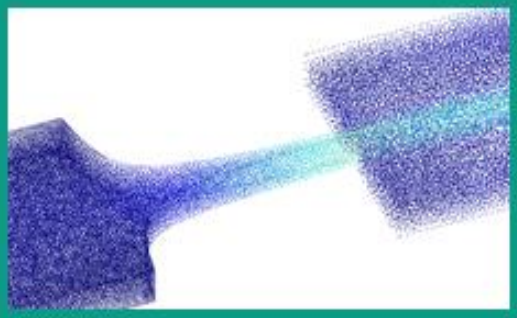
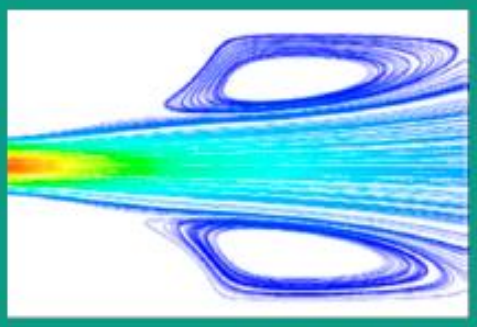
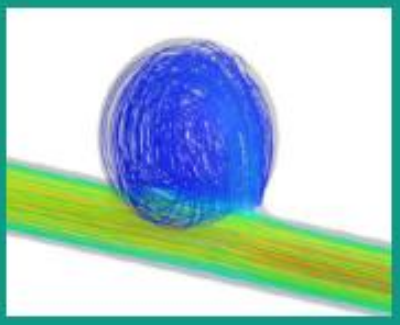
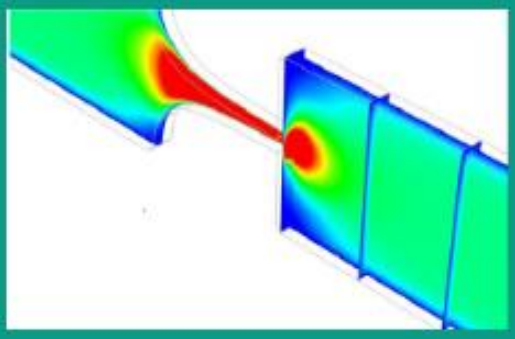
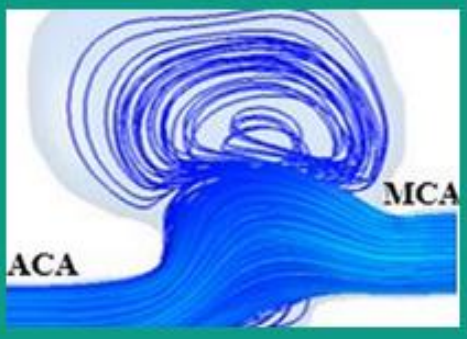
SEMINAR ON

COMPUTATIONAL FLUID DYNAMICS APPLICATIONS

IN BIOMEDICAL ENGINEEERING

Seminar on Computational

Fluid Dynamics Applications

in Biomedical Engineering

Book of Abstracts

Guimarães - Portugal

June 2023

Title: Seminar on Computational Fluid Dynamics Applications in Biomedical Engineering: Book of Abstracts

Editors:

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Publisher:

Instituto Politécnico de Bragança, **2024**
Campus de Santa Apolónia
5300-253 Bragança - Portugal
ISBN: 978-972-745-345-0
Handle: http://hdl.handle.net/10198/29385

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WELCOME

Computational fluid dynamics (CFD) is a technique employed by engineers for more than 50 years to analyze heat transfer and fluid flow phenomena. In last years, there have been rapid developments in biomedical and health research applications of CFD. It has been employed to assess drug delivery systems, analyze physiological flows, assist in surgical planning (e.g., management of intracranial aneurysms), and innovate medical devices (e.g., vascular stents and valve prostheses). The complexity of these flows necessitate an interdisciplinary approach involving engineers, computer scientists, and mathematicians to create computer programs and software required to solve the mathematical equations. The advancement and progression of computational medicine will necessitate collaboration among specialists in engineering, computer science, and biomedical research. This seminar brought together a diverse community of experts, researchers, and practitioners dedicated to explore the transformative potential of CFD in addressing some of the most complex challenges in biomedical engineering. By simulating complex physiological flows to design next-generation medical devices, the abstracts contained herein reflect the knowledge exchanged during this event.

The SCFDABE 2023 Organizing Committee,

Rui A. Lima

Conrado Ferrera

Senhorinha Teixeira

João Ribeiro

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Computational evaluation of the thrombosis risk in the left atrial appendage due to atrial fibrillation

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ABSTRACT

Atrial fibrillation (AF) is the most common type of cardiac arrhythmia, usually triggered by chaotic electrical impulses that enter the left atrium (LA) from the pulmonary veins (PV). Despite recent efforts using computational fluid dynamics (CFD) analysis, the specific flow patterns of AF are not fully understood, and the relationship between flow patterns, LAA morphology, and the thrombosis process is still elusive. The findings of this work illustrate the impact of several geometric and flow parameters on the formation of a stagnant volume within the LAA during an AF episode, paving the way for a generalized model to predict stasis under AF conditions, as well as the potential effect of atrial remodelling (AR) in a patient-specific manner.

INTRODUCTION

Cardiovascular disease is now the leading cause of death, even above cancer and respiratory diseases. In recent years, atrial fibrillation (AF) has attracted much attention, as it is the most common type of cardiac arrhythmia. In addition to its high incidence – affecting more than 1% of the European population - it is also considered an independent risk factor for stroke. During an AF episode, the electrical impulses that trigger the contraction of the left atrium (LA) become fast and irregular, causing the LA to contract irregularly and ineffectively.

AF episodes produce an increased risk of thrombus formation within the left atrial appendage (LAA), which is a small protruding appendix located on the side of the LA. If one of these thrombi manages to exit the LAA and enters the brain circulation, it can easily produce a stroke. On the other hand, AF produces long-term electrophysiological changes in the LA and LAA term, enlarging the volume of the LAA and reducing its contractility. This process is known as atrial remodelling (AR) and is also known to increase the risk of stroke in these patients.

