Title: Ray-tracing and CFD simulation for aiding design of Far UV-C based PPE

Authors: C. Bowers[1,4], E. Prast[1], C. Jones[1], K.G. Linden[1,2], E.R. Blatchley[1,3], D. Mosca[1], K. Kelley[1], W. Bryden[1,5], R. Rasansky[1], J. Ducoste[1,4]

chris@xcmr.co

[1]XCMR Inc. Narberth, PA 19072, USA
[2]University of Colorado Boulder, Boulder, CO 80303, USA
[3]Purdue University, West Lafayette, IN 47907, USA
[4]North Carolina State University, Raleigh, NC 27695, USA
[5]Zeteo Tech, Inc. Sykesville, MD 21784 USA

Body

Objective. There has been increased interest by the public and policymakers in the development of public health intervention technologies due to the recent global pandemic. N95 masks are currently the best defense against the spread of disease; however, under best-case scenarios, these only filter out pathogens, and only when used properly. Personal Protection Equipment (PPE) that disinfects the air in close-proximity would provide more effective treatment and safeguard against unknown future pathogens. The purpose of this work is to use numerical simulations to explore alternative PPE designs that use Far UV-C to inactivate airborne pathogens. An additional objective is to validate these modeling techniques using experimental measurements and assess the impact of optical enhancing strategies that magnify the potential fluence rate from UV sources. ***Methods*.** Optical simulations were performed using ray-tracing with Ansys Speos and Photopia, and radiative transfer modeling using Ansys Fluent. Computational fluid dynamics (CFD) simulations were performed using Ansys Fluent and OpenFOAM. Multiple CFD modeling techniques were used to provide real-time numerical validation and confidence in the simulation results. CFD was used to simulate the fluid flow and transport of airborne pathogens around PPEs. The simulated UV source was a KrCl lamp that has been custom built by Eden Park Illumination to emit narrow band filtered 222 nm UV radiance. The pathogen inactivation potential of the PPE design was investigated using T1 phage as a pathogen surrogate. ***Results*.** Computational modeling results were collected for a variety of systems and compared favorably to experimental results. Results showed that Ansys Speos and Photopia converged to similar outcomes; however, Photopia exhibited stochastic results that randomly varied by about 1% from the average regardless of simulation refinement. By contrast, Speos exhibited typical numerical convergence behavior, and thus was used for the airborne pathogen inactivation simulations involving alternative PPE designs. Radiative transfer models produced similar results to ray-tracing methods when reflective material was not present, but the inclusion of reflective material led to significant differences that suggest the need for ray tracing when such optical enhancing methods are employed. OpenFOAM and Ansys Fluent produced similar results and could be used interchangeably. ***Conclusion.*** Several numerical techniques

were used to simulate the inactivation of airborne pathogens and subsequently validated using experimental results. Of the different numerical methods, Ansys Speos was found to be the most effective optical simulation method, while OpenFOAM and Ansys Fluent were comparable and could be used interchangeably. The methods used here greatly accelerate the development of Far UV-C personal protection technologies, and may be considered a catalyst to fast track the designs of PPE.