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Kinetic multi-layer model of the epithelial lining fluid (KM-ELF): Reactions of ozone and OH with antioxidants and surfactant molecules

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Oxidants cause damage to biosurfaces such as the lung epithelium unless they are effectively scavenged. The respiratory tract is covered in a thin layer of fluid which extends from the nasal cavity to the alveoli and contain species that scavenge ozone and other incoming oxidants. The kinetic multi-layer model of the epithelial lining fluid (KM-ELF) has been developed in order to investigate the reactions of ozone and OH with antioxidants (ascorbate, uric acid, glutathione and α-tocopherol) and surfactant lipids and proteins within the epithelial lining fluid (ELF). The model incorporates different processes: gas phase diffusion, adsorption and desorption from the surface, bulk phase diffusion and known reactions at the surface and in the bulk. The ELF is split into many layers: a sorption layer, a surfactant layer, a near surface bulk layer and several bulk layers.

Initial results using KM-ELF indicate that at ELF thicknesses of 80 nm and 1×10^{-4}cm the ELF would become rapidly saturated with ozone with saturation occurring in less than a second. However, at an ELF thickness of 1×10^{-3}cm concentration gradients were observed throughout the ELF and the presence of antioxidants reduced the O_3 reaching the lung cells and tissues by 40% after 1 hour of exposure. In contrast, the antioxidants were efficient scavengers of OH radicals, although the large rate constants of OH reacting with the antioxidants resulted in the antioxidants decaying away rapidly. The chemical half-lives of the antioxidants and surface species were also calculated using KM-ELF as a function of O_3 and OH concentration and ELF thickness. Finally, the pH dependence of the products of reactions between antioxidants and O_3 were investigated. The KM-ELF model predicted that a harmful ascorbate ozonide product would increase from 1.4×10^{11}cm^{-3}at pH 7.4 to 1.1×10^{14} cm^{-3} at pH 4after 1 hour although a uric acid ozonide product would decrease from 2.0×10^{15}cm^{-3}to 5.9×10^{12}cm^{-3}.