Fluid-Structure Interaction Simulations of Mechanical Heart Valves with LS-DYNA ICFD

Mariachiara Arminio[1], Dario Carbonaro[1], Sara Zambon[1], Rodrigo Paz[2], Facundo Del Pin[2], Umberto Morbiducci[1], Diego Gallo[1], Claudio Chiastra[1]

[1]PolitoBIOMed Lab, Dept. of Mechanical and Aerospace Engineering, Politecnico di Torino, Turin, Italy
[2]Ansys, Inc., Canonsburg, PA, USA

1 Introduction

The aortic valve is responsible for allowing blood flow from the heart left ventricle into the aorta during the systolic phase of the cardiac cycle and for preventing backflow during the diastolic phase. The aortic valve is composed of three leaflets attached to the aortic root in proximity of three aortic dilations named sinuses of Valsalva. Leaflets open and close as a result of transvalvular pressure drop. Specifically, when the ventricular pressure is higher than the aortic pressure the leaflets open, whilst they close the valve orifice when the aortic pressure is higher than the ventricular pressure. Valve functionality may be impaired due to several conditions, such as aortic valve stenosis and aortic valve regurgitation, with a consequent increase in the risk of left ventricle hypertrophy and cardiac failure [1]. Among treatment options for aortic valve disease, a major role is played by the surgical replacement of the native valve with a prosthetic device.

Prosthetic heart valves can be classified into bioprosthetic and mechanical valves, which are composed by deformable biologic tissues and by rigid synthetic materials, respectively. Bioprosthetic valves are associated with a high failure risk in the long term due to leaflets calcification. Accordingly, current guidelines suggest that mechanical valves should represent the first choice for aortic valve replacement in patients younger than 50 years of age, when there is no contraindication to anticoagulation therapy [2]. In particular, anticoagulation therapy is needed to mitigate the thrombogenic risk entailed by mechanical valves which is impacted by the valve fluid dynamics. The design of mechanical valves determines blood flow features such as local high shear stress values which can cause platelet activation and aggregation. As a result, a thorough study of the fluid dynamics plays a key role in optimizing valve design and predicting valve performance, contributing to its long-term success. In this context, fluid-structure interaction (FSI) simulation has emerged as the most comprehensive *in silico* approach for investigating mechanical valves, accounting for both the structural mechanics of the valve and the associated fluid dynamics [3,4].

Within this context, this study presents a framework for the FSI simulation of mechanical aortic valves using the LS-DYNA ICFD solver. The capabilities of the ICFD solver are investigated in reproducing the key aspects of blood flowing through mechanical heart valves. Particular emphasis is placed on the use of **`*ICFD_CONTROL_GAP`**, a recently developed keyword which was here employed to explore the possibility of reproducing a full closure of the valve during the diastolic phase of the cardiac cycle [5]. Regarding this aspect, a simulation employing the **`*ICFD_CONTROL_GAP`** keyword is compared against one without its application. Moreover, the hemodynamic performance of mechanical aortic valves is investigated according to ISO standards (ISO 5840:2021) through the calculation of quantities such as the effective orifice area (EOA) and the regurgitant fraction (RF).

2 Methods

2.1 CAD model, structural and fluid domains

In order to perform an FSI simulation, a structural and a fluid domain need to be defined. In this study, the structural domain of the simulation was represented by the mechanical valve, while the fluid domain was represented by the aortic root. The two domains will be briefly described in the following paragraphs. Mechanical aortic valves are generally composed of four main parts: a sewing cuff, a housing and two leaflets. Leaflets are connected to the housing through two hinges each. During the cardiac cycle each leaflet rotates about the axis passing through its two hinges, determining the opening and closing of valve orifice. Here, a computer-aided design (CAD) model of a bileaflet mechanical heart valve was created using Solidworks (Dassault Systèmes, FR), resembling the commercially-available 25 mm Abbott Regent aortic valve (Abbott Laboratories, IL, USA) (Fig. 1A). The mechanical valve is composed of the sewing cuff (Fig. 1B), the housing (Fig. 1C), and the two leaflets (Fig. 1D).

