



Computational Modeling Approaches for Palliative Care in Infants with Ductal Dependent Pulmonary Flow

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Abstract— *The purpose of this biomedical engineering study is to examine interventional and surgical approaches for complex and palliative solutions in infants with patent ductus arteriosus and pulmonary atresia diagnosis with mathematical modeling and computational fluid mechanics methods. In the study, we visualized hemodynamically using patient-specific preoperative cross-sectional image data and computer-aided design techniques and discussed the differences between repair methods through mathematical models and virtual repairs. We discussed the significance of blood flow analysis in the treatment planning of infants with ductal-dependent pulmonary flow.*

Keywords— *Pediatrics, Congenital Heart Diseases, Fluid Mechanics, Hemodynamics, Blood*

I. INTRODUCTION

A biomedical digital twin is a virtual copy of a patient's anatomical structure generated with multi-planar medical image cross-sections [1], [2], [3]. The process involves obtaining the datasets in pixels, processing and segmenting the images to isolate relevant highlighted arteries using contrast agents and then producing a 3D virtual copy using image processing algorithms. The 3D digital twins technique has been very helpful in the treatment of complex vascular conditions in recent years [4], [5]. Technically, this creates virtual twins using patient-oriented medical imaging data as inputs that enable an analysis of complex flow fields in abnormal region blood pools via numerical visualization algorithms for hemodynamics [6], [7], [8]. This is because they have shown high support for clinical professionals who require comprehensive therapeutic planning aimed at improving the long-term results of patients with high mortality in congenital heart disease (CHD). The present study aimed at virtually demonstrating alternative configurations of interventions on patient-specific virtual vascular models, which were compared with each other in 3D blood flow simulations in

terms of the flow parameters including velocity, wall shear stress (WSS), and pressure distribution. The findings would be useful for comprehending CHDs as well as how to deal with them using engineering methods. The purpose of this investigation was to examine the use of computational modeling to predict the best way to approach repair surgery for 0-1-year-old cyanotic infants suffering from CHD with ductal-dependent pulmonary flow.

I. BACKGROUND

CHDs are one of the birth defects with a prevalence rate of approximately 0.8% to 1.2% worldwide [9]. These defects usually have complex anatomical or physiological abnormalities and require a variety of complex treatment measures that require highly specialized care by experienced, trained, and multidisciplinary professionals [10]. Since these defects in the neonatal circulatory system have a high mortality rate, they must be resolved quickly and effectively, considering the vascular growth. One of the most critical challenges in managing CHD is optimizing the therapeutic approach for neonates with ductal-dependent pulmonary circulation, especially those diagnosed with patent ductus arteriosus (PDA) and pulmonary atresia (PA). Traditional ways of managing PDA and PA in neonates include both surgical and interventional alternatives such as shunts and stents [11]. In this regard, vascular surgeons and pediatric cardiologists decide on the optimal solution according to their experiences, but it is not possible to find developed standards in this regard and solutions are being sought to suggest the most optimal solution by providing detailed patient-specific information. It is important to choose the right intervention strategy and personalize its planning according to the vascular anatomy and physiology of the infant [12], [13]. In the treatment of complex pediatric vascular diseases, thanks to the developments in the field of mathematical modeling and computational fluid dynamics (CFD), quite detailed and patient-

specific models and hemodynamic analyses have been developed recently, which has provided better accuracy in predicting and simulating many therapeutic interventions [14], [15].

In this study, it was aimed to investigate how stent and shunt interventions affect flow dynamics in newborns in terms of biomechanics in the treatment planning of ductal-dependent pulmonary flow cases. In this article, we present a comprehensive summary of the differences between stents and shunts supported by mathematical models and virtual repair simulations [9], [16]. We aim to provide a broad assessment of how these interventions affect key hemodynamic parameters such as blood flow velocity, wall shear stress (WSS), and pressure distribution through the application of CFD methods. The article examines the usefulness, and challenges of blood flow analysis for treatment planning in patients with PDA and PA, focusing on important considerations when developing personalized treatment plans for these patients.

