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On the role of aortic valve architecture for physiological haemodynamics and valve replacement. Part I: flow topology and vortex dynamics

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Research Article

Keywords: Aortic stenosis, Aortic valve replacement, Bioprosthetic aortic valve, Jet flow, Valve design, Vortical structures, Vorticity transport

Posted Date: September 27th, 2023

DOI: https://doi.org/10.21203/rs.3.rs-3385983/v1

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On the role of aortic valve architecture for physiological haemodynamics and valve replacement. Part I: flow topology and vortex dynamics.

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9 Abstract

4

Aortic valve replacement has become a growing concern due to the increasing prevalence 10 of a ortic stenosis in an ageing population. Existing replacement options have limitations, 11 necessitating the development of improved prosthetic aortic valves. In this study, flow charac-12 teristics during systole in a stenotic aortic valve case are compared with those downstream of 13 two newly designed surgical bioprosthetic aortic values (BioAVs) using advanced simulations. 14 Our findings reveal that the stenotic case maintains a high jet flow eccentricity due to a fixed 15 orifice geometry, resulting in increased vortex stretching in the commissural low-flow regions. 16 One BioAV design introduces non-axisymmetric leaflet motion, which reduces the maximum 17 jet velocity and forms more vortical structures. The other BioAV design produces a fixed 18 symmetric triangular jet shape due to non-moving leaflets and exhibits favourable vorticity 19 attenuation and significantly reduced drag. Therefore, this study highlights the benefits of 20 custom-designed aortic values in the context of their replacement through comprehensive flow 21 analyses. The results emphasise the importance of analysing jet flow, vortical structures, 22 momentum balance and vorticity transport for evaluating aortic valve performance. 23

24 Main

Aortic stenosis (AS) concerns the progressive deterioration and remodelling of the leaflet 25 tissue, which reduces its dynamics. This leads to an increased resistance for the blood to flow 26 from the left ventricle to the aorta, especially during systole, and to the possibility for blood 27 to flow back during diastole^{8,9,38}. The long-term consequences of such a pathology are very 28 serious including heart failure and mortality is more than 90% within a few years after the 29 onset of symptoms³⁴. Valvular prostheses made from either rigid materials such as titanium 30 or carbon, known as mechanical heart valves, or from biological tissue, known as bioprosthetic 31 aortic values (BioAV), have become a common solution for replacing the diseased aortic value 32 through a procedure called a ortic valve replacement (AVR). AS prevalence increases with 33 age and affects as many as 5% of the population after 75 years of age. AS is responsible for 34 300,000 surgical aortic valve replacements worldwide annually, a number that is expected to 35 double by 2050 with the ageing population²⁸. 36

The performance of aortic valves surgically implanted and made from biological tissue such as porcine or bovine pericardium has been extensively investigated in the literature^{2,3,8,38} but the link between valve design, flow features and leaflet motion has never been studied whether experimentally or computationally.

Bescek *et al.*³ presented a computational characterisation of the turbulent features of the 41 flow downstream of one bioprosthetic aortic valve model under peak systolic conditions. 42 To do so, they performed a statistical analysis on the flow data and found that the total 43 rate of turbulent dissipation was responsible for 26% of the total pressure loss across the 44 valve indicating that turbulence is a significant and detrimental factor for haemodynamic 45 performance. They also noted that the shedding of vortex rings periodically generated at 46 the leaflet tips at a frequency of 36 Hz as a consequence of the periodic leaflet motion leads 47 to peaks of viscous shear stresses, Reynolds' stress and dissipation rate of turbulence at a 48 distance of 30 mm from the leaflet tips. However, in their study, Becsek $et \ al.^3$ did not 49 analyse the downstream evolution of vortices from the specific aortic valve bioprosthesis 50 under consideration. They also did not establish a connection between valve design, leaflet 51

⁵² motion, the observed vortical structures and the spatial-temporal variations in vorticity.
⁵³ Furthermore, they did not quantify the drag forces associated with the presence of the
⁵⁴ mentioned bioprosthetic aortic valve.

Furthermore, Johnson *et al.*²¹ studied the impact of heart valve tissue thickness on the 55 presence, nature and extent of leaflet flutter. Under the assumption that the cyclic-strain 56 behaviour observed when valve leaflet free edge flutters over the lifetime of the valve causes 57 an additional induced cyclic loading that may contribute to non-uniform or accelerated leaflet 58 fatigue and deterioration, their study demonstrated that a major reduction in valve material 59 thickness can induce detrimental leaflet flutter. Relying upon an immersogeometric analysis 60 framework to simulate the fluid-structure interaction problem and on a flutter-quantification 61 methodology, their results exhibited the impact that a single parameter can have on both 62 the structural performance of the tissue and the blood flow behaviour throughout the whole 63 cardiac cycle. Nevertheless, flow quantities related to turbulence were not calculated and the 64 conclusions as to the impact of the flutter motion on the flow was limited to the visualisation 65 of iso-surfaces of instantaneous velocity and vorticity field close to the valve and in the curved 66 ascending aorta model. 67

Most recently, Morany et al.²⁵ conducted a computational study of the fluid-structure 68 interaction problem arising in healthy tricuspid and biscuspid aortic values (TAV and BAV). 69 For this purpose, they strongly coupled, using a partitioned approach, the lattice Boltzmann 70 method (LBM) to solve the blood motion equation to a Finite Element (FE) method to 71 solve the elastic body motion equation. To model the constitutive relationship of the porcine 72 leaflets, they considered a symmetric collagen fibre network (CFN) embedded in an elastin 73 matrix for each value leaflet. The distribution of these fibres was obtained by averaging 74 the maps of fibre bundles observed under a microscope for 15 porcine leaflets²³. Morany 75 et al. concluded that their LBM-FE FSI approach was able to reliably assess velocity, and 76 more specifically the velocity oscillations occurring at mid-diastole downstream of the TAV, 77 and wall shear stress throughout the whole cardiac cycle in the vicinity of a TAV and a 78 BAV. To state this, they conducted a comparison by evaluating the range of maximum 79

velocity achieved in the jet issuing from the leaflets at systole peak and compared it to 80 values documented in existing literature. Additionally, they compared the wall shear stress 81 values on the ventricular side of the leaflets during leaflet coaptation and at systole peak with 82 the range of values reported in previous studies. However, it is important to note that the 83 comparison was limited to expected ranges of values and no detailed examination of spatial 84 distributions for both velocity and wall shear stress fields was carried out. Furthermore, 85 the resolution of the fluid lattices considered in Morany *et al.* only permitted the analysis 86 of large-scale flow features, thus neglecting the small-scale velocity fluctuations that are of 87 great importance when characterising the transition to turbulence in the aorta. 88

The present work is the first part of a comprehensive two-part study. In this work, the analysis of blood motion focuses on characterising flow topology by describing the distribution of velocity magnitude and the dynamics of coherent vortical structures downstream of three different valvular configurations. The temporal evolution of the terms of the vorticity dynamics equation is also investigated. Besides, two novel quantities corresponding to the vortex advection and stretching terms, projected onto the eigenbasis of the vorticity gradient and rate-of-strain matrices, respectively, are introduced.