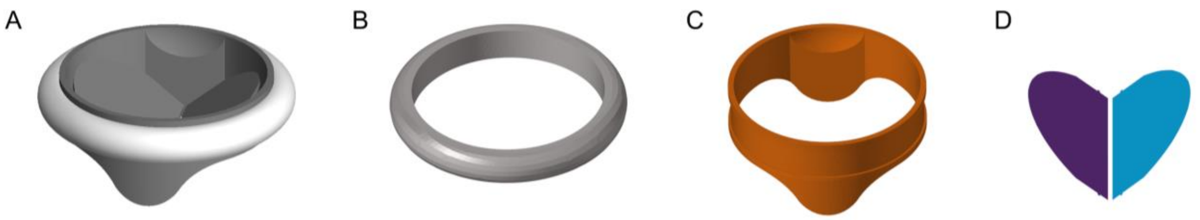

Fig.1: CAD model of the mechanical aortic valve (A) and its different components: sewing cuff (B), housing (C) and leaflets (D).

Regarding the fluid domain, the wall geometry was created based on an idealized model of the aortic root, including the sinuses of Valsalva, a portion of the left ventricular outflow tract and a portion of the ascending aorta [6]. Both the left ventricle outflow tract and the ascending aorta were simplified as straight tubes. The fluid domain was enclosed by the aortic wall, the inlet section located at the beginning of the left ventricle outflow tract, and the outlet section located at the end of the ascending aorta. Moreover, it was composed by two additional parts that represented the fluid counterparts of valve leaflets (Fig. 2). These fluid counterparts need to be defined to perform a FSI simulation using the ICFD solver and the **`*ICFD_BOUNDARY_FSI`** keyword, which requires specifying particular fluid parts intended to be in close proximity to the structures engaged in the FSI. A gap was intentionally introduced along at the edges of the leaflets, to prevent the fluid counterparts of the leaflets from touching each other and the fluid wall during the closure of the leaflets. The gap was not introduced in proximity of the hinges for leaflets in the structural domain. The size of the gap was set to 0.15 mm along the opposing sides of leaflets, and to 0.30 mm along the remaining perimeter. This selection ensured a consistent gap size between the two leaflets, and between each leaflet and the housing during valve closure, which in turn facilitated the proper functioning of the **`*ICFD_CONTROL_GAP`** keyword. In fact, this keyword relies on the definition of a global gap size threshold, and the presence of an almost constant gap size simplifies the selection of this threshold.

