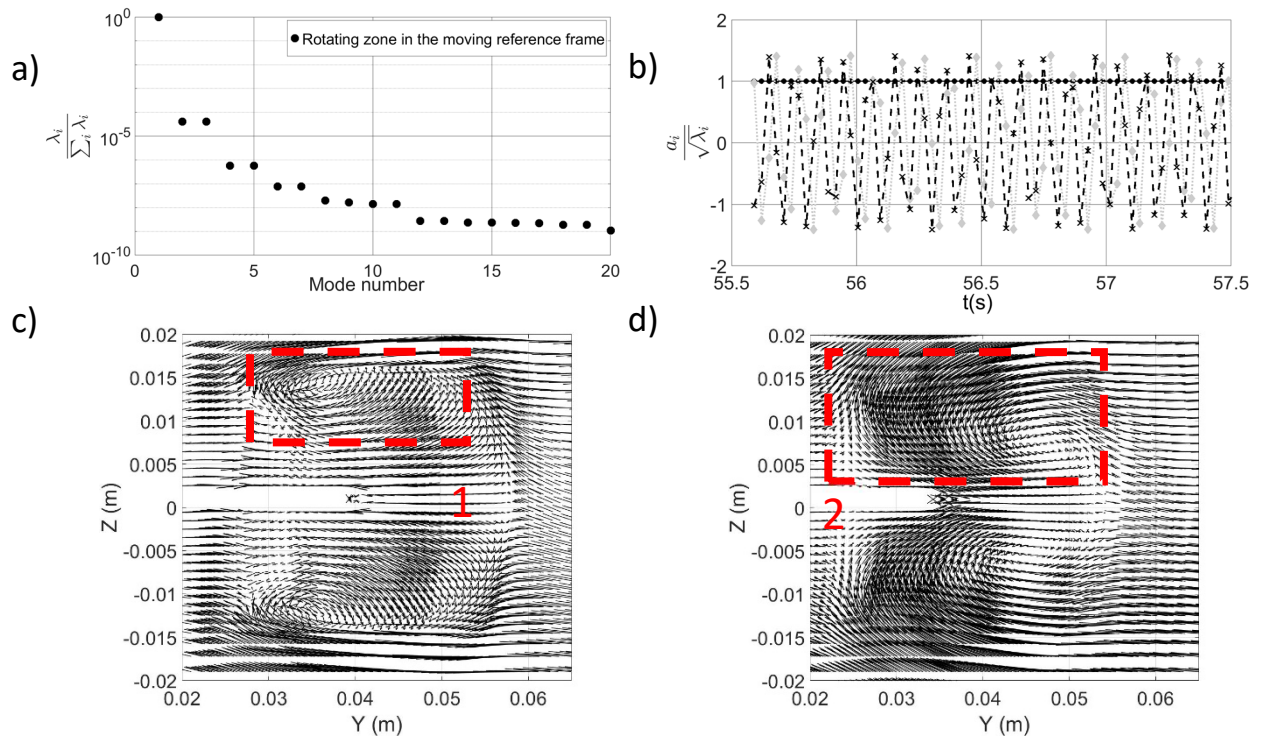
325 data. However, it can be seen, from the top view (Figure 6d) that the flow field reconstruction at  
326 every grid point of the computational mesh is actually obtained close to the shaft.

#### 327 4.2 POD in the rotating zone

328 Then, the POD analysis is performed using the velocity vectors belonging to the rotating zone of the  
329 mesh using again 386 snapshots. In this zone, the mesh rotates with respect to the inertial reference  
330 frame and the velocity fields  $\vec{U}_{IF}$  are obtained in different locations for each time instant.  
331 Consequently, the velocity fields must be expressed in a reference frame in which the velocity  
332 measurement coordinates do not change in time. We recall here that the CFD code export procedure  
333 gives access to the Cartesian velocity components in the inertial reference frame. The velocity  
334 components in the moving (or rotating) frame,  $\vec{U}_{MF}$ , were deduced performing the next steps:

$$\begin{aligned} \text{i.} \quad & \vec{U}'_{IF} = \vec{U}_{IF} + \vec{r}(t) \times \vec{\omega} \\ \text{ii.} \quad & \vec{U}_{MF} = \underline{M_{Rotation}} \vec{U}'_{IF} \end{aligned} \tag{11}$$

335  $\vec{r}$  is the position vector of any cell expressed in the inertial reference frame. Importantly, the vector  
336 position of a cell differs from one snapshot to the other due to the rotation of the mesh. This rotation  
337 takes place around the vertical axis (Z-axis) aligned with the shaft and the position vector is known  
338 from the current cell coordinates  $\vec{r}(t) = \vec{r}(x_{IF}(t), y_{IF}(t), z_{IF}(t))$ .  $M_{Rotation}$  is the time dependent  
339 rotation matrix that is used to express the velocity  $\vec{U}'_{IF}$  in a frame attached to the turbine (the  
340 position of the mesh in the first snapshot is used as a reference). Once the entire data set is treated,  
341 the snapshot database now contains a time series of the velocity components in the moving  
342 reference frame. Since the mesh is subjected to a solid rotation, the location of the cells, in the  
343 moving (rotating) frame, is now also time-independent. Once the transformations of (11) have been  
344 performed, the POD algorithm can be used. The POD results obtained are displayed in Figure 7.



