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A predictive multiscale computational tool for simulation of lung absorption and pharmacokinetics and optimization of pulmonary drug delivery

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Pulmonary drug delivery via oral inhalation is increasingly used for both treatment of lung diseases and for delivering drugs to the systemic circulation. Efficacy and safety of orally inhaled drugs is dependent on deposition and absorption of drugs in targeted region. However, due to the complex pharmaceutical and physiological factors involved in drug transfer from the administration site to the target region, it is difficult to experimentally capture the detailed mechanistic insights of involved pulmonary drug delivery processes.

In the present study, we have developed a novel predictive multi scale computational tool to simulate delivery, deposition, dissolution, absorption, distribution, metabolism, excretion, and actions of inhaled drug products within an integral framework of computational fluid dynamics (CFD) and PBPK-PD models. The tools and models will be used in predicting the effects of inhalation devices, drug formulation, compound physiochemical characteristics, physiological settings, and various pathological factors on drug deposition and distribution. Ultimately, we aim to provide not only the detailed mechanistic insights into key aspects affecting efficacy and safety of inhaled drug products, but also to guide optimal designs of pulmonary drug delivery systems, inhaled formulations, to prescribe these therapies optimally. Research reported in this study is supported by the U.S. Food and Drug Administration (FDA) under award number 1U01FD005214-01.

Biography

Ravishekar Kannan is a Principal Scientist at CFDRC. He obtained his Ph.D. degree in 2008 from the Department of Aerospace Engineering, Iowa State University. His research interests include particle transport methods, computational drug delivery, moving boundary problems, parallel programming, algorithm development for high order methods, fluid structure interactions and High Performance Computing (HPC). He has published a series of research papers on the above in well-known international journals. Some of his latest contributions include the development of the Wind-Kessel algorithm for truncated lung models, the Q3D model for lung airways, novel high order viscous flux schemes, optimized partitioning and communication routine for HPC and development of an algorithm to detect and quantify blast injuries. Currently Dr. Kannan works on the multiscale modelling of the pulmonary drug particle deposition, dissolution, clearance and systemic circulation, collaborating with the FDA, NIH and Merck teams. Dr. Kannan has been invited to present his research at several universities worldwide in the above mentioned areas. Dr. Kannan is in the editorial board of "Journal of Aerospace Engineering and Technology" and "International Journal of Biomedical Engineering".

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