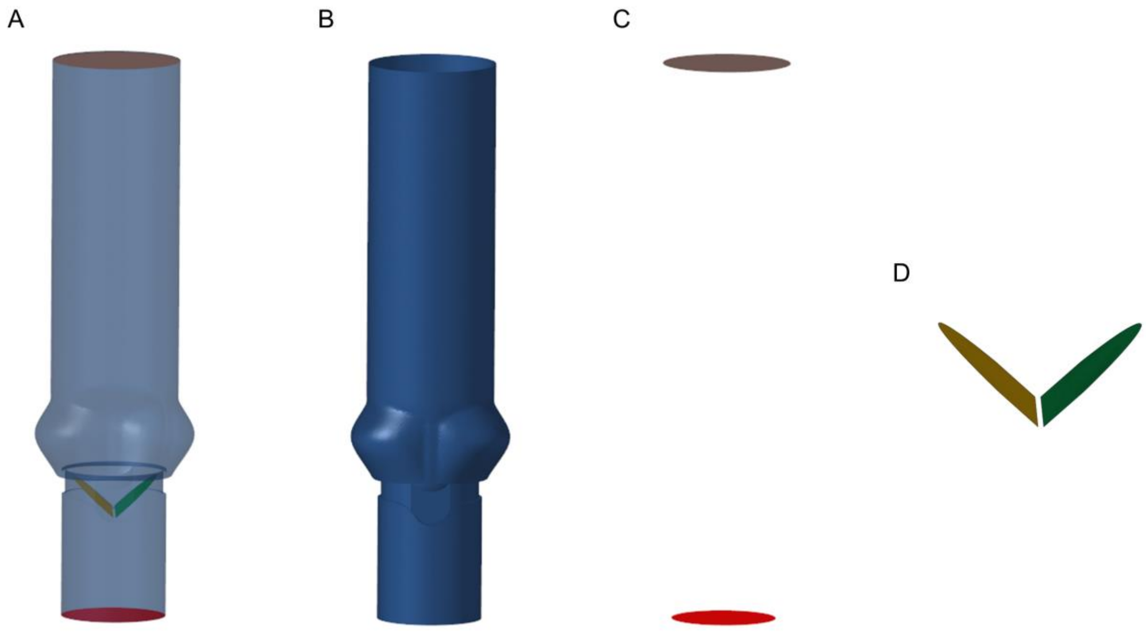

Fig.2: Fluid domain (A) and its different components: fluid wall (B), inlet and outlet (C) and fluid leaflets (D).

2.2 Meshing

Both the surfaces of the fluid domain and the valve model were meshed using Hypermesh (Altair Engineering, MI, USA). The surface of the fluid domain was discretized with ~82k triangular shell elements, with a size of 0.3 mm in the region of the valve housing and a size of 0.8 mm elsewhere. The fluid volume mesh was automatically built by the ICFD solver with a mesh growth scale factor of 1.6 (using the keyword **`*ICFD_CONTROL_MESH`**), except for the region of the valve housing, where the mesh size was set to 0.28 mm. This allowed obtaining a finer mesh in the valve region, where high accuracy in the fluid dynamic results is required, and a coarser mesh elsewhere. The fluid counterparts of the leaflets were meshed with ~6k quadrilateral shell elements each, with a size of 0.2 mm. Concerning the mechanical valve, the housing and the sewing cuff were discretized with ~16k and ~20k tetrahedral elements (size of 0.7 mm), respectively. The valve leaflets were discretized with the same mesh as their fluid counterparts.

2.3 FSI simulations

FSI simulations were conducted by coupling the LS-DYNA ICFD solver and the LS-DYNA implicit structural solver. This strong coupling mitigates numerical issues related to the added mass effect, which affects FSI simulations where the structural and fluid parts have similar densities [7]. Blood was modelled as a Newtonian fluid with a density of 1060 kg/m^3 and a viscosity of 4 cP. All valve parts were assumed as rigid, with a density of 2000 kg/m^3, which is close to the density of pyrolytic carbon, the material employed for both the Abbott Regent valve housing and leaflets. Since the interaction between blood and the sewing cuff was not of interest, the sewing cuff was also represented as rigid. The aortic wall was likewise assumed to be rigid, thus simulating only the fluid-structure interaction between blood and valve leaflets. A reference zero pressure was applied at the outlet of the fluid domain and a waveform representing the difference between the ventricular and the aortic pressure in physiologic conditions was applied at the inlet (Fig. 3). The no-slip condition was applied at the wall of the fluid domain and to the leaflets. The movement of valve housing and sewing cuff was constrained in all the directions. The time step was set adaptively based on the CFL condition. Two cardiac cycles were simulated to ensure the decay of any initial transients and that the solution is repeatable, computing the results only in the second cycle.

Two distinct FSI simulations were conducted, differing in their utilization of the **`*ICFD_CONTROL_GAP`** keyword: the first simulation was conducted without employing the keyword, whereas the second simulation incorporated its activation. **`*ICFD_CONTROL_GAP`** was employed with the aim of simulating a complete closure of valve leaflets during the diastolic phase of the cardiac cycle. This keyword artificially blocks the flow between two fluid parts having a distance lower than a defined threshold. Full closure of the valve could not be obtained using an alternative approach due to the inherent risk of volume mesh errors that would arise from allowing the fluid components representing the leaflet surfaces to come into contact with each other. A threshold value of 0.6 mm was chosen for the treatment of the gap closure. This threshold was intended to effectively obstruct flow through the gaps that were introduced along the edges of the leaflets when they are closed.

