Next Generation Personal Protective Equipment for Real-time Inactivation of Airborne Biological Threats
Part 2: Multi-physics computational fluid dynamics (CFD) simulation

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The recent COVID-19 pandemic has created a demand for expanded public health interventions against the spread of airborne disease. While N95 masks have been effective, the public response to masking has been unpredictable, sparking interest in novel technologies that are less intrusive. A possible alternative to filtration masking is UVC based personal protection equipment (PPE) that does not impede breathing, and also inactivates airborne pathogens rather than capturing them. Such technology has the potential for widespread adoption and would ensure that vulnerable populations can be safely protected from future airborne biothreats.

The development of UVC based PPE requires critical evaluation of the disinfection potential of several alternative designs. Although experimental evaluation provides the ultimate determination of disinfection performance, such methods can be cost prohibitive when exploring many design alternatives. Numerical multi-physics models that combine optical and computational fluid dynamics (CFD) simulations are a cheaper alternative to evaluate PPE configurations, with optimal designs being then selected to undergo physical and experimental prototyping. The primary objective of this work was to develop and validate such numerical methods to help expedite PPE development, especially when these PPE systems must be designed to minimize energy cost and exploit reflective surfaces.

Photopia and Ansys Speos, cutting edge software that use ray tracing to simulate light source emanation, were used along with the radiative transport equation (RTE) to evaluate the optical properties of a range of UVC spectrum sources in multiple PPE configurations. These light models were coupled with Ansys Fluent CFD simulations to evaluate the average UVC dose delivered to air as it is being breathed, allowing us to evaluate disinfection potential for dynamic systems that match real-world use case scenarios. Our results show that ray tracing models better predict the impact of reflective surfaces than the RTE model, a requirement for PPE that uses material exceeding 40% reflectance. Further, the use of an enclosed design with highly reflective walls was found to improve UVC dosing by up to 80 times, illustrating the importance of effective design. To validate these methods, simulated pathogen inactivation was compared to experimental tests carried out using T1 phage as a pathogen surrogate (as addressed in part-one of this three-part presentation), and the results were in good agreement with one another. This work shows how numerical simulations can play a vital role during iterative design and lays the groundwork to develop more complex and effective PPE in the future.