345

346 *Figure 7. POD results for the velocity fields in rotating zone measured in the moving frame. a) Mode spectrum: one mode*  
 347 *dominates the variance ranking; b) mode components associated to the three modes, circles: first mode, x's second mode*  
 348 *and rhomboids third mode (each data set is normalized by the variance corresponding to each mode). The modal component*  
 349 *of the first ranking mode is time independent and the second and third modes both oscillate with a frequency of 10 Hz.*  
 350 *These oscillations are related to the passage of the baffles observed from the moving frame. c) The first eigenvector in the*  
 351 *plane YZ three degrees behind one of the turbine blades reveal the presence of the trailing vortices (red box 1), d) The first*  
 352 *eigenvector in the plane YZ six degrees behind one of the turbine blades reveals the radial displacement of the trailing*  
 353 *vortices (red box 2).*

354 As shown in Figure 7 the variance ranking is dominated by a single mode. In addition, this mode  
 355 component is strictly time constant, as shown in Figure 7b. The second and third modes both  
 356 oscillate with a frequency of 10 Hz or a period of 0.1 s (see the table “Fitting for the second and third  
 357 modes for the moving frame” in Supplementary information). The impeller period is 0.4 s; since there  
 358 are four baffles, the period associated with each baffle is 0.1 s. The first eigenvector contains the  
 359 typical trailing vortices. They appear here as coherent structures attached to the turbine blades. The  
 360 presence of such structures is shown in Figure 7c and Figure 7d for different positions of one of the  
 361 turbine blades. The above results agree with the description of the fluid flow in a reference frame  
 362 moving with the turbine blades. However, transformation (11) modifies the energy content of the

363 initial data and there is no mathematical link between the kinetic energy in the rotating frame and  
364 the inertial frame.

#### 365 4.3 Reconstruction of the velocity field from the POD results per zone.

366 Once the procedure of reconstruction of the velocity field in the fixed and rotating zones has been  
367 carried out, the velocity field was constructed (expressed in the inertial reference frame) in the  
368 whole domain of the stirred tank. Since the two zones mentioned above were processed  
369 independently, the reconstruction of the velocity field was done by placing the reconstructed vector  
370 fields in each region. Special attention must be paid to two important details. First, the entire velocity  
371 field was built as a sum of the velocities reconstructed in each zone because the POD components  
372 involved are synchronized (the same snapshots were used). Second, all the data (fixed and moving  
373 zone) must be expressed in the inertial reference frame.

374 In the case of the fixed zone, no additional operation is necessary because the POD technique was  
375 applied on a fixed grid. Therefore, for this area, the reconstruction of the velocity field is already  
376 expressed in the inertial reference frame. The foregoing case is not valid for the moving zone  
377 because the CFD data were processed through the transformations (11). Consequently, the  
378 reconstructed velocity field in this region must be manipulated to express it back in the inertial  
379 reference frame. Concretely, inverse transformations of (11) must be applied to the reconstructed  
380 vector fields showed in Figure 7.

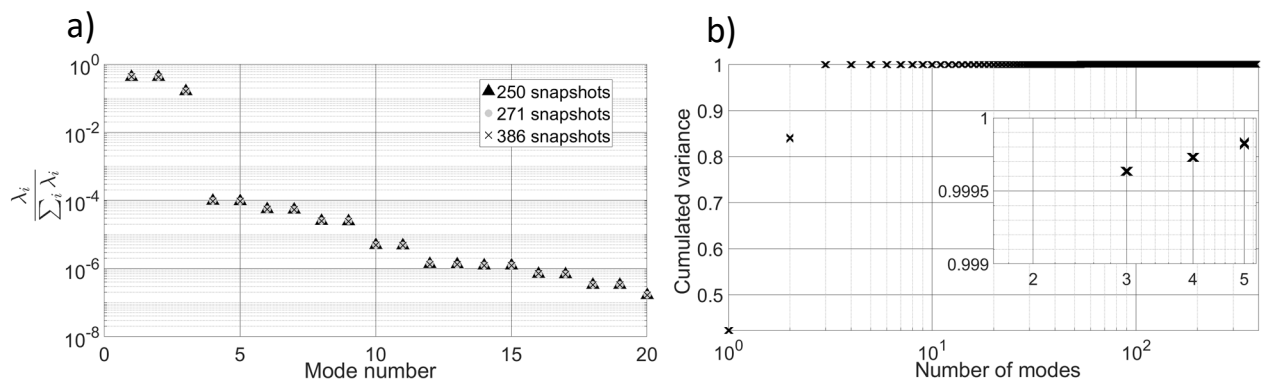
381 To sum up, in order to produce a 3D velocity reconstruction in the entire fluid domain, the recorded  
382 3D fields are split into two zones, the subset of data corresponding to the rotating or moving zone  
383 are transformed (through equation (11)), then typical POD is applied in each subset of data, velocity  
384 fields for both are reconstructed, velocities in the moving zone are transformed back to the inertial  
385 frame and finally, the two velocity fields are gathered in a single file. The procedure described is  
386 feasible but it is long, complex and cumbersome.

#### 387 4.4 Global POD treatment

388 In the previous treatments, velocities are expressed either in the fixed or in the moving or rotating  
389 frame. Such velocity fields are also referenced by a cell index, which does not change in time, i.e.  
390  $\vec{U}_{IF}(CI, t)$ ,  $CI = h(CI)$ . In addition, as indicated in the mathematical presentation of the technique,  
391 POD is a statistical method in which a correlation is sought between the different realizations and the  
392 procedure in itself does not require that all data are recorded at the same location. In the present  
393 case, the cell index is time independent while the relationship between the cell index and the  
394 location of that cell at any time is readily accessible. Therefore, it was postulated that a global POD  
395 treatment considering the entire mesh, with all the velocities expressed in the inertial frame of  
396 reference could make sense. The collected snapshots were analyzed using the numerical procedure  
397 described in the previous sections, producing a decomposition of the time varying 3D flow field on an  
398 orthogonal basis of 3D vector fields called modes. It is crucial to observe that such a POD  
399 decomposition is made in the space of cell indices which means that the associated POD modes are  
400 not spatial modes and their physical interpretation (as flow structure descriptors) has to be  
401 questioned. From a vector field reconstruction point of view the above methodology means that the  
402 velocity is reconstructed for the whole domain in the geometrical conditions (angle of rotation of the  
403 moving zone) corresponding to a given snapshot. Once the reconstruction is carried out in such  
404 conditions, the velocity vectors belonging to the rotating zone have to be placed at the appropriate  
405 location, considering mesh rotation. Presumably, this will not affect the velocity reconstruction  
406 derived from the POD method; this assumption will be evaluated according to the error values  
407 calculated in the results section.