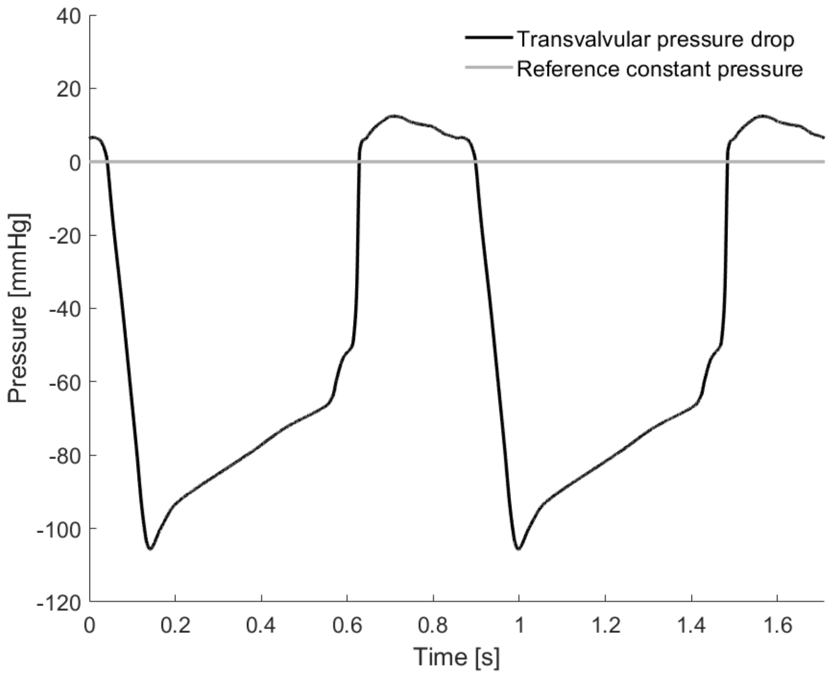

Fig.3: Pressure waveforms applied as boundary conditions: reference constant pressure (outlet) and transvalvular pressure drop (inlet).

2.4 Analysis of results

The hemodynamic results through the mechanical aortic valve were analyzed in terms of velocity and pressure. Moreover, the hemodynamic performance of the valve was assessed through the calculation of the EOA and the RF. These quantities are defined and proposed for the evaluation of prosthetic heart valves in the international standard ISO 5840:2021. The EOA and the RF differ in that the former is calculated considering the positive differential pressure period of the cardiac cycle, whilst the latter is calculated considering the whole cardiac cycle.

3 Results

The FSI simulation results reveal that both the simulation without gap control and the one utilizing the **`*ICFD_CONTROL_GAP`** approach successfully captured the most relevant aspects of valve leaflet kinematics and valve fluid dynamics. Figure 4 presents the configurations of the leaflets in closed and open states during diastole and systole, respectively. In the closed position, each leaflet formed an angle of 30° relative to the valve plane, while this angle rapidly increased up to 85° as the leaflets reached their fully open configuration.

