Computational Modelling of Bileaflet Mechanical Valves Using Fluid-Structure Interaction Approach

Han Hung Yeh1,2 Dana Grecov1,2,* Satya Karri3

1Department of Mechanical Engineering, University of British Columbia, Vancouver, BC, V6T 1Z4, Canada
2Biomedical Engineering Program, University of British Columbia, Vancouver, BC, V6T 1Z4, Canada
3Vitro Lab Inc, Victoria, BC, V8Z 1E7, Canada

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Abstract

This study presents numerical simulations of a minimally constrained mechanical valve model using a fully coupled fluid-structure interaction method with COMSOL Multiphysics, a finite-element-based software package. The model applies a physiological pulsatile pressure gradient across an aortic valve with an approximately symmetric aortic root. The complex hinge from the exact model is simplified with a pin joint and weak constraints to control the designated valve leaflet positions. The arbitrary Lagrangian-Eulerian method is applied in order to accommodate large mesh displacements due to leaflet motion. Constant material properties are applied to both the fluid and structure with the assumption that the flow is Newtonian and turbulent. The valve leaflet positions and flow patterns are verified against the results from literature. Hemodynamic performance in terms of flow velocity and shear stress is investigated. The maximum von Mises stress for each valve leaflet is calculated. Moreover, a simulation on a defective mechanical valve is conducted and hemodynamic and structural analyses are performed. It is found that vortices were generated with higher blood velocity passing through the unconstrained leaflet, which may lead to diagnostic confusion.

Keywords: Arbitrary Lagrangian-Eulerian (ALE) formulation, Bileaflet mechanical valve, Fluid-structure interaction (FSI)

1. Introduction

Heart valve stenosis is a serious heart valve disease that is characterized by the narrowing of the heart valve, which can potentially lead to several fatal complications, such as congestive heart failure. Patients who suffer from severer heart valve stenosis normally require surgical operation and replacement of the diseased native valves. According to the data from the U.S. Department of Health & Human Services, Agency for Healthcare Research and Quality, over a hundred thousand patients received heart valve procedures in 2012 [1]. A study conducted by Rizzoli et al. found that the overall survival rate for patients who received an artificial valve replacement dropped from 75% in year 5 to 29% in year 25 [2].

With ever increasing computing power, complex physical interactions have been simulated by many research groups [3-9]. Dasi et al. conducted a three-dimensional (3D) direct numerical simulation (DNS) to study the pulsatile turbulent flow of a bileaflet mechanical valve with particle image velocimetry (PIV) validation. The motion of valve leaflets was determined using a probability density function derived from experimental data [3]. Other study performed a 3D simulation with the fluid-structure interaction (FSI) method for a bileaflet mechanical valve; however, in order to maintain laminar flow, the inlet boundary was limited such that the Reynold’s number was roughly 2,400 [4]. Researchers simulated a 3D bileaflet mechanical valve using DNS coupled with the FSI method. In their study, Kolmogorov’s scale was not resolved and the motion of the leaflet was based on mesh distortion without the influence of structural stress [5]. The present study simulates the interaction between blood hemodynamics and the dynamics of an artificial heart valve with the fully coupled FSI method.

The arbitrary Langrangian-Eulerian (ALE) formulation approach was selected for handling large structural deformations due to leaflet motion. The ALE formulation has been applied for the FSI simulation of artificial heart valves for clinically related investigations on thrombosis [6] and subaortic stenosis [7], and for experimental validation [4].

The present study develops a generalized modeling scheme without additional artificial constraints or assumptions in order to capture not only the leaflet dynamics but also the stress within the leaflet under pulsatile turbulent flow. With a minimum artificial constraint imposed on the model, the freedom to investigate defective valves and clinically related problems, such as leaflet arrest, thrombosis, or pannus growth,
is increased. A simulation was conducted in order to investigate the flow patterns caused by a defective mechanical valve leaflet.

