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Computational Fluid Dynamics and Its Solicitation in Dentistry and Its Various Divisions – An Update and Review of Literature

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Abstract

Computational fluid dynamics (CFD) is a part of fluid mechanics that uses numerical means and algorithms to anticipate and resolve problems associated with fluid flow (gas or liquid). Boundary conditions that are set, intends to mimic the clinical condition. Fluid flow dynamics in the various aspects of the biological systems such as blood flow can contribute significantly to the area of research and development. Alteration in the flow dynamics in relation to gas or liquid may have important effects over the biological systems involved. The present review article aims to shed light upon the fundamental aspects of the modelling the digital clinical model or a 3-dimensional model in order to know about the behaviour of the system concerned and to acquire knowledge for carrying out future experimentation which would be beneficial in scientific field for various treatment modalities.

Keywords: *Computational fluid dynamics, Biological system, Dentistry, Fluid-system interaction.*

1. Introduction

Situations wherein experimental/clinical techniques are not able to provide with expected results, computational methods come into play. Few of the computational analysis in dentistry can be carried out in ways of stress analysis, dynamics analysis, fluid mechanics and thermal mechanics among others.[6] Finite Element Method (FEM) is one of the commonly employed applications in the field of engineering as well as dentistry for calculation of stress and strain related changes in the biological systems. Finite Element Analysis (FEA) allows us to unravel partial differential equations in a such a way that we are able to solve structural problems.[7] Computational Fluid Dynamics (CFD) is a similar method, but better suited for solving fluid-flow equations.

Computational Fluid Dynamics (CFD) is a technique of solving numerical problems, the governing equations of substances which are under continuous deformation as result of shear stress and acts as an alternative to predict responses of complex models of continuity, momentum and energy that are not possible to solve by analytical procedures.[1] In order to carry out any kind of experimentation related to human body it is being carried out through three types of approaches, in vivo studies, in vitro studies and in silico studies. Silico study involves the usage of a computational tool to simulate the fluid flow and dynamics of the blood vessels and to access the hypothesis for formation of any pathogen and structured conditions, in other words it is a numerical research to simulate the behaviour of the involved system of concern involving mainly fluids.[2] In the field of medicine, CFD is an universally applicable method with no scrutiny for guiding the treatment or design of a medical equipment that can be beneficial for the health of the patient and quality of life.[3]

Computational fluid dynamics is a method that has been successfully used to figure the mechanics of aero-dynamics of the airway space relating the pressure and flow within the airway space as it is analysed to be more sensitive than the actual anatomical model when it comes to evaluate the restrictions among obstructive sleep apnea patients (OSA).[4] Computational fluid dynamics (CFD) and computational aero acoustics (CAA) are the two kinds of simulations that are necessary to provide computational resources for the purpose of using simulations for dental treatment. CFD and CAA are a part of dental grid system which is used to evaluate the total computation time for performance of optimal CPU resource.[5]

History and Background

Computational fluid dynamics evolved during the period of World War II when scientists were developing a device to solve numerical equations concerned with flow. J. Von Newmann is considered as the father of computational fluid dynamics for his contribution in the artificial viscosity by capturing shocks in the numerical solutions. Among theoretical and experimental fluid dynamics, CFD has made its place stronger with this period of 65 years. As it contributes toward the problems of the various mathematicians, engineers and physicists it has gained popularity in the past and promises to do the same in future.[6]

Principles of Computational Fluid Dynamics

Fluids such as gases and liquids are flowing in a natural scenario all the time and in cases of our body it consists of blood flow, breathing and drinking. Laboratory made models provide a data for experimental studies and numerical method can be employed to find solutions. In the past CFD has been used to cure arterial diseases which came to be known as Computational Haemodynamic. In order to mention about the fluid, the area of interest include are density, viscosity, pressure and velocity which is possible with the help of Computational Fluid Dynamics.[7]

Density – It is the mass per unit volume of a fluid.

The behaviour of the fluid is affected under condition of buoyancy and pressure distribution. By the study of density, it is possible to gain access to the patterns of fluid flow, to detect patterns of stratification or mixing and to know about the fluid behaviour in certain environment.

Viscosity – It refers to the resistance of the fluid flow.

It is influenced by the factors of molecular interactions and temperature. Engineers can analyse the behaviour of the fluid from highly viscous substance like honey to the lowest viscous substance such as water.

