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CFD STUDY OF THE VOLUMATIC® SPACER: A REALISTIC APPROACH

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Abstract. *The asthma strong prevalence in the world is already affecting more than 300 million people. The inhalatory therapy is the more effective and used method worldwide, and inhalation devices are the ones to have a great deal of development. In children, where the asthma incidence is high and where a good coordination between the device actuation and the respiration is needed, the pressurized Metered Dose Inahaler (pMDI) has some problems. A solution was found with the introduction of an add-on spacer to the pMDI. The spacer attached to the pMDI is the cheapest and most effective way to treat asthma in children, being therefore important the improvement of its efficiency. The project herein reported was focused on the study of the air flux inside a well known and used spacer, as well as on the particles behaviour obtained from a pMDI spray. The present paper reports the application of Computational Fluid Dynamics techniques (CFD) to the analysis of flow inside the most sold expansion chamber, the Volumatic®, using the Fluent™ software. The geometry, including the valve, was tested with and without the pMDI spray particles. The spray was simulated using the Fluent Discrete Phase Model (DPM), tuned to the specific characteristics of the pMDI sprays. The drug influences the spray parameters and in this study the Ventolin® was used because it is the one associated to this particular spacer. The droplet diameter distribution in the spray was measured using the laser diffraction based instrument, Malvern. A Rosin-Rammler distribution proved to be representative of the spray. The most challenging feature to adjust in this model was the droplet-wall interaction. Fluent™ provides two boundary conditions, Reflect and Trap, although none of these two correspond to the real situation. The results obtained suggest that the interaction is a combination of the two phenomena. The results enable to assess the efficiency of the Volumatic®, by quantifying the number of particles that exit the spacer after the respiratory cycle as a function of the number of particles injected. The results show a good approach to the real-life situation using a transient CFD simulation.*

1 INTRODUCTION

Being asthma a chronic disease that affects over 300 million people in the world, the efficiency of the therapeutic has become a matter of emerging importance [1]. As the inhalatory therapeutic is the cornerstone of asthma treatment, drug delivering devices to the patient lungs are under constant improvement. The asthma treatment in public healthcare services also presents a high cost to the taxpayer, so it is important to increase the research on the asthma devices for inhalatory therapeutic, with the objective of reducing the waste of drug generated by poor efficiency devices.

The most used devices are the pMDIs, DPIs and nebulizers, although each one has its own range of application. The most innovative is, nevertheless, the pMDI, which is that being used by the majority of patients, often attached to another add-in device called spacer [2-3].

The spacer is the objective of the study herein reported, using realistic simulation parameters as for the velocity input and the pMDI spray. The main goal is to study the efficiency of the spacer device and to design a realistic computational model, allowing its use in the study of various and different spacers without any experimental costs.

The CFD model was created using the Fluent™ software, from Ansys®. The realistic parameters were obtained from several sources available in the literature or measured in laboratory. A DPM model was used to simulate the particle tracking in the air flow inside the spacer.

The influence of the geometry in the air flow inside the spacer, the behaviour of the dispersed phase and the differences between two walls conditions (Reflect and Trap) in the efficiency of the device will be reported in this paper.

2 GEOMETRY AND COMPUTATIONAL MESH

The initial phase of the project concerned the design of the geometry of the Volumatic® spacer using the Gambit™ software. Some simplifications were implemented on the original geometry: the inlet cross section shape was assumed as a circle with the same area as in the original model (approximately 400 mm^2) and the final segment, downstream the valve, was also simplified. A cross-section of the Volumatic® geometry along its axis is presented in Figure 1. The geometry origin point (0,0,0) is located at the center of the inlet face, while the *x*-axis is oriented as the air flows.

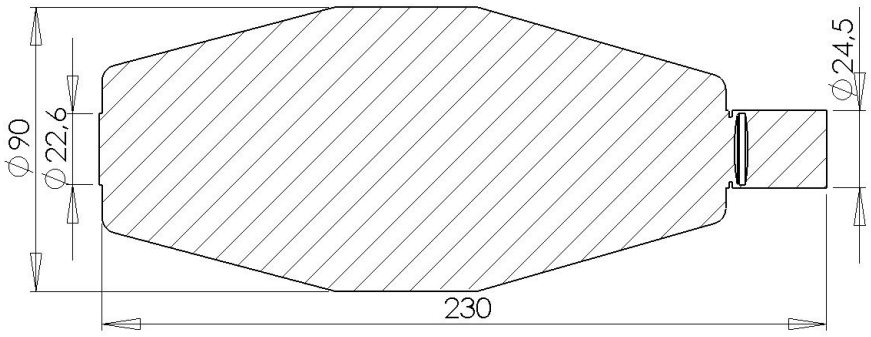

Figure 1: Longitudinal cross-section of the Volumatic® spacer geometry (dimensions in mm).

