Structural analysis of antiviral N95 filtering facepiece respirator VESTA

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Abstract. The pandemic caused by the coronavirus (SARS-CoV-2), which causes the disease COVID-19, forced health authorities and research institutes to propose solutions. An important and accessible tool to fight against the virus the use of masks. The VESTA respirator's designed product is the new antiviral N95 filtering facepiece respirator developed by the researcher team from the University of Brasilia. The facepiece mask is composed of three layers of non-woven that can retain up to 95% of solid, liquid, oily and aerosol particles besides inactivating the virus. The Vesta differential is the chitosan nanofilm, present in the intermediate layer, that works as a physical barrier for the virus. The nanofilm has antimicrobial action and greater ability to filter viruses, including the SARS-CoV-2 that causes COVID-19 and prevent infectious diseases with self-cleaning protection and drug delivery properties. This paper aims to perform structural simulations like tension, deformation, and vibration analysis on the respirator VESTA. It demonstrates the mechanical characteristic of the designed mask and certifies its resistance under the certain application. The numerical simulations were performed in the commercial finite element software ANSYS.

Keywords: Finite element method, Structural analysis, N95 filtering facepiece respirator, COVID-19.

1 Introduction

The speed of dissemination of COVID-19 led to an alert to the World Health Organization (WHO), which classified the emerging disease as a pandemic, characterised by an international health problem of an emergency nature [9]. The growing demand for obtaining personal protection equipment (PPE), including respirators, and the scarcity of such equipment for health professionals and society motivated researchers from different areas of the University of Brasília to develop protective equipment that would be effective in micro and nanoparticles filtration, such as the SARS-CoV2 virus, providing users with a safer environment. The adoption of emergency measures is necessary given the continuous increase in new SARS-CoV mutations. As measures to prevent the massive spread and worsening of the disease in the country, which has taken the Brazilian health system to the limit of its capacity, besides vaccines, it is extremely essential to use masks, respirators and constant hand hygiene. Healthcare professionals are highly exposed to SARS-CoV-2 because of the high demand from healthcare systems to deal with the pandemic. There is a consensus among public health agencies to adopt protective measures related to the use of PPE, such as face shields and semi-facial respirators with N95 particle filter, to reduce airborne disease transmission [7].

The new N95 class antiviral filter respirator developed by the team of researchers at the University of Brasília was called VESTA. This respirator is a face-piece composed of three layers of TNT-dental-hospital (non-woven fabrics) capable of retaining up to 95% of solid, liquid, oil and aerosol particles. The differential of the Vesta Respirator is the chitosan nanofilm present in the mask's intermediate layer, which besides working as a physical barrier against the virus, is also a barrier that, through chemical interaction, has the property of inactivating the virus. In addition, nanofilm has antimicrobial action and greater ability to filter viruses, including SARS-CoV-2. The nanofilm is produced from chitosan nanoparticles, a cationic polymer - a natural macromolecule - found in shrimp shells. The substance is a low-cost material, biodegradable, biocompatible, non-toxic and has properties that can stop the virus and inactivate him. Therefore, this PPE improves protection against contamination and reduction of SARS-CoV-2 infection in healthcare professionals working in hospitals and in the general population.

Facepiece respirator protects its wearer by sealing their face and filtering out hazardous particles from the environment. However, respirator wearers always present leaking of particles. Therefore, a numerical model was used to simulate the characteristics of the respirator and its mechanical behaviour under the condition of use, thus helping to optimise and improve its design. Zhipeng et al.[13] investigated the interaction between head shape and facepiece respirator with N95 filter according to contact pressure through simulation and experimental validation. Upon contact with the respirator, interactions take place mainly in the frontal maxilla and nasal regions. The nose clip, an item that makes up the respirator, improves protection against leakage between the respirator and the face [12], as well as the penetration of particles through the filter media. This work aims to carry out structural simulations such as stress, strain and vibration analysis in the Vesta respirator and in the nose clip. Aiming to study the mechanical characteristics of the respirator and clip in projected situations and analysis of their resistance under an application. Numerical simulations were performed in commercial finite element software ANSYS.

