COMPARISON OF PATIENT-VENTILATOR INTERFACES BASED ON THEIR COMPUTERIZED EFFECTIVE DEAD SPACE

R. Fodil^{1,2}, F. Lellouche³, J. Mancebo⁴, G. Sbirlea-Apiou^{1,2}, D. Isabey^{1,2}, L. Brochard^{1,2,5}, B. Louis^{1,2}

⁽¹⁾ Inserm Unite U955, Cell and Respiratory Biomechanics Group, Créteil, F-94010, France ;

⁽²⁾ Université Paris-Est, Faculté de Médecine, UMR_S955, Créteil, F-94010, France ;

⁽³⁾ Université Laval, Centre de Recherche de l'Institut Universitaire de Cardiologie et de Pneumologie de Québec, G1V4G5 Québec, QC, Canada ;

⁽⁴⁾ Servei Medicina Intensiva, Hospital Sant Pau, Barcelona, Spain

⁽⁵⁾ AP-HP, Groupe Henri-Mondor Albert-Chenevier, Service de Réanimation Médicale, Créteil, F-94010 France ;

Corresponding Author:

Bruno Louis Inserm U955, Eq. 13 Faculté de Médecine 8 rue du général Sarrail 94010 Créteil Cedex France

Tel: 33 1 49 81 36 76 Fax: 33 1 48 98 17 77 e-mail: <u>bruno.louis@inserm.fr</u>

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THREE-DIMENSIONAL SURFACE RECONSTRUCTION AND SET-UP OF A COMPUTATIONAL FLUID DYNAMICS (CFD) PROBLEM

Data acquisition and three-dimensional (3 D) surface reconstruction: The 3D computational geometry used for this numerical study was derived from computed tomography (CT) scan images, except in the case of the helmet type where the interface was reconstructed using a 3D modeller (3ds Max, Autodesk, Inc., CA, USA). The same mannequin head was used to delimitate the internal volume of each interface. Scans provided contiguous axial images which were 0.5mm apart. The stack of CT images in DICOM format was imported into a commercial software package: AMIRA[®] (VisageImaging, Richmond, Australia) for segmentation. Segmentation assigns a label to each pixel of the image, defining whether the pixel is in a solid or in an air region of the interface. Segmentation is a prerequisite for 3D-surface model generation. We used AMIRA[®] software to successively construct, for each interface, a triangular surface and a volumetric tetrahedral grid of the segmented object (see Figure 1).

Set-up of CFD problem: Mesh model. This original mesh, Amira normal mesh (A-NM), was used in a preliminary airflow simulation. The result was used to adapt the mesh via the CFD software to resolve large pressure gradients in the flow field. The quality of the resulting mesh (F-AM) was estimated by the triangle aspect ratio (< 10) and tetra aspect ratio (< 10), as usually reported in the literature [1]. To eliminate artifacts due to the boundary conditions, we added two further elements to each model. The first was a virtual cylindrical tube of 15 cm in length and a diameter equal to the inlet interface (\approx 1.9 cm). This was situated at the junction between the interface and the ventilator circuit. The second element was a virtual elliptical duct (3.6 cm in length, a 2 cm major axis and a 1 cm minor axis) at the

outlet of the mannequin's mouth. In the case of the helmet model, a third volume, identical to the first was added at the inlet of the expiratory circuit. This was done because of the presence of two distinct circuits in the helmet interface: one for the inspiratory and the other for the expiratory flow (Figure 1, panel d).

Set-up of CFD problem: Physical model. The incompressible flow was chosen to be unsteady, albeit with a constant flow rate for each inspiratory/expiratory phase. Based on the value of the Reynolds number computed in the inlet circular tube (2800 in case of inspiratory flow and 1400 in case of expiratory flow), a low Reynolds number (LRN) shear stress transport (SST) k- ω model was used in unsteady condition. This k- ω model has the advantage to fit with laminar-transitional-turbulent flows. Such model has also been used for extrathoracic flow studies [2, 3]. During inspiration, a uniform velocity profile was set at the extremity of the cylindrical tube, and during expiratory flow a similar uniform velocity profile was set at the extremity of the elliptical duct. An outflow boundary condition was set at the outlet of the mesh model. During inspiration and expiration, the outlet of the mesh model was at the extremity of the elliptical duct and at the extremity of the cylindrical tube respectively. In addition, a no-slip condition was assumed at the inner walls. Inspiratory and expiratory flow cycles were simulated using constant flow rates with a temporal step of 0.025 sec.

Set-up of CFD problem: 3D numerical model. Inspiratory and expiratory airflows were generated in the 3D mesh model. Governing equations for momentum and mass conservation were solved by a commercial CFD software package, FLUENT® (Fluent Inc., Lebanon, TN, USA), using a control-volume based method. The solution algorithm used was a segregated solver. The governing equations were made linear with an implicit method. The local mass fraction of each gas species ($O_2 - CO_2$) at a given time was predicted through the solution of a

convection-diffusion equation included in the FLUENT software. A uniform velocity profile was used as a boundary condition at the inlet of the mesh model. The CFD software package, FLUENT® (Fluent Inc., Lebanon, TN, USA), is a commercial software. It is extensively used in industry and academic fields. Our team used this software for several years. In previous studies we validated our use of this software measuring pressure drop and flow in nasal airway and human proximal airway tree [4, 5].

CFD Postprocessing: effective dead space

The CFD procedure allows estimating gas composition, flow and pressure at any locus of the interface gas region and at any time of the breathing cycle. Especially, gas composition at the mouth of the mannequin, allows determining the effective dead space (VD) of the interface gas region defined as the rebreathed gas volume resulting from the exhaled gas trapped in this interface gas region. Gas composition was described from CFD estimation of the mass fraction of each gas species, especially for oxygen (MF₀₂) and carbon dioxide (MF_{CO2}). The knowledge of the mean MF₀₂ at the mouth of the mannequin (calculated via CFD as shown in the online ESM), allows to estimate the inspired volume of oxygen (V₀₂):

$$\mathbf{V}_{O2} = \int_{t_1}^{t_2} \mathbf{MF}_{O2} \cdot \left(\frac{\rho_{air}}{\rho_{O2}}\right) \cdot \mathbf{\dot{t}}$$

where t_1 and t_2 are the beginning and the end of the inspiratory time respectively, ρ_{air} and ρ_{O2} the density of air and oxygen respectively and, $\dot{}$ is the flow rate.

 V_{O2} allowed to estimate the volume of fresh air (V_{fresh}) and the VD that are inhaled by the mannequin during each inspiratory cycle:

$$\begin{cases} V_{O2} = vF_{O2fresh} \cdot V_{fresh} + vF_{O2exhaled} \cdot VD \\ VT = V_{fresh} + VD \end{cases} \Longrightarrow \begin{cases} VD = \frac{V_{O2} - (VT \cdot vF_{O2fresh})}{vF_{O2exhaled} - vF_{O2fresh}} \\ V_{fresh} = VT - VD \end{cases}$$

where $vF_{O2fresh}$ and $vF_{O2exhaled}$ are the volume fraction of oxygen of fresh air (heated and humidified) and exhaled air (which contains CO₂) respectively and, VT is the tidal volume.

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3D volumetric meshes of the 4 interfaces positioned upon the adult polystyrene mannequin head. Panel a: the oronasal mask # 1 ; Panel b: the oronasal mask #2; Panel c: the integral mask; Panel d: the helmet interface.