408 Figure 8 depicts the POD mode spectrum obtained from the global treatment. The first three modes  
409 carry 99.99% of the total system variance. The first and second modes share the same variance  
410 content while the third mode has a slightly smaller variance. In addition, from mode 4 to mode 11,  
411 pairs of modes of equal variance are observed. In general, a pair of modes with the same variance  
412 content is typical of coherent structures propagating in space (the phase difference between the

413 time coefficients and the shifted distribution in space of the corresponding modes lead to the motion  
 414 of these structures). Thus, this decomposition reveals a strong spatial organization of the flow in the  
 415 form of multiple coherent structures with decreasing variance content. Interestingly, the third mode  
 416 is a single mode, which suggests that it will be associated to the reconstruction of the mean flow, the  
 417 time-independent component of the 3D velocity field. Similar results were obtained using either 250,  
 418 286, and 386 snapshots, which suggests a statistical convergence of the POD methodology.



419

420 *Figure 8. a) POD eigenvalue spectrum for the first twenty modes and three different time spans: the first three modes*  
 421 *represents almost the 100% of the total system variance. It is also evident a correlation between pairs in the upper modes*  
 422 *until the eleventh one. b) Cumulated variance POD spectrum for the time span of 386 snapshots. The cumulated variance*  
 423 *until the third mode already represents the 99.9% of the total system variance.*

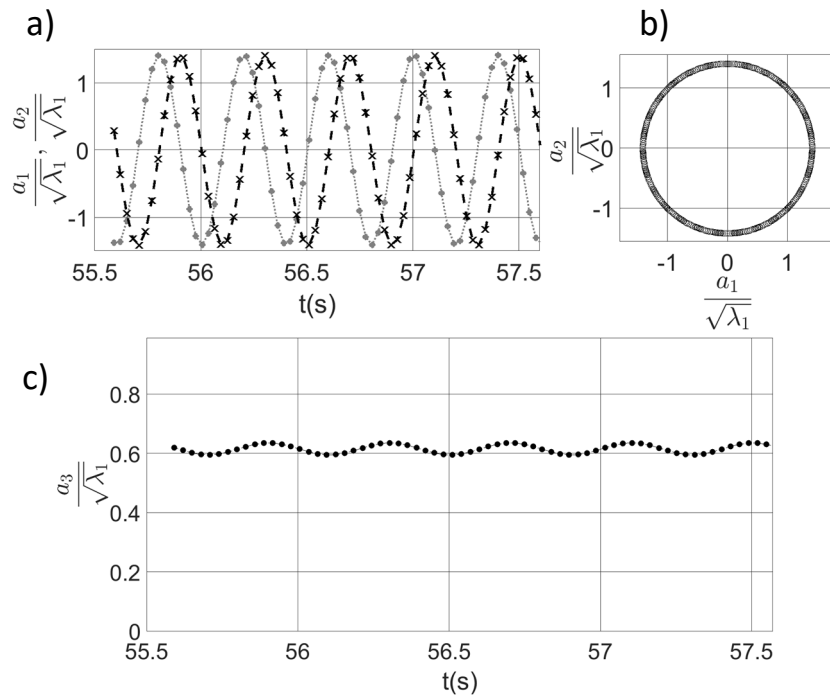
424 Since the first three modes contain practically the totality of system variance, the subsequent  
 425 discussion will first focus on them.

426 Figure 9a illustrates the time variation of the normalized amplitude factors associated to the first and  
 427 second modes over 28 impeller turns (time span 386 snapshots). The temporal organization of these  
 428 modes is clear; their behavior is oscillatory, with an identical period (0.4 s equal to the rotation  
 429 period of the turbine) and amplitude. In addition, the phase shift between these modes is  $\pi/2$  as can  
 430 be seen from the circular configuration of the Figure 9b. Likewise, the amplitude factor of the third  
 431 mode, presented in Figure 9c, shows a periodic time variation (again with a period of 0.4 s) but its  
 432 mean value is different from zero. This fact together with its variance content suggests that this third  
 433 mode will be associated to the reconstruction of the mean flow. The relatively small oscillations

434 presented in that POD component is related to the interaction between the periodic flow in the  
435 turbine region and the rest of the domain of the tank.

436 In order to verify statistically the periodic behavior of the coefficients  $a_1$ ,  $a_2$ , and  $a_3$  the pdf functions  
437 associated to each modal component are also provided (see “Examination of  $a_k$  statistical  
438 properties” in Supplementary information). It is evident that the functions are centered with respect  
439 to the origin (except  $a_3$ ) , proving their periodical character, which is in agreement with what is  
440 reported by (Liné et al., 2013). With such an idea in mind, a fitting of the first eleven modes  
441 components, using as reference the function  $A \sin(\omega t + \varphi)$  was performed with the Matlab curve  
442 fitting toolbox®. The results provided in Table 2 show that the considered modes exhibit a very  
443 organized time pattern as all the squared correlation coefficient  $R^2$  are equal to 1. The first three  
444 modes oscillate with a period of 0.4 s (2.5 Hz) corresponding to the impeller rotation speed while the  
445 remaining modes turn out to be associated with harmonic frequencies of the main frequency.