2 Finite element background

The finite element method (FEM) is a numerical tool that uses variational formulations and uses interpolation methods to solve difficult analytical formulation [8]. FEM concept solves a problem of balance where a complex global structure is divided into partitions, called elements. The elements are then connected, where boundary conditions of movement or rotation restriction and loading can be applied and results solution achieved by employing numerical methods of approximation. FEM formulation is a variational principle related to total potential energy as follows:

$$\int_V \boldsymbol{B}^T \mathbf{D} \boldsymbol{B}\, dV + \int_V \boldsymbol{N}^T \rho \boldsymbol{N} dV - \int_x \boldsymbol{N} P_x\, dx = 0 \tag{1.1}$$

where $\boldsymbol{N}$ is matrix of shape functions, $\boldsymbol{B}$ is the strain matrix, $\mathbf{D}$ is the matrix of material constants, and P_x vector of distributed load, which is found in [8]. Equation (1.1) is the basic equation for the finite element discretization and can be converted to algebraic equations of motion in the dynamic case as:

$$\left(\boldsymbol{K} - \omega_i^2 \boldsymbol{M}\right) u_i = \boldsymbol{f} \tag{1.2}$$

For the static approach, Eq (1.1) and (1.2) reduce to the expressions

$$\int_V \boldsymbol{B}^T \boldsymbol{D} \boldsymbol{B}\, dV - \int_x \boldsymbol{N} P_x\, dx = 0 \tag{1.3}$$

and

$$\boldsymbol{K} \boldsymbol{u}_i = \boldsymbol{f} \tag{1.4}$$

2.1 ANSYS Mechanical simulation

The analysis process in ANSYS is divided into three key steps: pre-processing, processing and post-processing. The pre-processing step includes defining the elements, the system mesh, assigning material properties to each element, defining boundary conditions and loads. Understanding the physical principles behind the problem is always more important than the modelling technique itself. If the boundary conditions are incorrect or the element type is not chosen correctly, the results may be incorrect. The processing step is where the MEF is applied computationally in the model made previously. The pre-processed model is imported into a solver that will then assemble the stiffness matrix and calculate all degrees of freedom (GDLs) and solve the problem of extracting the result given the choice analysis.

A static analysis calculates the effects of steady loading conditions on a structure while ignoring inertia and damping effects, such as those caused by time-varying loads. The static analysis includes steady inertia loads such as gravity and rotational velocity. Also, time-varying loads can be approximated as static equivalent loads (such as the static equivalent wind and seismic loads commonly defined in many building codes) [3]. Static analysis determines the displacements, stresses, strains, and forces in structures or components caused by loads that do not induce significant inertia and damping effects. Steady loading and response conditions are assumed;The loads and the structure's response vary slowly regarding time.

Modal analysis is used to determine the vibration characteristics (natural frequencies and mode shapes) of a structure or a machine component while it is being designed. It can also serve as a starting point for another, more detailed, dynamic analysis, such as transient dynamic analysis, a harmonic response analysis, or a spectrum analysis [4]. The natural frequencies and mode shapes are important parameters in the design of a structure for dynamic loading conditions. It also required them to do a spectrum analysis or a mode superposition harmonic or transient analysis [4]. The extraction of eigenvalue and eigenvector, using numerical methodologies, the main ones being Block Lanczos, PCG Lanczos, Supernode, Reduction (Householder), as presented by [4]. In this paper, we decided on the Block Lanczos method. The eigenvalue extraction process can take from seconds to several days, depending on the number of elements and the computational capacity of the computer where the analysis is solved.

3 Product information

The new Vesta respirator is of the N95 PFF-2 class that contains in its composition an antiviral nanofilm. Vesta's differential is this chitosan nanofilm, present in the intermediate layer, which has antimicrobial action and greater capacity to filter viruses, including SARS-CoV-2 which has a diameter of 120 nanometres. It acts as a physical barrier to the virus, besides having the property of inactivating it by chemical interaction, as illustrated in Figure 3.1(LHS). We performed the 3D scan of the physical Vesta respirator used in the numerical simulation, as shown in Figure 3.1(RHS). The respirator is a semi-facial piece of filter material that covers the nose, mouth and chin under the specification of NBR-13698:2011 [2]. Two rubber straps fixed the mask to the user's face and the nose clip that has the functionality to reinforce the seal on the face, ensuring its frontal fit. Figure 3.2 demonstrates the usability of the respirator, where the actual 3D model of the respirator is attached to the wearer's face. The NIOSH standard [6,7] standardises the long-long type face CAD model.