On the other hand, computational fluid dynamics (CFD) analysis of atrial flow in patient-specific models is gaining recognition as a tool to investigate the hemodynamic substrate for stroke in AF conditions (García-Villalba, 2021). From a prescribed combination of flow inlet/outlet boundary conditions and atrial wall motion, CFD simulations produce a 3D time-resolved representation of the atrial flow, which allows to compute hemodynamic metrics known to be related with the risk of thrombosis, e.g. residence time, time-average shear-stress (TAWSS) or oscillatory shear index (OSI).

However, as AF is a complex and multifactorial process, these metrics are sensitive to parameters like LA wall motion, pulmonary vein (PV) flow split, or cardiac conditions, which may experiment significant variations over the course of the day for a given patient. Furthermore, the variability between patients in LA and LAA morphologies makes it difficult to extract general conclusions, and even to compare simulation results between different patients and cardiac conditions (Dueñas-Pamplona, 2022).

All of these uncertainties have made it difficult to achieve a generalizable understanding of the relationship between atrial flow patterns, LA and LAA geometrical parameters, and the

LAA thrombosis process. To address the challenges described above, we introduce a methodological advance: in an effort to model the potential effect of AR associated with AF, we apply plausible geometric and flow variations to patient-specific atrial models. In this way we generated a data-augmented atrial database that allowed us to gain knowledge of how AR exacerbates the hemodynamic substrate for LAA thrombosis.

METHODS AND RESULTS

Six cardiac patients were CT-imaged, injecting a contrast dose to each patient following standard clinical protocols. Three of the patients were AF patients with a thromboembolic history, while the other three were cardiac patients without AF or a thromboembolic history. The CT images were segmented to obtain 3D anatomical models, which were rigged and morphed to parameterize the atrial surface, generating a data-augmented atrial database. These geometries were used to launch CFD simulations and calculated thrombosis-related metrics such as stagnant volume, TAWSS, and OSI.

CONCLUSIONS

We present a methodological advance to compare and classify phenotypic hemodynamic signatures between patient cohorts using CFD atrial simulations in a data-augmented atrial database. Rigging and morphing patient-specific atrial geometries provided us with a framework to identify patterns related to normal and impaired atrial function, illustrating some features associated with thrombi formation.

ACKNOWLEDGMENTS

This work was supported by the Ministerio de Ciencia, Innovación y Universidades of Spain under contract DPI 2017-83911-R and by Junta de Castilla y León under project “Proyecto de apoyo a GIR 2018” with reference VA081G18, and the US National Institutes of Health (grant numbers 1R01HL160024 and 1R01HL158667). We thank the Programa Propio - Universidad Politécnica de Madrid, and the Ayuda Primeros Proyectos de Investigación ETSII-UPM. The autors also thank the Programa de Excelencia para el Profesorado Universitario de la Comunidad de Madrid for its financial support and the CeSViMa UPM project for its computational resources.

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CFD study for an alternative treatment in non-conventional aortic regurgitation patients

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ABSTRACT

Heart Failure is one of the leading causes of death worldwide. This disease can appear because of a maintained Aortic Regurgitation. In that illness, an abnormal function of the aortic valve does not prevent blood from returning to the left ventricle through the aortic valve. Therefore, the aortic valve should be replaced either surgically or via transcatheter. C. A. Hufnagel introduced the first procedure to treat this disease in the 1950's. However, this procedure has become outdated and abandoned. Nevertheless, a group of patients is not eligible for transcatheter aortic valve replacement. Moreover, a surgical replacement is not possible in a subset of this group because of age, comorbidities, or repeated surgeries in the aortic root.

Rescuing Hufnagel's procedure with a modern approach could be possible for those patients. This alternative has only been employed in a patient with a long surgical history who needed the less invasive procedure. However, there is neither any report quantifying the percentage of reduction in the aortic regurgitation nor an analysis of the flow inside the aorta when Hufnagel's technique is employed.

Here, we have used the combination of Computational Fluid Dynamics and Fluid-Structure Interaction to analyze how the flow is modified when a bileaflet heart valve is deployed in the descending aorta instead of the normal orthotopic location (aortic root).

A reduction of 52% on the regurgitation fraction is achieved, and the streamlines can be visualized. Although more tests (both simulations and experiments) will be needed to confirm this commiserate treatment, the results promise a vast improvement in the left ventricle function.

INTRODUCTION

Heart Failure is expected to affect nearly 8 million people by the end of this decade (Virani et al. 2021). Aortic Regurgitation is an illness that can cause Heart Failure when it is permanent. In this disease, the blood previously pumped by the left ventricle contraction is returned through the ascending aorta. Its incidence is mainly concentrated in the population older than 60 (Singh et al. 1999).

An aortic valve malfunction causes this regurgitation. A conservative treatment only succeeds in 20% of the affected population (Carabello 2008). Therefore, a surgical or transcatheter aortic valve replacement must be done. The new valve replaces the affected one in its identical position.

However, the transcatheter procedure is challenging for correcting aortic regurgitation in particular cases (El-Gamel 2021), and surgery is the only alternative. Unfortunately, a specific group of people cannot withstand surgery (ancient, previous surgery history, concomitant cardiac pathologies accumulation, or active endocarditis (Dhurandhar et al. 2016).

Therefore, the aortic valve replacement in the orthotopic position cannot be performed, and a valve placement in a heterotopic position has been suggested (descending aorta) (Fantidis et al. 2014). The procedure would consist of recovering Hufnagel's procedure (Rose et al. 1954; Hufnagel et al. 1958) employing a modern approach and equipment.

Recently, we have employed a combination between Computational Fluid Dynamics and Fluid Structure Interaction to study the effect of placing a bileaflet heart valve in the descending aorta (García-Galindo et al. 2023). The valve reduces a 52% of the blood volume that returns to the left ventricle.

The present manuscript reports the effect of the valve on the flow by visualizing the streamlines.

RESULTS

Figure 1 shows the valve effect in the velocity contours. The valve is fully opened when the blood is pumped from the left ventricle. These contours are altered when the valve is fully closed to prevent regurgitation. Acceleration can be noticed in the gaps between leaftlets and the valve housing and between themselves. A stagnation is observed both upstream and downstream of the valves.