446 Moreover, the presence of paired modes with the same frequency and amplitude is evidenced. This  
447 modal configuration implies a strong correlation between duets and is usually an indicator of  
448 coherent flow structure being present. Additionally, Figure 10 presents the relationship of the first  
449 mode with modes fourth to tenth. In agreement with the results of Table 2, each pair of modes is  
450 correlated with the first one in terms of Lissajous patterns. For each pair, represented by one  
451 member of each pair, the number of loops is related to the corresponding harmonic mode. Thus, for  
452 example, the fifth mode presents three loops since this is the third harmonic of the main frequency  
453 associated with the first mode. The same reasoning is applicable to the sixth, eighth and tenth mode.



454

455 *Figure 9. Graphical representation of the first three modes identified with the global treatment. For clarity, results are*  
 456 *illustrated during 2 seconds only. a) Normalized time variation of the first and second mode. The circles and the crosses*  
 457 *correspond to the modal component  $a_1$  and  $a_2$  respectively. The dotted and continuous lines correspond to their fitting by*  
 458 *continuous sinusoidal functions. b) The circular configuration reveals a phase shift of  $\pi/2$  between the first and second*  
 459 *modes. c) Normalized time variation of the third mode. The solid circle corresponds to the modal component  $a_3$ . The dotted*  
 460 *line corresponds to the sinusoidal fitting of the third mode.*

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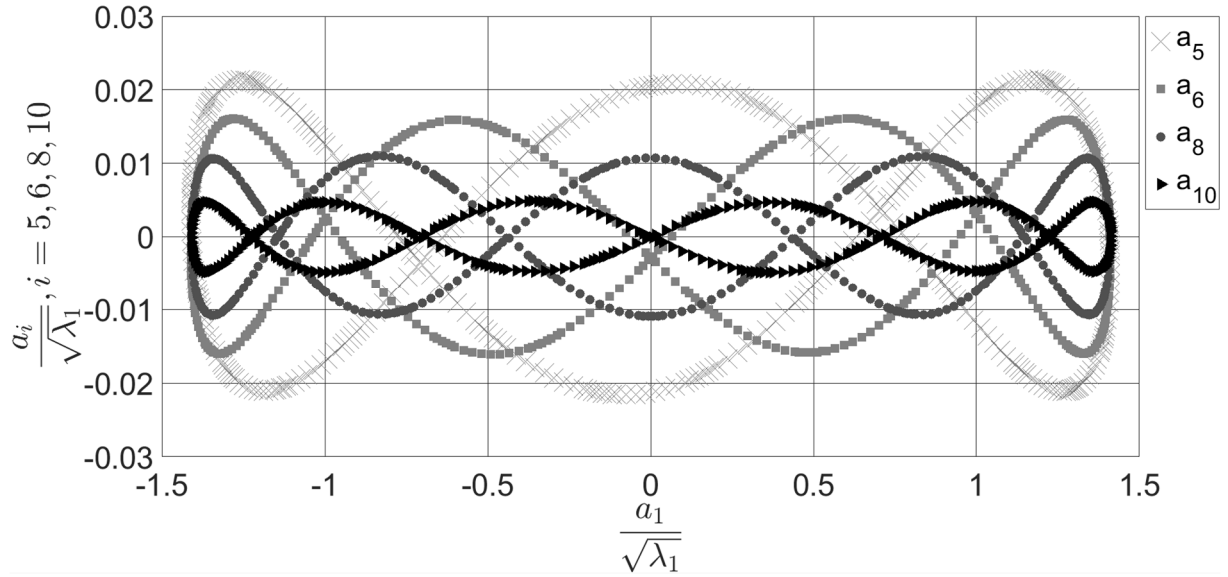
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470



471 Table 2. Sinusoidal fitting of the mode components,  $a_k(t)$  associated to the first eleven POD modes.

Modal coefficient	$A_k$ : Amplitude (m/s)	$\omega_k$ : Angular frequency (rad/s)	$f_k$ : Frequency (Hz)	$\varphi_k$ : Phase (rad)	$R^2$	$\frac{f}{(2.50 \text{ Hz})}$
$a_1$	454.50	15.71	2.50	17.21	1.00	1.00
$a_2$	454.60	15.71	2.50	15.65	1.00	1.00
$a_3$	6.51	15.71	2.50	15.64	1.00	1.00
$a_4$	6.84	47.12	7.50	7.84	1.00	3.00
$a_5$	6.84	47.12	7.50	12.55	1.00	3.00
$a_6$	5.15	62.83	10.00	21.91	1.00	4.00
$a_7$	5.15	62.83	10.00	26.62	1.00	4.00
$a_8$	3.47	78.54	12.50	5.97	1.00	5.00
$a_9$	3.47	78.54	12.50	4.39	1.00	5.00
$a_{10}$	1.53	94.25	15.00	21.61	1.00	6.00
$a_{11}$	1.53	94.25	15.00	23.17	1.00	6.00



473

474 *Figure 10. Lissajous patterns obtained from the temporal variation of the first to tenth modes.*

475 The information provided above concerning the mode components  $a_k$ , clearly shows that the global  
 476 POD approach produces an unexpected pattern regarding the temporal behavior of the  
 477 corresponding modes. Indeed, the strong correlation between all frequencies and the impeller  
 478 rotation speed suggests that the mode components actually reflect some information related to the  
 479 mesh rotation rather than to the flow structure.