To the best of our knowledge, a comprehensive computational study and detailed analysis 96 encompassing various designs of a ortic valve bioprostheses along with a comparative analysis 97 to a severe stenotic case have not been previously undertaken. This work makes a significant 98 contribution to the advancement of optimally designed and patient-customised aortic valves. 99 Through dedicated flow analysis, it comprehensively investigates the flow topology near 100 a pathological aortic stenosis, comparing it to the flow characteristics downstream of two 101 surgical valve bioprostheses. These two bioprostheses have undergone modifications in their 102 leaflet geometry by changing thoughtfully selected geometric parameters. The connection 103 between the two valve designs, subsequent leaflet motion and encountered aortic flow features 104 is established. 105

¹⁰⁶ Jet flow topology

Fig. 1 presents the velocity magnitude in a plane at a distance of 10 mm from the STJ (plane 1) as well as the evaluation of the eccentricity of the jet centre (white dots in Fig. 1) in relation to the centre of the circular cross-section (black dot in Fig. 1).

In the stenotic case, the eccentricity angle α_c of -5° to 5° and eccentricity distance ε_c of 110 about 2 mm do not significantly vary over time as the orifice geometry is immobile due to 111 the calcified leaflets (see Fig. 5 (f)). Moreover, the regions situated between commissures 1-2 112 and 2-3 (cf. Fig. 1) exhibit elevated velocity magnitudes that extend from the jet, in contrast 113 to the region between commissures 1-3. This trend is further highlighted in Fig. S4 of the 114 supplementary material illustrating vortex stretching magnitude in the proximal plane p1. 115 In fact, we observe that elevated values of vortex stretching magnitude are predominantly 116 located between commissures 1-2 and 2-3. Conversely, within the area between commissures 117 1-3, the magnitude of vortex stretching is negligible. At time instant t=0.12 s, the velocity 118 magnitude in the trilobal jet drops, which is represented by a 30% decrease in the maximal 119 velocity magnitude. The corresponding shear layers present smaller velocity gradients at 120 this instant and are thicker. In Fig. S4, this trend is indicated by a decrease in the vortex 121 stretching magnitude. From 0.21 s until 0.3 s, the velocity magnitude in Fig. 1 indicates 122 a more ordered separation between the main high velocity jet flow and the surrounding 123 secondary low velocity flow. In Fig. S4 and Fig. 4 (a), this is revealed by a decrease in the 124 values of $||S_{\omega}||$ over the proximal plane or averaged over the volume of investigation (VoI). 125 Concerning the VLth30 BioAV case, the eccentricity distance and angle vary throughout 126 the systolic phase with higher eccentricity distances observed from t=0.21 s onward. This 127 is a direct consequence of the three leaflets moving asymmetrically with a displacement 128 magnitude amplitude of 1.5 to 2 mm (see Fig. S1 in the supporting information). From 129 Fig. S1, it is also noteworthy that the amplitude and difference in the three leaflets' position 130 in relation to their initial position is more pronounced from t=0.21 s onward. Besides, as 131 compared to the stenotic case, the motion of the leaflets and of the connected flow motion 132 leads to a 10 to 20% smaller maximum velocity in the jet reaching peak values between 133

t=0.12s and t=0.15s as shown in Fig. S2 (a). The velocity magnitude distribution in the region surrounding the jet is much less organised and presents larger velocity values as compared to the stenotic case due to the leaflet motion pushing blood in this region and promoting mixing of high and low velocity zones.

With regard to the Ulth0 bioprosthesis case, given the almost immobile leaflets at peak 138 systole (see Fig. 8 (c) and Fig. S1), the eccentricity distance ε_c is negligible. The shape of the 139 jet is well defined and triangular. Between time instants t=0.15 and t=0.21 s, an instability 140 is observed in the shear layer between the high-velocity jet (with a maximum velocity of 141 2 m/s, as shown in Fig. S2 (a)) and the surrounding quiescent region. This instability 142 is characterised by the emergence of wavy irregularities in the velocity distribution at the 143 borders of the triangular jet. It arises from the entrainment of high-velocity fluid elements 144 into the region of lower velocity, subsequently pushing the low-velocity fluid towards the high-145 velocity flow region. This change in the velocity distribution and the creation of vortices 146 along the shear layer interface is known as the Kelvin-Helmholtz instability (KHI)¹⁴. In the 147 Ulth0 case, this instability, which breaks the flow axisymmetry, is likely to be accentuated 148 by the flow deceleration that begins at t=0.1 s and is imposed by the inflow conditions (see 149 Fig. 7). 150

Finally, it is of relevance to mention that the fixed triangular-shaped jet described in the 151 Ultho valvular case issuing from the valve leaflets has been also noted in Corso *et al.*⁸ 152 throughout systole and by means of three-dimensional particle tracking velocimetry measure-153 ments, downstream of a Medtronic (Minneapolis, Minnesota, USA) Evolut R transcatheter 154 aortic valve. In the study by Corso et al.⁸, another transcatheter valve, namely the CoreValve 155 from Medtronic, was tested. Worthy of noting that the phase-averaged flow analysis revealed 156 a jet of moderate velocity with an elliptical shape, the position of which varied in relation to 157 the aorta wall during systole. This observation is congruent with the moving jet of moderate 158 to high velocities noted for the VLth30 valvular case characterised by a varying eccentricity 159 distance and angle of the jet over systole. 160

[Figure 1 about here.]