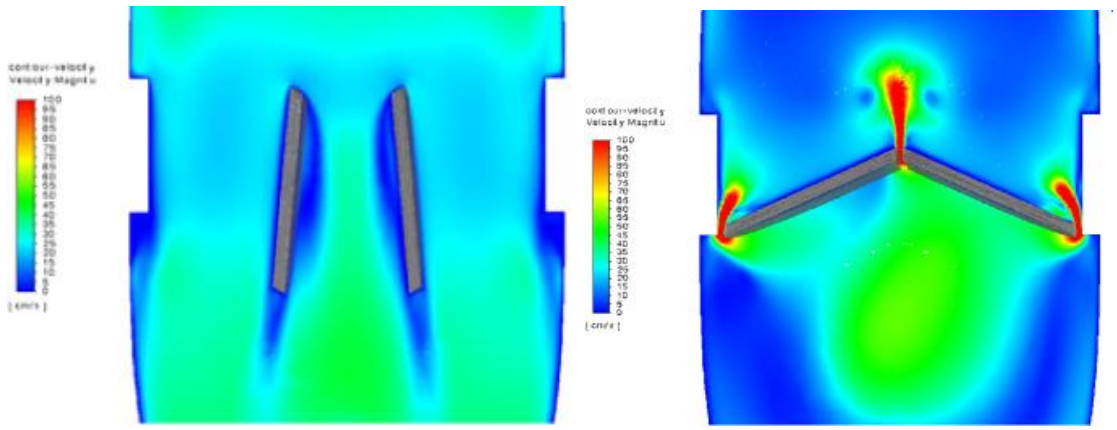

Figure 1 - Velocity contours when the valve is deployed: (a) Leaflets allowing flow circulation, (b) Leaflets preventing flow regurgitation.

Regarding streamlines showing in Figure 2, flow is nearly undisturbed when the valve is opened. The stagnation effect and the recirculation downstream can be visualized when the leaflets are fully extended.

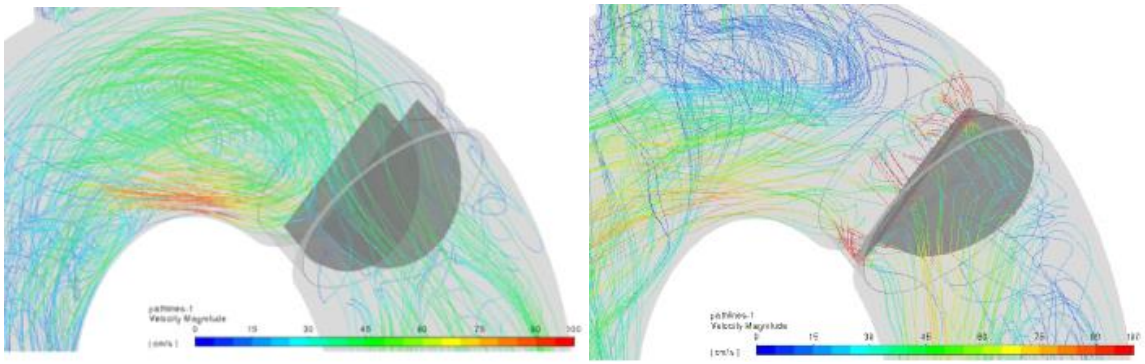

Figure 2- Velocity streamlines when the valve is deployed: (a) Leaflets allowing flow circulation, (b) Leaflets preventing flow regurgitation.

CONCLUSIONS

CFD/FSI is a valuable tool to analyze the flow when applied in biomedical engineering. Quantifying the effect of placing a valve in the heterotopic position at the descending aorta is helpful because it allows treatment for terminal patients. When a valve is deployed, the flow analysis allows valve design and improvement. More simulations and in-vivo tests will

be needed to confirm this commiserate treatment. Its confirmation will ameliorate the left ventricle function and the life expectancy in otherwise considered terminal patients.

ACKNOWLEDGMENTS

Partial support from the Junta de Extremadura through Grants No. GR21091 and IB20105 (partially financed by FEDER funds) is gratefully acknowledged.

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RANS vs LES turbulent flow models comparison in a clinical case

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ABSTRACT

This work compares Reynolds-Averaged Navier-Stokes (RANS) models and Large Eddy Simulation (LES) models for simulating blood flow in a stenosed brachiocephalic trunk using patient-specific boundary conditions derived from Doppler measurements. The study finds that RANS models are significantly faster computationally but struggle to predict Turbulent Kinetic Energy accurately compared to LES. Among RANS models, k-ε shows the poorest agreement with LES results, while k-ω and SST k-ω models perform better, especially for near-wall variables like pressure and Wall Shear Stress.

INTRODUCTION

Turbulence in fluid dynamics involves chaotic, irregular fluid motion with significant fluctuations in variables like vorticity and dissipation (Huang, 1998). Reynolds-Averaged Navier-Stokes (RANS), Large Eddy Simulation (LES), and Direct Numerical Simulation (DNS) are key methods in Computational Fluid Dynamics (CFD) for turbulent flows.

DNS stands out as the most accurate method, capable of resolving all turbulent scales by directly solving the Navier-Stokes equations without turbulence modeling assumptions. However, its high computational cost limits its application to small-scale simulations (Doran, 2013). In contrast, LES captures large-scale turbulent structures directly while modeling smaller scales, offering a balance between accuracy and computational efficiency. This makes LES particularly suitable for studying phenomena like vortex shedding and flow separation downstream of arterial stenoses.

RANS models are computationally less expensive as they only solve for mean flow properties, relying on empirical turbulence models to approximate turbulent effects (Rodi, 2017) [3]. Despite their simplifications, RANS models are widely used due to their efficiency in simulating large-scale blood flow patterns and their applicability to clinical scenarios such as predicting the Fractional Flow Reserve (FFR) from medical imaging data (Taylor, 2013) and (Malota, 2018).

This work compares Reynolds-Averaged Navier-Stokes (RANS) models and Large Eddy Simulation (LES) models for simulating blood flow in a stenosed brachiocephalic trunk using patient-specific boundary conditions derived from Doppler measurements.

METHODS AND RESULTS

3D Slicer software was used to segment a patient-specific (PS) geometry of a stenosed Brachiocephalic Trunk from Magnetic Resonance Angiography (MRA) images obtained at Hospital Universitario de Badajoz. The MRA procedure involved gadobutrol injection and specific imaging parameters to enhance contrast and detail. Expert radiologists supervised the lumen segmentation, which was then refined with CAD tools to ensure accuracy. Boundary conditions were set using Doppler measurements from a Siemens S2000 device, detailing velocity profiles at the stenosis and Right Common Carotid Artery (RCCA).