Using the Gambit™ software for meshing the 3D geometry with elements with 2.5 mm resulted in 64766 nodes and 357855 tetrahedrical/hybrid (TGrid) elements.

Mesh quality reports obtained from Gambit™ are presented in Table 1 [4].

	EquiAngle Skew	EquiSize Skew
Very good	15%	36.5%
Good	77%	54%
Normal	8%	9.5%
Bad	0%	0%

Table 1: Mesh quality report for the Volumatic®'s geometry.

3 CONFIGURATION

3.1 Velocity input

To improve the computational model, an User Defined Function (UDF) for the air flow input to the geometry was created, in C language and compiled using the Fluent™ Interpreted option [5].

The UDF function was defined in two distinct parts: the inspiration and the expiration. The inspiration was simplified by using a sine function and the expiration was defined having null velocity, to simulate the closure of the one way valve in the spacer. According to literature information about the Peak of Inspiratory Flow (PIF) in children with asthma [6], the duration of the respiratory cycle in children [7] and the recognized fact that inspiration phase is 1/3 of the total cycle duration. The resulting sine function was derived and used in the UDF, describing the velocity profile presented in Figure 2.

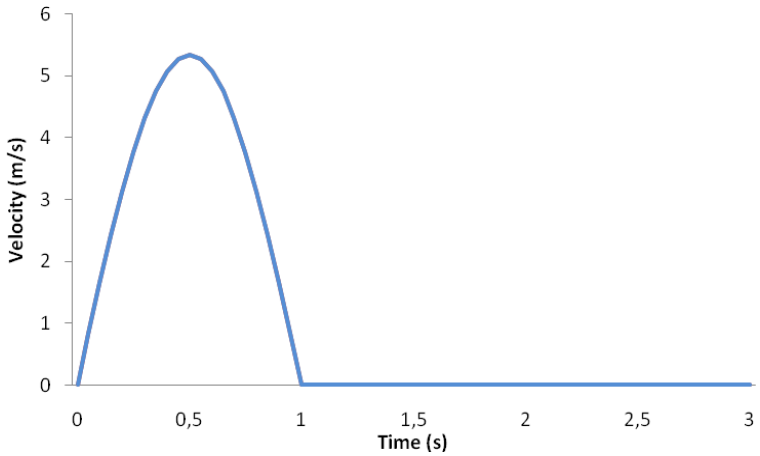

Figure 2: Velocity of the respiratory cycle used in the simulations.

3.2 Fluent™

The discretization models used were Standard for pressure and Second Order Upwind for momentum, turbulent kinetic energy and turbulent dissipation rate [8]. The absolute convergence criteria used for all variables was 10^{-3}.

Due to the nature of the velocity input, the simulation was transient, with a time step of 0.05 seconds using a maximum number of 200 iterations per time step. The results were obtained and analyzed from the second respiratory cycle onwards. Each simulation was performed in 6 seconds, resulting in a total of 120 time steps per simulation.

The results presented over the following sections were obtained at 0.2 s, 0.5 s and 0.8 s for the second respiratory cycle and from a symmetry plane, Z=0, which corresponded to the acceleration and deceleration peaks of the velocity function depicted in Figure 2.

3.3 DPM

The DPM was used in the Fluent™ simulation to study the efficiency of the Volumatic® using the CFD methodology. To configure the pMDI spray, using the DPM, it was necessary to obtain some experimental information about the spray, such as, the particle diameter distribution, cone angle (from high speed imaging), duration, nozzle diameter and spray shape. The other necessary parameters were obtained from various sources in the literature.

The Ventolin® was used since it is a common Short Acting Beta Agonist (SABA) drug applied in the treatment of asthma and delivered with the Volumatic®. The characteristics of the Ventolin® are listed in Table 2.

Characteristic	Value	Refs.
Propellant	HFA 134a	[9-10]
Salbutamol density (kg/m3)	1230	[9]
Actuation dose (µg)	100	[10-12]
Actuation time (s)	0.1	[13]

Table 2: Ventolin® properties.

The DPM allows the user to choose among three different particle diameter distributions [8]. For this project the Rosin-Rammler distribution model was used. The actual particle size distribution was also measured by the laser diffraction particle sizer Malvern 2600, always showing a good experimental fit to the data. This experimental data provided the parameters needed to configure the dispersed phase injection in Fluent™ – see Table 3.