The velocity magnitude in a distal plane (at a distance of 24 mm from the STJ) is 162 presented in Fig. 2. In the stenotic case, the stratified organisation between two clear 163 flow zones, i.e. a trilobal jet of high velocities and the surrounding quiescent flow, is not 164 present anymore. Instead, scattered high velocity patches resulting in longer and disorganised 165 shear layer interfaces are pushed toward the outer wall of the aorta model from t=0.12 s. 166 We speculate that the shift of the high velocity jet toward the outer wall results in the 167 impingement of the vortices against the wall leading to a break-up of these vortices. In 168 addition, the separation between a helical flow motion in the time-averaged velocity field 169 along the inner wall¹⁰ and the shattered initial jet along the outer wall creates at the interface 170 between these zones a sustained entrainment of fluid momentum in the high velocity zone. 171 Concerning the VLth30 case, the jet flow structure with the moving high velocity region is 172 still noticeable and the maximum velocities in the distal plane p2 are similar to the ones 173 encountered in the proximal plane p1. The most striking features in the distal plane are 174 the thickening of the interface between the high flow regions, corresponding to the tail of 175 the jet and the low flow regions resulting in smaller velocity gradients at the shear layers. 176 Furthermore, the time-varying position of the jet tail follows the one remarked in the proximal 177 plane through the analysis of jet eccentricity emphasising the importance of leaflets' motion 178 effect also on distal flow structures. 179

In the Ulth0 BioAV case, similarly to the case with the VLth30 BioAV, the central jet can still be observed in the distal plane. Unlike the well defined triangular jet noted in the proximal plane, irregularities and thickening of the shear layer interface are observed at all the time instances over systole as a result of the shedding of the vortices created in the shear layers upstream.

[Figure 2 about here.]

185

¹⁸⁶ Vortical structures

In Fig. 3, the image sequence of the intricate coherent vortical structures downstream of the aortic stenosis and the two BioAVs is visualised using the λ_2 -criterion²⁰.

In the stenotic case, we note a starting vortex ring hugging the shape of the stenotic orifice. 189 The high difference in velocity between the accelerating flow (maximum velocity in the 190 stenotic jet of 1.9 m/s) and the quiescent flow close to the wall of the aorta brings about 191 zones of high shear at the interface propitious for the roll-up and shedding of eddies. This 192 initial vortical structure is then shed and broken into smaller vortices that occupy the whole 193 straight aorta volume under the push of a high velocity jet. From time t=0.09 s onward, due 194 to the impingement of the jet on the outer wall of the curved ascending aorta, as presented 195 in Corso $et \ al.^{10}$, a secondary retrograde helical mean flow motion with smaller velocities is 196 created in the curved portion of the aorta and pushes the majority of the vortical structures 197 towards the outer aortic wall accentuating the asymmetry in the spatial distribution of the 198 vortical structures. The high velocity jet is thus confined in the outer wall region throughout 199 the whole systole. At the interface between the high-velocity jet and the low-flow regions 200 near the inner wall, the entrainment of fluid with low momentum at the shear layers leads 201 to intermittent increases in the number of small-scale densely distributed vortices at times 202 t=0.12, 0.18, 0.21, and 0.27 s. This intermittent surge in vortex break-up is mainly located 203 close to the outer wall. The times at which it occurs coincide with the time instants at which 204 slightly decelerating inflow velocities upstream of the stenosis are imposed (see Fig. 7). 205

With regard to the VLth30 BioAV case, initial coherent vortices are found along the free edge 206 of the leaflets (t=0.03 s). These vortices quickly dissipate due to leaflet motion. However, 207 starting at t=0.03 s, new vortical structures resembling hairpin vortices (as seen in the inset 208 of Fig. 3 at t=0.06 s) form in the gaps between the leaflet commissures and above the ring 209 posts. In fact, the movement of the ring posts, resulting from the unstable motion of the 210 leaflets, initiates the generation of hairpin-like vortical structures, particularly when the gaps 211 widen. At t=0.09 s, we note large vortical structures stretched in the axial direction issuing 212 from the moving leaflet free edges. Between t=0.12 and 0.21 s (after the inflow conditions 213

reach the peak flow), due to flow deceleration, the coherent vortical structures are broken 214 down into small vortices uniformly distributed over the whole straight ascending aorta as 215 a consequence of the moving leaflets and valve orifice promoting higher mixing and vortex 216 merging further downstream. Besides, large coherent eddies are displayed close the leaflet 217 free edges and in the low velocity regions whereas stretched and smaller eddies are found 218 in the shear layers, i.e. at the interface between the high velocity jet and the surrounding 219 quiescent fluid close to the aorta wall. Between t=0.24 s and t=0.3 s, the breakdown of 220 the vortex is diminished as compared to previous times due to a reduction in jet velocity. 221 However, the presence of large-scale vortical structures, induced by the motion of the leaflets, 222 is still observable. 223

In the Ulth0 BioAV case, a pattern reminiscent of the VLth30 case emerges, characterised 224 by an initial vortex ring at the leaflets' free edge. It is interesting to note that up until 225 t=0.06 s, the jet of fluid maintains a circular shape, aligning with the contours of the orifice. 226 Due to the flow acceleration, beyond t=0.06 s, the shape of the jet becomes triangular. The 227 initial vortex ring sheds and fades after t=0.03 s owing to the formation of new eddies at the 228 the ring posts. In fact, akin to the VLth30 BioAV case, hairpin-shaped vortices are found 229 at the ring post at t=0.06 s due to the commissural gap between the leaflets (see inset at 230 t=0.06 s in Fig. 3). Unlike the other BioAV case though, between t=0.12 s and t=0.21 s, 231 these hairpin-shaped vortices demonstrate a tendency to elongate axially before being broken 232 down into smaller vortices further downstream. This change in vortex shape is instigated by 233 heightened shear between the triangular jet of elevated velocities (peaking at 1.8 m/s) and 234 the surrounding zones of low velocity. Consequently, the presence of the three ring posts 235 under stable leaflet motion condition, as the one observed in the Ulth0 BioAV case (cf. Fig. 8 236 (c)), has a pivotal influence on the distribution and size of the vortices downstream of the 237 valve. From t=0.21 s onward, the number of coherent vortical structures dwindles as a result 238 of the flow deceleration as illustrated in Fig. 7. 239

240

[Figure 3 about here.]