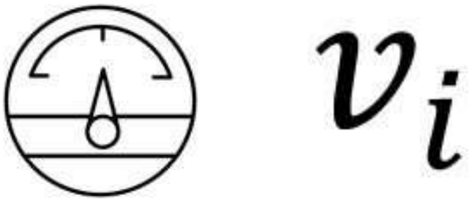
Pressure – It is the force exerted by a fluid per unit area.

Change in pressure can result in fluid motion and helps to understand behaviour of the fluid, pressure distributions to evaluate forces acting on structures, design efficient fluid transport system and optimise performance.

Velocity –It is the rate of fluid flow.

It helps us to understand fluid dynamics and flow pattern, impact of fluid on structures and analyse factors like turbulence and boundary layer formation. Regions of high and low flow rates can be identified which can lead to problem solving in fluid dynamics.

$$\rho \quad \tau = \mu \frac{du}{dy}$$

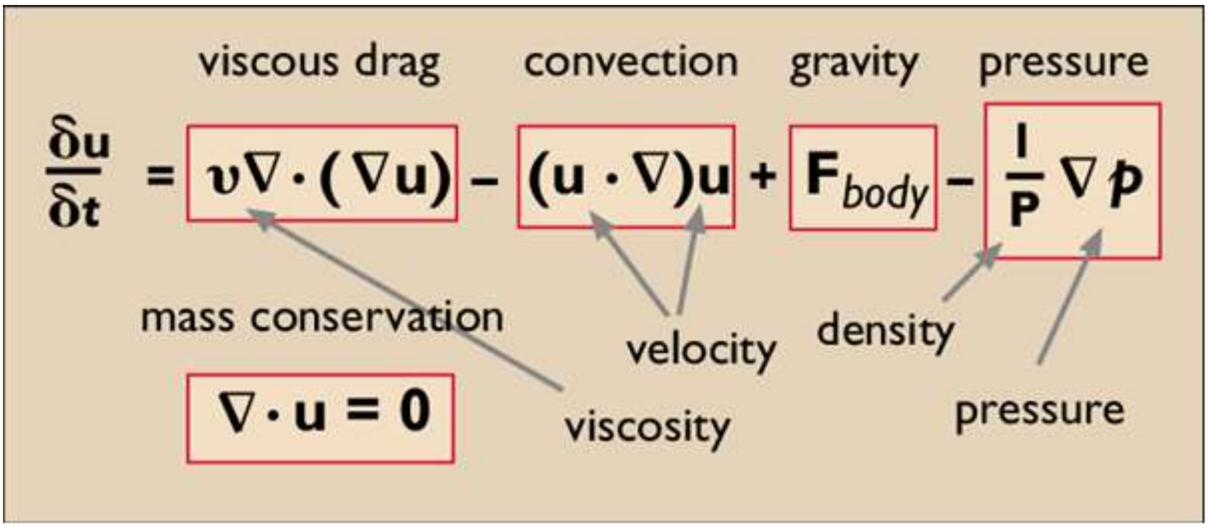


Numerical methods used in fluid dynamics

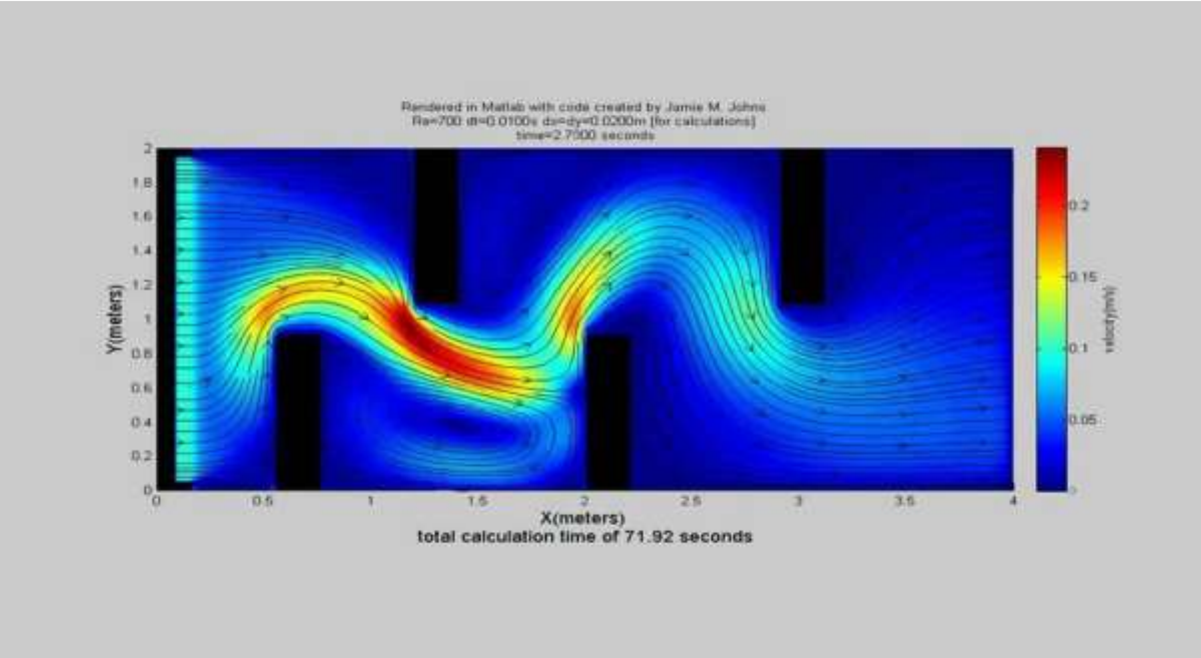
Numerical methods serve as a tool for CFD simulations which help engineers and scientists to solve the governing equations of fluid flow. We explore the various numerical techniques used to discretize these equations, with a primary focus on the Navier-Stokes equations. By breaking down the continuous equations into discrete form, numerical methods pave the way for solving complex fluid flow problems through computation. Three mainly employed numerical technique in CFD are the finite difference method, the finite volume method and finite element methods. Each has certain set of advantages, disadvantages, and suitable applications.[8]