2. Materials and methods

2.1 Numerical method

The advantage of using the fully coupled FSI method is that relevant physical parameters, such as wall shear stress and leaflet deformation, can be evaluated during a simulation with additional computational resources. Additionally, with the established fully coupled FSI model, further analysis can be conducted on a more complicated geometry such as tissue valves with arterial walls, which require information from the structural domain for an accurate simulation. COMSOL Multiphysics was chosen for the simulation since both the fluid and structural domains can be fully coupled using the FSI method with the flexibility of simulating additional physics without extensive modifications. The discretization of the fluid domain was set such that the velocity component was second-order and the pressure component was first-order. Combined with the FSI method, the moving mesh approach was integrated using the ALE formulation with automatic re-meshing for high mesh quality in order to maintain high solution accuracy. The coupling between the fluid and structural domains was achieved by transferring boundary velocity and stress between the fluid-structure boundaries, as shown in Eqs. (1) and (2).

\[ \mathbf{u}_{\text{fluid}} = \mathbf{u}_{\text{solid}} \]  
\[ -p + \mu \left( \nabla \mathbf{u}_{\text{fluid}} + (\nabla \mathbf{u}_{\text{fluid}})^T \right) n = \sigma \cdot n \]  

where \( \mathbf{u} \) represents the velocity for the fluid or solid domain and \( p, \mu, \) and \( \sigma \) are the fluid pressure, viscosity, and solid stress, respectively.

2.2 Geometrical model

The geometrical model used in this study is the simplified 25-mm St. Jude Medical bileaflet mechanical valve presented by Choi [8]. The computational domain (Fig. 1) comprises an aortic valve with a symmetrical realistic aorta root, which was constructed using a combination of quadratic rational Bézier curves. The overall length of the computational domain is 75 mm with an arterial diameter of 25 mm and an entry length of 16.5 mm. For the valve leaflet, the length is 12.8 mm, the thickness is 0.65 mm, and the free rotational angle is 25° to 85°. The gap between artificial valve joints is 3 mm.

2.3 Simulation conditions

The material properties for the fluid and structural domains are summarized in Table 1. The valve leaflets are assumed to be an isotropic and linear elastic material and the blood is assumed to be an unsteady, isothermal, incompressible, and Newtonian fluid.

![Illustration of computational domain.](image1)

![Pressure profiles for boundaries.](image2)

The imposed inlet and outlet boundaries are governed by the physiological pressure profile, which was approximated with a Fourier series (Fig. 2). Because of the physiological pressure gradient imposed on flow boundaries, flow is observed to enter the transition region, which introduces solver instability; hence, the two-equation, \( k-\omega \) turbulent model is incorporated. However, the turbulent model can be replaced by a DNS model using a mesh configuration based on Kolmogorov’s scale with additional computational resources.
pressure are applied as initial conditions at the start of simulation at 0.14 s, which has smaller pressure difference compared with 0 s.

2.4 Mesh convergence study

The x-direction velocity was analyzed at three locations downstream away from the artificial valve. The first location for the mesh convergence study was chosen to be at the widest diameter within the aortic root, approximately 10 mm away from the valve. The two other locations were chosen to be 20 and 40 mm further downstream from the first location, respectively. These three locations were approximately located at the middle, three-quarters, and at the exit of the domain, respectively. The total numbers of mesh elements for the mesh configurations used are 9900 for coarse, 17300 for normal, 21200 for fine, and 39200 for finer. The overall difference between two mesh configurations was computed by averaging the errors in the x-direction velocity at three designated locations. This velocity error was calculated by averaging the difference at each time step, which was computed by taking the mean errors from the point by point velocity difference. The variations in each configuration at three locations are summarized in Table 2. The overall percentage errors, based on the three locations, are 2.82%, 1.5%, and 1.58% for the mesh configuration between coarse and normal, fine and normal, and finer and normal, respectively; therefore, the fine mesh was used as the final configuration for the current model. Additionally, the mesh element was carefully constructed with five rectangular elements across boundaries in order to account for the boundary layer. Additional mesh refinements around any curvatures were also made, including the edges of the valve leaflet and the interavalvular gaps.

3. Results and discussion

3.1 Leaflet dynamics

The leaflet dynamics for one cardiac cycle is shown in Fig. 3(a). The approximate durations required for both leaflets to reach the fully opened position are 70 ms (at 0.23 s from 0.16 s). The duration the leaflets remained open is 90 ms (from 0.23 s to 0.32 s). The duration the leaflets were closed is 40 ms (from 0.32 s to 0.36 s). Leaflet rebounds at closure were also captured, as reported by Chio and Mohammadi [8,9]. With a minimized reaction time of approximately 6 ms under the optimized numerical constants from the current model, the results agree with the value presented by Chio (8.3 ms) [8]. However, the trade-off of the imposed numerical constraints was that the leaflets traveled beyond the designated closure angle of 25° to approximately 23° (Fig. 3(b)). This overshoot of the leaflet position was due to the back pressure from the aorta after the leaflets were fully closed at 0.36 s. One objective for future study is to minimize the magnitude of overshoot. Overall, the valve leaflet dynamics is in good agreement with the results of other studies [5-8].

