**Heuristic Optimization of a Continuous Flow Point-of-Use UV-LED Disinfection Reactor
using Computational Fluid Dynamics**

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Alternative disinfection sources such as ultraviolet light (UV) are being pursued to inactivate pathogenic microorganisms such as *Cryptosporidium* and *Giardia*, while simultaneously reducing the risk of exposure to carcinogenic disinfection by-products (DBPs) in drinking water. UV-LEDs offer a UV disinfecting source that do not contain mercury, have the potential for long lifetimes, are robust, and have a high degree of design flexibility. However, the increased flexibility in design options will add a substantial level of complexity when developing a UV-LED reactor, particularly with regards to reactor shape, size, spatial orientation of light, and germicidal emission wavelength. Anticipating that LEDs are the future of UV disinfection, new

methods are needed for designing such reactors. In this research study, the evaluation of a new design paradigm using a point-of-use UV-LED disinfection reactor has been performed. ModeFrontier, a numerical optimization platform, was coupled with COMSOL Multi-physics, a computational fluid dynamics (CFD) software package, to generate an optimized UV-LED continuous flow reactor. Three optimality conditions were considered: 1) single objective analysis minimizing input supply power while achieving at least (2.0) $\log_{10}$ inactivation of *E. coli* ATCC 11229; and 2) two multi-objective analyses (one of which maximized the $\log_{10}$ inactivation of *E. coli* ATCC 11229 and minimized the supply power). All tests were completed at a flow rate of 109 mL/min and 92% UVT (measured at 254 nm). The numerical solution for the first objective was validated experimentally using biodosimetry. The optimal design predictions displayed good agreement with the experimental data and contained several non-intuitive features, particularly with the UV-LED spatial arrangement, where the lights were unevenly populated throughout the reactor. The optimal designs may not have been developed from experienced designers due to the increased degrees of freedom offered by using UV-LEDs. The results of this study revealed that the coupled optimization routine with CFD was effective at significantly decreasing the engineer's design decision space and finding a potentially near-optimal UV-LED reactor solution.

Keywords

disinfection; UV Light Emitting Diodes; Numerical model; Numerical optimization; Biodosimetry

47 Abbreviations

DBP: Disinfection By-Product
CFD: Computational Fluid Dynamics
cfu: colony forming unit
cm: centimeter
D: Diffusion coefficient ($\text{m}^2\cdot\text{s}^{-1}$)
F: Fluence ($\text{mJ}\cdot\text{cm}^{-2}$)
FW: Flat Window
g: gravity ($\text{m}\cdot\text{s}^{-2}$)
HRT: Hydraulic Retention Time (s)
I: fluence rate ($\text{mW}\cdot\text{cm}^{-2}$)
k_λ : kinetic rate constant at wavelength λ ($\text{t}^{-1}\cdot\text{cm}^2\cdot\text{mW}^{-1}$)
LED: Light Emitting Diode
LP: Low Pressure mercury UV lamp
LPHO: Low Pressure High Output UV lamp
m: meter
mL: milliliter
MP: Medium Pressure UV lamp
MPSS: Multiple Point Source Summation Model
mW: milliwatt
N: microbial concentration ($\#\cdot\text{m}^{-3}$)
nm: nanometer (m^{-9})
p: fluid pressure ($\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-2}$)

P: Light Power (W)
pfu: plaque forming unit
r: radial distance from light source (m)
Re: Reynolds number (unit less)
R_N : Microbial fluence response term (# of cells* m^{-3} * t^{-1})
s: second
t: time (s)
u : fluid velocity ($m*s^{-1}$)
UNEP: United Nations Environment Program
UV: Ultraviolet
UVT: Ultraviolet Transmittance
W: Watts
α : viewing angle (degrees)
λ : wavelength (m)
μ : dynamic viscosity ($kg*m^{-1}*s^{-1}$)
ρ : fluid density ($kg*m^{-3}$)

48

49 **1 INTRODUCTION**

50 UV has become an increasingly important drinking water disinfection process due to its ability to
51 inactivate chlorine resistant protozoa (*Cryptosporidium* and *Giardia*) without the formation of
52 known disinfection by-products (DBP). In addition, UV does not result in taste/odor compounds
53 and over-dosing will not compromise public health (Chatterley and Linden, 2010). Currently,
54 mercury vapor lamps are the most widely-used technology for UV water treatment. While other

UV light emitting sources do exist, the three most common mercury-based UV sources are medium-pressure (MP), low-pressure (LP), and low-pressure high output (LPHO) lamps. MP lamps emit polychromatic UV light (200-400nm) and operate at much higher temperature, pressure, and intensity than LP and LPHO lamps, which emit monochromatic light at 253.7 nm (USEPA, 2006). Most microorganisms have a peak DNA absorbance to UV light near 260-265 nm, which results in the LP and LPHO lamps having a higher germicidal efficiency compared to MP lamps. Much of the MP lamp emission spectrum falls outside the ideal 240-280 nm wavelength range (USEPA, 2006).