The simulations, conducted in Ansys Fluent 2019 R3, employed non-structured tetrahedral meshes built for RANS and LES. Mesh refinement studies confirmed convergence, ensuring an accurate representation of flow dynamics near the stenosis. The LES meshes demonstrated a minimum of 80% of directly solved Turbulent Kinetic Energy (TKE), a threshold validation requirement in this approach. Computational efficiency varied significantly between RANS and LES models, reflecting their respective capabilities and computational demands.

The results show that the geometry of the bifurcation initially directs flow towards the right common carotid artery (RCCA) but redirects it towards the right subclavian artery (RSA) due to downstream stenosis. This redirection causes significant flow disruption and recirculation, which is particularly noticeable in LES models compared to RANS (RANS models approximate turbulence effects).

Time-averaged velocity profiles show good agreement between RANS and LES models upstream of the stenosis but highlight RANS models' limitations in capturing post-stenosis flow disturbances, as can be seen in Figure 1. TKE profiles emphasize that LES models better resolve larger eddies than RANS, which is crucial for predicting turbulence intensities near stenosis and bifurcation regions. Pressure profiles demonstrate consistent results across all models, with slight discrepancies observed in the RSA branch for some RANS models.

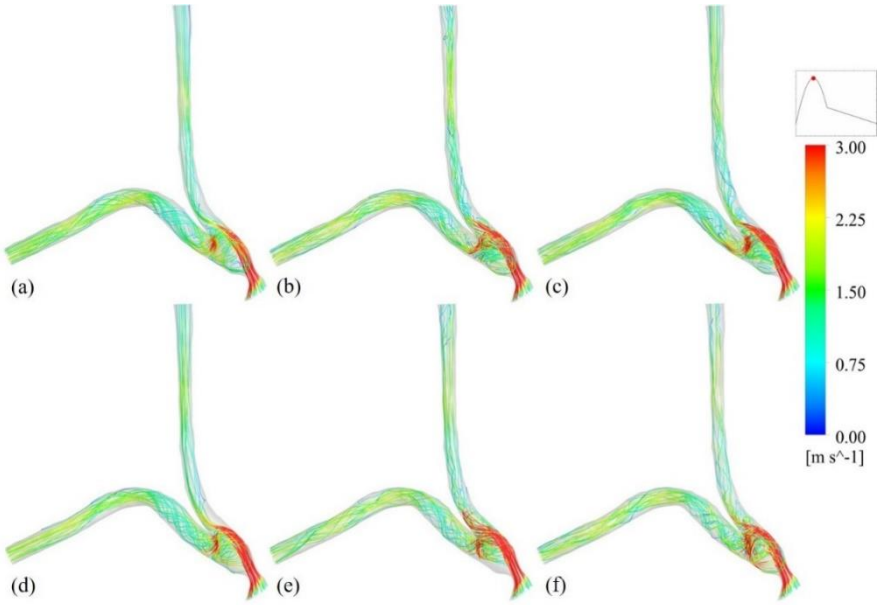

Figure 1: Velocity streamlines at the systolic peak (a) k-ε; (b) k-ω; (c) SST k-ω; (d) Transition SST; (e) LES SL; (f) LES DKE.

OSI profiles reveal high recirculation zones downstream of the stenosis, accurately predicted by LES models but less so by RANS, particularly the k-ε model. Similarly, RRT profiles show that LES models provide better insights into regions prone to atherosclerosis development (low TAWSS, high OSI). In contrast, RANS models, especially k-ε, show deviations in predicting RRT values. Figure 2 shows the residual residence for all the studied models.

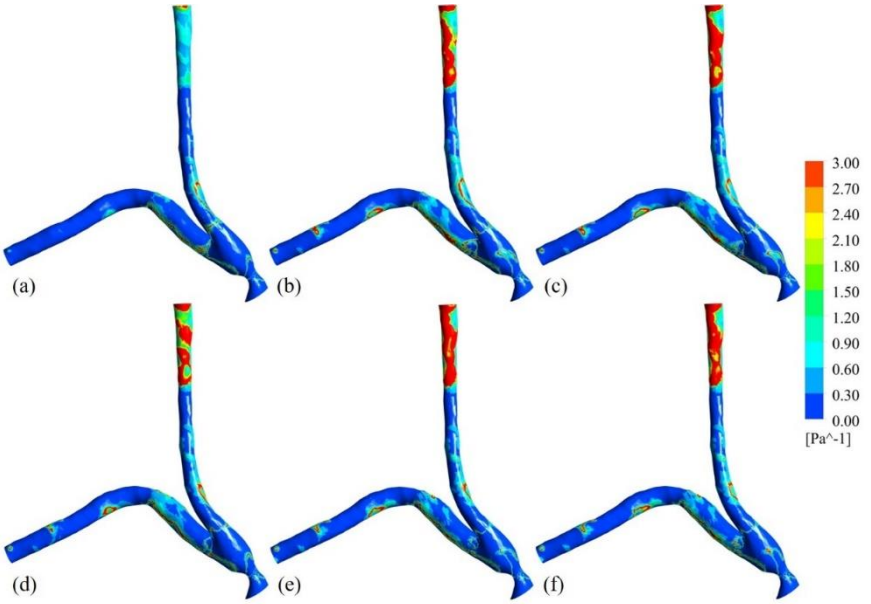

Figure 2: Residual Residence Time (RRT). (a) k-ε; (b) k-ω; (c) SST k-ω; (d) Transition SST; (e) LES SL; (f) LES DKE.

CONCLUSIONS

This work emphasizes the superiority of LES models in providing detailed insights into turbulent flow phenomena critical for understanding hemodynamic factors influencing atherosclerosis in carotid bifurcation stenosis. While RANS models are computationally efficient, they demonstrate limitations in accurately capturing turbulence effects and flow disturbances near stenosis and bifurcation regions. These findings highlight the importance of selecting appropriate turbulence models in CFD simulations for clinical applications to improve cardiovascular outcomes and optimize treatment strategies.