²⁴¹ Momentum balance

To compare the results downstream of the three valvular configurations examined in this 242 study with the findings of Chen and Luo^7 and Becsek *et al.*³ and to evaluate the flow 243 resistance resulting from the presence of prosthetic or stenotic values, we compute each 244 term of the flow momentum balance in the streamwise direction within a control volume, 245 V_{con} , which corresponds to the fluid present in both the ascending aorta and the sinus. The 246 examined quantities, derived from the momentum balance equation and non-dimensionalised 247 using the maximum pressure flux difference over systole, are listed below and presented in 248 Table 1: 249

• the pressure term ΔPA averaged over the systole;

• the acceleration term $\dot{p} = \frac{\partial}{\partial t} \iiint_{V_{con}} \rho u_z \, dV$ averaged over the systole with V_{con} , the control volume;

• the mean and maximal drag coefficient $C_D = (2F_{\text{leaflets}}) / \left(\iint_{in} \rho u_z^2 dA \right)$ with F_{leaflets} , the total hydrodynamic force acting on the leaflet surfaces and the denominator being the inlet momentum flux;

• the mean equivalent length of accelerated fluid column $h_{F_{\text{leaflets}}} = (LF_{\text{leaflets}})/\dot{p}$ made dimensionless by dividing it by the reference diameters $\mathscr{D}_{\text{sten}} = 0.011$ m and $\mathscr{D}_{\text{BioAV}} =$ 0.018 m. *L* is the length (in the Z-direction) of the control volume.

Table 1 shows that the time-averaged dimensionless pressure flux difference is of a comparable magnitude for the bioprosthetic cases (lines 2, 3, 4 in Table 1) and the flexible aortic valve case (line 5 in Table 1) but it is 67% higher in the stenotic case. This larger value can be attributed to stenosis, which introduces larger pressure loss as well as to the curved aorta geometry in the stenotic case, which modifies the position where pressure recovery arises³⁶. In addition, in the stenotic case, the time-averaged acceleration term is two to four times as small as that calculated in the four prosthetic aortic valve cases.

With regard to the drag coefficient C_D , the mean and maximal values for the cases presented

in Becsek *et al.* (line 4 in Table 1) and Chen and Luo (line 5 in Table 1) are in good 267 agreement. This can be attributed to the observed strong periodic flutter of the leaflets 3,7 . 268 This type of flutter motion leads to the generation of a sequence of vortex rings, whose 269 shapes vary over time⁷. For the other two BioAV cases studied in this work (lines 2 and 270 3), the drag coefficient (C_D) values are one-fourth to one-fifth of those calculated from the 271 data presented in⁷ and³. The VLth30 case presents higher C_D value compared to the Ulth0 272 case as a consequence of the non-axisymmetric but moderate flutter motion (see Fig. S1 in 273 the supplementary information). This underscores the influence of leaflet geometry on the 274 resistive forces introduced by the aortic valve prosthesis and its correlation with the type of 275 flutter motions exhibited by the leaflets. 276

In relation to the equivalent length of the fluid column $\overline{h_{F_{\text{leaflets}}}}$ decelerated due to the reaction 277 forces at the leaflet surfaces, the stenotic case displays the highest value. However, for the 278 valvular cases demonstrating periodic flutter of the leaflets with substantial displacement 279 magnitudes (lines 4 and 5 in Table 1), the decelerated fluid column due to the presence 280 of the valve falls within a similar range as that observed in the case of aortic stenosis for 281 the flexible valve scenario presented by Chen and Luo^7 and is 50% smaller in the case 282 investigated by Becsek et al.³. The newly designed BioAV cases, namely VLth30 and Ulth0, 283 exhibit values for $\overline{h_{F_{\text{leaflets}}}}$ that are 4 and 6 times smaller than the value calculated in the 284 stenotic case, respectively. 285

286

[Table 1 about here.]

²⁸⁷ Vorticity transport and vortex stretching

Finally, we analyse the vortex stretching term S_{ω} and advection due to the flow velocity A_{ω} of the vorticity transport equation (cf. Eq. 2). This transport equation is central for the characterisation of the evolution and distribution of vortices, especially pertaining to their amplification or decay at the considered time instance.

²⁹² In Fig. 4 (a), the evolution of the magnitude of the vortex stretching tensor averaged over

the VoI is presented. In the stenotic case, $\langle ||S_{\omega}|| \rangle$ generally decreases over systole with 5 peaks occurring at t=0.125, 0.143, 0.193, 0.25 and 0.28 s. The peaks observed, ranging between 1.85×10^5 and $2.8 \times 10^5 s^{-2}$, correspond to instances when a higher density of vortical structures were identified in Fig. 3.

In the VLth30 case, between t=0.135 s and 0.156 s, peak values of $1.76 \times 10^5 \, s^{-2}$ are exhibited following the trend of the inflow rate time series consisting of an acceleration until t=0.1 s and a two-third less deceleration until t=0.21 s (cf. Fig. 7).

In the Ulth0 case, a peak value of 1.38×10^5 , s^{-2} is observed at t=0.186 s. The rate of change over time for the vortex stretching magnitude in this case is nearly identical. Finally, the time-averaged $< ||S_{\omega}|| >$ presented in the table of Fig. 4 (d) is twice as large for the stenosed aorta case compared to the values calculated in the two BioAV cases.

The time series of the ensemble-averaged projected vortex stretching as defined in Eq. 3 304 is shown in Fig.3 (b). It is noteworthy that the majority of values are highly positive in 305 the case of calcific stenosis, especially up to t=0.23 s. Positive projected vortex stretching 306 reaching a maximal value of $1.33 \times 10^4 \ s^{-2}$ in the stenotic case suggests an alignment of 307 the vorticity vector and the principal directions of the rate-of-strain tensor multiplied by 308 the eigenvalues of this tensor. It represents a phenomenon called vorticity amplification or 309 intensification³⁷ characterised by the elongation of vortical structures and an increase in the 310 rotational motions in the flow. In the VLth30 bioprosthetic case, positive levels of $<\Pi^{S_{\omega}}>$ 311 are found between t=0.11s and 0.156s and between t=0.19 s and 0.22 s with a maximum 312 of $3.5 \times 10^3 \, s^{-2}$ and on average over systole, the projected vortex stretching is positive (see 313 Fig. 4 (d)). In contrast, the levels of $\langle \Pi^{S_{\omega}} \rangle$ for the Ulth0 case are mainly negative. 314 This results, as shown in the table of Fig.4 (d), in a negative time-averaged value, which 315 is 4.7 times smaller in magnitude than that for the stenotic case and 4.4 times larger than 316 the one obtained for the VLth30 BioAV case. It is worth noting that negative projected 317 vortex stretching is associated with an anti-parallel alignment of the vorticity vector and the 318 strain rate, resulting in a decrease in overall vorticity acceleration, a phenomenon known as 319 vorticity attenuation³⁷. This attenuation is linked to the favourable reorganisation of the 320

³²¹ flow and the suppression of flow disturbances.