II. METHODS

Medical image datasets from three patients with CHD diagnosis representing the study were obtained retrospectively from the hospital's Image Archiving and Communication System (PACS). Thoracic scans of the patients performed with Siemens SOMATOM Scope computed tomography (CT) were selected from the PACS system of Mehmet Akif Ersoy Thoracic and Cardiovascular Surgery Training Research Hospital. Ethical approval was obtained following ethical guidelines for non-invasive research and the datasets were anonymized. Minimum imaging requirements such as the device (Siemens SOMATOM Scope) and imaging protocol were standardized to ensure consistency in data processing.

Python-based techniques and 3D Slicer software were used for the segmentation of contrast-enhanced thoracic image slices. Otsu algorithm was used in image processing to obtain the optimum threshold value. This algorithm ensured accurate segmentation by reducing the intra-class variance between the foreground (contrast-enhanced vascular structures that can be defined as blood pools) and the background. After the thresholding process, regulatory image processing filters were used to improve the identification of vascular structures in these images (Fig.1). The obtained separated 2D slices were then transferred to the open-source software 3B Slicer for 3D reconstruction of filtered vascular structures and were obtained as STL outputs in 3D form [17].

Digital replicas in STL format were adjusted with computer-aided design (CAD) tools and made suitable for simulation solvers. SketchCAD tool was used for virtual configuration scenarios of shunt and stent options and they were designed and placed at the determined anastomy points with appropriate diameters for the patient. Autodesk Fusion 360 Student, FreeCAD, Ansys Discovery Student, and Geomagic software tools were used to give the surface models their initial form. In this process, pediatric cardiology specialists, cardiovascular surgeons, and biomedical engineers collaborated to accurately represent the intervention approach.

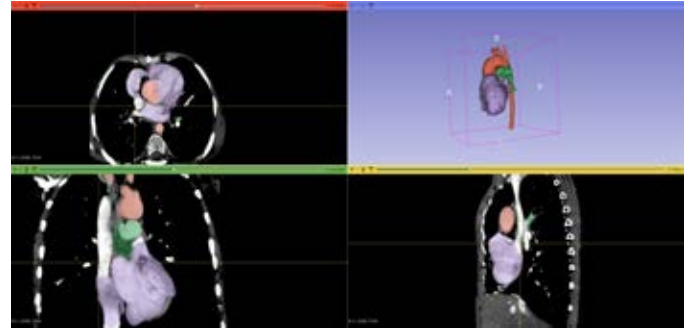


Fig.1 This image shows the process of 3D reconstruction from patient-specific images using the 3D Slicer tool. It includes windows representing the axial, sagittal, and coronal views, where anatomical structures are identified and segmented with different thresholds. The reconstructed volume is displayed in the top right corner.

Blood is assumed to be a Newtonian fluid with constant viscosity, while Navier-Stokes equations governing mass conservation, momentum conservation, and energy conservation were used as the basis for the investigations using simulations. The mathematical model used in our study is based on the assumption that blood behaves as a Newtonian fluid. In this model, the viscosity of blood is considered to be a constant value, and the Navier-Stokes equations are used, relying on the principles of mass conservation Eq.(1) and momentum conservation Eq.(2). Here, $\mathbf{v}$ represents the velocity vector, p represents the pressure, μ represents the dynamic viscosity, and $\mathbf{f}$ represents external forces.

$$\partial \rho / \partial t + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (1)$$

$$\partial (\rho \mathbf{v}) / \partial t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \mu \nabla^2 \mathbf{v} + \mathbf{f} \quad (2)$$

This included performing volume mesh operations for CFD calculations on SimScale, an open-source simulation cloud platform based on CalculiX algorithms with a hexagonal dominant partitioning strategy. No slip wall boundary condition and pressure outlet setup were performed. Blood viscosity was 3.5×10^{-3} to 4.0×10^{-3} Pa·s., density was 1060 kg/m³, and inlet mean velocity was generated using velocity gradients obtained from patients' archived Doppler echo data. CFD analyses including pre-operative, post-operative, and virtual shunt and virtual stent configurations were performed for each case and visualized in the post-processing platform created with OpenFOAM solver in Simscale Academic [18].

III. RESULTS & DISCUSSION

Velocity streamlines, WSS distribution, and blood pressure distribution were visualized and evaluated in 3D on the post-processing platform. Three simulations were performed for each patient, with at least one pre-operation, one stent, and one shunt configuration (Table.1).