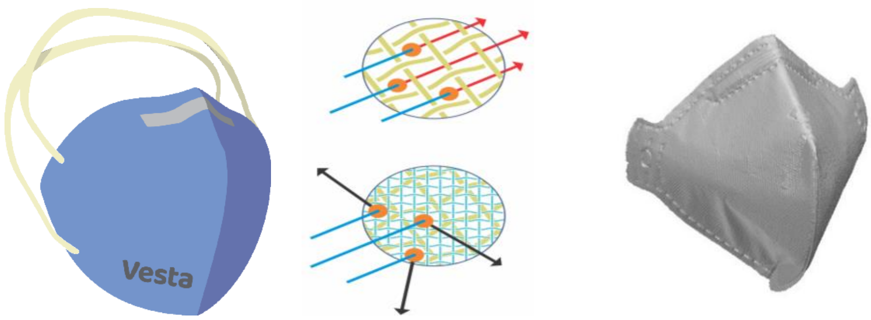


Figure 3.1 Antiviral Vesta respirator N95: Infographic (LHS) and 3D Vesta scan (RHS).

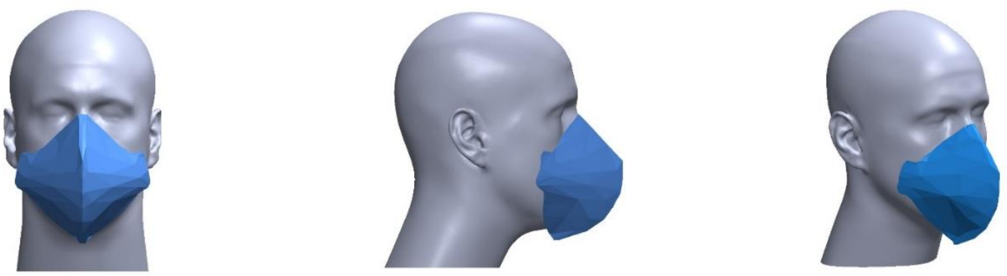


Figure 3.2 Real 3D model of the respirator attached to the user's face.

3.1 Respirator Vesta design

Vesta is a facepiece respirator N95 class which indicates retention of up to 95% of solid, liquid, oil and aerosol particles. It is composed of three layers of non-woven fabric with the outer layer of non-woven weight 40 plus felt, the middle layer of non-woven weight 60 plus MELT with CHITOSAN, and the inner layer of non-woven weight 40, as shown in Figure 3.3(a). The middle layer is the filtering element that contains nanotechnology, the chitosan nanofilm, which is Vesta's differential. Nanofilm is produced from chitosan nanoparticles, a cationic polymer that is a natural macromolecule found in shrimp shells. The substance has properties that can stop the virus and inactivate. Figure 3.3 (b), shows the nose clip, where was analyzed in [16].

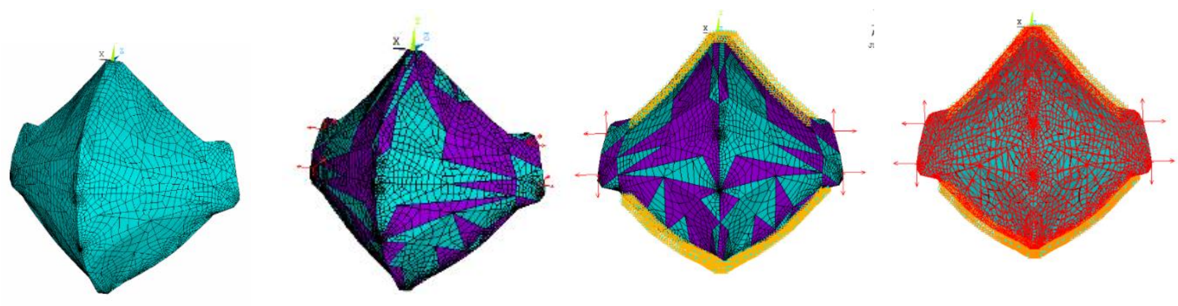
(a) (b)

Figure 3.3 Vesta components: a) Three layers of dental-hospital TNT and b) Nose clip.

The design of VESTA [15] follows the recommendations of the resolution ANVISA RDC N 356/2020 [5], establishing that the filtering respirator N95 must have the mask's edge free of burrs and tips. VESTA's manufacturing material is non-woven fabric for dental-medical-hospital use, same specification for surgical mask [1]. The technology developed and applied in the filter layer is based on chitosan nanoparticles proposing to reduce SARS-CoV-2 contamination and infection among users. This application increases the filtering power of the respirator, aiming to mitigate the harmful effects of bacteria and viruses, especially in the hospital environment. Chitosan is a low-cost natural cationic polymer derived from chitin, with biodegradable, biocompatible and non-toxic characteristics, besides its antimicrobial activity. Virucidal activity works as an attraction factor of its cationic charge to negative charges, as with viruses. Thus, chitosan can act as a viral absorption and inactivation surface. Using nanomaterials in facial respirators can decrease particle permeability and promote an effective antiviral effect compared to conventional respirators such as class N95 [11]. A detailed analysis of the nose clip is presented in [16].