Fig.4 (c) shows the time evolution of the projected vorticity advection, which repre-322 sents the intensity whereby vorticity is transported by the velocity field. In fact, a positive 323 (negative) value indicates that the velocity vector is parallel (anti-parallel) to the principal 324 directions of the vorticity gradient tensor and the magnitude is the result of the multiplica-325 tion of the latter by the eigenvalues of the vorticity gradient tensor. In other words, positive 326 ensemble-averaged projected vorticity advection values indicate that spatial variations in 327 the vorticity field primarily occur along the flow direction, while negative values suggest 328 that the deformation in the vorticity field predominantly opposes the flow direction. For 329 the aortic valve stenosis case, we observe that $\langle \Pi^{A_{\omega}} \rangle$ levels are, for the most part of 330 systole, positive leading to a large time-averaged value of 9,157 s^{-2} as shown in the table 331 of Fig. 4 (d). We also note that this time-averaged $\langle \Pi^{A_{\omega}} \rangle$ is 3.65 times as large as the 332 time-averaged $\langle \Pi^{S_{\omega}} \rangle$ and of the same sign. Concerning the VLth30 bioprosthetic value 333 case, $<\Pi^{A_{\omega}}>$ alternates between positive and negative values over systole resulting in a 334 negative time-averaged value. The times at which these negative and positive peaks occur 335 are coincident with the times of the peaks observed in Fig. 8 (c) and Fig. S2 for the area 336 at the vena contracta and vorticity deficit, respectively. Thereby, the asymmetric leaflet 337 motion does play an important role in the transport of vortices in the region downstream 338 of the value albeit not necessarily by promoting the advection of the vorticity field in the 339 flow direction but in an opposite direction as well. Finally, the magnitude of time-averaged 340 $<\Pi^{A_{\omega}}>$ is in this case 2.8 times as large as as the time-averaged $<\Pi^{S_{\omega}}>$. For the Ulth0 341 case, the most favourable conditions are met to fulfil vorticity weakening in the bulk of the 342 flow downstream of the valve with a positive time-averaged $\langle \Pi^{A_{\omega}} \rangle$, whose magnitude is 343 26% less than the magnitude of time-averaged $\langle \Pi^{S_{\omega}} \rangle$. As previously stated, the latter is 344 negative highlighting a more pronounced vorticity attenuation over the VoI. 345

[Figure 4 about here.]

346

347 Outlook

These findings emphasise the complex interplay between valve geometry, leaflet motion and aortic haemodynamics. They highlight the importance of understanding jet flow topology, vortical structures close to the valvular orifice and of analysing momentum balance and vorticity transport for assessing the performance of aortic valves.

In fact, the comprehensive analysis conducted in this first part of the study contributes to our understanding of the critical geometrical features of valve design that promote a more organised and physiological flow. This, in turn, leads to a reduction in pressure loss and decreased haemodynamic forces acting on blood cells and on the aortic wall.

The two-part computational study, which comprehensively analyses aortic flow data, paves the way for the development of innovative and patient-customised valve designs that can optimise systolic flow patterns and minimise detrimental effects associated with aortic valve replacement.

360 Methods

³⁶¹ Geometrical models and leaflet geometry parametrisation

As far as the severely calcified aortic valve case is concerned, the geometry of the curved 362 aorta was obtained from an MRI scan (cf. Fig. 5 (a, b)) and has a diameter at the sino-363 tubular junction (STJ) d_{STJ}^{sten} of 25 mm (see Fig 5 (e)). A patient-based geometry of stenosis 364 was added to the sino-tubular extremity and the eccentric stenotic orifice subsequent to the 365 calcification of a tricuspid aortic valve is shown in Fig. 5 (f). The reduction in cross-sectional 366 area through the orifice is about $80\%^{9,10}$. Within the scope of this study, only the straight 367 section of the ascending aorta is considered when comparing the jet flow structures present 368 in the vicinity of the orifice for the stenotic and bioprosthetic cases (see Fig. 5 (b, c)). 369

³⁷⁰ Concerning the bioprosthetic valve cases, the geometry of the aortic root (AR) including ³⁷¹ the sinus of Valsalva (SOV) geometry is similar to the one presented in Bescek *et al.*³. The main dimensions of the sinus portion and the straight aorta are shown in Fig. 5 (g, h). The geometry of the bioprosthetic heart valves, including three leaflets and a supporting ring, corresponds to an approximate reproduction of the commercial valve *Edwards Intuity Elite 21mm* (Edwards Lifescience, Irvine, CA, USA). The leaflets are made from glutaraldehydefixed bovine pericardium and are mounted on a rigid ring made of polymer supported by a nitinol wireframe and covered with fabric. The BioAV models are introduced in the AR, as shown in Fig. 5 (d).

379

[Figure 5 about here.]

To test the influence of different leaflet geometries of BioAV on their kinematics and on 380 the flow characteristics at peak systole, two new geometrical configurations (with reference 381 VLth30 and Ulth0) for the 500-micron-thick leaflets have been designed (cf. Fig. 6 (b, c)). 382 Besides, it is assumed that the designed initial leaflet position corresponds to the stress-free 383 configuration. As shown in Fig. 6 (b) and (c), the two geometries of the newly designed 384 leaflets vary with each other based on three features of the leaflet: (i) the belly curve, i.e. 385 the curve obtained by longitudinally cutting the leaflet in half (cf. Fig. 6 (b, c, e); (ii) the 386 free edge, i.e. the leaflet extremity not attached to the ring (Fig. 6 (a)); (iii) the scallop or 387 attachment curve, i.e. the leaflet extremity attached to the ring (Fig. 6 (d)). Each feature of 388 the designed leaflets is defined based on different parameters that are summarised in Fig.6 389 (f). The belly curve with centred and normalised coordinates is defined by two parameters 390 a and b of the hyperbolic sine function as shown in Fig.6 (e). Depending on the geometry 391 of the ring and on the other two features, the belly curve is dimensionalised leading to two 392 radial lengths (ΔX_{Ulth0} , ΔX_{VLth30}), two axial lengths (Δh_{Ulth0} , Δh_{VLth30}) and two belly 393 curve lengths (l = 13 mm and L = 14.5 mm). 394

The free edge is characterised by the angle θ between the plane perpendicular to the centreline of the straight aorta passing through the intersecting points of the free edge and scallop curve and the plane defined by the centre point of the free edge and the intersecting points of the free edge and scallop curve. The shape of the scallop curve of the leaflets to the valve ring is classified as V- or U-shaped depending on its resemblance to the corresponding letter.