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Computational simulations of oxygen transport in an organ-on-a-chip

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ABSTRACT

Organ-on-a-chip (OoC) technology has revolutionized the way human diseases are studied. These miniature devices mimic the structure and function of human organs, providing a more accurate alternative to traditional in vitro and animal models. Computational simulations play a crucial role in OoC research, enabling researchers to investigate fluid flow phenomena, mass transport, and cellular interactions within these microfluidic devices. These facilitate the exploration of a wide range of experimental conditions that might be impractical or costly to replicate in in vitro experiments alone.

Herein, fluid flow and oxygen transport within an OoC was performed only considering the diffusive process. The results demonstrated that turning off the convective term in oxygen transport simulations leads to lower oxygen concentrations in the cell culture chambers compared to simulations that account for convective flux. Moreover, a uniform oxygen distribution along the OoC device.

INTRODUCTION

Organ-on-a-chip (OoC) technology seeks to bridge the gap between traditional in vitro cell culture models and in vivo physiological complexity by replicating the microenvironment and functions of specific organs in a controlled environment (Fan, Demirci, and Chen 2019; Leung et al. 2022). Due to their potential to revolutionize drug development, disease modeling, and personalized medicine these have been gained significant attention. The integration of numerical simulations has also contributed to the success of these platforms, by allowing researchers to explore in detail the fluid flow, mass transport, and cellular interactions occurring within the microfluidic channels (Carvalho et al. 2021). Furthermore, simulations facilitate the exploration of a wide range of experimental conditions, allowing researchers to examine scenarios that might be challenging or costly to replicate in physical experiments alone (Jafarzadeh and Oscuii 2019; Zheng et al. 2022).

Herein, a computational model of a OoC device was developed, and oxygen transport was evaluated within it. It should be noted that the OoC numerical model used in the present work was previously validated by the authors (Carvalho et al. 2024).

METHODS AND RESULTS

The mesh used to run the computational simulations, and the boundary conditions are schematized in Figure 1. The fluid flow was modelled considering the properties of culture medium with a density of 1007 kg/m^3 and viscosity of 0.958×10-3 kg/(m·s). The fluid was considered incompressible and Newtonian, and a laminar flow condition was assumed. The oxygen concentration was simulated by including a scalar, and different user-defined functions (UDFs) were developed to better represent the experimental conditions (Carvalho et al. 2022). These UDFs allowed to simulate the oxygen recirculation, the oxygen consumption at the organoid and different diffusivities at the organoids and culture medium. It should be noted that, in the present work, all bodies were treated as fluids, and at the inlet, a constant velocity was set (11.14 mm/s). To run the numerical simulations, the commercial software Ansys Fluent was used. More details about the geometry, dimensions and computational simulations can be found elsewhere (Carvalho et al. 2022).

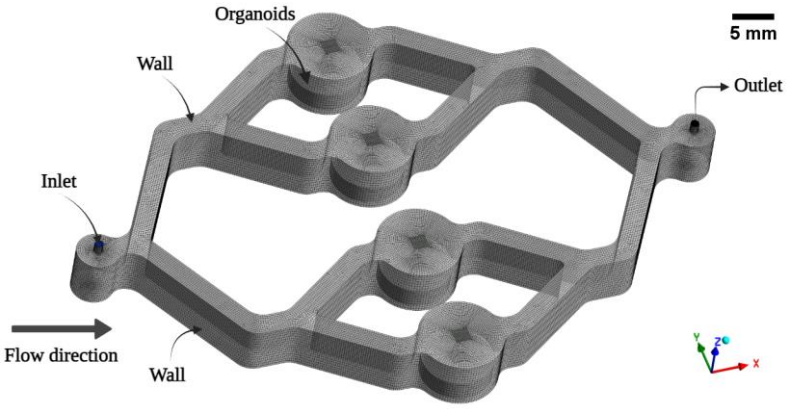

Figure 1 – Hexahedral mesh with 325,068 elements and boundary conditions considered for numerical simulations.

Figure 2 shows the oxygen distribution along the OoC device. One can see that, when the convective term is neglected the oxygen transport is uniform along the domain and the influence of oxygen consumption by cells in the region after the organoid is not observed as previously stated. Furthermore, the oxygen concentration that reaches the cells is lower when compared to the case with the convective flux (Carvalho et al. 2022).

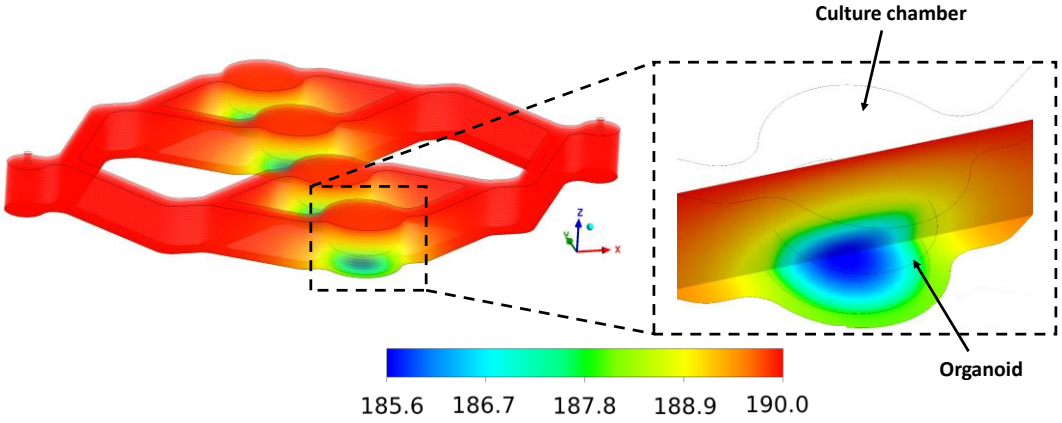

Figure 2 – Oxygen distribution along the device (mmol/m3).

CONCLUSIONS

In this study, numerical simulations within an OoC were conducted to assess the oxygen transport, but only diffusive transport was taken into account. The findings reveal that when the convective term in oxygen transport simulations is disabled, the resulting oxygen concentration within cell culture chambers is reduced compared to simulations that incorporate convective flux. This investigation underscores the importance of using computational simulations to investigate and test diverse conditions without the need for physically fabricating models. This can significantly accelerate the research and development of improved OoC models while minimizing resources.

