

**Computational fluid dynamics simulation of cavitating propellant flow inside a pressurised metered dose inhaler expansion chamber, using volume of fluid method**

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Atomisation quality of pressurised metered dose inhaler (pMDI) devices is directly linked with the complex two-phase flow dynamics and vapour/liquid structure of the pre-atomised propellant inside the valve stem and actuator sump. Fundamental understanding and predictability of such flow is instrumental in pMDI performance optimisation where large quantities of respirable particles are highly desirable.

Flow visualisation studies of various kinds have emphasised on the inhomogeneity of vapour/liquid phase distribution inside the expansion chamber. These studies revealed the sensitivity of atomisation quality to the precursor vapour/liquid structure travelling through the spray nozzle. Current pMDI phenomenological models are unable to account for spatial phase distribution and hence more sophisticated computational fluid dynamics (CFD) framework should be adopted to predict such flow parameters. We have developed a CFD model using STAR-CCM+ of cavitation propellant flow, inside a pMDI valve stem and sump, using volume of fluid (VOF) framework. Cavitation phenomenon is accounted in the model using full Rayleigh-Plesset equation.

In-line with previous visualisation studies, our CFD model shows the existence of a vapour rich region that travels from the valve stem into the sump. The liquid initially impacts the bottom surface of the sump and creeps through the spray nozzle and forms high velocity jet. Moreover, evidence of the annular flow regime in the spray nozzle, with a vapour core and an unsteady wall film consisting of evaporating liquid has been captured by the model. CFD models of this kind can run in parallel with focused experimentation for understanding and optimisation of future inhaler devices.