401

[Figure 6 about here.]

The following nomenclature consisting of a sequence of letters and digits is used to refer to the two leaflet geometries: attachment curve shape - length of the belly curve - th - value of θ (cf. Fig. 6 (b, c, f)).

405 Numerical setups

The direct numerical simulation (DNS) of blood flow in the stenosed aorta was conducted 406 with the open-source code NEK5000²⁶. This code is based on a spectral element method¹³ 407 solving the Navier-Stokes equations for Newtonian and incompressible flows. Details on the 408 numerical methods used and on the implementation of the direct numerical simulation can 409 be found in Corso *et al.*⁹. It is worth noting that the Reynolds number Re_o calculated at the 410 stenotic orifice averages at 3,800 over systole. Re_o is determined by considering the diameter 411 of the circular area corresponding to the stenotic orifice area and the spatially averaged 412 velocity at the orifice. The Dirichlet inflow boundary conditions on the three components 413 of velocity over the inflow cross-section upstream of the stenosis are prescribed such that 414 pseudo-steady systolic conditions (taking into account flow variations measured during in 415 vitro experiments) are simulated reaching a mean systolic flow rate of $12 \text{ L/min}^{9,10}$ (cf. 416 Fig. 7). 417

With respect to the simulation of the bioprosthetic aortic valve cases, the computational method for the high-fidelity simulation of the blood flow and the mechanics of the leaflets relies on a fluid-structure interaction (FSI) approach based on a modified immersed boundary method taking into account a deformable structure (i.e. the valve and the aorta) embedded into a fixed fluid domain^{31,27}.

The Navier-Stokes equations for incompressible flows of Newtonian fluid are solved on a Cartesian grid (of dimension $40 \ge 40 \ge 80 \ [mm^3]$ with $120 \ge 120 \ge 288$ points for each direction)

using sixth-order compact finite differences on staggered grids for each velocity components 425 and pressure³⁵. Grid stretching is applied so that the cell dimension close to the jet shear 426 layers is about 100 μm . Moreover, an explicit low-storage third-order accurate Runge-Kutta 427 time stepping scheme for the advective term and a semi-implicit Crank-Nicolson scheme 428 for the temporal discretisation of the diffusive term¹⁷ are used. An iterative solution tech-429 nique was developed to solve the large linear system of discretised equations for the fluid 430 sub-problem¹⁷. This technique is based on the Schur complement formulation of the orig-431 inal linear system and relies on the resolution of two Poisson problems on pressure solved 432 with the Krylov subspace bi-conjugate gradient stabilised method (BiCGstab) with right 433 preconditioning (geometric multigrid V(3,3)-cycle scheme as a preconditioner). A dedicated 434 highly efficient commutation-based preconditioner matrix is indeed applied for the pressure 435 iterations^{17,24}. A Helmholtz problem on velocity is then solved with the unpreconditioned 436 BiCGstab method. The termination of the Helmholtz iterations and the convergence of the 437 residuals in order for the continuity constraint to be met is controlled through an absolute 438 threshold parameter $\varepsilon_U = 10^{-10} m/s$ or s^{-1} while the accuracy level in the Poisson iterations 439 is dependent on the supremum norm of residuals out of the velocity divergence computation 440 between two consecutive iterates and a tolerance value set to 10^{-417} . The presented Navier-441 Stokes solver was tested for transitional and turbulent channel flows and the accuracy of the 442 solver was verified by comparing the results with solutions from a pseudospectral solver¹⁷. 443 Direct numerical simulation of transitional blood flow in the straight ascending aorta for the 444 two valvular cases is then considered in this study. 445

The elastodynamics equation is solved on a moving tetrahedral mesh (i.e. on a Lagrangian frame of reference) of about 200,000 affine elements using the finite-element formulation and a second-order accurate semi-implicit central difference time-stepping scheme^{27,30,35}. All the structural parts (i.e. aorta, leaflets and ring) share element nodes at their intersection. The Newton method is used to linearise the system of non-linear equations for the solid subproblem and the linear system of equations is solved using a generalised minimal residual iterative method (GMRES) with an additive Schwarz preconditioner^{30,33}. The relative and absolute tolerance value on the residuals to stop the iterations for the resolution of the linear and non-linear systems is set to 10^{-6} and 10^{-8} , respectively³.

The strong coupling of the Navier-Stokes and elastodynamics equations is based on a parallel 455 variational transfer²² of velocities (from fluid grid to solid mesh) and of reaction forces 456 (from solid mesh to fluid grid) between non-matching discretisation points and elements' 457 nodes. The fluid and solid sub-problems are solved synchronously with a time-step of $5 \times$ 458 10^{-6} s. The formulation of the variational transfer corresponds to the equalities of the L^2 -459 projections of velocity or forces between two non-overlapping meshes by defining a suitable 460 space of Lagrange multipliers. The transfer operator is then assembled from mortar matrices 461 computed by numerically integrating the Lagrange basis functions of the three spaces. A 462 linear system is ultimately solved to obtain the projected velocities imposed as Dirichlet 463 boundary condition at the fluid-structure interface of the solid sub-problem and the projected 464 force density added as a source term to the blood flow momentum equation. An iterative 465 procedure, stopped when a prescribed relative tolerance of 10^{-6} is reached, is implemented 466 to ensure velocity and force continuity at the fluid-structure interface 27,22 . 467

Concerning the material properties for the structural elements of the investigated FSI prob-468 lems, a fibre-based model is used to characterise the nearly incompressible anisotropic ma-469 terial properties of the glutaraldehyde-pretreated bovine pericardium leaflets^{1,18,27,35}. The 470 six parameters of this constitutive model, including two families of fibres oriented at a fitted 471 angle of 60° to each other, were regressed to match experimental bi-axial tensile test data¹. 472 The material properties of the aortic wall and the supporting ring of the leaflets are described 473 by a linear elastic constitutive relationship (density: $1500 kg/m^3 (ring)$; $1100 kg/m^3$ (leaflets, 474 aortic root and aorta), bulk modulus: 3 MPa and shear modulus: 0.3 MPa)³. Following a 475 well-established assumption⁵, blood is modelled as a Newtonian fluid with a constant kine-476 matic viscosity ν of $3.77 \times 10^{-6} m^2/s$, equal to the blood viscosity in the ascending aorta at 477 the largest shear rate and a density ρ_f of 1060 kg/m^3 . 478