![Figure 3. Leaflet position for (a) one cardiac cycle and (b) near fully closed region.](image)

The maximum von Mises stresses were calculated for each valve leaflet. The results are plotted in a semi-log plot for the systolic phase in Fig. 4. During the systolic phase, the maximum stress was found to remain below 0.1 MPa; however, a peak value of 37.6 MPa of the maximum stress was calculated during the first rebound period when the leaflets reached the fully closed position at 0.361 s. Since the yield strength of the material is approximately 400 MPa, according to the calculated peak von Mises stress, the valve leaflet is unlikely to fail by yielding.

3.2 Hemodynamics

The velocity contours of the artificial valve in different isolated time frames are plotted with fully opened and closed valves at 0.23 s and 0.36 s, respectively, in Figs. 5(a) and 5(b). The maximum velocity for the fully opened valve is 1.36 m/s.
and that for the fully closed valve is 1.82 m/s. The higher velocity, found in fully closed valve, is due to the reversed leakage jet and squeeze flow by the valve leaflet. The maximum velocity of 1.36 m/s at peak systole from the current model is comparable with those reported in the literature (1.38 m/s [5], 1.25 m/s [8], and 1.32 m/s [10]). In addition, given that the distance between the leaflet hinges is small, limited blood flow was observed between the valve leaflets downstream at 0.23 s (Fig. 5(a)). Furthermore, the maximum shear stress distribution of the blood flow was also calculated (Figs. 6(a) and 6(b)). According to Yeleswarapu et al., the critical shear stress experienced by a blood cell should be maintained below 1500 dPa with moderate shear stress exposure time [11]. Based on this criterion, the maximum shear stresses at 0.23 s and 0.36 s were found to be greater than the critical limit of 1500 dPa near the valve leaflet surfaces (Figs. 6(a) and 6(b)). This implies that blood cells would likely be damaged and thrombosis might occur, and thus the patient should follow anticoagulant therapy.

The effects of the tuning parameters, such as the turbulent length scale, on the turbulent model are currently under investigation. Given that the experiments will be conducted using a 3D simplified human aortic model using PIV, the simplified symmetric aortic root geometry was assumed in order to compare the numerical result with experiments.

### 3.3 Clinical application

To extend this study further, an additional simulation was conducted to investigate a defective mechanical valve (Fig. 7). With one leaflet totally constrained for the simulation of a severe defective mechanical valve, the simulation identified vortices generated during the systolic phase, similar to the results found by Smadi et al. [12]. The generated vortices and
the asymmetrical blood velocity for the defective valve could lead to further diagnostic complication and decrease diagnostic accuracy for clinicians. The simulation also identified a high-velocity jet passing through the normal leaflet that might potentially create additional difficulties for accurately measuring the blood pressure gradient during a cardiac catheterization. Given that vortices were generated within the aortic root further downstream with low flow velocity on the defective side, any invasive probe measurements could be affected by the lower velocity at the vortex center and the asymmetric blood flow. Moreover, comparing the maximum velocity magnitude of the normal and the defective valves (Figs. 5 and 7), the defective valve had a maximum increase of 25% in the velocity magnitude. A leaflet position comparison between the normal and the defective aortic valves was also conducted (Fig. 8). It is shown that the defective valve experienced both early peak opening and closure at approximately 0.19 s and 0.34 s, respectively. Although the opening time for the defective valve was slightly longer, the leaflet started closing after 0.19s and the maximum leaflet position was not able to be maintained.

4. Conclusion

The proposed model can accurately predict leaflet dynamics with the additional evaluation of leaflet stress. The computed structural stress can be used for further investigations on artificial valve damage due to leaflet motion for the presented mechanical valve model or a bioprothetics valve model. Furthermore, the valve leaflets were properly constrained with the reduction of geometrical complexity. Additional simulation on the defective mechanical valve identified the generation of vortices, which suggested regions of high and low velocity for further evaluation. Moreover, a comparison of leaflet position between the normal leaflet and the defective leaflet throughout one cardiac cycle indicated a significant difference. Nevertheless, the fully coupled FSI simulation with a realistic aortic root provided additional information on hemodynamics and valve leaflet dynamics. Experiments will be conducted to verify and further improve the accuracy of the current model such that a 3D FSI model can be developed.

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References