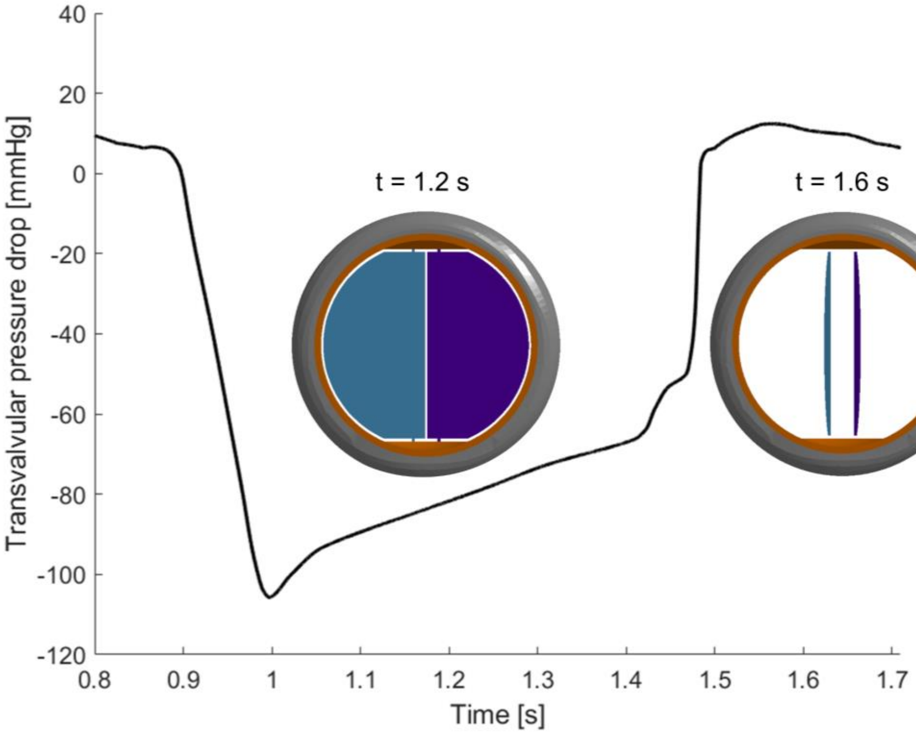

Fig.4: Closed and open configuration of the valve at mid-diastole and mid-systole.

Considering the diastolic phase of the cardiac cycle, the two simulations gave similar results in terms of pressure (Fig. 5). The closed valve configuration was characterized by a gap of almost constant size (~0.3 mm) between the leaflets and between the leaflets and the housing. This led to a blood flow leakage, clearly visible in Fig. 6A, 6C and 7A. Although **`*ICFD_CONTROL_GAP`** was employed with the aim of blocking this backflow, this purpose was not fully reached. In particular, in Fig. 6B, 6D and 7B it is visible that the flow was almost fully blocked between each leaflet and the housing, but not between the two leaflets.

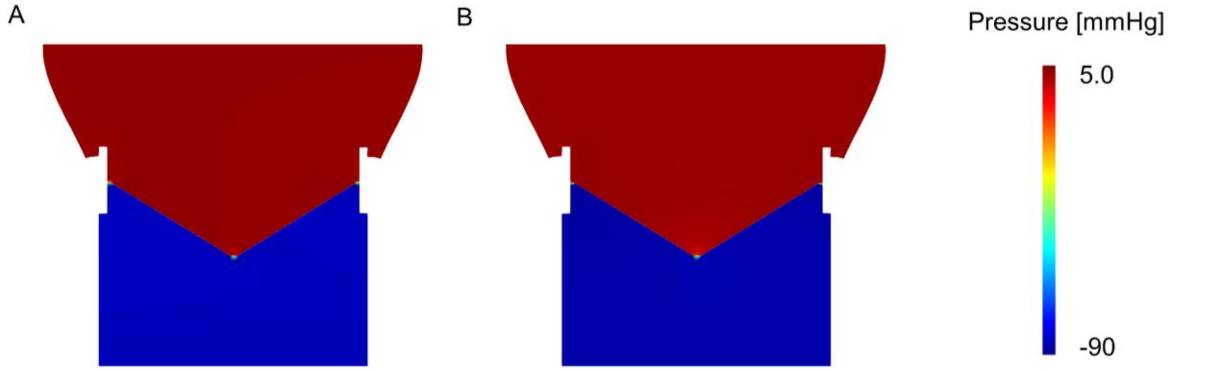

*Fig.5: Pressure in the fluid domain on a long-axis section at t = 1.2 s for the simulations without gap closure treatment (A) and with *ICFD_CONTROL_GAP (B).*

