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Large Eddy Simulation of Pharmaceutical Aerosol Deposition in Complex Geometries

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Numerical investigations of aerosol deposition onto adjacent walls from turbulent flows are being performed using CFD (Computational Fluid Dynamics) techniques. In particular, the deposition of pharmaceutical aerosols in extra-thoracic airways (nose-mouth-throat) is being investigated. The continuous primary fluid flow of air can be calculated using DNS (Direct Numerical Simulation), LES (Large Eddy Simulation), or RANS (Reynolds Averaged Navier-Stokes) equations and the particulate phase simulation can be performed using Lagrangian techniques, where individual particles are numerically released in the computational flow domain. DNS and LES provide the actual and filtered instantaneous values of fluid velocities, respectively, for the calculation of the particle trajectory. In contrast, simulations using RANS equations, where only averaged values of mean velocities, pressure and other turbulence characteristic values (such as turbulence kinetic energy and turbulence eddy dissipation) are calculated, require eddy interaction models (EIM, or random walk models) to randomly generate the fluctuation components of the fluid velocities at the particle location.

Previous simulations using standard RANS with Lagrangian random-walk EIM (eddy-interaction models) to track individual particles in the computational domain have shown poor agreement with experimental data on deposition in an idealized mouth-throat region. More recently, a near-wall correction in the EIM was proposed, yielding significant improvement over previous results, but still falling short from the desired accuracy. Overall, the RANS/EIM results may indicate that the model is not capturing relevant features of the flow. Because memory and computational requirements are less for LES than DNS, and that particle trajectories can be calculated without eddy-interaction models as in the RANS/EIM approach, LES is adopted here in the study of deposition of particles in nose-mouth-throat geometries. Simulated particle deposition results are compared with separate experimental data.

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admission is free

17:30 – 19:00 pm

Mackenzie Building 4359

Carleton University

Light refreshment will be served



Dr. Matida was born in Brazil and completed his undergraduate studies at Sao Paulo University. He has pursued his master's and doctorate at Yokohama National University, Japan. From there, he came to Canada as a postdoctoral fellow at the University of Alberta, leading to research collaboration and time spent in Germany. His current focus is on pharmaceutical aerosols used in the treatment of lung diseases (such as asthma and bronchitis) and also in nasal drug delivery.



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