Finite difference methods approximate derivatives using discrete difference equations, making them straight forward and intuitive. Finite volume methods, on the other hand, focus on the conservation of mass, momentum, and energy within control volumes, offering accurate and robust solutions. Lastly, finite element methods utilize variational principles and element discretization to achieve flexibility in handling complex geometries and boundary conditions. In addition to numerical methods, CFD simulations, such as grid generation and boundary conditions are a major aspect of modern engineering. Grid generation involves dividing the computational domain into discrete cells or elements, which play a vital role in accurately representing the geometry and capturing the fluid flow features. Boundary conditions define the behaviour of the fluid at the domain boundaries and are essential for obtaining realistic and reliable results. Different types of boundary conditions have implications on simulation accuracy and stability.[8]

All these methods form the basis for conducting accurate and stable CFD simulations, helping engineers and researchers gain valuable insights into fluid flow phenomena, optimize designs, and make informed decisions in various engineering and scientific applications.[8]



NAVIER-STOKES EQUATION



NAVIER-STOKES INCOMPRESSIBLE FLOW

STEPS OF COMPUTATIONAL FLUID DYNAMICS

COMPUTATIONAL FLUID DYNAMICS

SIMULATION OF FLUIDS

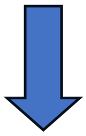
MODELING

DISCRETIZATION METHOD

SOLVERS

NUMERICAL PARAMETERS

GRID GENERATION



SIMULATION RESULTS

Procedure For Computational Fluid Dynamics

Preprocessing

The geometry and physical bounds of the problem can be defined using computer aided design (CAD). From there, data can be suitably processed (cleaned-up) and the fluid volume (or fluid domain) is extracted.

The volume occupied by the fluid is divided into discrete cells (the mesh). The mesh may be uniform or non-uniform, structured or unstructured, consisting of a combination of hexahedral, tetrahedral, prismatic, pyramidal or polyhedral elements.

The physical model is defined – for example, the equations of fluid motion + enthalpy + radiation + species conservation. Boundary conditions are defined. This involves specifying the fluid behaviour and properties at all bounding surfaces of the fluid domain. For transient problems, the initial conditions are also defined.

The simulation is started and the equations are solved iteratively as a steady-state or transient. Lastly, postprocessor is used for the analysis and visualization of the resulting solution.

