CFD Simulation and Validation of a Redesigned Paediatric Inhaler Spacer

GROUP:
HEALTHCARE 1

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Project Brief

Background:

- Computational Fluid Dynamics is carried out to explore the trajectory of drug particles from the inhaler to the throat. This is performed on a pressurised metered-dose inhaler targeted towards children.

Aims:

- Evaluate the effect of changing the size/shape of the inhaler spacer.
- Analyse the efficiency of the inhaler through the particles that travel to the throat.

Inhaler Spacers and Asthma.

- Metered-Dose Inhaler's (MDIs) are a way of providing a standardized dose of medication during an asthma attack.
- The medicine is typically a corticosteroid or bronchodilator and is absorbed via the lungs.
- A spacer improves the efficiency of the MDI by reducing the amount of medicine wasted in the throat and mouth.
- Spacers do require constant cleaning, with soap and water and there is a misunderstanding regarding the target audience for a spacer – any age can benefit from them.

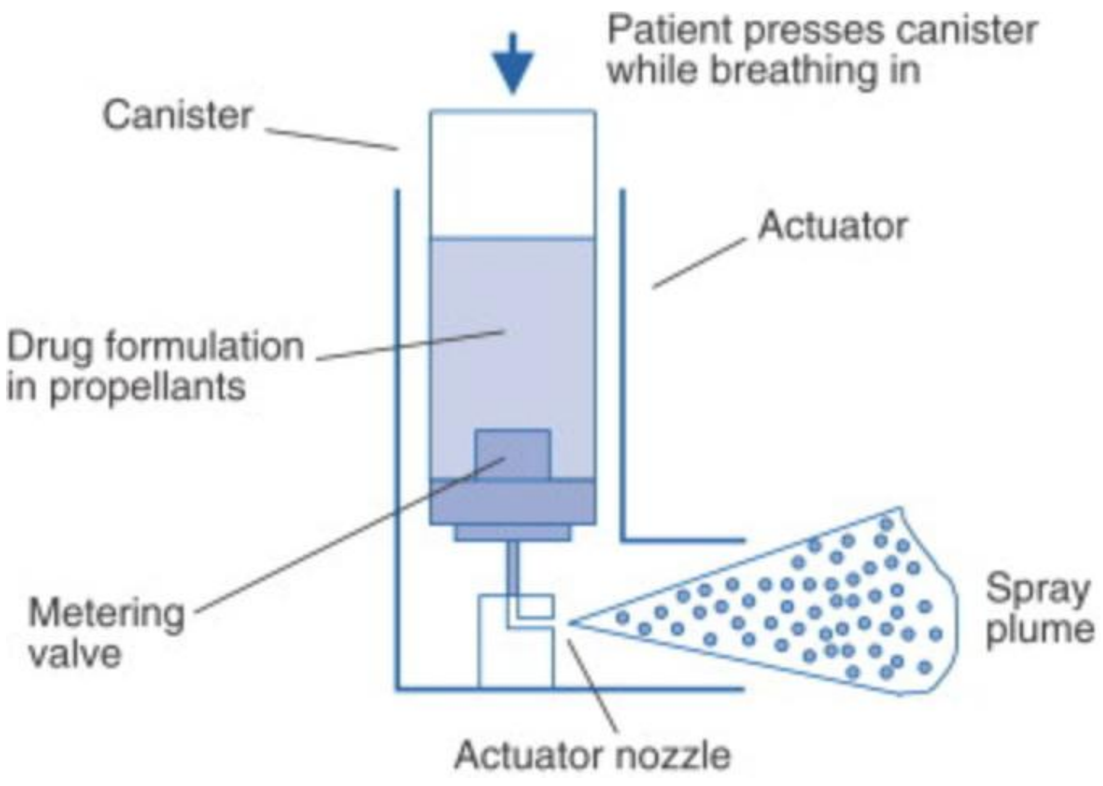
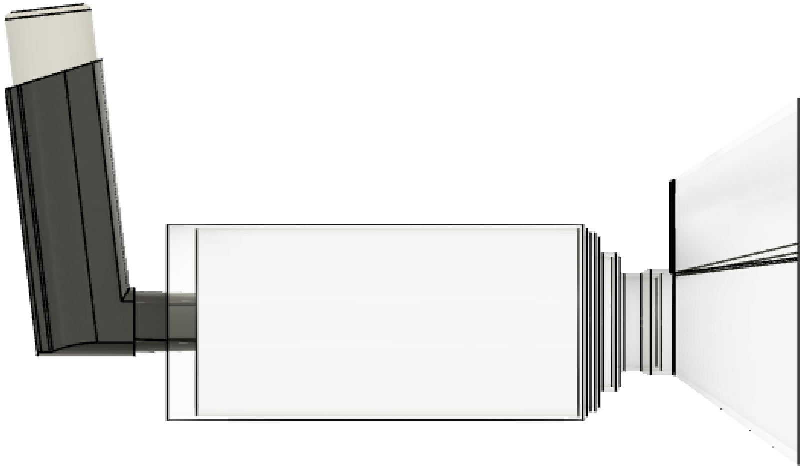


Figure 1: Pediatric Inhaler Delivery

Muchão, F.P., Perín, S.L.R.R., Rodrigues, J.C., Leone, C. and Silva Filho, L.V.R.F., 2008. Evaluation of the knowledge of health professionals at a pediatric hospital regarding the use of metered-dose inhalers. *Jornal Brasileiro de Pneumologia*, *34*, pp.4-12.

Volerman, A., Balachandran, U., Siros, M., Akel, M. and Press, V.G., 2021. Mask use with spacers/valved holding chambers and metered dose inhalers among children with asthma. *Annals of the American Thoracic Society*, *18*(1), pp.17-22.

Geometry of Initial Design of Inhaler Spacer



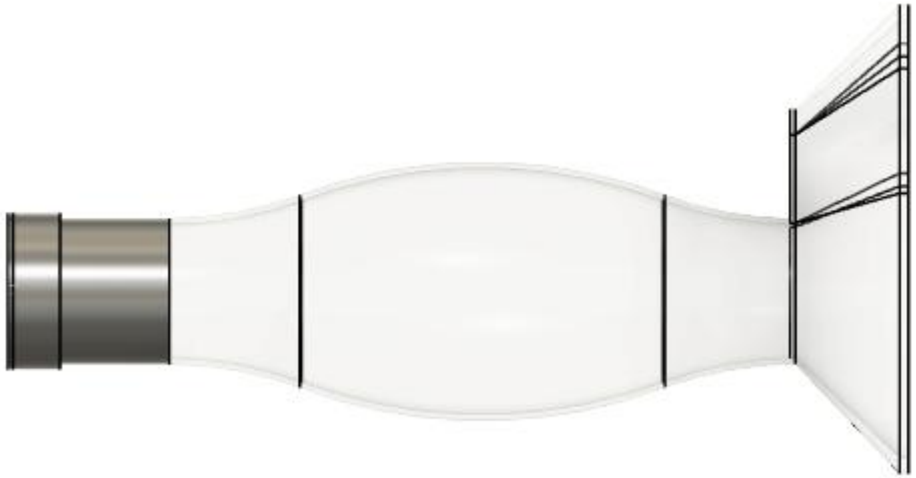
Geometry of Initial Design

Dimensions	Value
Length of Spacer	119 mm
Spacer Diameter	48 mm
Mask Insertion Diameter	24 mm

Geometry of Redesigns

Design 1 – Tapered Spacer (Skyler)

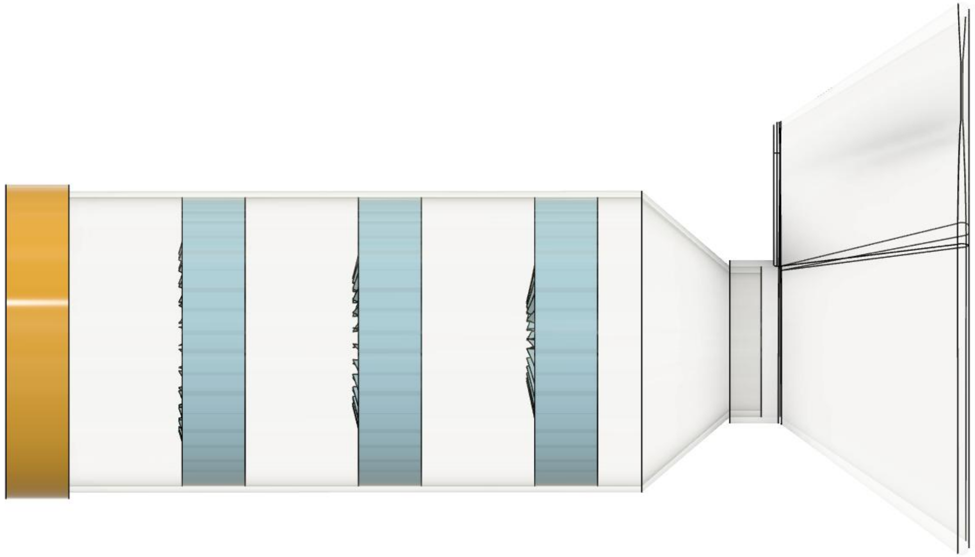
Design 2 – Pear-shaped Spacer (Brandon)



Geometry of Redesigns

Design 3 – Inclined Outlet Spacer (Diljit)

Design 4 – Internal Guide Vanes Spacer (Harkirat)



Concept for Redesign 4

Design is inspired by: Stator blades in turbine jet engines

- Usually act to diffuse air, however in some cases they can act as compressors

The geometry of the compressive ring is loosely based on two diagrams below

- Key points:
  - Curved blade > Straight Blade
  - Equally spaced thin blades

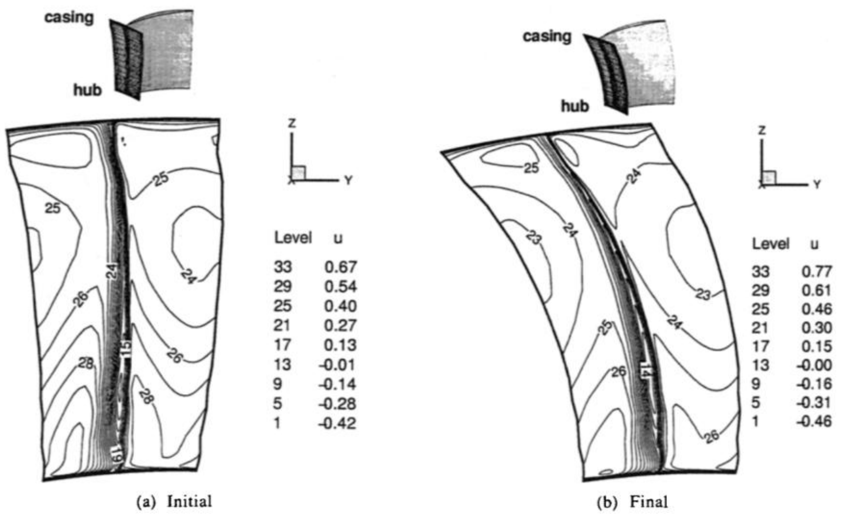


Figure 2: Initial and final designs for a stator blade (Lee S.Y and Kim K.Y, 2000)