4 Numerical results

In the simulation analysis the Vesta respirator non-woven fabric properties related to the polypropylene material [10] are density of 900 kg/m3, Young's Modulus of 1100 MPa, and Poisson of 0.45. Mask thickness is 1 mm. The tensile yield strength limits are 35 MPa, compressive rupture strength 60 MPa and flexural rupture strength 40 MPa.

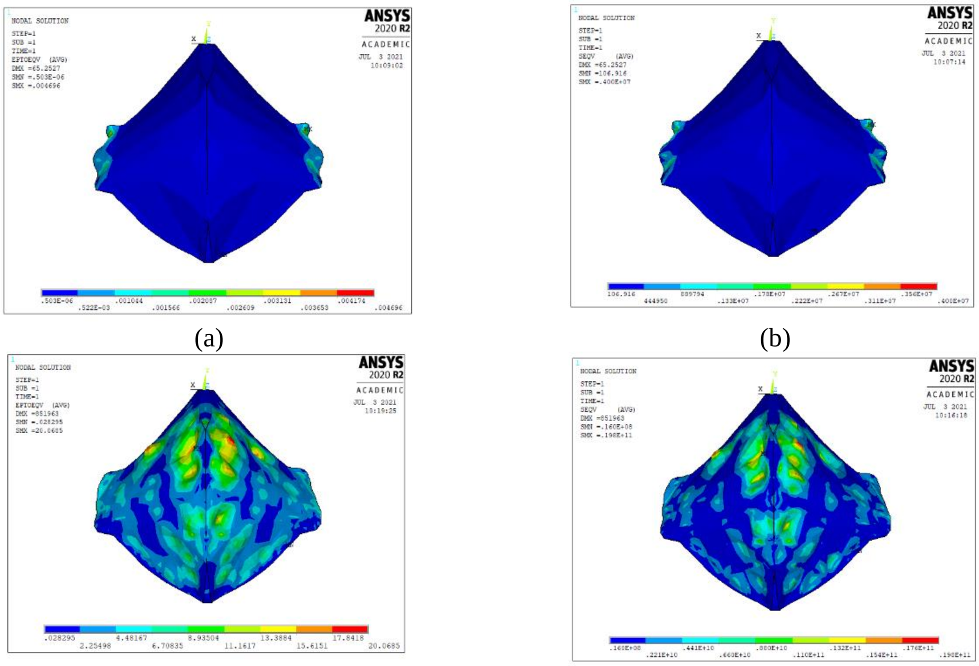


(a) (b) (c) (d)

Figure 4.1 Vesta model used in the ANSYS simulation: (a) Mesh with 3296 elements; (b) Simulating the strength of the elastics securing Vesta to the wearer's face; (c) Simulating the strength of the elastics and condition representing the Vesta in contact with the wearer's face. (d) Pressure application and boundary condition;

Loads assumed in the simulation are the breath pressure of 300 Pa [14] applied on the entire area of the respirator in the z-direction (Figure 4.1b) and punctual loads simulating the rubber straps used to fix the respirator on the face. These rubber straps forces are applied at four points on the respirator, as illustrated in Figure 4.1 (b), on x-direction with a value of 20N, y-direction of 10N, and z-direction of 40N [14]. This static study shows the tension analysis performed for the Vesta. The aim is to evaluate the limit values for each loading type in the pre-yield stage. It is assumed that the edge of the respirator is always in contact with the user's face while using the respirator (Figure 3.2), hence, the boundary condition applied is simply supported contains on the GDLs of the respirator's edges, as shown in Figure 4.1.

We used 3296 SHELL type elements in the mesh, as in Figure 4.1(b). The results of the static analysis performed on the respirator shown in Figure 4.2(a-d) are relative to the Von Mises stress for tension. In Figure 4.2(a) we have the Von Mises equivalent stress of the total strain (EPTOEQV) associated with the rubber straps forces, where the maximum value is 0.00469MPa and in Figure 4.2(b) we have the Von Mises equivalent stress (SEQV) as a maximum value of 4 MPa, much lower than the material's limit values. Figure 4.2 (c) shows the equivalent Von Mises stress of the total deformation due to the strap's forces combined with the pressure on the entire area of the respirator, where the maximum value is 20MPa. Figure 4.2 (d) shows the Von Mises equivalent stress reaching a minimum value of 16 MPa and a maximum value of up to 19.8 GPa.