Computational fluid dynamics in Biomedical Engineering

Aortic flow characteristics were also analysed using computational fluid dynamic method in the past surpassing the experimental methods. Models of the human vascular systems were created using CAD models with help of MRI and computed tomography so that the fluid flow is documented and properties such as viscosity, density and pressure can be recorded.[9]

Evolving applications of computational fluid dynamics in dentistry and its related divisions

Analysis of the upper airways after rapid palatal expansion: Rapid palatal expansion (RME) is a process of expanding the maxillary arch using orthodontic mechanics in patients reporting with constricted arch forms. These patients pose with problems related to dental crossbites and breathing difficulties because of reduced airway volume or space. A comparison of pre and post treatment CFD models were made based on the 3dimensional models of the upper airway. Constant volume flow rate was used for simulating the inhalation process in which the walls were set to be stationery and rigid using turbulent and laminar analysis. Increase in the volume were seen at the region of nasal cavity and nasopharynx and at the constricted part of the airway. In comparison to laminar flow, turbulence was seen at the region of nasal and oro-pharynx and also greater pressure and velocity was observed in comparison to laminar flow. Therefore, use of RME can essentially provide with reduction in resistance of airflow, pressure and velocity in a patient.[10]

Evaluation of pharyngeal airway space using computational fluid dynamics after treatment with Herbst appliance: A longitudinal study was conducted using a total number of 40 patients in which twenty-one patients underwent treatment with Herbst appliance (class II malocclusion subjects with fixed orthodontic mechanotherapy) while the remaining nineteen patients were kept as control group (class I malocclusion subjects with fixed orthodontic mechanotherapy). All patients underwent cone beam computed tomographic (CBCT) investigation prior to and after the treatment. The oropharyngeal airway velocity was larger in the Herbst appliance treated group, similarly a decrease in the laryngopharyngeal airway velocity in the Herbst group was larger when compared to the control group. Hence treatment of obstructive sleep apnea (OSA) during growth period using Herbst appliance can cause significant improvement in ventilation by improving oropharyngeal and laryngopharyngeal airways.[11]

Assessment of mini screw assisted rapid palatal expansion (MARPE) in obstructive sleep apnea (OSA) patients using computational fluid dynamics (CFD): Cone beam computed tomography assisted modelling was performed of an adult patient with obstructive sleep apnea syndrome for CFD analysis. Changes in node displacement, velocity and pressure of the airflow, total resistance at inspiration, rest and expiration was examined after carrying out expansion (MARPE). Expansion with this technique was considered to be of significance as it depicted an improvement of airflow and less resistance of upper airway.[12]

Posterior airways analysis using computational fluid dynamics in patients with maxilla-mandibular advancement (MMA) surgery for correction of obstructive sleep apnea: A study of eight patient who underwent maxilla-mandibular advancement surgery was done using computed tomography for creating 3dimensional models for computational fluid dynamics. These models were simulated to assess the difference between the pressure effort and airway anatomy suitable for breathing. 3-dimensional pre and post models were assessed for pressure effort, apnea-hypopnea index, dimension of airway and skeletal changes. After MMA it was observed that there was an increase in dimension of the airways as well as the distance between the pogonion to the occipital base. There was a significant decrease of laminar and turbulent flows and increase in the cross-sectional areas at the base of the tongue and soft palate. Decrease in the pressure effort and improvement in apnea-hypopnea index that reduced the breathing load and overall improvement of obstruction in sleep apnea was seen.[13]

Analysis of upper airway in patients with unilateral cleft lip and palate (UCLP) using computational fluid dynamics: In this study 21 children with UCLP and 25 children (control group) requiring orthodontic treatment without the presence of UCLP were evaluated for upper airway ventilation and nasal resistance using CBCT data for CFD. Maximal pressure of the upper airway, pharyngeal airway and nasal resistance were seen to be higher in the UCLP patients as compared to the control group predisposing them to the obstruction in nasal and pharyngeal airway causing obstructive sleep apnea syndrome.[14]

Analysis of shear stress on nerve endings in dentinal microtubules by computational fluid dynamics: A study was performed taking into account quantitative interpretation of hydrodynamic theory of dental pain to analyse the shear stress produced on the intra-dental nerve endings that may excite the pulpal mechanoreceptors responsible for causing dental pain sensations. It relied on the fact that any kind of thermal or mechanical stimulus on the dentin can cause flow of fluid in the dentinal microtubules. A CFD model was prepared having innervated dentinal microtubules with dentinal fluid flow. Odontoblastic process movement, dentinal velocity, fluid viscosity were found to have a significant effect over the shear stress however density of the fluid showed no irrelevance. It was concluded that odontoblastic movement change caused by dentinal fluid flow caused changes in the dimensional space and affected the shear stress on the nerve endings.[15]

Computation fluid dynamics employed to check for the changes in the upper airway response after incisor retraction in cases of dental bimaxillary protrusion involving premolar extraction: A sample of 30 patient who completed orthodontic treatment participated in the study with their CBCT scans for 3D model reconstruction. It was analysed that pressure drop in the minimum area, oropharynx and the hypopharynx were increased significantly. In pre-treatment the minimum pressure and the maximum velocity those were located in the hypopharynx were seen in the oropharynx after treatment. All these findings suggested that there is a higher chance of pharyngeal collapse in patients undergoing extraction treatment protocol for bimaxillary protrusion with maximum anchorage.[16]