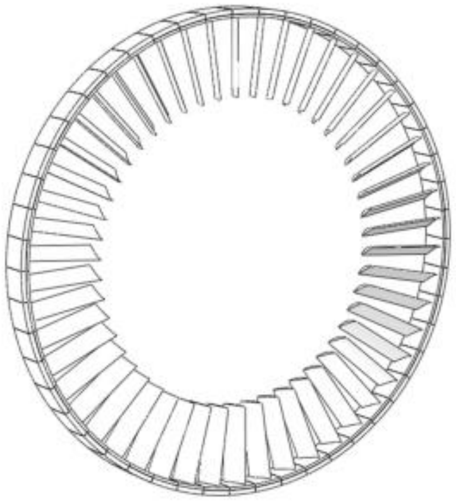


Figure 3: Full circle compressor stator blade ring model (Ma J, Liu Z, Zhang D and Xie Y, 2023)

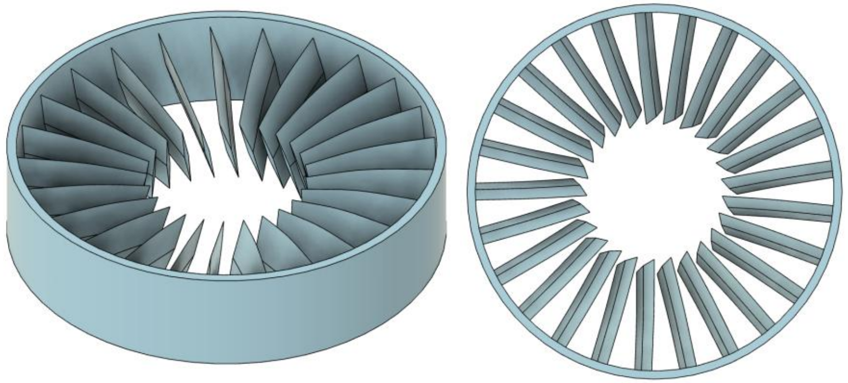


Figure 4: Isometric and top view of the guide vanes CAD render

Lee, S.Y. and Kim, K.Y., 2000. Design optimization of axial flow compressor blades with three-dimensional Navier-Stokes solver. *KSME International Journal*, *14*, pp.1005-1012.

Ma, J., Liu, Z., Zhang, D. and Xie, Y., 2023. Numerical Study on Vibration Response of Compressor Stator Blade Considering Contact Friction of Holding Ring. *Applied Sciences*, *13*(11), p.6380.

Mouth Anatomy

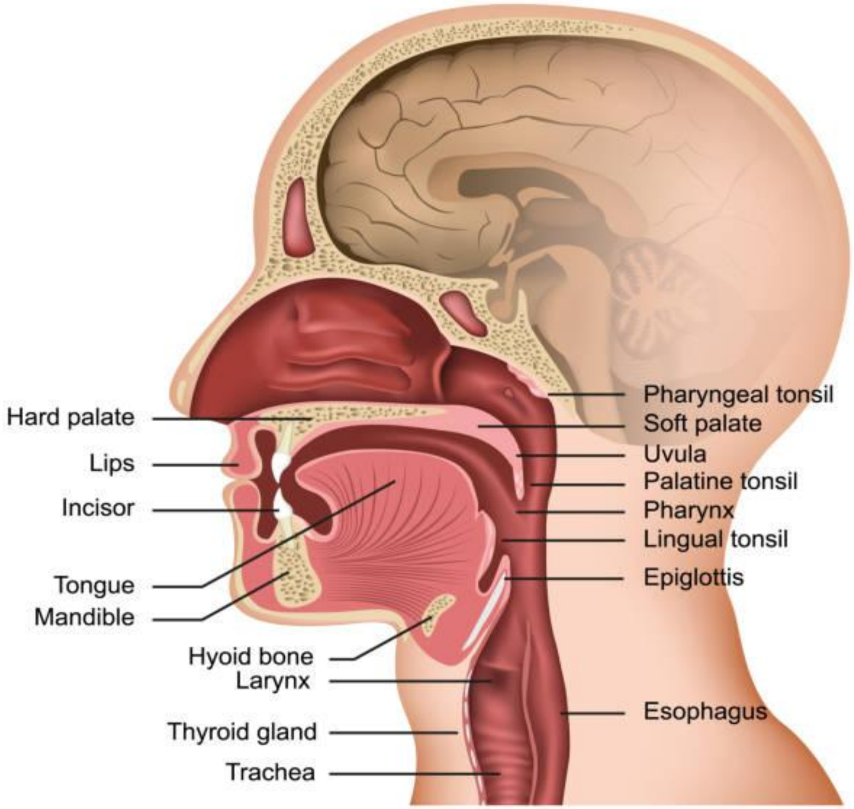
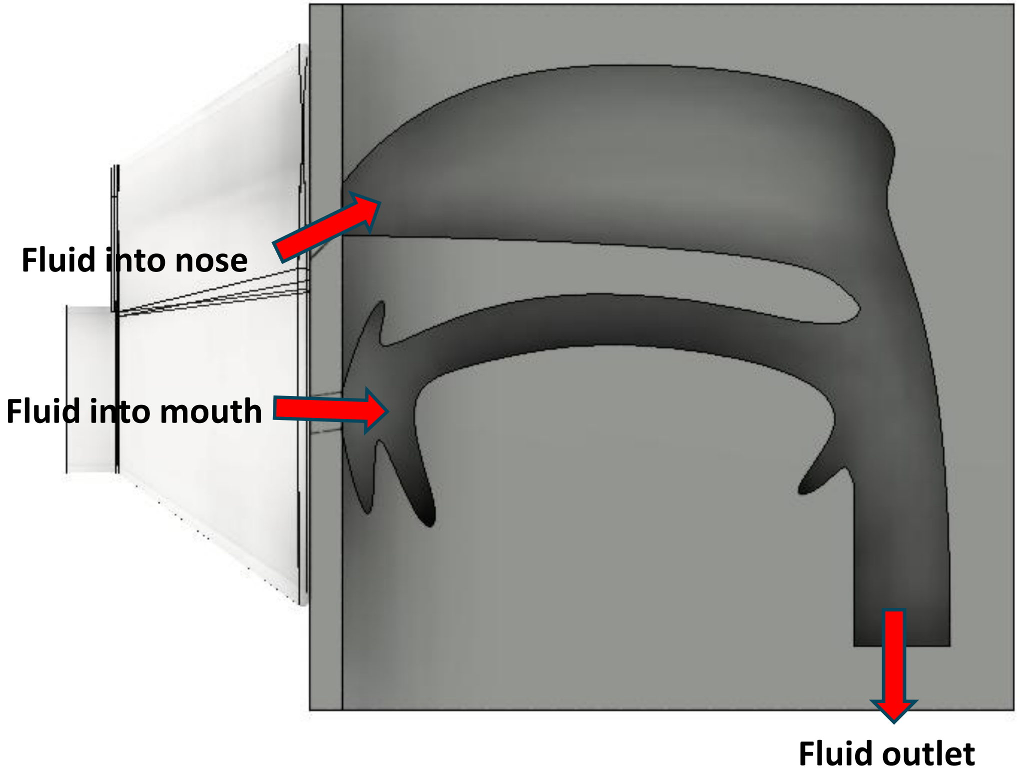


Figure 5: Mouth and Tongue Anatomy



Direction of Fluid Into and Out of the Cavity of Mouth and Nose.

ISTOCK (N.D.) ANATOMY OF THE MOUTH AND TONGUE - MEDICAL VECTOR ILLUSTRATION.
AVAILABLE AT: HTTPS://MEDIA.ISTOCKPHOTO.COM/ID/1141280498

Regulations

- The National Institute for Health and Care Excellence (NICE) guideline emphasises the importance of using Pressure Metered Dose Inhalers with a spacer device for young children.
- They also highlight the need to select the right device to ensure consistent drug dosing.

NATIONAL INSTITUTE FOR HEALTH AND CARE EXCELLENCE (NICE) (2000) GUIDANCE ON THE USE OF INHALER SYSTEMS (DEVICES) IN CHILDREN UNDER THE AGE OF 5 YEARS WITH CHRONIC ASTHMA. AVAILABLE AT: HTTPS://WWW.NICE.ORG.UK/GUIDANCE/TA10/RESOURCES/GUIDANCE-ON-THE-USE-OF-INHALER-SYSTEMS-DEVICES-IN-CHILDREN-UNDER-THE-AGE-OF-5-YEARS-WITH-CHRONIC-ASTHMA-PDF-2294389002949

Fluid and Material Properties

- Due to insufficient information around the properties of salbutamol except density, air properties from Ansys Fluent are used to replace the missing ones.