480 Now that the amplitude factors associated with each mode are expressed as continuous sinusoidal  
 481 functions, it becomes possible to perform a continuous reconstruction of the 3D velocity field at any  
 482 instant and not only at the instants corresponding to the snapshots. However, it is crucial to note  
 483 that the mode produced by the global POD treatment are *cell index modes* and not spatial modes as  
 484 is typically the case in POD analysis:

$$\vec{U}_{POD}(\mathbf{CI}, t) = \sum_k A_k \sin(\omega_k t + \varphi_k) \vec{\phi}_k(\mathbf{CI}) \quad (12)$$

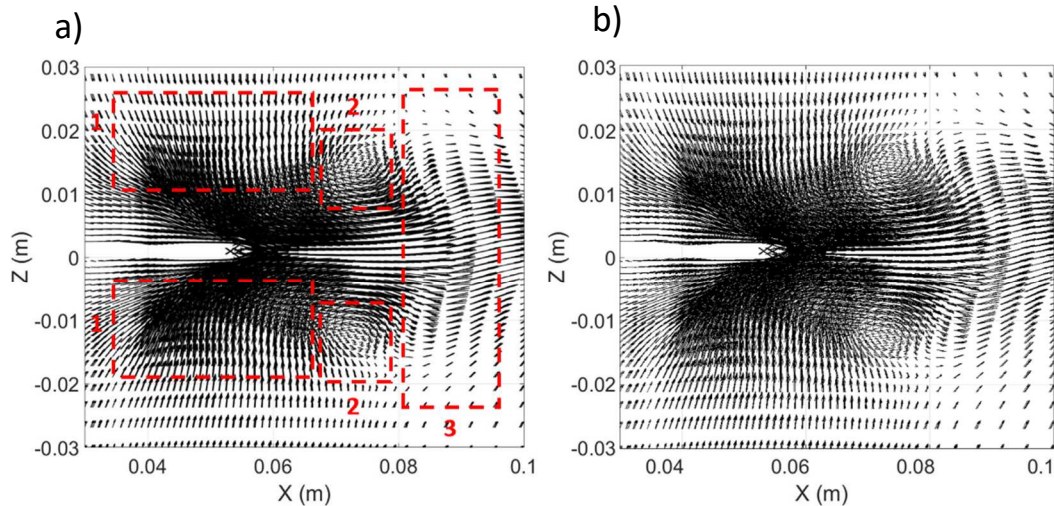
485

486 The exact location of any cell at any instant can be easily recovered from its initial position knowing  
 487 the rotation speed of the moving zone. For those cells belonging to the fixed zone, the relationship  
 488 between the cell index and the spatial location is time independent. For those cells belonging to the  
 489 rotating zone, the relationship between the cell index and the location in the inertial reference frame

490 is a rotation around the z-axis. The angle of rotation is  $\theta(t) = \omega (t - t_0)$  where  $t_0$  is the instant  
491 corresponding to the first snapshot. As a result, the global procedure to perform the velocity field  
492 reconstruction contains only three steps:

- 493 i. Perform the POD on the entire domain
- 494 ii. Reconstruct the velocity field in the entire domain using *cell index POD modes*
- 495 iii. Relocate the velocity vector of the rotating zone at their actual location.

496 Figure 11a provides a close up of such a reconstructed flow field in the region of the blade impeller.  
497 Reconstruction is here performed at the instant when the blade is located in the middle of the  
498 angular sector, the first, second and third POD modes are included. The three major features of a  
499 flow field generated by a Rushton turbine are clearly visible. Firstly, there is an axial flow moving  
500 towards the blade as consequence of the suction produced by the passage of the blade turbine (red  
501 boxes n° 1). Secondly, a pair of symmetrical vortices develop behind the blade (red box n° 2). These  
502 very organized structures represent a manifestation of the well-known trailing vortices, which play  
503 an extremely important role in mixing and transport processes. Noteworthy, these organized flow  
504 structures would not be present if a time averaging of instantaneous velocity field (snapshots) was  
505 performed. This fact represents an important advantage in the use of POD for velocity field  
506 reconstruction in comparison to a mean flow field description based on the time averaging of  
507 velocity fields. Thirdly, an axial jet flow is produced at the periphery of the turbine (red boxes n° 3).  
508 Although wiggling, the jet flow is, on average, slightly deflected upwards in concordance with  
509 (Delafosse, 2008; Escudié & Liné, 2004). This flow feature is present in the third mode and can  
510 therefore be related to the mean flow. Figure 11b shows the velocity field obtained from the CFD  
511 simulation at the same instant of the POD reconstruction (Figure 11a). A simple inspection of both  
512 figures shows a very close resemblance between the reconstructed field and the field generated by  
513 the simulator.



514

515 *Figure 11. a) Reconstruction of the velocity using the first three modes. From the left to the right side the most important*  
 516 *features of the field are marked by numbered dot rectangles: Upward and downward axial pumping flow (red boxes #1),*  
 517 *vortices generated by the passage of the blade (red boxes #2), and radial flow out of the impeller-sweeping zone (red box*  
 518 *#3), b) Velocity field from the CFD data in the same snapshot of the POD reconstruction.*

519

## 520 5 Discussion

### 521 5.1. On the Global POD treatment eigenvectors

522 Having shown that the proposed treatment allows an accurate reconstruction of the fluid flow, we  
 523 now comment on the mode decomposition. As already indicated, the global POD approach yields  
 524 results that are not as intuitive as those usually provided by the typical POD approach are. In  
 525 particular, the eigenvector obtained through the global treatment do not reveal the structure of the  
 526 flow. Nevertheless, this “non-standard” treatment offers some striking features worth noting.

527 Firstly, the resulting modes preserve the variance content and allow a direct reconstruction without  
 528 applying the per-zone method. This fact is an advantage in terms of computational resource savings  
 529 by avoiding the use of equation (11).