Parameter	Value
Diameter distribution	Rosin-Rammler
Minimum diameter (µm)	1.22
Maximum diameter (µm)	49.5
Mean diameter (µm)	12.82
Spread parameter	1.44
Point of injection (*x*,*y*,*z*)	0,0,0
Spray type	Solid-cone
Angle (º)	8
Velocity (m/s)	40
Radius (m)	$2.5e^{-4}$
Flow rate (kg/s)	$1e^{-6}$

Table 3: Particle diameter distribution and spray parameters.

The spray parameters used to configure the "Injection" menu were obtained from various references. The angle of the spray was assumed as 8º, after detailed analysis of a few high speed digital movies.

The spray particles were considered to be solid, rather than liquid droplets. The reason for this consideration is simple: when the drug exits the nozzle of the pMDI, it undergoes a flash evaporation. That can be defined as the instantaneous transformation of a liquid phase into a vapour phase due to a sudden decrease in pressure. Because this is an instantaneous process, it is assumed that no heat transfer between the gas and liquid phases occurs [2, 14-15].

Subsequently, the spray flow rate was determined with the information presented in Table 2, dividing the dose over the duration of the spray.

The DPM model assumes spherical particles dispersed in the continuous phase. Fluent™ computes the trajectories of these discrete phase particles, as well as heat and mass transfer to/from them [8].

The injection model used for turbulence dispersion of particles was the Stochastic Tracking, with Random Eddy Lifetime and 0.3 for the Time Scale Constant.

The parameters used to configure the DPM menu in Fluent™ are listed in Table 4.

Parameter	Value
Interaction with Continuous Phase	On
Unsteady Particle Tracking	On
Inject Particles at	Particle Time Step
Particle Time Step Size (s)	0.001
Drag Law	Spherical
Two-way coupling turbulence	On

Table 4: Parameters for the DPM model.

Based on an extensive experimentation of different configuration parameters, these proved to be the best fit for this simulation. As the injection occurred over a limited period in time (0.1 s), the unsteady particle tracking was used, also the injection of particles has their own time step of 0.001 s, the simulation has accurate results.

The spherical drag law used is the most well-know law and is the one that better fits this model amongst the four different options in Fluent™. This assumes the particles as spheres, which is an acceptable simplification for the drug particles that exit the pMDI nozzle [8, 15].

In the present calculations, the dynamic drag model was not used, as no models for droplet collision and break up were introduced [8]. This simplification is justified because the spray is dilute. The total number of particles streams injected during the simulation was approximately 82000.

3.4 Boundary conditions

The boundary conditions applied to the geometries tested were a Velocity Inlet, in the entrance, and an Outflow in the exit of the spacer. The UDF function was associated to the Velocity Inlet.

The k-ε Standard turbulence model was used, with k=0.2 and ε=0.2 in the Velocity Inlet.

The objective of this study is to compare the efficiency of the CFD model using the Trap and Reflect conditions for the wall boundary. Therefore all the particles that hit a wall either will get trapped or get reflected, so the configuration of this parameter is the only one that will be changed.

4 RESULTS AND DISCUSSION

4.1 Gas phase pathlines and contours

Representative cases of the Fluent™ simulation results were post-processed and are represented in Figure 3. The results were obtained from the second respiratory simulation cycle, because the flow only stabilizes from this point onwards. They were also obtained from three important instants during the breathing in phase, which has

duration of 1 s, at 3.2 s (acceleration in air input), 3.5 s (maximum velocity point) and 3.8 s (same velocity as in 3.2 s but during deceleration). They are represented using pathlines and velocity contours.