Property	Salbutamol / Air
Density	1.07 kg/m^3
Specific Heat	1006.43 J/kgK
Thermal Conductivity	0.0242 W/mK
Dynamic Viscosity	1.7894 x 10^{-5} kg/ms

Property	Polycarbonate
Density	63.987 kg/m^3
Specific Heat	1198.5
Thermal Conductivity	0.034606 W/mK

CHEMICALBOOK (N.D.) PRODUCT CHEMICAL PROPERTIES: CB3129524. AVAILABLE AT: HTTPS://WWW.CHEMICALBOOK.COM/PRODUCTCHEMICALPROPERTIESCB3129524_EN.HTM

Governing Equations

- Assuming that density is constant: $\nabla \cdot (\rho \vec{v}) \equiv \rho \nabla \cdot \vec{v} + \vec{v} \cdot \nabla \rho$
- Assuming that momentum is constant:

$$x\text{-component:} \quad \frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u \vec{V}) = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x$$

$$y\text{-component:} \quad \frac{\partial(\rho v)}{\partial t} + \nabla \cdot (\rho v \vec{V}) = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} + \rho f_y$$

$$z\text{-component:} \quad \frac{\partial(\rho w)}{\partial t} + \nabla \cdot (\rho w \vec{V}) = -\frac{\partial p}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} + \rho f_z$$

- Energy is conserved:

$$\begin{aligned}
&\frac{\partial}{\partial t}\left[\rho\left(e + \frac{V^2}{2}\right)\right] + \nabla \cdot \left[\rho\left(e + \frac{V^2}{2}\right)\vec{V}\right] \\
&= \rho \dot{q} + \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) \\
&\quad + \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z}\right) - \frac{\partial(up)}{\partial x} - \frac{\partial(vp)}{\partial y} - \frac{\partial(wp)}{\partial z} + \frac{\partial(u\tau_{xx})}{\partial x} \\
&\quad + \frac{\partial(u\tau_{yx})}{\partial y} + \frac{\partial(u\tau_{zx})}{\partial z} + \frac{\partial(v\tau_{xy})}{\partial x} + \frac{\partial(v\tau_{yy})}{\partial y} \\
&\quad + \frac{\partial(v\tau_{zy})}{\partial z} + \frac{\partial(w\tau_{xz})}{\partial x} + \frac{\partial(w\tau_{yz})}{\partial y} + \frac{\partial(w\tau_{zz})}{\partial z} + \rho \vec{f} \cdot \vec{V}
\end{aligned}$$

ANDERSON, J.D., 1992. GOVERNING EQUATIONS OF FLUID DYNAMICS. COMPUTATIONAL FLUID DYNAMICS: AN INTRODUCTION, PP.15-51.

Governing Equations

- Computational approach: Reynolds-Averaged Navier Stokes (RANS) with k-epsilon model.

- Navier-Stokes –Body and Surface forces present:

$$-\rho\left(\frac{D\vec{v}}{Dt}\right) = \rho\nabla\Phi + \nabla p + \eta\nabla^2\vec{v} \qquad \frac{D}{Dt} \equiv \frac{\partial}{\partial t} + (\vec{v}\cdot\nabla)$$

- Turbulence – For internal flow: $Re \geq 2300$

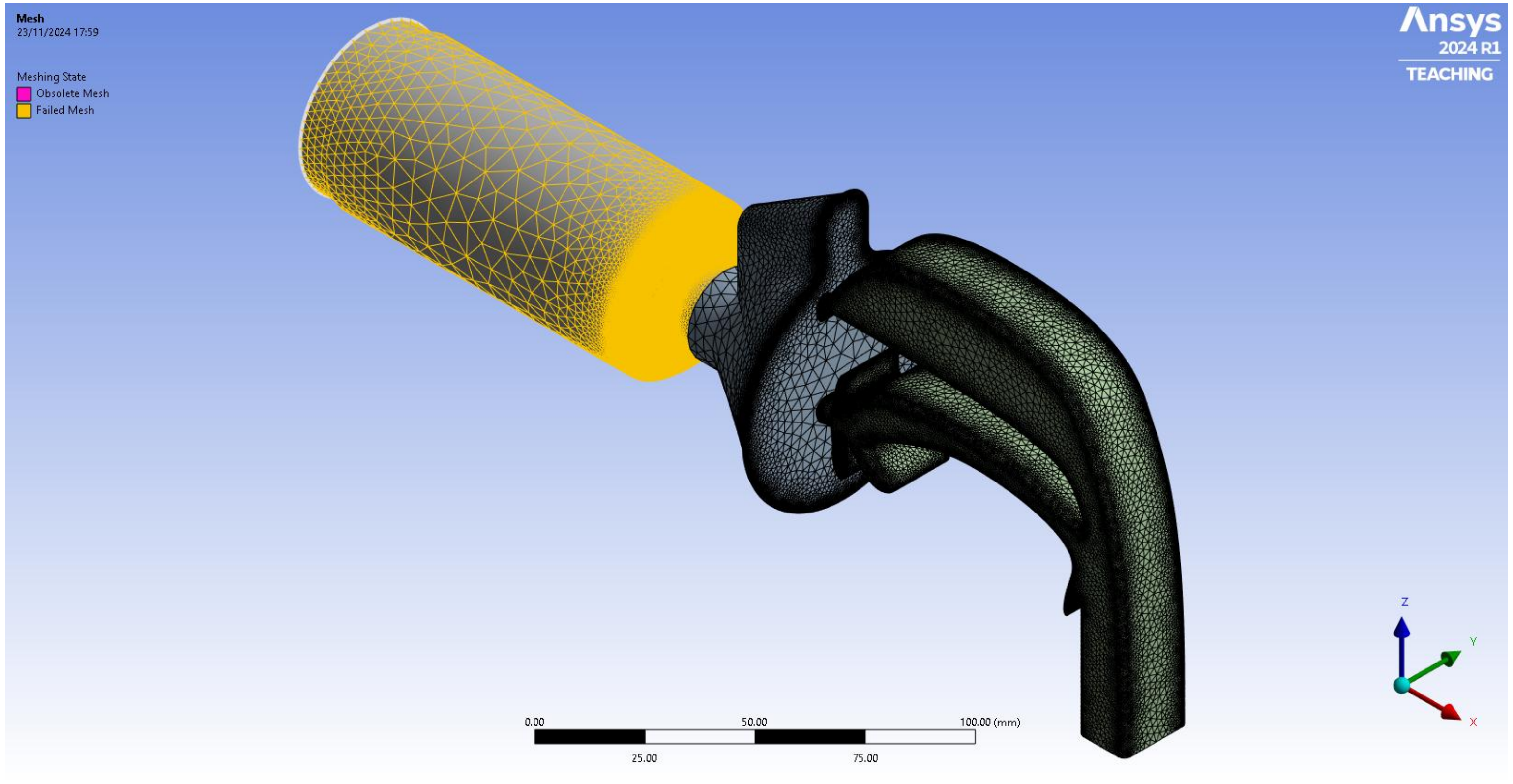
- $Re_{Salbutamol/Air} = \frac{\rho u L}{\mu} = \frac{1.07 \times 1.724 \times 119 \times 10^{-3}}{1.7894 \times 10^{-5}} = 12269$

ANDERSON, J.D., 1992. GOVERNING EQUATIONS OF FLUID DYNAMICS. COMPUTATIONAL FLUID DYNAMICS: AN INTRODUCTION, PP.15-51.

Default Mesh for Initial design

The default meshing option is inadequate:

- High number of Elements
- The Mesh fails



Mesh Size (mm)	Number of Elements	Aspect Ratio	Skewness	Orthogonal Quality	Element Quality
Default	1,141,767	1.9014	0.2419	0.7568	0.8274

Finding optimum Mesh Size – Method

Details of "Mesh"

Solver Preference	Fluent
Element Size	16.0 mm
Export Format	Standard
Export Preview Surface Mesh	No
Sizing	
Use Adaptive Sizing	No
Growth Rate	1.2
Max Size	32.0 mm
Mesh Defeaturing	Yes
Defeature Size	0.1 mm
Capture Curvature	Yes
Curvature Min Size	0.2 mm
Curvature Normal Angle	Default (18.0°)
Capture Proximity	No
Bounding Box Diagonal	287.31 mm
Average Surface Area	522.4 mm²
Minimum Edge Length	1.3306e-002 mm
Quality	
Check Mesh Quality	Yes, Errors
Target Skewness	0.5
Smoothing	Medium
Mesh Metric	Element Quality
Min	6.4624e-003
Max	0.9994
Average	0.80534
Standard Deviation	0.11973
Inflation	
Use Automatic Inflation	None
Inflation Option	Smooth Transiti...
Transition Ratio	0.3
Maximum Layers	5
Growth Rate	1.2
Inflation Algorithm	Pre
View Advanced Options	No
Advanced	
Statistics	
Nodes	119185
Elements	503308
Show Detailed Statistics	No

Will be varied to find the optimum size

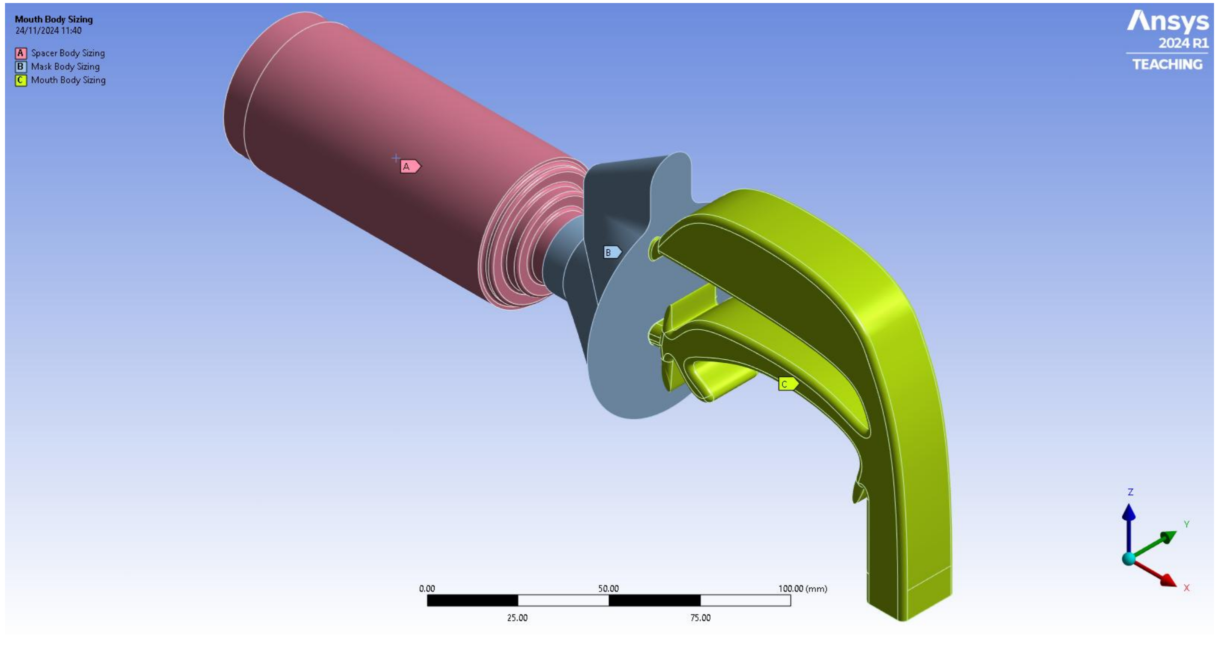
Standard growth rate to avoid abrupt changes in adjacent mesh elements