530 Secondly, the rotational frequency of the mesh appears in the temporal behavior of all modes. In  
 531 contrast with the typical treatment, this does not reveal a periodic fluid motion but rather reflects a  
 532 correlation between velocity data when the mesh occupies the same location. In that sense, this  
 533 observation is related to the statistical nature of POD. Although, the snapshot method is not aimed

534 at identifying temporal correlation, this type of correlation emerges here in the mode component  
535 that are all scaled by the mesh rotation frequency: the velocity field in every cell is strongly  
536 correlated with that obtained one turn later. Higher frequencies can be related to a strong angular  
537 periodicity of the mesh.

538 Thirdly, the inspection of the local features of the cell index modes helps understanding the  
539 outcomes of the global POD treatment. The first and second modes are significant in the rotating  
540 region and almost negligible outside this zone (the same apply to high order modes also). It was  
541 observed that both of them contain only radial and angular components and practically no axial  
542 component. Since such modes do not come out from a typical POD procedure, and refer to a cell  
543 index, it makes no sense to try to visualize them as such. However, as already emphasized, their  
544 contributions to the reconstructed velocity field can be identified. It appears that these first two  
545 modes are involved in the description of trailing vortices. The third mode is present throughout the  
546 tank, including the rotating zone, and the three components (axial, radial and angular) are present in  
547 this mode. However, the three components are not present everywhere. In the area swept by the  
548 rotating mesh, the third mode contains essentially an axial component above and below the turbine  
549 and a strong radial component away from the blades (see Figure 11a, Figure 3a from Supplementary  
550 Information). Considering that the related mode component is almost constant, the third mode  
551 seems to contain the axial flow corresponding to the pumping flowrate of the turbine and a radial  
552 flow rate associated to the jet flow created by the radial impeller. Note that both of them are, on  
553 average, independent of the actual mesh position. Accordingly, the reconstruction of the actual flow  
554 field in the rotating zone requires using the first three modes altogether. In the fixed zone, the third  
555 mode of the global treatment is very similar to the first mode of the POD treatment of the fixed zone  
556 only (first mode of the per-zone treatment). In that zone, the contribution of the third eigenvector  
557 can be physically interpreted, since the cell position is time independent. This result is sounded  
558 because in a fixed domain, the per-zone and global approaches are equivalent. Indeed, the  
559 configuration of this mode is very similar to the spatial mode presented in Figure 6d, Figure 6c. In the

560 upper part of the fixed zone, within a layer between 0.05 m and 0.1 m, this third eigenvector reveals  
561 the presence of clockwise vortices behind each baffle as is marked with the red boxes n°1 and n° 2  
562 (see “Flow structure analysis using cell index modes” in Supplementary information).

563 Thus, the global treatment of the entire volume leads to identical results in those regions where the  
564 cell location is not changing in time. In the particular case studied here, it was observed that the  
565 constant mode in the moving zone contains a contribution to the flow, which is independent of the  
566 mesh rotation. Possibly, the structured mesh configuration played a role here since the Z location of  
567 the cell in the rotating zone is truly time independent while the mesh is invariant by rotation outside  
568 the zone swept by the impeller.

569 5.2. Dynamical representation of the reconstructed flow using the three first POD  
570 modes

571 The sinusoidal fit of the amplitude factor (Table 2) associated to each mode allow reconstructing the  
572 flow field at any instant. Therefore, a reconstruction was performed for a complete turn of the  
573 turbine, using a temporal resolution of the CFD ( $\Delta t_{CFD} = 0.5 \text{ ms}$ ), which corresponds to 715  
574 snapshots. These snapshots were then superposed to generate a dynamic visualization or video of  
575 the plane reconstruction shown in Figure 11a. The video is provided in the complementary material  
576 (1+2+3 POD\_Reconst stp 0.03s\_XZ\_5.5degrees\_FITTING\_6.avi). Such dynamic representation makes  
577 visible the dynamic or temporal evolution of the structures presented in Figure 11a. As can be seen in  
578 the video, both the axial flow (box n° 1 in Figure 11a) and the jet flow (box n° 3 in Figure 11a) are  
579 essentially constant. Finally, it is possible to identify the appearance of traveling vortices. These  
580 appear behind the blades every time they pass. Once such vertical structures are generated, they  
581 move radially away from their point of origin.

582 It is worth mentioning that all this dynamic information is contained in arrays whose size is much  
583 smaller than the CFD analogous. More explicitly, each POD vector has a dimension of  $3L \times 1$  and its  
584 respective modal coefficient has a size of  $N \times 1$ . In the present case study,  $L = 1.129.140$  elements,  $N$

585 = 386 snapshots, and only the first three POD eigenvectors with their respective modal components  
586 are necessary to recover 99% of the total variance of the system. This represents a storage  
587 requirement of  $(3L \times 3) = 9L$  for the POD vectors plus the temporal components  $(N \times 3) = 3N$ , the total  
588 number of elements being  $1 \times 10^7$  or 0.08 Gb in total. The CFD data size  $3 \times L \times N = 1.3 \times 10^9$  elements  
589 which is equivalent to a data storage of 9.7 Gb. Thus, 121 times more storage capacity is required  
590 when using CFD data.