ACKNOWLEDGMENTS

This work has been supported by the projects, EXPL/EMD-EMD/0650/2021, PTDC/EEI-EEE/2846/2021 and 2022.06207.PTDC (https://doi.org/10.54499/2022.06207.PTDC), through national funds (OE), within the scope of the Scientific Research and Technological Development Projects (IC&DT) program in all scientific domains (PTDC), through the Foundation for Science and Technology, I.P. (FCT, I.P). The authors also acknowledge the partial financial support within the R&D Units Project Scope: UIDB/00319/2020, UIDB/04077/2020, UIDB/04436/2020. Violeta Carvalho thanks for her Ph.D. grant from FCT with reference UI/BD/151028/2021. Raquel O. Rodrigues thanks FCT for her contract funding provided through 2020.03975.CEECIND.

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Flow visualizations in a semi-rigid aneurysm biomodel

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ABSTRACT

Intracranial aneurysms (IAs) affect approximately 3-5% of the population. The dynamics of blood flow in aneurysms can be influenced by physiological factors, increased blood pressure, aging of the arteries and artery geometry. Of the existing forms of research, the numerical and experimental approach using phantom flow models has been the most used. With the evolution of materials, these models have been increasingly improved, with the aim of simulating and carrying out experiments with more reliable geometry and behavior of arteries. One of the materials used due to its flexibility, transparency, ability to replicate geometries and ease of manufacturing is polydimethylsiloxane (PDMS). However, this material has the disadvantage of interacting with some materials, causing it to become opaque, making flow analysis difficult. Therefore, finding easy-to-manufacture materials that can replicate the lumen geometry is extremely important in the evolution of flow phantom Biomodels. In this work we present different materials that proved to be suitable for manufacturing semi-rigid intracranial aneurysm models and flow visualization experiments.

INTRODUCTION

With a rate of 3-5% of the population affected by intracranial aneurysm and a mortality associated with its rupture varying between 50 and 60%, intracranial aneurysm has been shown to be a serious disease of the cerebral arteries (Rodriguez-Régent et al., 2014). Although you know that the appearance of aneurysms and rupture of aneurysms can be associated with several factors, including high blood pressure, weakening of the artery with age, alcoholism, among others. Even today we cannot predict the location of the appearance and whether an aneurysm will rupture or not. Today the most used risk classification to determine the greatest probability of an aneurysm rupturing is its size (Saqr et al., 2019). Aneurysms classified as large have a greater possibility of rupture, requiring surgical intervention. However, many current authors show that the flow dynamics within AIs can have a great influence on the appearance and rupture of intracranial aneurysms (Miranda I et al., 2022). The approach used in these studies is mostly numerical and experimental, however, the difficulties presented in creating flow phantom biomodels suitable for in vitro experiments mean that many numerical works are published without any experimental validation (A. V. Souza et al., 2019). Therefore, demonstrating means of manufacturing Biomodels that use accessible technologies and materials that allow flow visualization is important for advancing intracranial aneurysm research. In this work we present two intracranial aneurysm models, we report the manufacturing techniques used, and the flow tests performed.

METHODS AND RESULTS

The first step in manufacturing idealized aneurysm biomodels is to define the model to be studied. The idealized models are obtained using 3D CAD software, and Inventor was used for this work. The geometries were based on real aneurysms from the work carried out by (Parlea et al., n.d.) The real models are obtained through a computed tomography and, by carrying out the steps reported in (A. Souza et al., 2020) work, the STL model can be obtained.

With the two STL models obtained, the next stage of the work consists of printing these models on a 3D printer. The Ultimaker S3 3D printer and Polysmooth printing filament were used. With the physical models already printed, which correspond to the lumen of the arteries, the next step consists of positioning them inside an acrylic box where the PDMS will be poured by gravity. After pouring the PDMS, the set remained at room temperature for a period of 48 hours, enough time for the PDMS to cure. Finally, the aneurysm models were immersed in isopropyl alcohol until all material in the lumen was dissolved. Figure 1 below shows the final PDMS models obtained with the process.

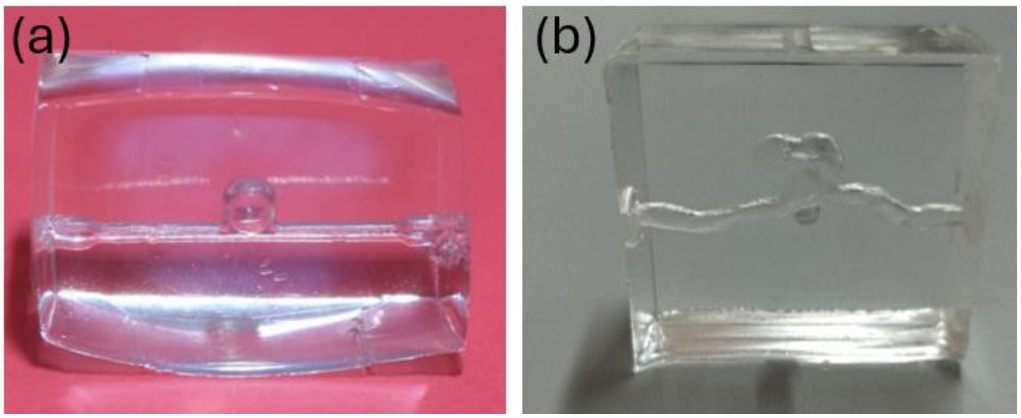

Figure 1 – Phantom biomodels of flow from intracranial aneurysms. (a) Idealized; (b) Real.

The Biomodels must be suitable for flow visualization testing, which in short consists of simulating the flow of arteries with a fluid with tracer particles inside the Biomodels. There are several techniques that can be applied to obtain images and video processing, such as PIV, PTV and image microscopy.

In this work, an Olympus inverted microscope, model IX71, was used, using the N-Achroplan 2.5x/0.07 objective. coupled to the Photron FASTCAM high-speed camera. This camera is associated with visualization software that allows you to work and obtain results later. The flow was injected by a syringe pump at 100 mL/min. At the end of the process, the videos obtained were processed in ImageJ software with the Zproject plugin. We can see below the images of the results obtained in the idealized and real Biomodels.