Limited to the geometry of the CAD

Lowest possible value with valid mesh

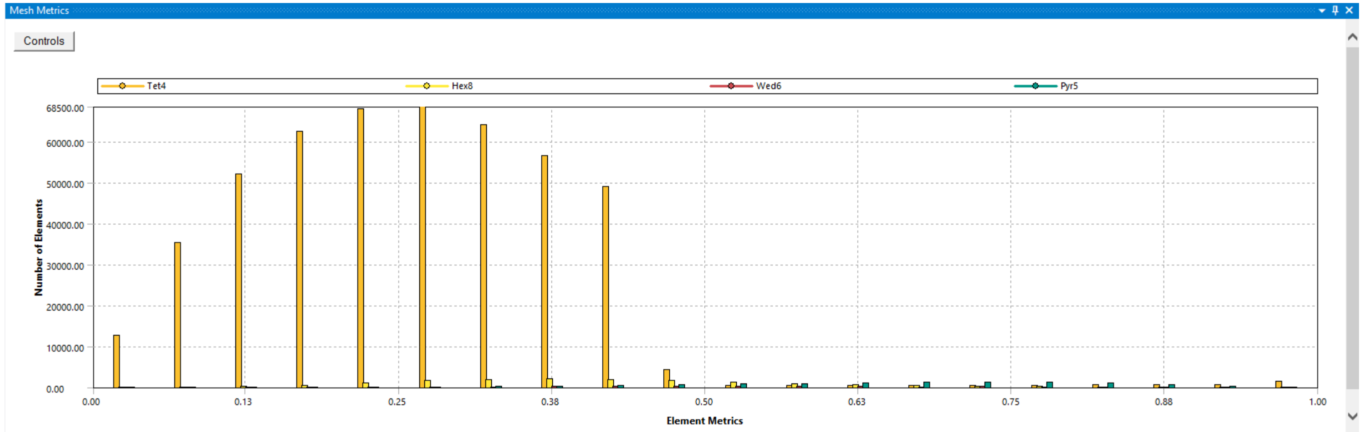
Properties and their values can be found for each mesh

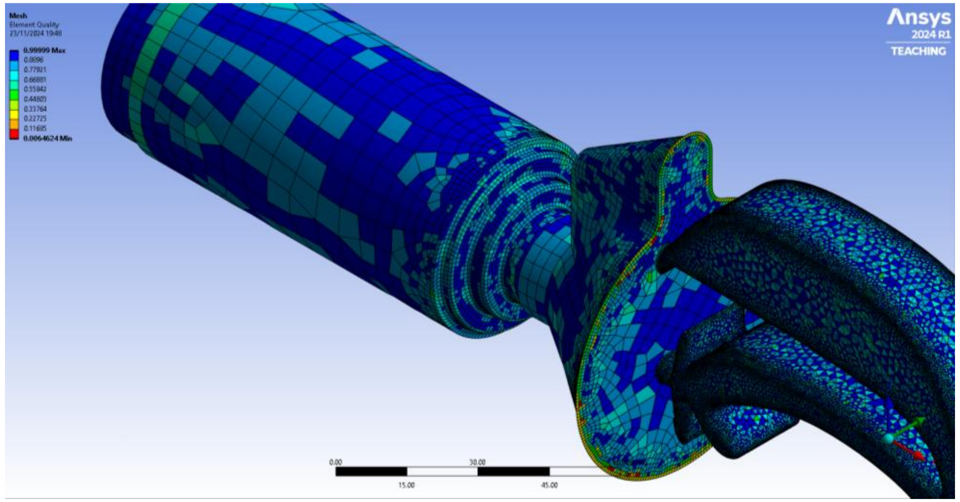
Detailed of the number of nodes and elements can be seen.



Location	Mesh Method	Defeature size	Local Minimum Size
Spacer Volume	Hex Dominant	0.75 mm	1.2 mm
Mask Volume	Hex Dominant	0.5 mm	0.8 mm
Mouth Volume	Patch Conforming	0.3 mm	0.5 mm

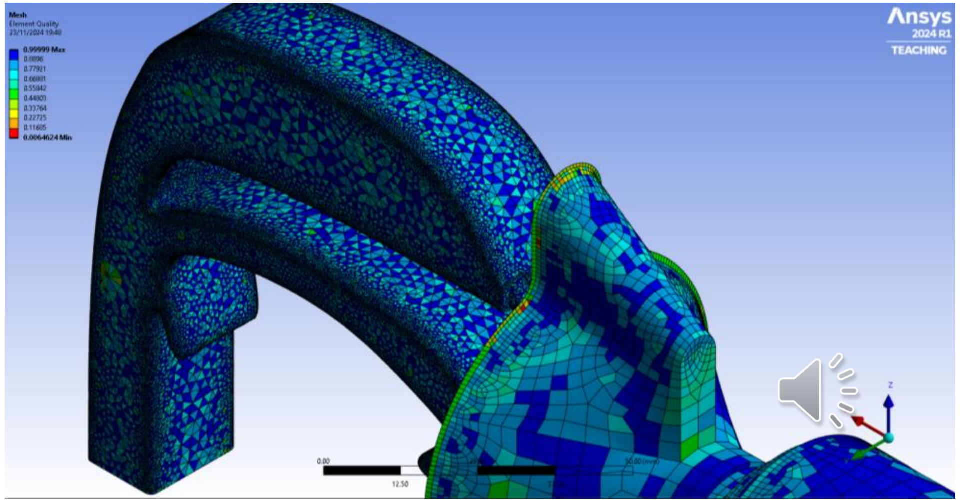
Varying Mesh Size for Initial Design



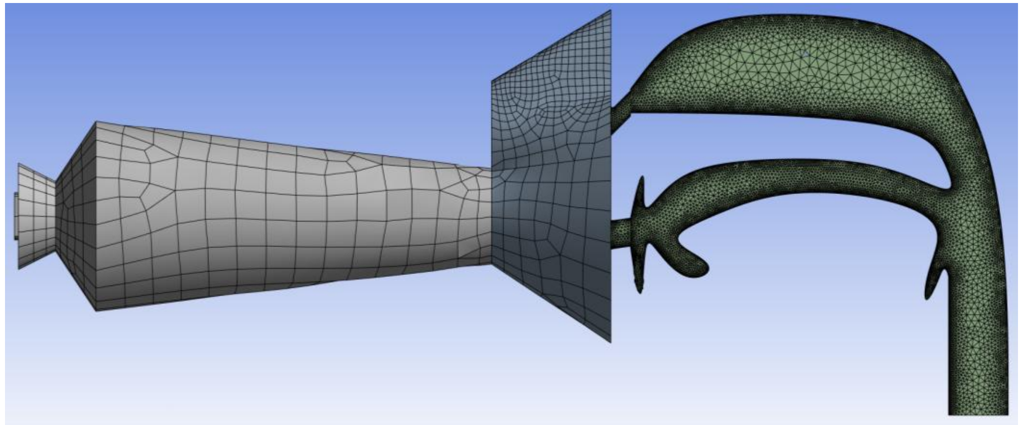


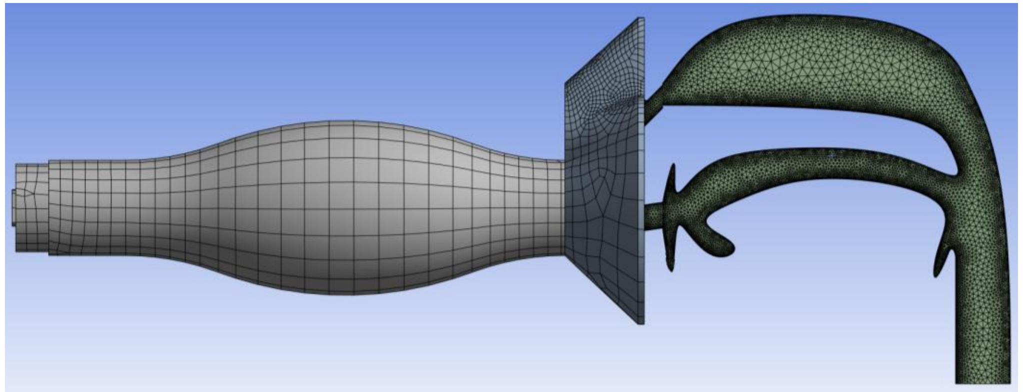
$$Average\ Metric = \sum \frac{Metric\ \times n_i}{n}$$

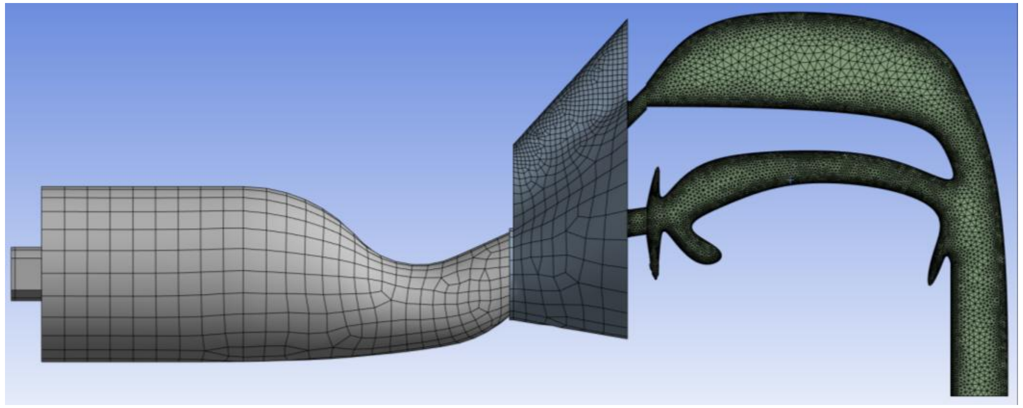
$$where\ n\ is\ the\ number\ of\ elements$$