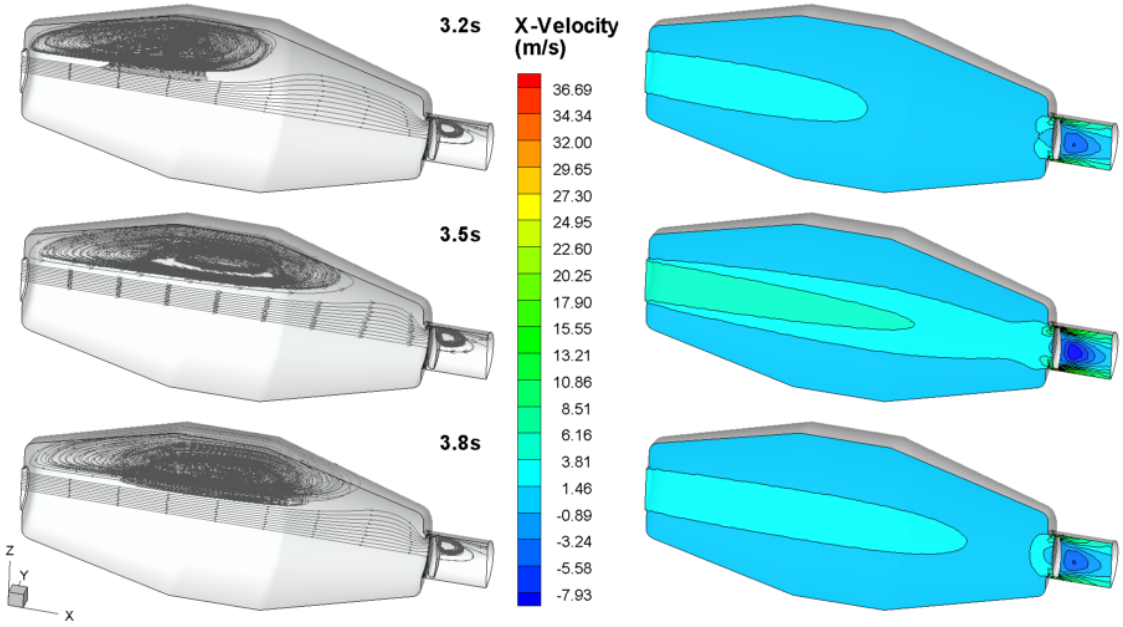

Figure 3: Results of the air flow behaviour inside the Volumatic® geometry, obtained in 3 different instants. On the left hand side, the air flow pathlines in half of the z=0 cutting plane. On the right hand side, the air axial velocity contours in the z=0 cutting plane.

The velocity contour results show, as expected, a behaviour corresponding to an acceleration zone in the centre, where the maximum value is reached at 3.5 s. In the valve zone, where the cross section is smaller, the air undergoes a sudden increase in velocity. Although the figure is not detailed enough, the maximum value in this section is approximately 37 m/s. In the downstream face of the valve a recirculation zone is created, which is clearly shown in Figure 3: the lowest gas velocities are reached in this precise zone, confirmed by the axial negative values (of -8 m/s).

By a detailed analysis of the air pathlines, it is easy to understand the air behaviour inside the holding chamber. Basically a large recirculation zone is created right after the inlet section. As the entrance walls are at 90 º with the direction of the injected flow, it can be considered a classic fluid dynamics case of sudden expansion of a fluid inside a pipe, so as expected the air recirculates there. As the air velocity increases with time during the respiratory cycle, the recirculation zone grows. Also a smaller recirculation zone, already noticed in the contours section, is easy to observe appearing downstream the valve. However, its size seems to be almost constant throughout the cycle.

The recirculation zones will surely retain the drug particles and will lower the efficiency of the holding chamber [16].

4.2 Particles position

The positions of the particles inside the Volumatic® for the same time intervals previously considered are represented in Figure 4.

