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Regional aerosol deposition in the human airways: The SimInhale benchmark case and a critical assessment of in silico methods

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Abstract

Regional deposition effects are important in the pulmonary delivery of drugs intended for the topical treatment of respiratory ailments. They also play a critical role in the systemic delivery of drugs with limited lung bioavailability. In recent years, significant improvements in the quality of pulmonary imaging have taken place, however the resolution of current imaging modalities remains inadequate for quantifying regional deposition. Computational Fluid-Particle Dynamics (CFPD) can fill this gap by providing detailed information about regional deposition in the extrathoracic and conducting airways. It is therefore not surprising that the last 15 years have seen an exponential growth in the application of CFPD methods in this area. Survey of the recent literature however, reveals a wide variability in the range of modelling approaches used and in the assumptions made about important physical processes taking place during aerosol inhalation. The purpose of this work is to provide a concise critical review of the computational approaches used to date, and to present a benchmark case for validation of future studies in the upper airways. In the spirit of providing the wider community with a reference for quality assurance of CFPD studies, in vitro deposition measurements have been conducted in a human-based model of the upper airways, and several groups within MP1404 SimInhale have computed the same case using a variety of simulation and discretization approaches. Here, we report the results of this collaborative effort and provide a critical discussion of the performance of the various simulation methods. The benchmark case, in vitro deposition data and in silico results will be published online and made available to the wider community. Particle image velocimetry measurements of the flow, as well as additional numerical results from the community, will be appended to the online database as they become available in the future.

Keywords: inhaled drug delivery, respiratory airways, regional deposition, computational fluid particle dynamics, benchmark case

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