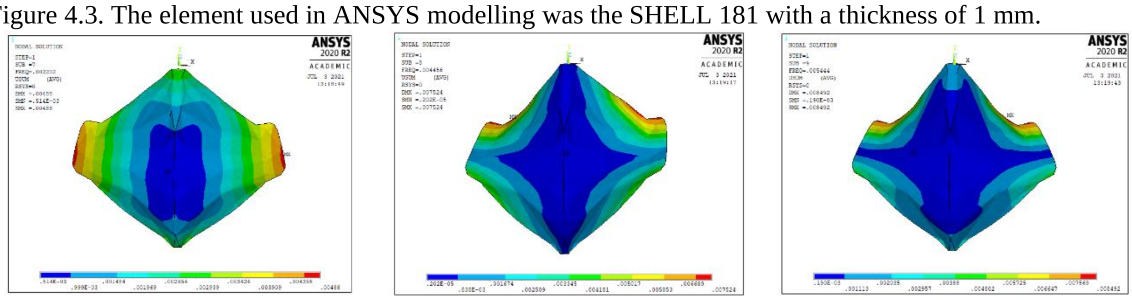


(a) (b)

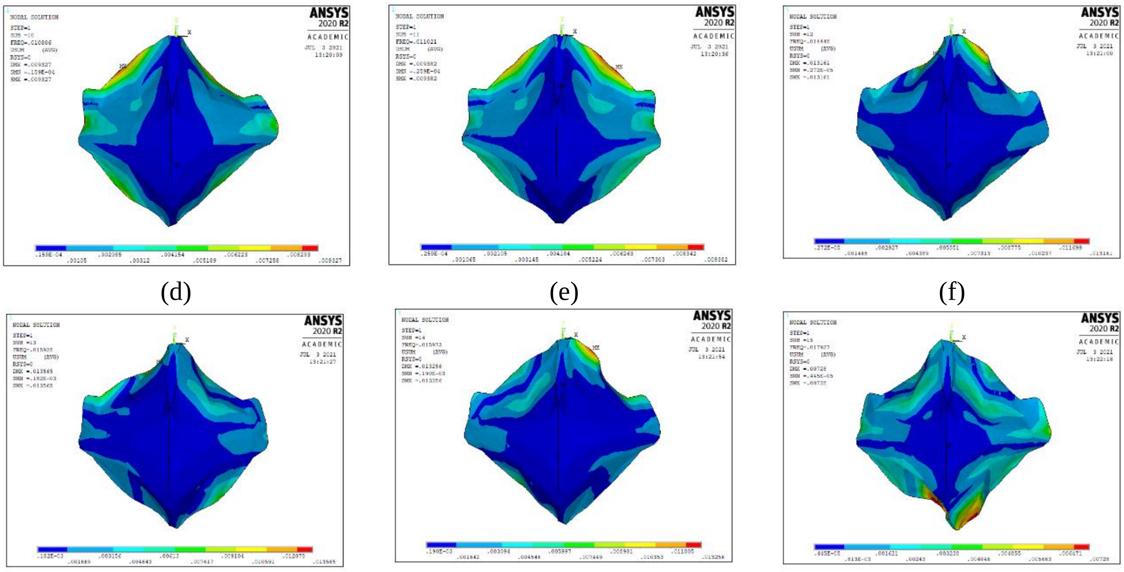
(c) (d)

Figure 4.2 Von Mises deformation due to the strap force (a); Von Mises tension due to the strap force (b); Von Mises deformation associated with the strap force and pressure (c); Von Mises stress associated with the strap and pressure (d);

Dynamic analysis explores the modal parameters (natural frequencies and modal shape) of the respirator. Vesta's modal parameters are estimated for the free-free boundary condition and the support condition. In this second, the entire contour of the mask has the GLDs constrained, except by the region of the flaps where the connection of the fixation straps is found. The free vibration in both cases and number of elements, as shown in Figure 4.3. The element used in ANSYS modelling was the SHELL 181 with a thickness of 1 mm.