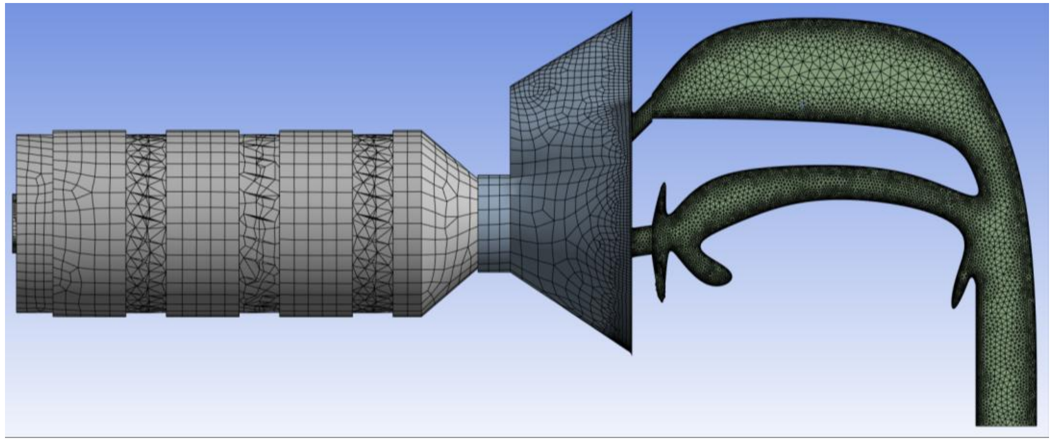


Mesh Size (mm)	Number of Elements	Aspect Ratio	Skewness	Orthogonal Quality	Element Quality
16	503,308	2.0772	0.2730	0.7334	0.8053
12	503,456	2.1290	0.2747	0.7318	0.8042
8	503,813	2.0613	0.2731	0.7331	0.8056
4	507,966	2.1024	0.2742	0.7334	0.8030



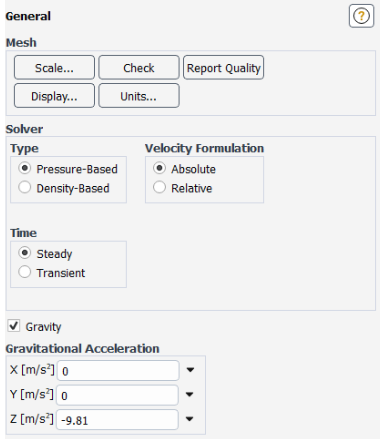




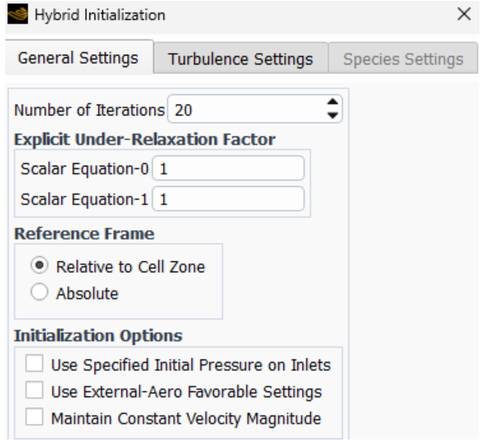


Design	Number of Elements	Aspect Ratio	Skewness	Orthogonal Quality	Element Quality
Tapered	481,829	1.9265	0.25776	0.74292	0.81704
Pear Shape	486,293	1.9434	0.25948	0.74178	0.81528
Inclined Outlet	488,125	1.9409	0.25942	0.74207	0.81565
Guide Vanes	508,911	2.2861	0.27787	0.72855	0.80159

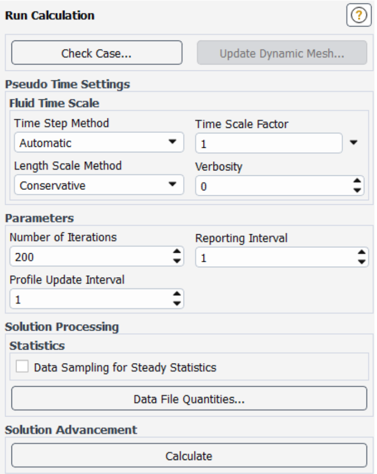
Calculation, Initialisation and Setup Conditions



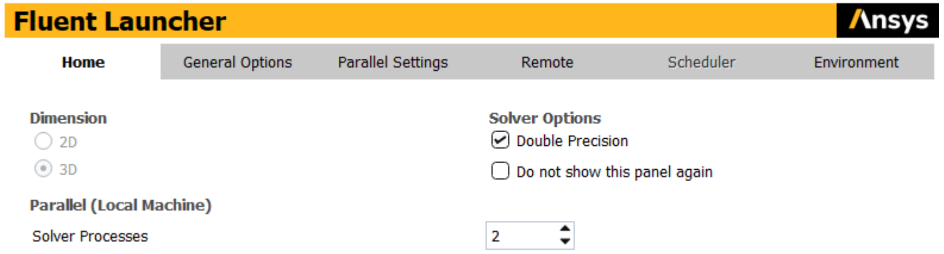
Gravity and Time Conditions



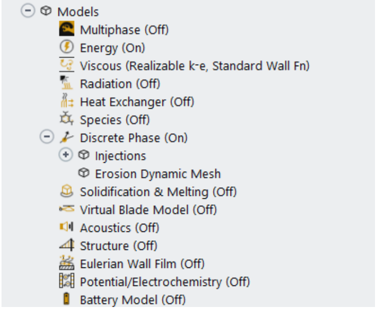
Hybrid Initialisation Conditions



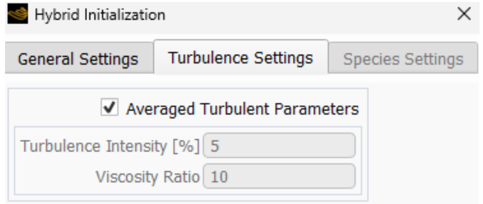
Run Calculation Conditions



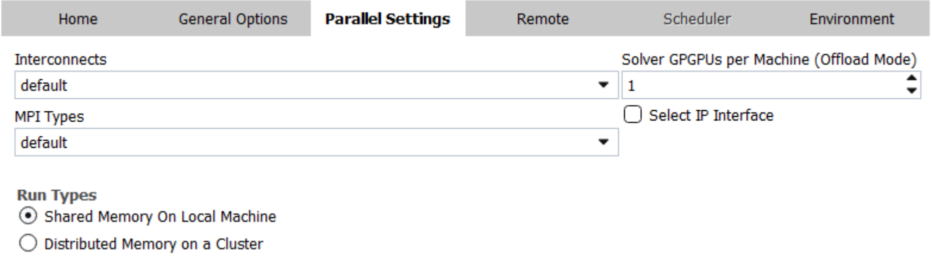
Solver Processes Input Parameters



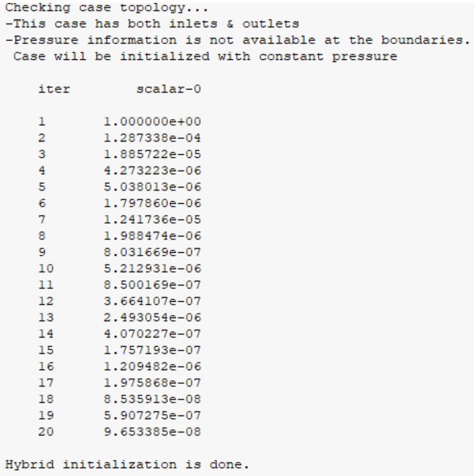
Energy and Viscous Input Parameters



Hybrid Initialisation Turbulence Conditions



Solver GPGPUs per machine Input Parameters



Hybrid Initialisation Iterations

Boundary Conditions

Inlet Conditions	
Velocity Magnitude (m/s)	1.724
Specification Method	Intensity and Viscosity Ratio
Turbulent Intensity (%)	5
Turbulent Viscosity Ratio	10
Temperature (°C)	25
Discrete Phase Type	Escape

Outlet Conditions	
Backflow Reference Frame	Absolute
Gauge Pressure (Pa)	0
Specification Method	Intensity and Viscosity Ratio
Turbulent Intensity (%)	5
Turbulent Viscosity Ratio	10
Backflow Total Temp (°C)	25
Discrete Phase Type	Escape

Wall Conditions	
Wall Motion	Stationary
Shear Condition	No Slip
Roughness Model	Standard
Roughness Height (m)	0
Roughness Constant	0.5
Temperature (°C)	25
Discrete Phase Type	Trap

$$Average\ number\ of\ breaths\ for\ 3-5\ year\ olds = 28\ breaths\ per\ minute$$

$$Inspiratory\ Flow\ Rate\ for\ 2-12\ year\ olds\ (Q_1) = 30\frac{L}{min} = 0.0005\ \frac{m^3}{s}$$

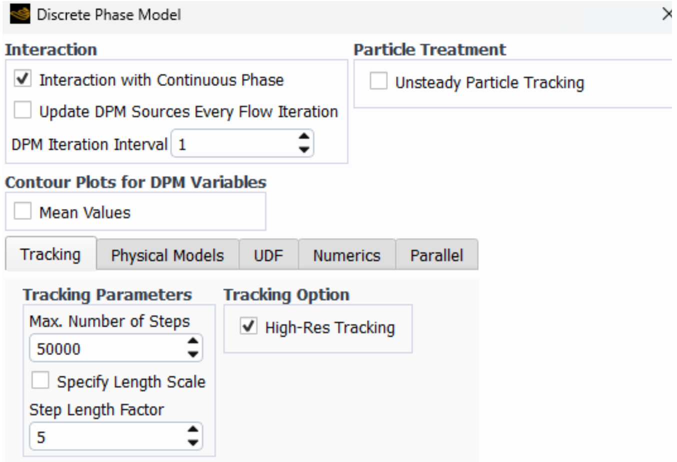
$$Inlet\ Area\ of\ Spacer(A_1) = 0.00029\ m^2$$

$$Inlet\ Velocity = \frac{Q_1}{A_1} = \frac{0.0005}{0.00029} = 1.724\frac{m}{s}$$

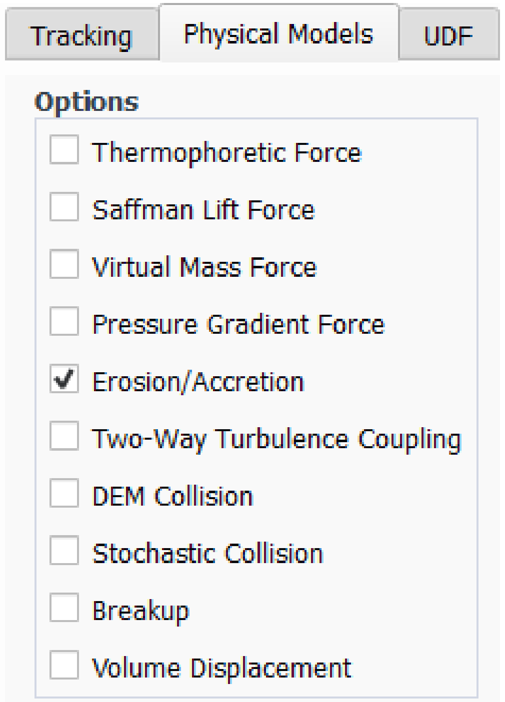
VOGELBERG, C., KREMER, H.J., ELLERS-LENZ, B., ENGEL, M., MAUS, J., CONRAD, F. AND HERMANN, R., 2004. CLINICAL EVALUATION OF THE PEAK INSPIRATORY FLOW GENERATED BY ASTHMATIC CHILDREN THROUGH THE NOVOLIZER®. RESPIRATORY MEDICINE, 98(10), PP.924-931.