### 591 5.3. Assessing the accuracy of the flow field reconstruction using global POD approach

592 The accuracy of the reconstruction obtained from a global treatment is now examined. The equation  
593 (13) estimates the quality of the approximation as a function of the number of modes  $p$  used for the  
594 flow field reconstruction from global approach. The expression (13) estimates a maximum average  
595 relative error  $E_{MNE}$ . First, the average of the maximum error between the reconstructed velocity  
596 field and the CFD velocity field is calculated for every snapshot. Then by dividing this quantity by the  
597 tip blade velocity ( $U_{tip} = 1.18 \text{ m} \cdot \text{s}^{-1}$ ), a normalized averaged error is obtained. This quantity is  
598 relevant because the POD technique is designed to minimize the average error between the  
599 reconstructed data and the experimental data (CFD data in this case).

$$E_{NAE} = \frac{\sum_{i=1}^N \max(\|\vec{U}_{POD}^i(\mathbf{x}, p) - \vec{U}_{CFD}^i(\mathbf{x})\|)}{N U_{tip}} \quad (13)$$

600

601 The relation (13) was calculated using 2, 3, 5 and 10 POD modes (time span of 386 snapshots). The  
602 results are provided in the Table 3 and presented graphically in the supplementary information  
603 (“Visual representation of the normalized error”):

604 *Table 3 : Normalized Averaged Error as a function of the number of modes used for the reconstruction.*

Number of modes	2	3	5	10
Normalized error (%)	62	6	5	3.5

605

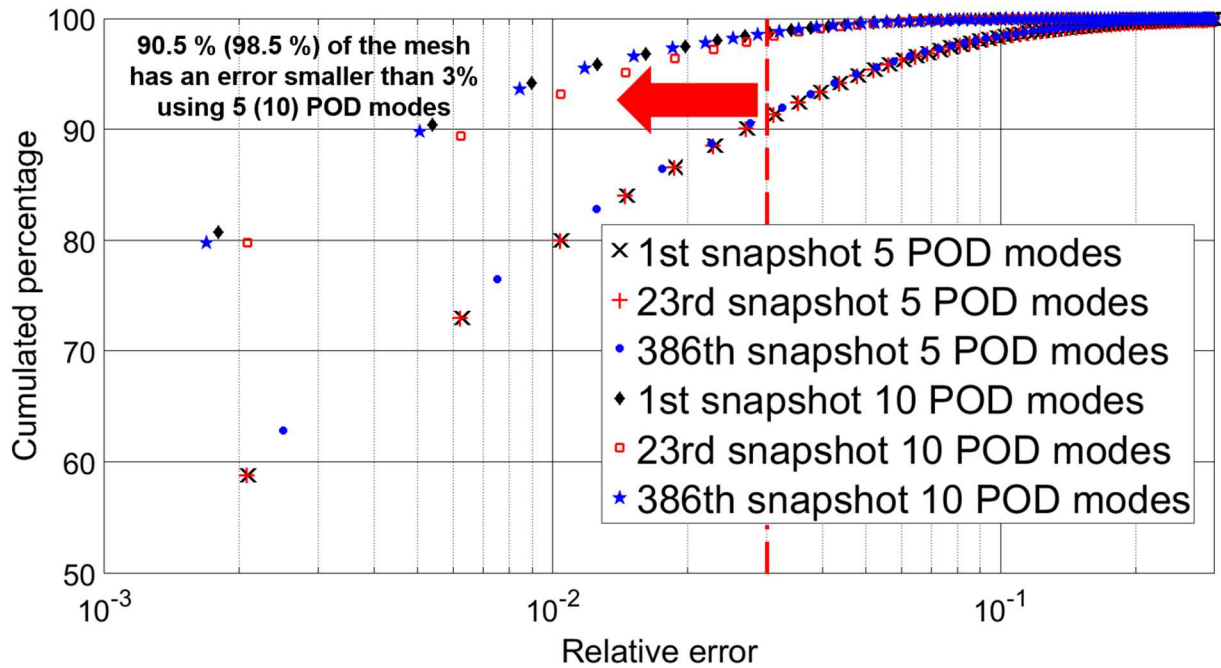
606 The use of the first and second modes produces an average error of 62% with respect to the tip  
607 velocity of the turbine. Such components are independent of the third mode, which is associated  
608 with the reconstruction of the average flow. In this way the POD reconstruction associated with the  
609 two first modes do not contain the mean flow information, implying a considerably high average  
610 error. When the third mode is included in the reconstruction, the error decreases noticeably, which  
611 is fully consistent with the previous analysis. As can be seen in the Table 3, the maximum error  
612 becomes approximately 6.0 %. Adding more modes to the reconstruction only slightly reduces the  
613 error down to 3.5 %. The above information shows that the global treatment allows the  
614 reconstruction of the velocity field with a low average error.

615 Beside the normalized error, it seems interesting to quantify the error considering the number of  
616 cells in which the error is significant, i.e. the error as a function of the cumulative percentage of cells.  
617 Equation (14) estimates a local error between the global POD reconstruction of the velocity field and  
618 the CFD velocity field for each cell in the domain. From this, the error distribution is built and  
619 represented in Figure 12. Unlike expression (13), (14) provides the error due to the reconstruction in  
620 a localized and instantaneous manner because the respective calculation is performed for each cell.  
621 The definition of (14) allows a more adequate and accurate evaluation of the POD reconstruction for  
622 the unsteady case studied in the present work.

$$E(\mathbf{x}, t, p) = \frac{\|\vec{U}_{POD}(\mathbf{x}, t, p) - \vec{U}_{CFD}(\mathbf{x}, t)\|}{\|\vec{U}_{CFD}(\mathbf{x}, t)\|} \quad (14)$$

623 Error distribution obtained through equation (14) for three different snapshots and using  $p = 5$  and  
624  $p = 10$  POD modes for the reconstruction is presented in Figure 12. For the case of 5 POD modes, it  
625 was found that around 90.5% of the total number of cells exhibit an error smaller than 3%. The  
626 relative error of the rest of the cells is distributed according to the following categories: 4.5% of the  
627 cells have an error greater than 3% and less than 5%. The final 5% has an error greater than 5% and  
628 less than 27%.