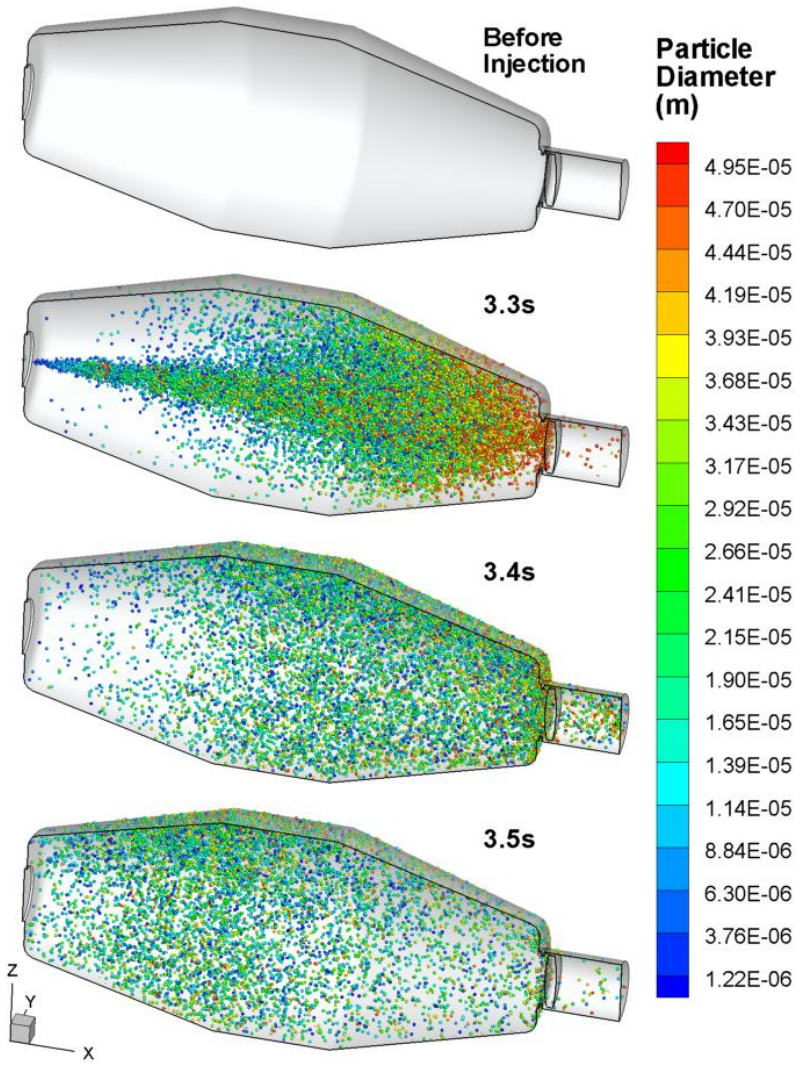

Figure 4: Positions of drug particles inside the Volumatic® (as a function of time), using the Reflect boundary condition.

The injection of the particles has duration of 0.1 s, as already described, and started at the instant of 3.2 s from the start. It is observed that the particles are moving forward, towards the walls and valve, where the boundary condition starts to work. These results were obtained using the Reflect condition with a coefficient of restitution of 1 (as the particle hits a wall, its collision energy is fully restored, as in an elastic collision).

As observed with the pathlines analysis, the large recirculation area in the body of the holding chamber is making the particles to move, from the instant 3.4 s to 3.5 s, as expected.

4.3 Particles statistics

An UDF was written to collect all the particles diameters that pass through the outlet of the Volumatic®, to a *.txt file, as well as to compute the number of particles of each diameter that exits the geometry. As the built in UDF macro for particles diameter in Fluent™ only enables the report of the diameter of the streams used by the Fluent™ for statistical calculations of the particles trajectories, it was necessary to rebuild the Fluent™ particles calculations of the injected Rosin-Rammler distribution to determine the amount of mass that exits for each particle diameter. For this purpose a specific algorithm was developed. Therefore one was able to compare the results obtained with

the experimental method for measuring particles. Because a particle impactor was used (made up by a filter for each stage of diameter intervals) to measure the particle mass distribution, the mass was divided in four stages. The filter's 1st stage is tuned for particles smaller them 3.1 µm, the 2nd stage is for particles between 3.1 µm and 6.8 µm, the 3rd stage from 6.8 µm to 13 µm and the 4th stage for particles greater than 13 µm [1]. In this way the amount of drug that was retained inside the holding chamber could also were determined.

Using this method, the Trap and Reflect conditions were tested, and also other Reflect conditions using different values for the restitution coefficient.

	1st Stage	2nd Stage	3rd Stage	4th Stage	Stay inside
Injected	10.833	20.669	30.807	37.689	0.000
Trap	0.166	0.016	0.000	0.000	99.816
Reflect	7.195	13.429	20.495	25.972	32.905

Table 5: Mass percentages for the four stages that exit the Volumatic® at t=4 s.

The values obtained from the simulation with particles in Fluent™ are depicted in Table 5. It is possible to observe that 32% of particles are kept inside the Volumatic® using the Reflect condition and 99% using Trap, after t=4 s. These two simulated conditions represents the hypothetical limits of the real amount of drug hold in the spacer, which was determined experimentally to be around 50% [1].

5 CONCLUSIONS

Based on the study herein reported, the following conclusions can be drawn:

- The simulation of a realist approach to a real-life situation of the drug flow inside a spacer using CFD tools was carried out, using realist parameters;
- The geometry is proved to be of great influence regarding the air flow inside the spacer, which is closely related to the formation of recirculation zones;
- The behaviour of the particles trajectories are affected by the recirculation zones, and
- The two wall interaction conditions tested (Trap and Reflect) produced very different results, which are not the real ones. With this in mind, a special care has to be undertaken to the development of an UDF function to better simulate the wall interaction and the particles behaviour after the collision with the spacer wall.

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