 $_{479}$ Systolic flow conditions are considered in the computational study. A pressure drop across $_{480}$ the valves and in the ascending aorta of 8 mmHg is imposed over a time span of 0.3 s³⁵. In ⁴⁸¹ order to prescribe a pressure difference within a cylindrical region upstream of the valve³⁵, ⁴⁸² which corresponds to the left ventricle outflow tract (LVOT), a forcing term is introduced ⁴⁸³ on the right-hand side of the fluid momentum equation. This method is adapted from ⁴⁸⁴ the concept of fringe regions or sponge layers as described in^{4,6}. Consequently, the inflow ⁴⁸⁵ velocity undergoes gradual acceleration due to the pressure difference imposed by means of ⁴⁸⁶ the additional forcing term given by the following equation:

$$\mathbf{f}_{inflow} = \begin{bmatrix} \frac{\lambda(l)}{\lambda_{max}} \frac{\Delta p_{inflow}}{h_{cyl}} \frac{1}{\rho_f U_{ref}^2} \\ \lambda(l) \left(0 - u_2/U_{ref}\right) \\ \lambda(l) \left(0 - u_3/U_{ref}\right) \end{bmatrix} \quad [-]$$
(1)

where $\lambda(l)$ is a damping function vanishing in the physical domain, flat in most of the interior 487 of the cylindrical fringe region, while decaying smoothly to 0 at the boundaries of the fringe 488 region⁶. λ_{max} is the magnitude of the damping function. Δp_{inflow} is equal to 16 mmHg (= 489 2133.2 Pa). U_{ref} is the reference velocity used to non-dimensionalise the velocity vector **u** in 490 the Navier-Stokes equations. h_{cyl} is the length of the cylindrical fringe region. A coordinate 491 system projection is performed such that the pressure difference imposed by \mathbf{f}_{inflow} along 492 direction l aligns with the normal to the inflow cross-section and in the streamwise direction. 493 u_2 and u_3 are then the velocity components perpendicular to the axis of the cylindrical fringe 494 region. 495

In addition, a second cylindrical fringe region is positioned at the outflow extremity of the aorta model. Its purpose is twofold: firstly, to emulate the resistance (by applying a resistive pressure) arising from the curved portion of the aorta (which is not modelled in the pericardial bioprosthesis cases) and secondly, to attenuate the flow fluctuations that might otherwise flow back due to the periodic boundary conditions prescribed on the fluid Cartesian grid³⁵. The expression governing the forcing term in the second cylindrical fringe region shares a similar form with Eq. 1, except that $\Delta p_{outflow}$ is set to -8 mmHg (= -1066.6 Pa).

⁵⁰³ A third cylindrical fringe region cancelling out the radial velocity components with a ⁵⁰⁴ reduced width and placed before the inflow fringe region is finally added from time instant ⁵⁰⁵ 0.1 s onward (after reaching a peak flow rate of about 16 L/min^8) to model the gradual flow deceleration occurring from time instances 0.1 s to 0.3 s (see Fig. 7). Similarly to the simulation setup for the aortic stenosis case, the reference Reynolds number at the valvular orifice Re_o is equal to 3,800 in the BioAV cases. This Re_o corresponds to the Reynolds number computed by taking the average velocity at the valvular orifice and the diameter of the circular area corresponding to the BioAV orifice area over the acceleration and deceleration phases occurring throughout systole (see Fig. 7). These phases result from the use of the three fringe regions.

[Figure 7 about here.]

⁵¹⁴ Vortex structures, dynamics, stretching and circulation

The instantaneous vorticity transport equation, which is obtained by taking the curl of the three-dimensional momentum Navier-Stokes' equation and using vector identities, is:

$$\frac{D\boldsymbol{\omega}}{Dt} = \underbrace{\frac{\partial\boldsymbol{\omega}}{\partial t}}_{L_{\boldsymbol{\omega}}} + \underbrace{\mathbf{u}\cdot\nabla\boldsymbol{\omega}}_{A_{\boldsymbol{\omega}}} = \underbrace{\boldsymbol{\omega}\cdot\mathbf{L}}_{S_{\boldsymbol{\omega}}} + \underbrace{\nu\nabla^{2}\boldsymbol{\omega}}_{D_{\boldsymbol{\omega}}}.$$
(2)

with L_{ω} , the local vorticity acceleration, A_{ω} , the vorticity advection; S_{ω} , the vorticity 517 stretching and D_{ω} , the vorticity diffusion. Of particular interest in this study is the vortex 518 stretching term as the latter represents the rotational acceleration (or deceleration) brought 519 about due to strain L parallel (or anti-parallel) to the vorticity vector $\boldsymbol{\omega}$. As shown in Eq. 2 520 for three-dimensional viscous flows, the rate of change of vorticity is dependent on both the 521 stretching and diffusion terms. In fact, a high and positive stretching term increases the rate 522 of change of vorticity (phenomenon called amplification) and because of the conservation of 523 the angular momentum, vortex filaments are confined as a consequence of the decrease in the 524 coherent vortex radius.³². At moderate Reynolds numbers, the diffusion term is predominant 525 in the smallest length scales of the flow except at the wall where viscous forces dominate. 526

⁵²⁷ The magnitude of the advection A_{ω} and stretching terms S_{ω} is investigated. Nonetheless, ⁵²⁸ in order to take into account the orientation of both the rate of strain in the blood flow in ⁵²⁹ relation to the vorticity vector, a projected vortex stretching $\Pi^{S_{\omega}}$ is introduced and defined as the vorticity vector projected onto the eigenvectors of the rate-of-strain tensor and multiplied
by the eigenvalues of this tensor:

$$\Pi^{S_{\boldsymbol{\omega}}} = (\boldsymbol{\omega} \cdot \mathcal{V}_{\mathbf{L}}) \cdot \boldsymbol{\lambda}_{\mathbf{L}},\tag{3}$$

with \mathcal{V}_{L} , the eigenvectors of L and λ_{L} , the eigenvalues of L.