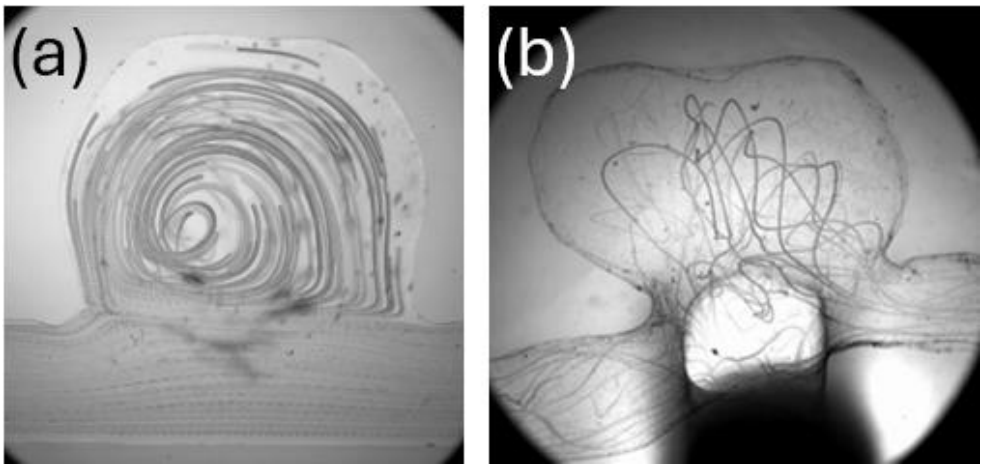

Figure 2 – Flow visualization tests. (a) idealized flow phantom; (b) Real flow phantom.

CONCLUSIONS

In this work, a material that does not interact with PDMS in the manufacture of AI flow phantom was presented. The manufactured real and idealized flow phantoms proved to be suitable for flow visualization tests, which, allows the analysis of different flow behaviors.

Furthermore, it was possible to visualize and compare the effects of geometry on flow behavior. The flow of the idealized flow phantom corresponds to only one area of vortices, whereas in real models we can see a flow characterized by several areas of vortices, providing a more comprehensive view of the blood flow patterns within the aneurysms. For the development of new techniques applied to surgeries and materials, the real model appears to be more appropriate.

ACKNOWLEDGMENTS

C. Ferrera gratefully acknowledges funding from the Junta de Extremadura through grant IB20105 (partially funded by FEDER). The authors additionally acknowledge the projects EXPL/EME-EME/0732/2021 and 2022.06207.PTDC for the financial support, through national funds (OE), within the scope of the Scientific Research and Technological Development Projects (IC&DT) program in all scientific domains (PTDC), PORTUGAL 2020 Partnership Agreement, European Regional Development Fund (FEDER), via the Foundation for Science and Technology, I.P. (FCT, I.P) and the R& D Units projects UIDB/00690/2020,UIDB/04077/2020, UIDB/04436/2020, and UIDB/00532/2020. Andrews Souza acknowledges FCT for the Ph.D. scholarship 2021.07961.BD.

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The Role of Computational Fluid Dynamics and Molecular Dynamics in Biomedical Engineering Applications

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ABSTRACT

Advances in computational simulations have revolutionized biomedical engineering, providing detailed insights into the complex fluid dynamics within the human body. Two significant techniques—Computational Fluid Dynamics (CFD) and Molecular Dynamics (MD)—are widely employed to study biofluid mechanics at both the macroscopic and microscopic scale. CFD is used to simulate blood flow, drug delivery, and artificial organ design, while MD is used to provide particle-level insights into cellular behavior, fluid-solid interactions, and large deformations. The present work gives an overview of how CFD and MD are applied to biomedical engineering, exploring their complementary nature through case studies on red blood cell (RBC) dynamics and aneurysm modeling. The integration of both techniques enables more accurate simulations and enhanced medical device design. Challenges, such as computational requirements and accuracy limitations, are discussed, along with prospects for the field.

INTRODUCTION

Biomedical engineering has increasingly embraced advanced computational techniques to tackle complex physiological problems, from the understanding of cardiovascular diseases to the design of advanced medical devices. Over the past two decades, Computational Fluid Dynamics (CFD) has become a core tool for studying macroscopic level fluid dynamics in biological systems, including blood flow, respiratory mechanics, and tissue perfusion (Karmonik et al. 2009). CFD allows for the simulation of fluid flow in complex geometries like blood vessels, providing valuable insights into parameters such as velocity fields, pressure distribution, and shear stresses, which are critical for understanding diseases like aneurysms (Campo-Deaño et al. 2015). On the other hand, Molecular Dynamics (MD) has more recently emerged as a powerful method for studying microscopic processes in the biomedical field, including cell membrane interactions, particle dynamics, and deformation behaviors of biological materials (Yong et al. 2023).

Recent developments in biomedical research have seen a growing interest in integrating both CFD and MD. State-of-the-art applications include the simulation of microvascular blood flow, where CFD offers a macro-level analysis, while MD provides detailed information on cell deformation and interactions at the microscopic level (Toma 2017). The synergy between these two methods is particularly effective in modeling biofluids in microchannels, where MD captures intricate details like cell membrane dynamics and stress responses (Karampelas et al. 2022). One key challenge, however, is the significant computational power required for MD simulations, which necessitates access to high-performance computing clusters like the SeARCH7 Cluster used in this study.

CFD APPLICATIONS IN BIOMEDICAL ENGINEERING

CFD is commonly applied to simulate the dynamics of biofluids in large biological systems such as arteries, veins, and respiratory airways. In cardiovascular simulations, CFD helps assess parameters such as wall shear stress, blood velocity, and pressure gradients, which are essential in understanding and predicting the development of atherosclerosis or aneurysms. For example, in aneurysm modeling, CFD has been used to simulate blood flow patterns to predict rupture risk, providing critical information for surgical interventions (Ong et al. 2020).

ANSYS Fluent®, a widely used CFD tool, has been instrumental in validating fluid velocity profiles within hyperbolic microchannels, often used for biofluid flow studies and cells deformability assessments. This macroscopic perspective complements molecular-level insights gained from MD simulations, providing a comprehensive understanding of biofluid behavior (Barbosa et al. 2023).