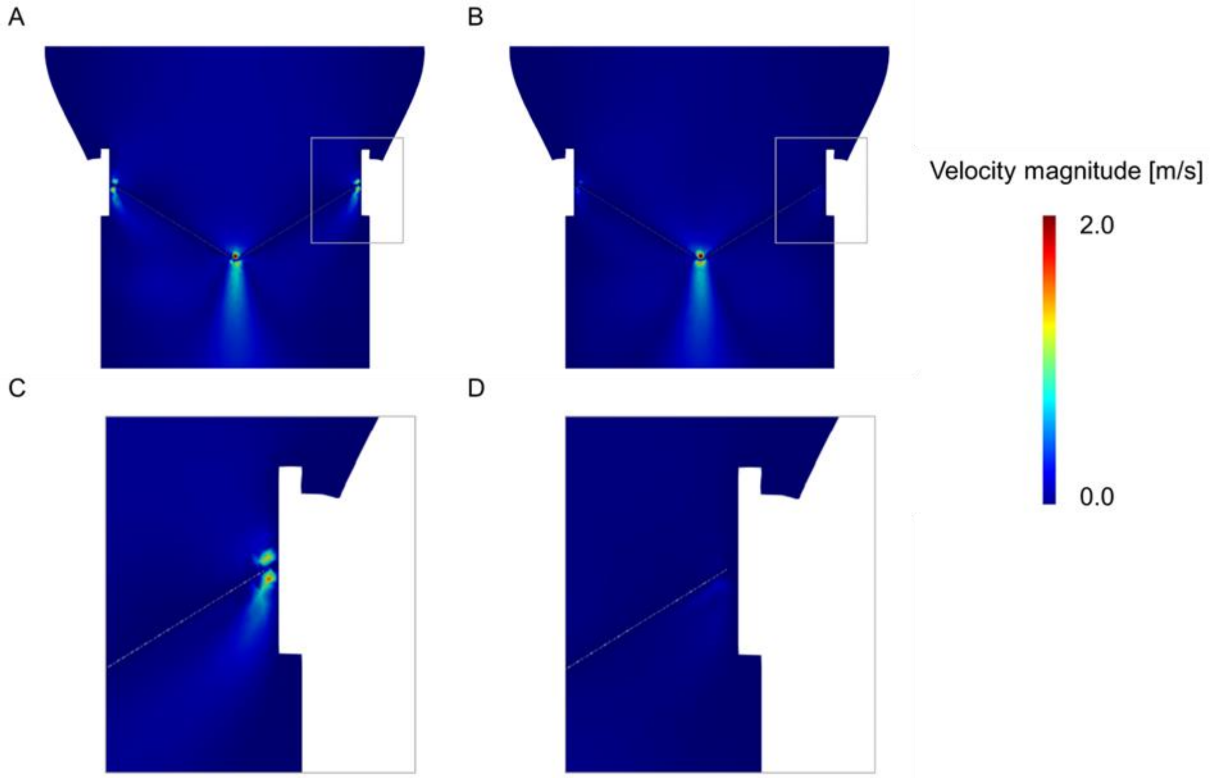

Fig.6: Velocity magnitude in the fluid domain on a long-axis section at t = 1.2 s for the simulations without gap closure treatment (A, C) and with **`*ICFD_CONTROL_GAP`** *(B, D).*

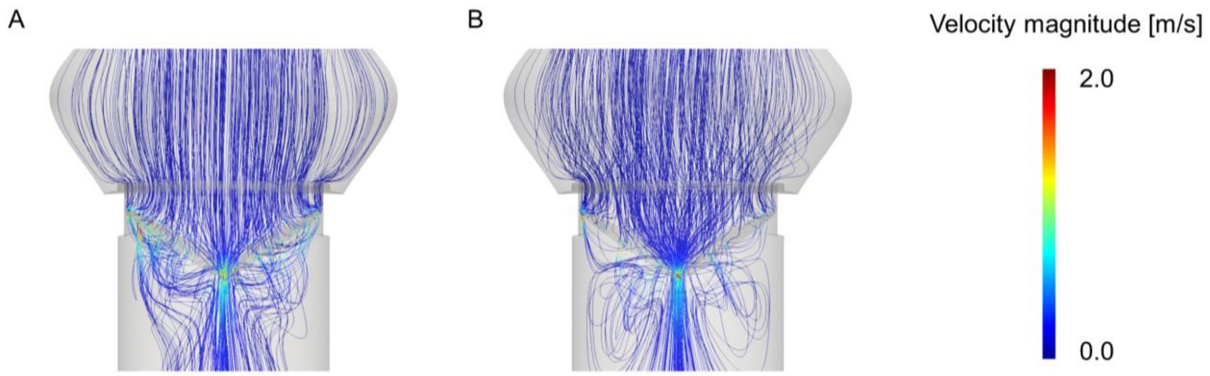

Fig.7: Streamlines at t = 1.2 s for the simulations without gap closure treatment (A) and with **`*ICFD_CONTROL_GAP`** *(B).*