629

630 *Figure 12. Cumulative percentage of the number of cells as a function of the relative error calculated by equation (14), using*  
 631 *either 5 and 10 POD modes. An increase in the number of POD modes leads to an upward shift of the curve. The vertical red*  
 632 *line indicates 3% relative error.*

633 The previous results are improved when 10 POD modes are used to perform the flow reconstruction:

634 98.5% of the total number of cells have an error less than 3%, 1% of the cells have an error between

635 3% and 5%. The final 0.5% has an error greater than 5% and less than 27%. Table 4 proposes the

636 same results in terms of percentage of cells with an error comprised in a given range.

637 *Table 4 : Percentage of cells with an error  $E(x, t, p)$  comprised in a given range for  $p = 5$  and 10 modes.*

Snapshot #	$E(x, t, p) < 3\%$		$3\% < E(x, t, p) < 5\%$		$5\% < E(x, t, p)$	
	$p = 5$	$p = 10$	$p = 5$	$p = 10$	$p = 5$	$p = 10$
1	90.5	98.5	4.5	1	5	0.5
23	90.4	98.0	4.5	1.4	5.1	0.6
386	90.5	98.5	4.5	1	5	0.5

638

639 It was observed that the cells in which the relative error is high are mainly located on the interface

640 between the fixed and rotating mesh grids (see 'locations of cell with significant error' in

641 Supplementary Information).

642 5.4. Numerical cost of a spatio-temporal reconstruction using the global POD  
 643 technique

644 The use of order reduction methodologies is not justified solely in terms of flow structure analysis.  
 645 Another relevant aspect is the efficiency in the implementation of the method compared with the  
 646 standard use of CFD tools. At this point of the present work, it is possible to propose a continuous  
 647 spatio-temporal reconstruction of the 3D unsteady flow field, i.e. at a higher temporal resolution  
 648 than the initial CFD data. Starting from the previous POD results and after identifying the continuous  
 649 function associated with the mode components, the 3D field reconstruction was performed 714  
 650 times over 0.4 s, the duration of one turn. The time necessary to perform these reconstructions is  
 651 compared with the time necessary to perform the CFD calculation with the same temporal  
 652 resolution. Table 5 presents a summary of the physical time required for the CFD simulation of a full  
 653 turn on the complete tank and the corresponding time necessary to perform the POD reconstruction  
 654 via a global treatment using 5 and 10 modes. The first two lines provide the results for five and ten  
 655 modes respectively. For both cases, the set-up time (time to read data and perform POD  
 656 decomposition) is equal because the input data and numerical operations are identical. The  
 657 reconstruction of a single 3D flow field is longer when ten modes are considered, 133.6 seconds for  
 658 10 modes against 64.5 seconds for 5 modes reconstruction. The corresponding time for the CFD  
 659 simulation is  $2.7 \times 10^4$  seconds, which corresponds to 58 and 50 times the duration of the POD  
 660 reconstruction using 5 and 10 POD modes respectively.

661 *Table 5. Comparative summary of the time duration for the CFD and POD reconstruction procedure.*

Procedure	Number of POD modes	Set up time (s)	Reconstruction time (s)	Total time (s)	$\frac{t_{Recons\_POD}}{t_{CFD}}$
POD	5	400	64.5	464.5	$1.7 \times 10^{-2}$
Reconstruction	10		133.6	533.6	$2.0 \times 10^{-2}$
CFD				$2.7 \times 10^4$	

662

663 This saving of calculation time is important especially considering that the reconstruction process is  
664 carried out only once. As indicated in the last column of the table it is also advantageous to use POD  
665 reconstruction with respect to CFD data. The difference in processing time between the two  
666 numerical methodologies evidences the advantage of using the POD technique for flow  
667 reconstruction and its subsequent use as input to other physical and biochemical models.

668 In particular, a continuous 3D reconstruction of the velocity field at a minimal computational cost can  
669 be particularly interesting to perform Lagrangian Particle Tracking and/or a compartmentalization of  
670 the fluid domain.

## 671 Conclusions

672 By using a per-zone and global POD approaches, it is possible to reconstruct the 3D mean and  
673 organized unsteady flow of a four-baffled agitated tank equipped with a Rushton turbine.

674 The per-zone method turns out to be an option to reconstruct the velocity field but such a  
675 methodology involves a larger number of steps compared with the global treatment of the entire  
676 volume.

677 For the global POD approach, the fact that in an inertial reference frame, the spatial coordinates of  
678 the cells belonging to the rotating zone are changing does not actually matter for the POD  
679 reconstruction. Such findings show the feasibility of using the POD technique for velocity field  
680 reconstruction using a CFD simulation on a mesh with a stationary zone and a rotating zone without  
681 zone separation.

682 The global POD decomposition results provide a series of components with different variances and  
683 frequencies. The top ranking modes present temporally periodic, these ones are associated with the  
684 reconstruction of coherent structures. The frequency associated to the first three modes (carrying  
685 99.9% of the total system variance) is identical to the rotation frequency of the turbine. The first and

686 second modes are localized in the rotating zone and their axial component is essentially zero. The  
687 third mode carries the information related to the mean flow so its contribution is present in the  
688 whole domain. The largest horizontal (circulation loops) and vertical vortices are contained in it.

689 The coherent structures found by means of global POD reconstruction do not depend on the number  
690 of snapshots implying a statistical convergence of such organized movements. There exist modes of  
691 very low variance associated with the reconstruction of very organized structures. Such modes  
692 turned out to be harmonic frequencies of the main frequency associated the rotation of the turbine.

693 When three modes are considered for the reconstruction of the mean and organized velocity field,  
694 the maximum average error is of the order of six percent with respect to the CFD data. The addition  
695 of higher modes reveals an improvement in the maximum average error but it is not large unless  
696 several modes are considered.

697 The POD technique proves to be accurate even when evaluating a localized and instantaneous error.  
698 As expected, such accuracy is greatly improved when a larger number of POD modes are included.

699

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