Healthline. (2023). *Normal respiratory rate: What is normal and when to be concerned*. Healthline. Available at: https://www.healthline.com/ealth/normal-respiratory-rate#normal-rate-in-kids [Accessed 26 Nov. 2024].

DPM/ Injection Conditions

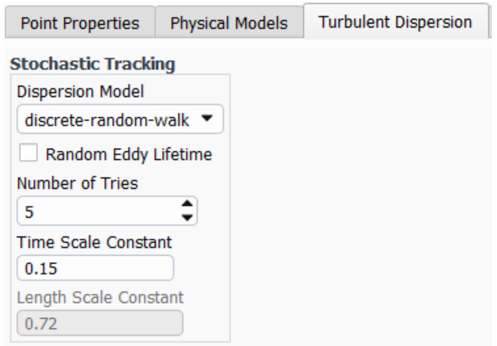


DPM Tracking Conditions

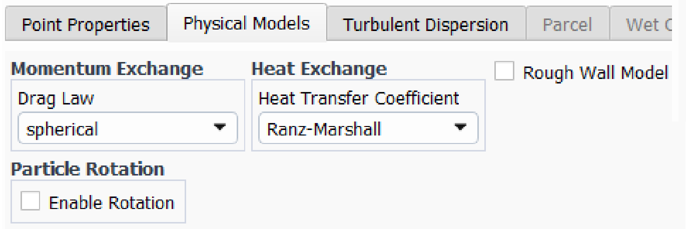


DPM Erosion/ Accretion Conditions

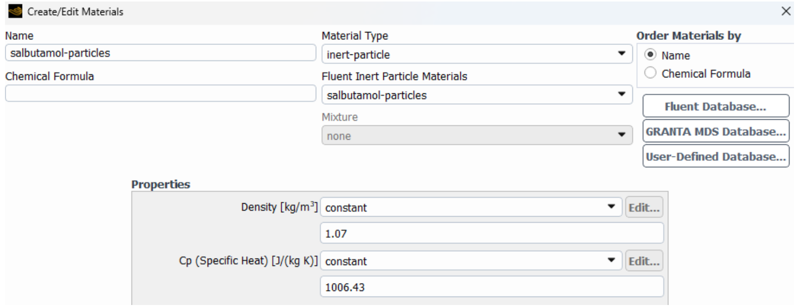
DPM Injection Properties	
Injection Surface	Inlet
Injection Type	Surface
Particle Type	Inert
Diameter Distribution	Uniform
Velocity (m/s)	1.724
Diameter (m)	0.0004
Temperature (°C)	25
Total Flow Rate (kg/s)	1
Surface Options	Scale Flow Rate By Face Area