In the first patient, a graft of 3 mm diameter and 15 mm length was designed and its dimensions were determined specifically for the patient. It was shown that a 4.2 mm stent positioned approximately 2-3 mm distal to the PDA provided the most favorable hemodynamic results.

Comparative analysis of the simulations showed that the stent configuration consistently reduced hemodynamic values across all tested parameters and therefore backed up the suggestion for placement of a stent in this patient (Fig.2).

TABLE.1 THE RESULTS TABLE SHOWS THE MINIMUM AND MAXIMUM VELOCITY RANGES FOR SHUNT AND STENT OPTIONS FOR THREE CASES.

		Patient 1	Patient 2	Patient 3
STENT	Velocity m/s	0.1– 2.5	0.245 – 0.986	0.09 – 2.5
SHUNT		0.1-2.6	0.1 – 4.90	20– 40

For the second patient, a 9 mm long and 2.5 mm diameter stent configuration was created that was positioned approximately 2 mm proximal to the PDA. This configuration produced the optimal aortic pressure drop. Aortic pressure reached its maximum level in the shunting model among all configurations used in comparison with others. A comparison of shunt and stented models indicated slightly better hemodynamic performance by stents with patent PDA.

The third patient had an unusual “U” shaped PDA resulting in considerable stenosis which is further complicated by the associated transposition of great arteries. Virtual stenting simulation ascertained that WSS on vascular tissues significantly increased due to substantial elevation of pressure caused by PDA upon positioning it about 3mm before the midpoint between the left pulmonary artery and descending thoracic aorta. The best intervention strategy involved total removal of PDA, reversal of the TGA, and introduction of a 3.4mm shunt. This arrangement led to an increase in the flow of blood through the aortic branches and pulmonary arteries reducing the mixture of deoxygenated blood while relieving both high pressures and WSS observed in the stented configuration.

The treatment strategy for case four involved placing a modified 2.8mm Blalock-Taussig shunt, and occlusion of the main aortopulmonary collateral arteries. Stenting simulation results for the 3rd patient were performed in association with satisfactory hemodynamic conditions, as this treatment strategy was best reflected by observed velocities between 0.3 m/s and 1.5 m/s.

IV. CONCLUSION

This experiment aimed to evaluate the mechanical effects of stent and shunt procedures on blood flow dynamics and structural changes in neonates with ductal-dependent pulmonary circulation through hemodynamic modeling and digital twin simulations which were successful.

These findings have the potential to provide strong proof that accurate pre-operative planning made possible by a digital twin approach that can replicate and predict clinical outcomes will go a long way in deciding treatment options. Based on the research, even though WSS, velocity, and pressure seem more beneficial for stenting under simpler cases, shunting is typically advocated in anatomically challenging ones where stents could raise mechanical stresses as well as pressures [19].

Some key factors identified from this study for consideration when making patient-specific treatment plans include the size/condition of the pulmonary artery, orientation of the aortic arch together with clinical history alongside long-term prognosis for each patient.

Among patients who have narrower pulmonary arteries, catheter interventions may reveal whether such people are candidates for the placement of a stent. However, if pulmonary arteries are wider, blood flow in the lung could be improved through a Blalock-Taussig shunt [20].

Furthermore, the anterior surgical option is usually considered when catheter-based stenting is complicated by the retro aortic arch location. This is why individual anatomical and physiological considerations must be taken into account when choosing between shunting and stenting approaches.

Therefore, one approach to managing complex congenital heart disorders that affect systemic circulation and oxygen saturation in children should employ multidisciplinary teams. The findings show how advanced simulation techniques can be incorporated into this process to identify patient-specific cardiovascular structures and develop tailored therapeutic options. This means that digital twins and mathematical models will allow the simulation of different intervention scenarios and novel medical device solutions under patient-specific conditions. Using this facility, the best treatment plan could be chosen for better long-term outcomes.

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Fig.2 The figure presents the simulation results for the first case. The velocity streamlines (top left) and WSS distribution (bottom left) for the flow visualization through the PDA are shown. The velocity streamlines (top right) and WSS distribution (bottom right) are visualized for the scenario where the PDA is closed and the flow is provided through a shunt.



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