(a) (b) (c)

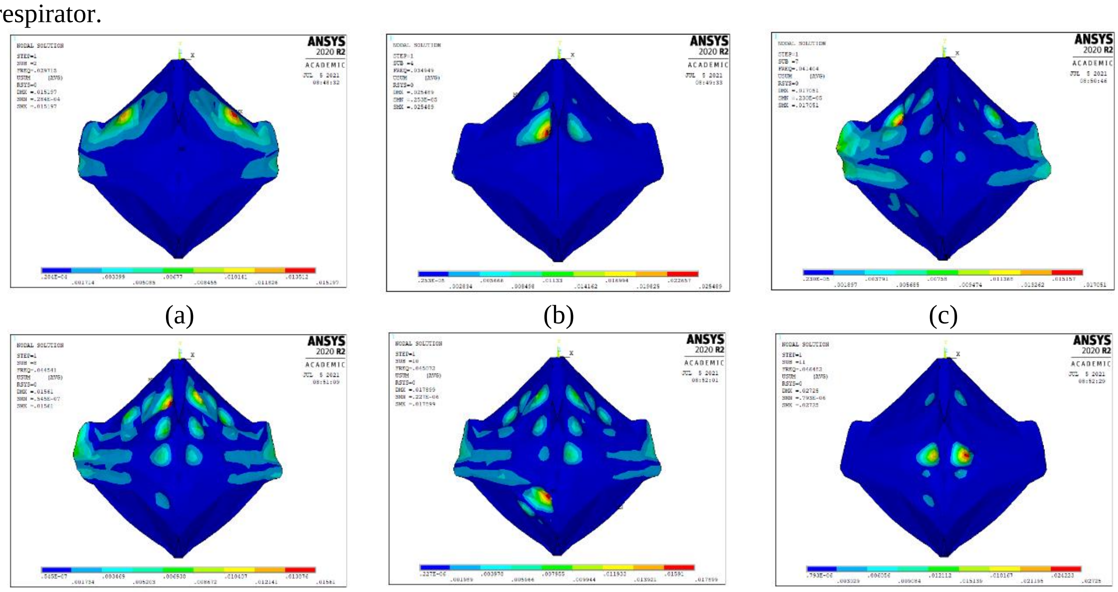


(d) (e) (f)

(g) (h) (i)

Figure 4.3 Vesta respirator natural frequencies and modes shaped under free-free condition.

The first nine vibrating modes associated with the respirator's natural frequencies for the free-boundary condition are shown in Figure 4.3(a-i). The nine natural frequencies are 0.004, 0.0044, 0.0054, 0.0108, 0.010, 0.0144, 0.0159 and 0.0179 Hz. The rigid body modes were discarded, even though the first frequency followed by the others are relatively low, this effect is because of the high flexibility of the material and geometry of the respirator.



(a) (b) (c)

(d) (e) (f)

Figure 4.4 Vesta respirator natural frequencies and modes shaped under supported boundary condition.

For the second case, where the breath has its contour in the condition of supported contours and the region of the free flaps simulating the use of the product, the first six modes shapes associated with natural frequencies were estimated. Figure 4.4(a-f). shows the natural frequencies associated with modes shapes are 0.0151, 0.0254, 0.0414, 0.0445, 0.045 and 0.0464 Hz. The rigid body modes have been discarded, in this case the frequencies have increased because of the boundary condition. The first, third and fifth modes are symmetric with a maximum amplitude of 0.017 mm in the z-direction and the asymmetric modes reach a maximum vibration amplitude of 0.0254 mm in the second mode.

5 Conclusions

This paper presented a static and modal simulation of antiviral N95 filtering facepiece respirator VESTA using the finite element method through the ANSYS software. The respirator was 3D scanning and a CAD model was generated and used in the simulations. A brief description of the product is presented in section 2. The analysis provided by simulations aiming to characterise the structural behaviour of the Vesta under pressure and force simulating one case of use. Static and vibration analysis performed on the mask defined the loads acting during the use of the product, which was considered the breathing pressure in the entire area of the respirator and loads of the rubber straps used to fix the respirator on the user's face. The strap forces are applied at four points on the respirator flap and the Von Mises equivalent stress of the total strain (EPTOEQV) and total stress (SEQV) preformed. The maximum values were under the material limits excepted by the maximum SEQV. Natural frequencies and modal shape were estimated for the mask in free-free vibration and supported boundary conditions. Therefore, the natural frequencies are low due to the high flexibility of the mask material and its geometry. The knowledge of modal parameters is essential for the design as it demonstrates the dynamic deformation of the product associated with its characteristic natural frequency. In summary, obtaining the mechanical parameters such as tension, deformation, bending, and vibration values of the respirator help the researchers to improve the VESTA design and understand the Vesta respirator material limits. Therefore, the analysis shows Vesta level of quality and simulated mechanical tests.

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