DPM Turbulence Conditions



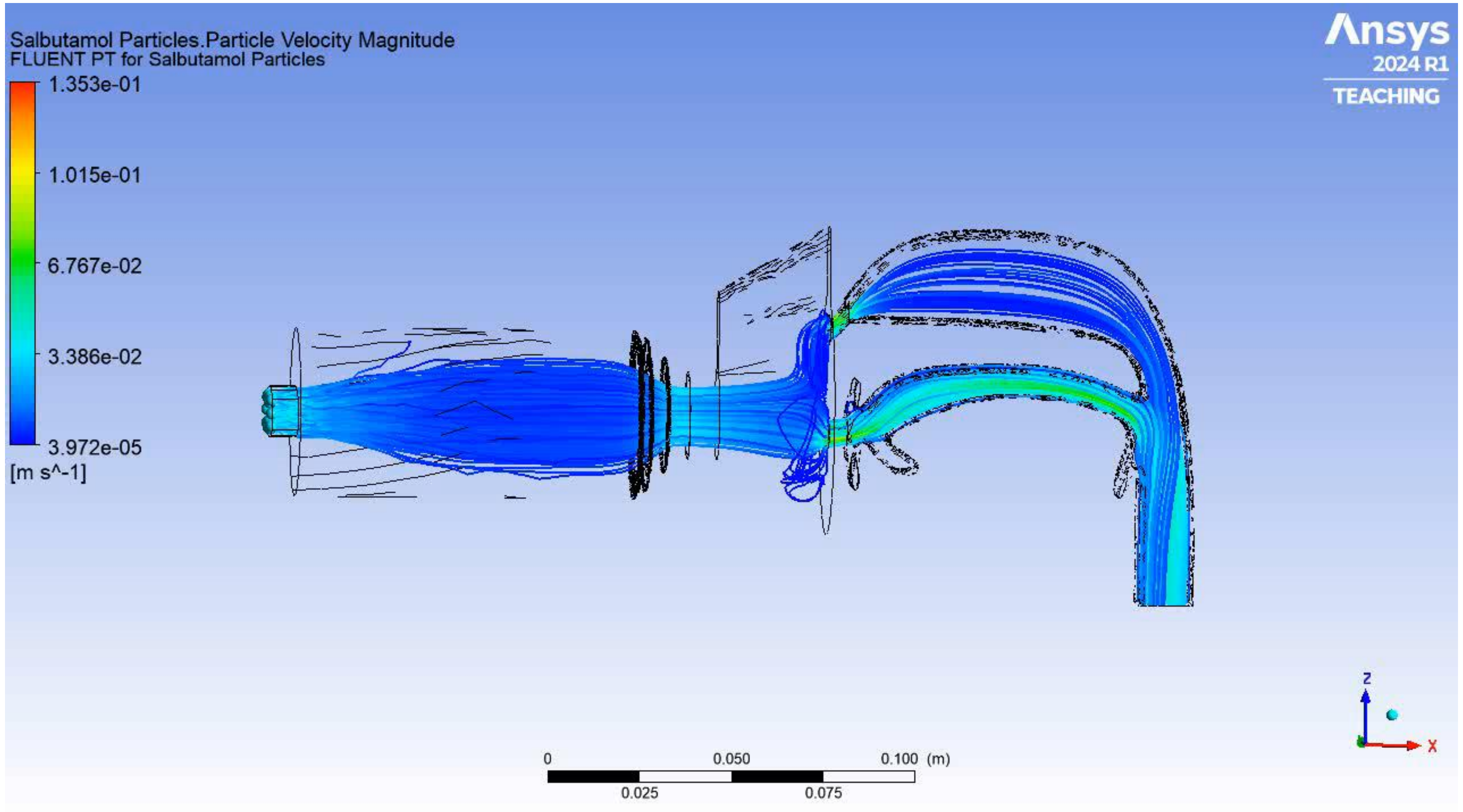
DPM Physical Model Conditions



Salbutamol Injection Material Properties

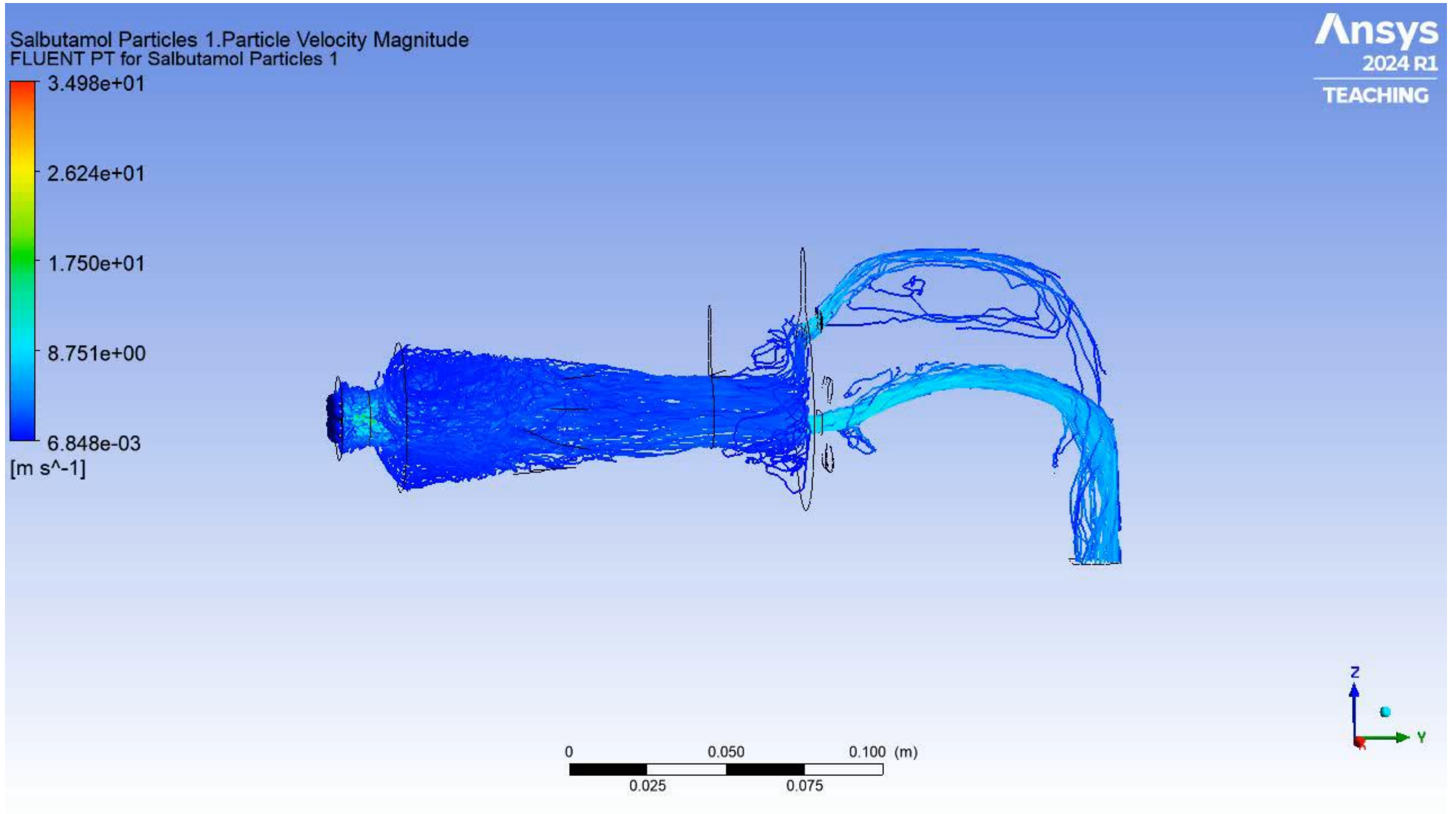
Initial Design Result

$$Efficiency\ of\ Spacer = \frac{Particles\ Escaped}{Particles\ Tracked} = \frac{562}{1200} = 46.83\%$$



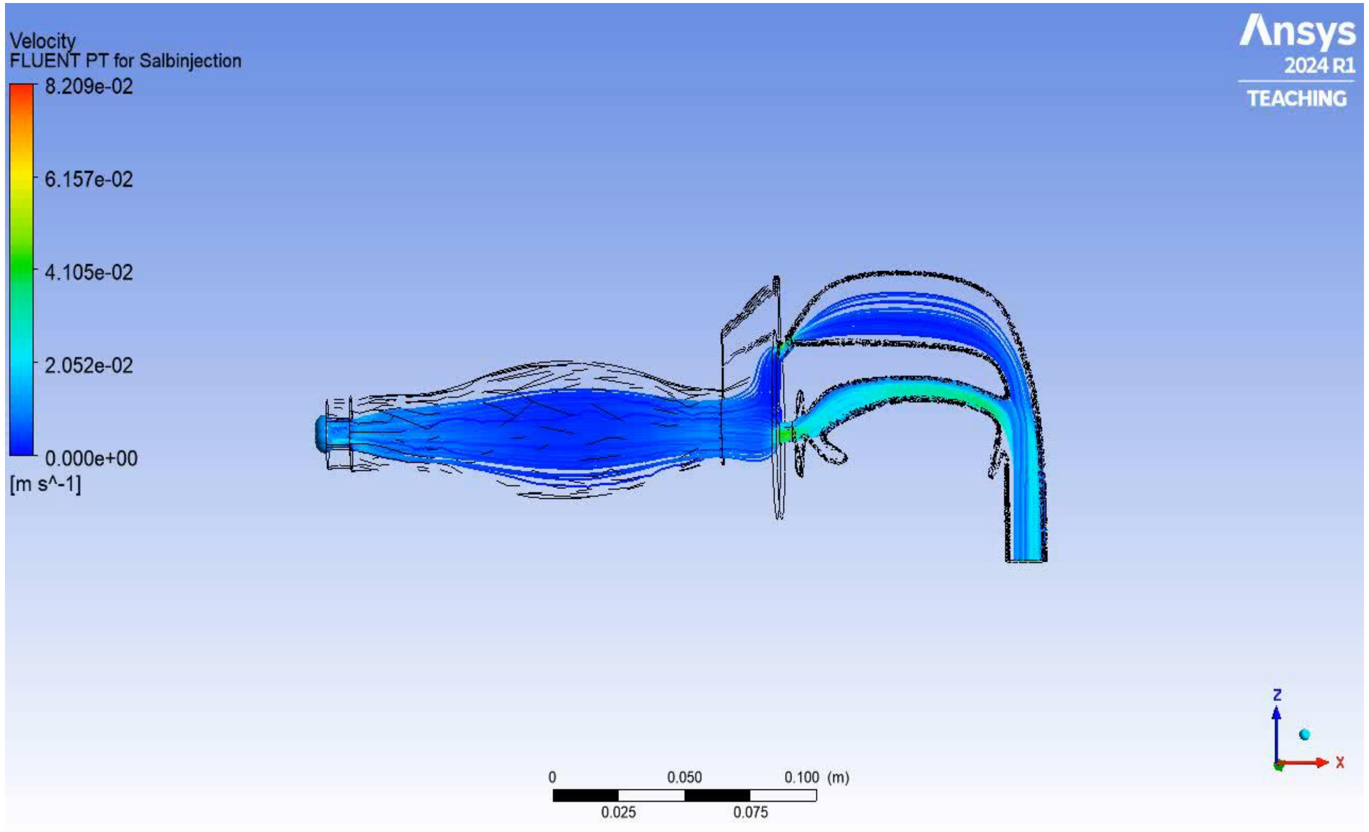
Tapered Spacer Result

$$Efficiency\ of\ Spacer = \frac{Particles\ Escaped}{Particles\ Tracked} = \frac{2109}{4400} = 47.93\%$$



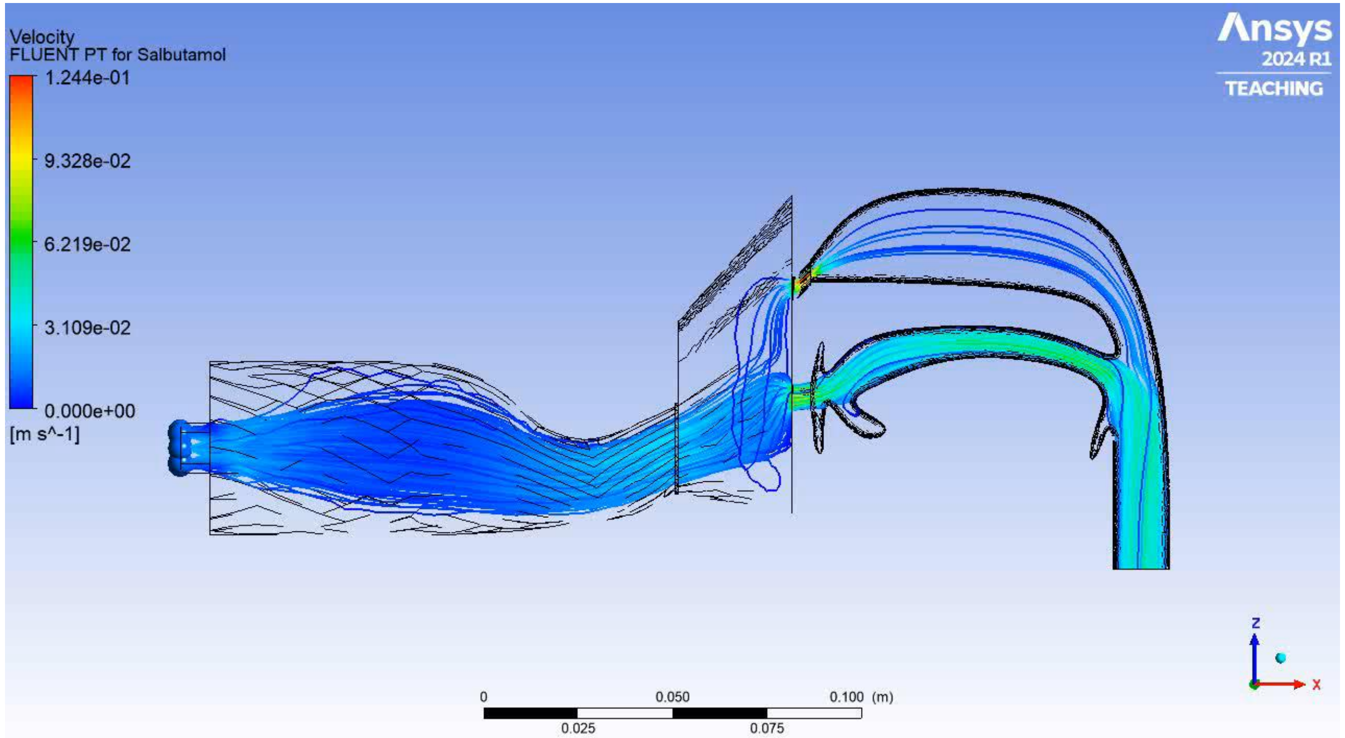
Pear-Shaped Spacer Result

$$Efficiency\ of\ Spacer = \frac{Particles\ Escaped}{Particles\ Tracked} = \frac{658}{900} = 73.11\%$$



