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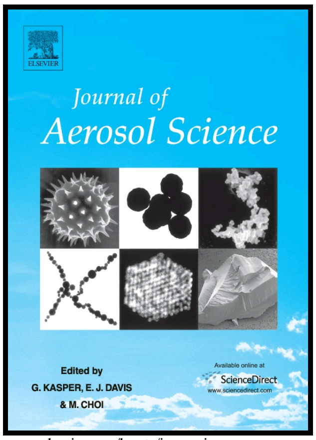

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Computational transport, phase change and deposition analysis of inhaled multicomponent droplet-vapor mixtures in an idealized human upper lung model

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Abstract

Numerous inhalable aerosols consist of multiple nano-to-microscale solid or liquid particles with dissolved or embedded compounds, as well as associated vapors. In general, of interest are the transport and conversion phenomena leading to local particle/droplet/vapor depositions. Selected examples include inhalation of aerosols from use of inhalers, cigarettes and electronic cigarettes. In this study the focus is on hygroscopic growth of nano-size multi-component droplets and droplet-vapor interactions during transport with subsequent deposition in a human upper lung-airway model. For that purpose a comprehensive and efficient computational fluid-particle dynamics model has been developed. It is capable of simultaneously analyzing multi-component droplet-vapor and airflow interactions with evaporation and condensation effects for different sets of inhalation conditions. Selecting inhaled electronic cigarette (EC) aerosols as an application, the simulation results include detailed transport, deposition and absorption data for different constituents (i.e., water, propylene glycol, glycerol and nicotine) in both vapor and liquid forms for an idealized human upper lung airway geometry, i.e., from mouth to generation 3. Results indicate that liquid-vapor phase change induces hygroscopic growth of droplets, which in turn impacts significantly the deposition concentrations of aerosols via inertial impaction, secondary flows, Brownian motion, and the vapor-specific absorption rates. Parametric sensitivity analyses were performed to evaluate the influence of different inhalation flow waveforms on EC-aerosol transport, interaction, and deposition.

Keywords: Hygroscopic droplet growth; Multi-component droplet-vapor interaction modeling; Multi-component mixture plus discrete-droplet (MCM-DD) model; Inhaled droplet-reduction (IDR) method; Electronic cigarettes

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