The two simulations showed similar results also in the systolic phase, when valve leaflets are open. In this case, the three blood flow jets determined by the bileaflet design of the valve were correctly captured and the use of **`*ICFD_CONTROL_GAP`** did not significantly impact the fluid dynamics (Fig. 8). The two simulations were similar also in the vortical structures generated in the valve region during systole (Fig. 9).
The EOA for the simulation without gap closure treatment and for the one with **`*ICFD_CONTROL_GAP`** were 4.10 cm^2 and 4.12 cm^2, respectively. This confirms that the systolic phase of the simulation was not markedly influenced by the gap closure treatment. On the contrary, the RF decreased from 16.04 to 13.23 when **`*ICFD_CONTROL_GAP`** was introduced, as a result of the partial blocking of the backflow. The EOA values satisfied the minimum requirement of the ISO standard for both cases, while the RF was acceptable only for the case with gap closure treatment.

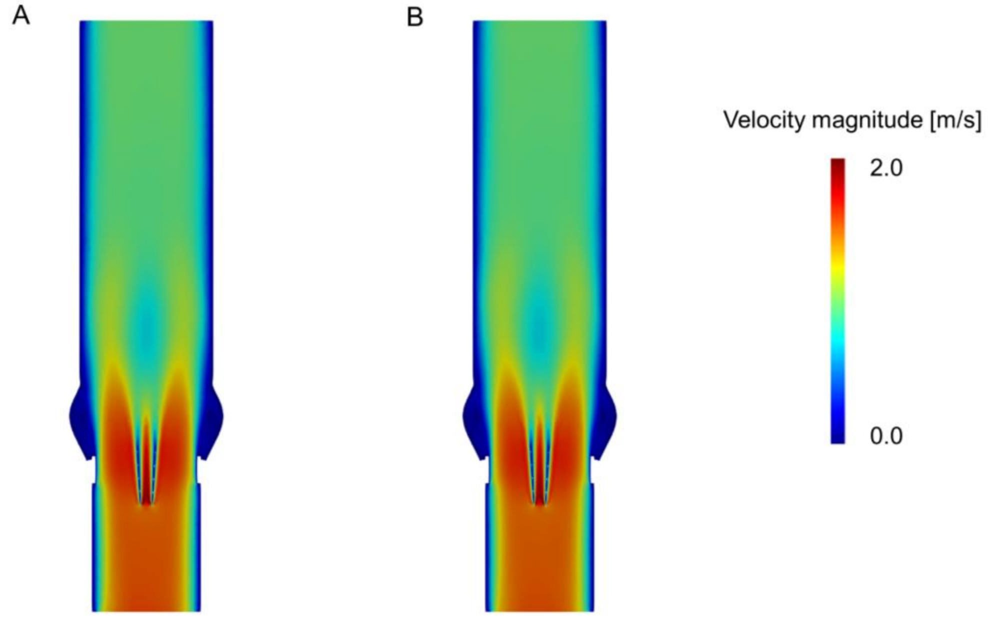

Fig.8: Velocity magnitude in the fluid domain on a long-axis section at t = 1.6 s for the simulations without gap closure treatment (A) and with **`*ICFD_CONTROL_GAP`** *(B).*

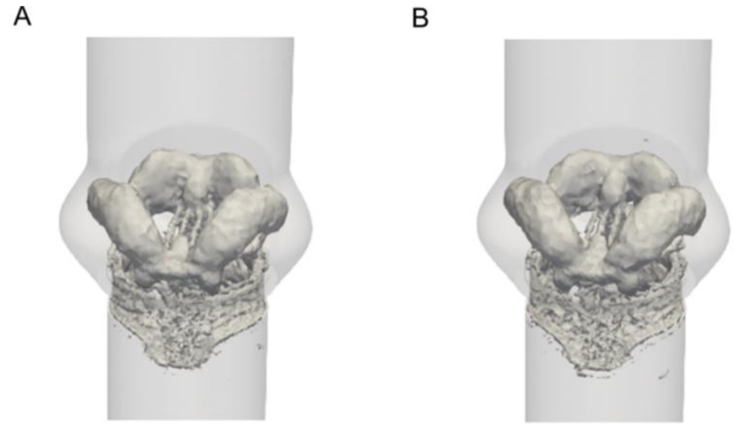

Fig.9: Isosurfaces depicting swirling strength in the valve region at t = 1.6 s for the simulations without gap closure treatment (A) and with **`*ICFD_CONTROL_GAP`** *(B).*