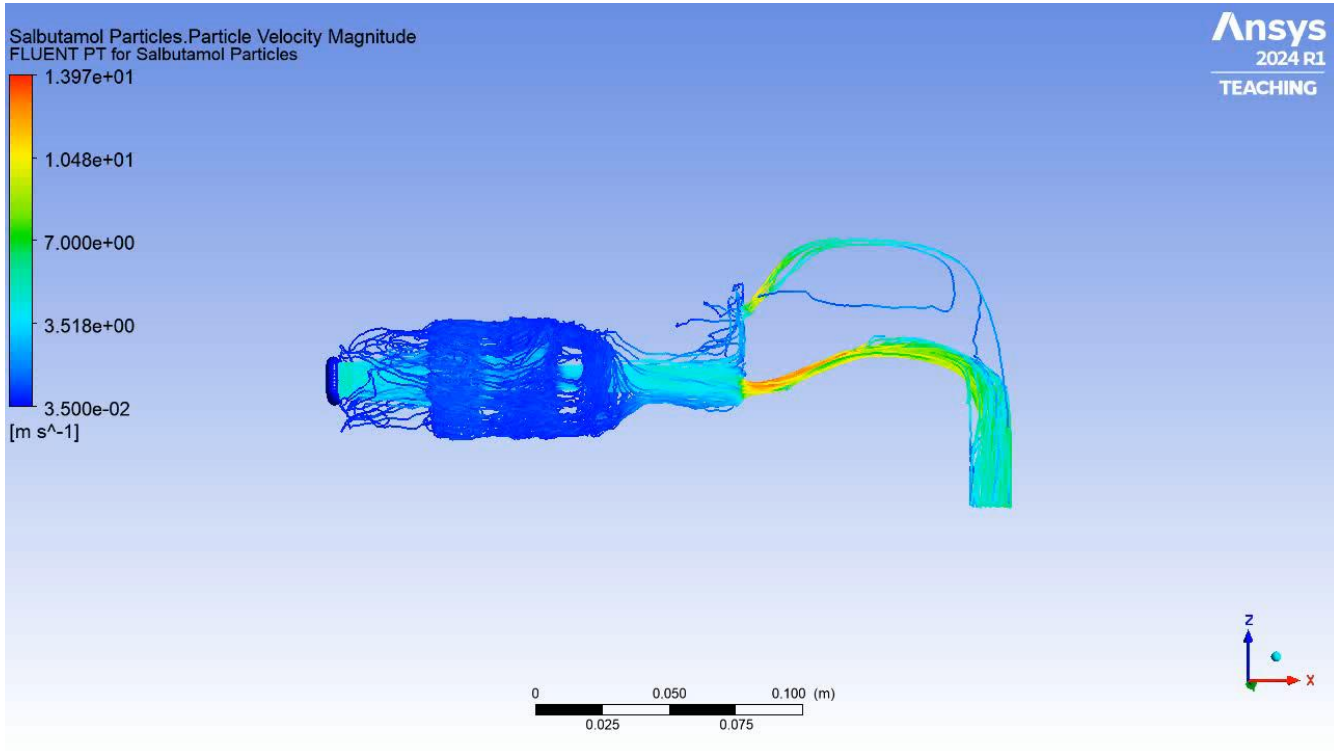
Inclined Outlet Spacer Result

$$Efficiency\ of\ Spacer = \frac{Particles\ Escaped}{Particles\ Tracked} = \frac{686}{990} = 69.29\%$$



Internal Guide Vanes Spacer Result

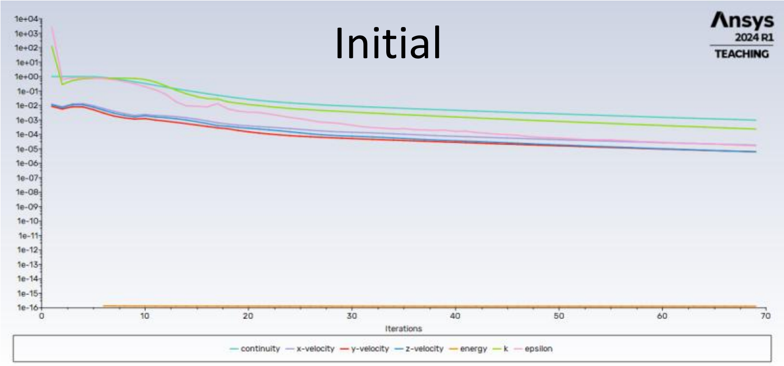
$$Efficiency\ of\ Spacer = \frac{Particles\ Escaped}{Particles\ Tracked} = \frac{283}{1120} = 25.27\%$$

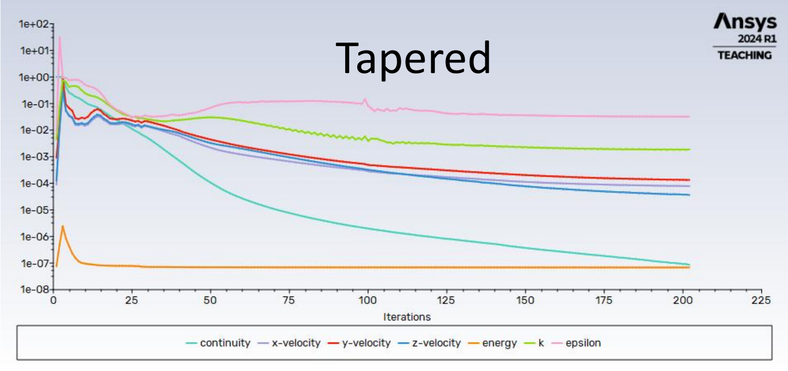


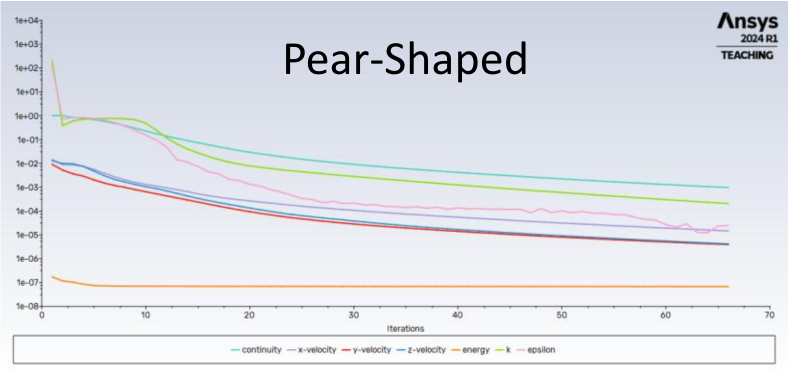
Comparison of Results

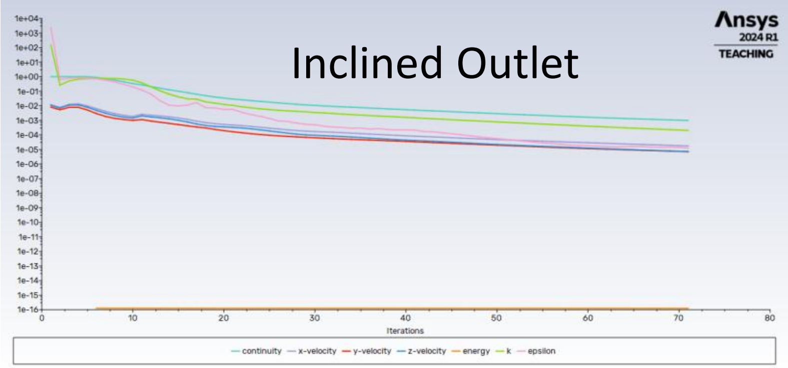
Spacer Type	Tracked Particles	Escaped Particles	Efficiency (%)
Initial	1200	562	46.83
Tapered	4400	2109	47.93
Pear-shaped	900	658	73.11
Inclined Outlet	990	686	69.29
Internal Guide Vanes	1120	283	25.27

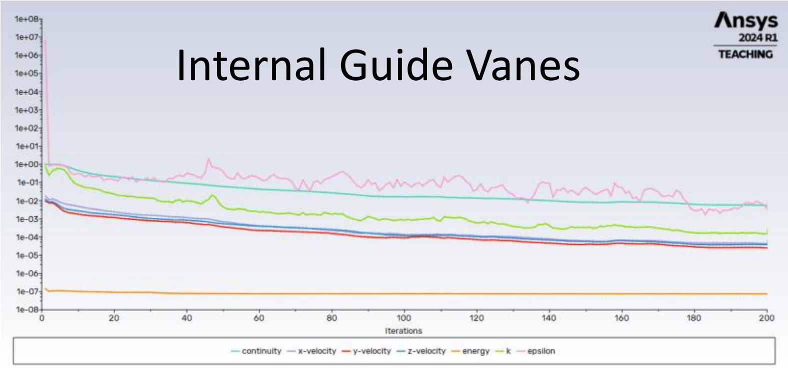
Solver


Initial
Ansys
2024 R1
TEACHING
Iterations
continuity x-velocity y-velocity z-velocity energy k epsilon


Tapered
Ansys
2024 R1
TEACHING
Iterations
continuity x-velocity y-velocity z-velocity energy k epsilon


Pear-Shaped
Ansys
2024 R1
TEACHING
Iterations
continuity x-velocity y-velocity z-velocity energy k epsilon


Inclined Outlet
Ansys
2024 R1
TEACHING
Iterations
continuity x-velocity y-velocity z-velocity energy k epsilon


Internal Guide Vanes
Ansys
2024 R1
TEACHING
Iterations
continuity x-velocity y-velocity z-velocity energy k epsilon

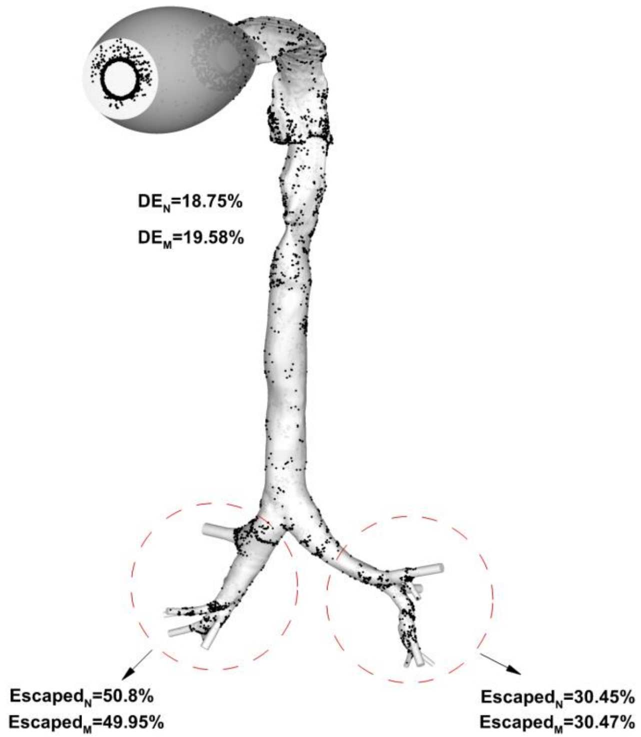
Validation

Advantages:

- Complies with regulations
- Turbulent model – k epsilon
- Mesh Resolution – default meshing

Things to Consider:

- Accuracy of human anatomy
- Using transient model instead of steady state
- Material and fluid properties



Limitations of model

- The computational cost of a transient model is too high (simulations take hours or crash). To address this, the model is simplified by choosing the steady-state option.
- The model for the mouth makes simplifications in CAD. We could outsource a more anatomy-correct model.
- The material for the wall boundary was chosen to be "honeycomb polycarbonate plastic" and modelled as smooth. Ideally, the mouth should be another material and have the associated roughness model.
- The fluid properties are mainly accounting for air instead of salbutamol, which slightly affects our efficiency values when solving.