Another study by Boutsioukis C et al to evaluate the effect of tip design of the needle on the flow of the irrigant into a prepared root canal was done by computational fluid analysis. Three open ended and three closed ended needles were tested in this study to evaluate the velocity, apical pressure and shear stress on the wall of the root canals. Pattern of flow in open and closed ended needles differed in a way that there was more irrigant replacement by open ended needles and also high apical pressure, whereas the closed ended group caused less efficient irrigant replacement.[17]

Computational fluid dynamics to check for the salivary flow around an orthodontic bracket for microbial and periodontal parameters: A model of the lower central incisor and with orthodontic appliance in place were created and salivary flow was simulated. There was significant decrease of salivary flow velocity and increase of bacterial count (total peri-bracket bacterial count and periodontal status were tested parallelly). Areas of inflammation was formed gingival to the bracket which acted as site of plaque accumulation and retention which is a causative factor for inflammation.[18]

Intra-arterial chemotherapy for oral cancer studied by computational fluid dynamics: The distribution of flow of anti-cancer agent into the branches of external carotid artery by intra-arterial chemotherapy (IAC) technique was investigated through computational fluid dynamics. From CT images of two patients with tongue cancer, 3dimensional (32) models of the blood vessels were created with varying horizontal and vertical positions of the catheter tip, which were patient specific and combined with the catheter models. Streamline of blood was followed and traced from the common inlet towards each outlet to observe the flow of anti-cancer agents and to calculate the shear stress of the vessel walls with the use of zero-dimensional resistance model of conventional IAC and supers-selective IAC into 30 and 2 models respectively. According to the findings, the anti-cancer agent was delivered to the target artery only when the tip of the catheter was located below the bifurcation of external carotid artery and each target artery and when the catheter tip was shifted towards the target artery. Flow of anti-cancer agent was only in the supers-selective IAC whereas high shear wall stress was seen at the target artery in one patient's model which can cause complications during the treatment.[19]

Fibrinogen simulation around the dental implant surface using computational fluid dynamics: Titanium implants are hydrophilic for osteointegration because of their ultraviolet treated surface. Their degree of hydrophilicity plays an essential part in the aggregation of fibrinogen which is required in the blood clot formation and healing of wound. Using the CFD model the level of hydrophilicity was expressed between the surface of the implant and blood plasma showing that there was a flow of fibrinogen into the interfacial implant surface which was time dependent with a steeper slope, however the mass of blood plasma was also absorbed in the same manner but it was rapid and non-time dependent. On comparison of fibrinogen and blood plasma it was observed there was no linear correlation, hydrophilic implant surface promoted their infiltration onto the implant surface which was non proportional implying that fibrinogen has greater affinity for recruitment by the hydrophilic surface of implant.[20]

Dentinal fluid flow in the dental pulp during mastication by fluid simulation-structure interaction: A study was done to investigate the interaction between dental pulp fluid flow and mastication. 3dimensional simulation of a premolar tooth and its surrounding structures and food particles were created. The stress, displacement and fluid flow indices were selected for evaluation. It was concluded that masticating food with high elastic modulus caused high stresses, displacement and faster fluid flow compared soft food and fast chewing of food was associated with faster fluid flow with dental pain occurrence.[21]

2. Conclusion

Occupational hazards of mercury while removing amalgam restoration and its risk assessment on air quality studied with computational fluid dynamics: A CFD model with particle size, density and compositional data was obtained from aerosolization experiments that simulated the clinical breathing conditions in a dental scenario where removal of an amalgam restoration may be performed. Study revealed that about 58% of the mercury in the restoration is vaporized with 0.85-570 microns particles size, which are aerosolized may remain in the air for 2 mins. Taking into consideration that many such events are performed in a day, hence it is a must that a dental professional follows a strict respiration protective protocol.[21] In another study by Chen C et al they measured the aerosol contamination in a clinical environment spread through patients' mouth and the effectiveness of air cleaner. For this they simulated energy, airflow and different dispersion of aerosol particles and particle removing efficiency of the air cleaner using CFD simulations and found that the location air cleaner and the distance of the air cleaner from the droplet source are important to consider for adequate protection of the dental health care workers[22].

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