MOLECULAR DYNAMICS: A MICROSCOPIC APPROACH

MD simulations are particularly suited to study microscopic interactions between biofluids and solid particles, such as red blood cells (RBCs) in narrow capillaries. MD models the system at the molecular level, allowing for the exploration of physical phenomena that cannot be analysed by continuum models like CFD. For instance, MD simulations provide detailed insights into how red blood cells deform as they pass through capillaries or microfluidic devices (Sikkandar et al. 2019).

In bioengineering, MD simulations are implemented through highly parallelized codes like LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), which is capable of running simulations with millions of particles (Thompson et al. 2022). Using the Smoothed Mach Dynamics (SMD) package of LAMMPS to model the interactions between liquids and solid structures, which is a model related to the total Lagrangian technique of the Particle Hydrodynamics (SPH) method used for liquids, MD can model complex deformations and interactions in biofluids. SMD, a mesh-free method, handls large deformations such as those found in tissue modeling, which traditional CFD struggles to capture (Williamson et al. 2022).

A case study discussed in the seminar utilized SMD/LAMMPS code to simulate biofluid flows through a hyperbolic microchannel. The simulations demonstrated the deformation and stress responses of RBCs as they encountered varying flow rates and channel dimensions. This particle-level detail, including strain and stress distribution, is critical for applications like drug delivery, where understanding the mechanical behavior of cells is essential (Malviya and Sharma 2021).

CASE STUDIES IN BIOFLUID SIMULATIONS

One of the most prominent applications discussed during the seminar was the comparison of strain rates and velocity profiles between CFD (using ANSYS Fluent®) and MD (with SMD/LAMMPS) simulations in microchannels. While Fluent software provided accurate macroscopic flow features, MD simulations offered detailed particle interactions, such as the deformation of red blood cells (RBCs) and their stress responses. This multi-scale approach allowed for a comprehensive understanding of fluid behavior, from macro to the microscale. An illustrative example obtained from LAMMPS simulations of the deformation and stress response of an RBC flowing in a hyperbolic contraction, can be seen in Figure 1. The observed behavior for the deformation of the solid corresponds to a linear-elastic material strength model implemented in the SMD package, while a linear model was used for the equation of state.

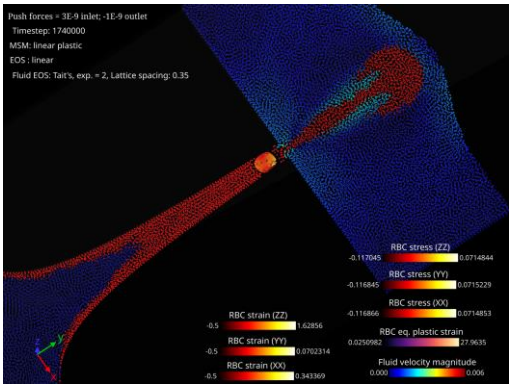
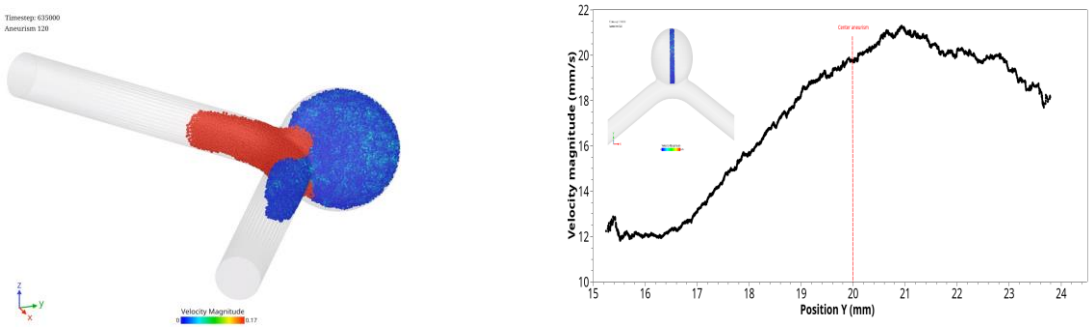


Figure 1. Snaphot of a LAMMPS/SMD simulation showing the deformation and stress response of an RBC flowing in a hyperbolic contraction.

Fig. 2 shows a snapshot of a simulation using the mesh-less code SMD in LAMMPS, to study the fluid distribution and velocity profiles in a simple aneurysm model.



(a) **(b)**

Figure 2. Molecular dynamics simulation of a simple aneurysm using the SMD package in LAMMPS: (a) snapshot of the fluid distribution in the aneurysm region; (b) velocity profile of a cross-section inside the aneurysm.

ADVANTAGES AND LIMITATIONS OF CFD AND MD

CFD is used in macroscopic simulations of biofluid dynamics, especially in large-scale systems like blood vessels. However, when it comes to capture the behavior of highly deformable systems, such as cells in narrow capillaries or tissues under stress, its limitations become apparent. MD, particularly when combined with SPH methods, allows for more flexibility in handling these scenarios. MD simulations provide particle-level insights into the interactions between biofluids and cells, making it an invaluable tool for understanding phenomena such as cell deformation, rupture, and adhesion.

CONCLUSION

The integration of CFD and MD provides a powerful tool for biomedical engineers, enabling comprehensive simulations that range from macroscopic fluid flow to particle-level interactions. By combining these two approaches, researchers can better understand the complexities of biofluid dynamics and enhance the design of medical devices. Future developments in computational power and algorithm efficiency will likely further strengthen the role of CFD and MD in biomedical applications, making them even more relevant for advancing healthcare solutions.

ACKNOWLEDGMENTS

The authors acknowledge the projects 2022.02085.PTDC (https://doi.org/10.54499/2022.02085.PTDC), 2022.06207.PTDC (https://doi.org/10.54499/2022.06207.PTDC), and PTDC/EEI-EEE/2846/2021 (https://doi.org/10.54499/PTDC/EEI-EEE/2846/2021) for the financial support, through national funds (OE), within the scope of the Scientific Research and Technological Development Projects (IC&DT) program in all scientific domains (PTDC), PORTUGAL 2020 Partnership Agreement, European Regional Development Fund (FEDER), via the Foundation for Science and Technology, I.P. (FCT, I.P) and the R&D Units projects UIDB/04077/2020, UIDB/04436/2020, and UIDB/00532/2020.

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