⁵³³ A similar definition is used to calculate a projected vorticity advection $\Pi^{A_{\omega}}$ by computing ⁵³⁴ the eigenvectors and eigenvalues of the vorticity gradient.

535 Experimental validation of the numerical model

The validation of the direct numerical simulation results in the stenosed aorta case from the 536 comparison with *in vitro* time-resolved three-dimensional flow magnetic resonance imaging 537 can be found in Corso et al.¹⁰. With respect to the experimental validation of the fluid-538 structure interaction computational model of the bioprosthetic aortic valve case from *in vitro* 539 experiments, Figure 8 shows the very good agreement both qualitatively and quantitatively 540 between the numerical FSI results and *in vitro* measurements 2,16 . The leaflet kinematics 541 during valve opening for the VLth30 BioAV (see Fig. 6 (c)) is in very good agreement with 542 the images recorded at three time instants with a high-speed camera and presented in² (cf. 543 Fig. 8 (b)). Furthermore, the comparison of the area at the vena contracta between the 544 numerically and experimentally evaluated values over systole is presented in Fig. 8 (c). We 545 notice a good agreement of the VLth30 curve obtained from the numerical flow velocity 546 data with the diamond-shaped markers representing the area calculated based on the phase-547 averaged velocity field obtained from tomographic particle image velocimetry (tomo-PIV) 548 measurements¹⁶. From the graph at Fig. 8 (c), we also observe that, for the VLth30 BioAV 540 case, the area where the flow velocity is the highest periodically varies in time at variable 550 frequencies between 18 and 30 Hz¹¹. Conversely, the BioAV with Ulth0 design does not 551 exhibit periodic motion of the three leaflets during peak systole (refer to Fig. S1 (a, c) in the 552 supporting information), unlike the VLth30 case where the three leaflets move periodically 553 at distinct frequencies¹¹ and asymmetrically relative to the centerline of the aortic root (see 554

Fig. S1 (b, d) in the supporting information). A more in-depth analysis of the correlation 555 between the kinetic energy carried by the leaflets and the kinetic energy calculated in the flow 556 over spherical regions is presented in the second part of this study¹². The flow characteristics 557 highlighted by the streamlines of the time-averaged velocity field obtained from the 3D FSI 558 simulation are in line with those observed in experimental tomo-PIV data. The tomo-PIV 559 data were acquired using a silicone phantom model of the ascending aorta with the *Edwards* 560 Intuity Elite BioAV (Edwards Lifesciences, Irvine, CA, United States) positioned in the sinus 561 of Valsalva portion of the aorta model¹⁶. For comparison, the experimental velocity field 562 was phase-averaged over peak systole. Notably, a high-velocity jet is present in the middle 563 of the aorta, as indicated by streamlines aligned with the aorta's centreline. Additionally, 564 recirculation zones are observed and align with the three posts of the BioAV ring. The curves 565 in Fig. 8 (f) showing slice-averaged turbulence intensity, which represent the magnitude of 566 velocity fluctuations owing to turbulence relative to the strength of the mean flow velocity, 567 are nearly coincident for various slices perpendicular to the centerline of the ascending aorta. 568 This observation underscores the remarkable consistency between the *in vitro* experiment 569 utilising the silicone phantom model and the numerical simulations including the VLth30 570 BioAV model. 571

572

[Figure 8 about here.]

573 Acknowledgements

This work was supported by the computational resources from the Swiss National Supercomputing Centre (CSCS) under project IDs c12, s1012 and sm56.

P. Corso would like to thank F. B. Coulter (ETH Zürich) for providing the computer-aided
sketch of the sheet-like leaflet geometry. This sketch was instrumental in generating the final
three-dimensional and volumetric geometrical model of the VLth30 BioAV for the present
study. P. Corso also acknowledges the support of M. G. C. Nestola from Università della

⁵⁸⁰ Svizzera italiana (USI) on the solid solver and on the part of the code dealing with the ⁵⁸¹ coupling of the two solvers.

582 Author contribution

P. Corso: Conceptualisation, Data curation, Formal analysis, Interpretation of the results,
Investigation, Methodology, Software, Visualisation, Writing - original draft. D. Obrist:
Funding acquisition, Input on the results and on the original draft.

566 Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Figure 1: Jet geometries (highlighted by velocity magnitude) for the three valvular cases at 8 time instances. The plane of investigation is positioned at a distance of 10 mm from the sino-tubular junction (STJ). The eccentricity from the centre of the circular cross-section is quantified by the distance ε_c and the azimuthal angle α_c in the plane. The centre of the cross-section is displayed by a black dot while the centre of mass of the jet region is represented by a white dot.



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Figure 8: Experimental validation of the FSI numerical model under peak systolic conditions. Leaflet opening (a) simulated for the VLth30 bioprosthetic valve case and (b) recorded by a high-speed camera during *in vitro* experiments² (c) Area at the vena contracta downstream of the two simulated BioAV cases obtained from the FSI numerical simulations and downstream of the *Edwards Intuity Elite* BioAV extracted from the flow field measured using the tomographic particle image velocimetry technique¹⁶. (d) Streamlines along the velocity field averaged over systole downstream of the VLth30 valve model. (e) Streamlines along the phase-averaged velocity obtained from tomo-PIV measurements. (f) Non-dimensional slice-averaged turbulence intensity from the simulation (VLth30 BioAV case) and from tomo-PIV experiments.

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Table 1: Table of the non-dimensional quantities based on the terms of the momentum conservation along the streamwise direction for the three valvular cases presented in this work and for the cases presented in Chen and Luo^7 and Becsek *et al.*³.

	$\overline{\Delta PA}$	$ $ $\overline{\dot{p}}$	$\overline{C_D}$	$\max C_D$	$\overline{h_{F_{\texttt{leaflets}}}}/ \mathscr{A}$
1. Stenotic - Corso et al. ⁹	0.746	0.037	1.42	3.36 at t=0.083 s	2
2. BioAV - VLth30	0.432	0.14	0.175	0.24 at t= 0.108 s	0.5
3. BioAV - Ulth0	0.459	0.072	0.103	0.14 at t= 0.154 s	0.33
4. BioAV - similar case as that presented in Becsek et al. ^{3}	0.387	0.081	0.502	0.94 at t= 0.122 s	1.12
5. Flexible AV - Chen and Luo^7	0.477	0.16	0.47	1.04 at t= 0.18 s	2.23

Supplementary Files

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