4 Discussion

The results of the present study confirmed the capability of LS-DYNA ICFD solver to effectively replicate the main features of both the kinematics and fluid dynamics within an aortic bileaflet mechanical valve. The solver can handle the high-displacement FSI simulation of these devices, offering a powerful tool

for investigating their hemodynamic behavior. Achieving an accurate simulation of the diastolic phase potentially becomes attainable through the utilization of **`*ICFD_CONTROL_GAP`**. However, it is important to note that this keyword requires a careful selection of the global gap closure threshold to ensure the dual objectives of full gap closure and the successful execution of the simulation.
The LS-DYNA ICFD solver emerged as a powerful tool for the FSI simulation of mechanical heart valves, owing to a variety of attributes, including (i) the capability to strongly couple the ICFD solver with the implicit structural solver, effectively addressing numerical challenges stemming from the added mass effect; (ii) the implementation of the boundary-fitted approach of the mesh kinematics at the interface between the structural and the fluid domain and the automatic remeshing of the fluid domain, which ensure accurate fluid dynamic results at the interface; (iii) the potential to explore a wide range of scenarios related to specific aspects of the fluid dynamics simulation, such as boundary condition types, rheological models and turbulence models. However, these valuable characteristics come at the cost of high computational times and high sensitivity of the successful execution of the simulation to parameters. These parameters include the adaptive time step settings, mesh size and the threshold for gap closure treatment. With regard to the latter aspect, some simulations were conducted using a threshold value higher than the one adopted in this study, but they failed due to a fluid volume mesh error while leaflets were closing. In future research, the aspects impacting the successful execution of the simulation will be further analyzed, with the objective of enhancing the robustness and accuracy of our model, extending the current study through a more comprehensive analysis of valve fluid dynamics.

5 Summary

Aortic valve disease can impair the proper functioning of the aortic valve, with a high burden on patients' lives. The surgical replacement of the native diseased valve with a mechanical valve is a common treatment option in younger patients. Accordingly, an in-depth study of the hemodynamics of mechanical aortic valves is essential to predict their performance and optimize their design. FSI simulation has emerged as the most complete *in silico* tool in this field. In this context, this study aims at exploring the use of LS-DYNA ICFD solver for the FSI simulation of mechanical aortic valves.
The CAD of a commercially available mechanical valve and an idealized aortic root geometry were created. FSI simulations were conducted by coupling the ICFD and the implicit structural solvers. The difference between the ventricular and the aortic pressure in physiologic conditions was applied at the inlet of the fluid domain. A constant zero pressure was imposed at the outlet. A FSI simulation where **`*ICFD_CONTROL_GAP`** was adopted to artificially block blood flow through the valve during diastole was compared with a simulation without **`*ICFD_CONTROL_GAP`**.
Results showed that the ICFD solver successfully captures the main hemodynamic features determined by the valve, both in the systolic and in the diastolic phase of the cardiac cycle. Concerning **`*ICFD_CONTROL_GAP`**, it emerged that the choice of the gap control threshold influences the successful execution of the simulation and that a threshold value higher than the gap size does not necessarily guarantee full flow blockage. Finally, the effective orifice area and the regurgitant fraction of the mechanical valve were computed as defined by ISO 5840:2021. Both the simulation without **`*ICFD_CONTROL_GAP`** and the one with its activation presented a value of EOA satisfying ISO requirements, while the RF was acceptable only in the case with **`*ICFD_CONTROL_GAP`** activation.
To conclude, this preliminary study highlights the capability of the ICFD solver in simulating the FSI behavior of mechanical aortic valves. In the future, this capability will be exploited for an in-depth hemodynamic study of these devices as well as for their characterization according to the ISO standard.

6 Literature

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