Mercury UV lamps, however, are long, typically cylindrical in stature, and do not offer a high degree of design flexibility. Further drawbacks to traditional UV lamps include its toxic components. Mercury is hazardous to both human health and the environment, and its vapor may enter the drinking water supply or may expose plant personnel if the lamps are broken during installation, maintenance, disposal, or by foreign-object strike (USEPA, 2006). In addition, the United Nations Environment Program (UNEP) has signed an agreement to significantly limit the mining and usage of mercury by the year 2020 (UNEP, 2013). The agreement will significantly affect the manufacturing of all products that contain mercury, including UV lamps.

Recent technological advances have led to the development of small Light Emitting Diodes (LEDs), around 5 mm in diameter, to generate light in the germicidal range (Bettles et al., 2007; Chatterley and Linden, 2010; Bowker et al., 2012, Jenny et al., 2014). However, the current state of UV-LED technology only allows for low-flow, point-of-use applications due to their inefficiency (less than 1%) and low optical output power (typically around 1 mW LED⁻¹ for the

germicidal wavelengths). Nonetheless, UV-LEDs have the potential to be spatially distributed in UV reactors in a seemingly infinite number of ways, due to their small size. Additionally, UV-LEDs can be manufactured to produce a targeted wavelength of light (from 255 nm to 405 nm), which further increases design flexibility over traditional lamp technologies (Shur and Gaska, 2008). The design variability offered by UV-LEDs provides an opportunity to engineer a more efficient disinfection process by strategically placing the UV-LEDs at locations that lead to a narrow UV fluence distribution.

UV-LED disinfection research has grown steadily, particularly in quantifying the kinetic response to germicidal light exposure (Vilhunnen et al., 2009; Chatterley and Linden, 2010; Gaska et al., 2011; Bowker et al., 2011; Würtele et al., 2011; Oguma et al., 2013; Jenny et al., 2014). Conversely, some studies have incorporated LEDs within the UV-A spectrum, or a coupled system that uses light emission from both the UV-A and UV-C ranges (Hamamoto et al., 2007; Chevremont et al., 2012). Additionally, computational fluid dynamics (CFD) has become a common method to characterize UV reactor physics (Downey et al., 1998; Ducoste et al., 2005; Zhao et al., 2009; Wols et al., 2010). However, only a small fraction of published research has experimentally validated CFD numerical predictions of a UV-LED reactor system (Wang et al., 2012; Jenny et al., 2014).

As mentioned previously, traditional mercury lamp UV sources are long and cylindrical in nature, are often arranged either parallel or perpendicular to the direction of fluid flow, and offer only two UV emission profiles: monochromatic (254 nm) or polychromatic (200-400 nm). Thus, the design degree of freedom for cylindrical UV lamps is relatively small, making it reasonable

for engineers to determine (with the assistance of CFD) the optimal lamp type, number, and spatial arrangement in a disinfection reactor. UV-LEDs are point sources of light able to potentially emit at any targeted monochromatic wavelength. The combination of UV wavelength options and spatially discrete light locations provides a significant number of design options that will make it difficult for engineers to optimally design such a system. Coupling CFD models with optimization software will offer an opportunity to heuristically determine the most efficient UV-LED reactor design under specified design constraints. For these reasons, ModeFrontier, commercial optimization software, was coupled with COMSOL Multi-physics, commercial CFD software, to numerically optimize a continuous flow UV-LED reactor. The numerical representation of the hydraulic flow, light distribution, and microbial inactivation through the UV-LED reactor was experimentally validated in a prior study (Jenny et al., 2014). For the optimized reactor design, the optimization routine was designed to vary the placement, number (0-30), and wavelength (260 nm or 275 nm) of UV-LEDs irradiating through the system under three optimality criteria: 1) minimizing the total input UV-LED power while achieving a target $\log_{10}$ inactivation (2.0) of *E. coli* ATCC 11229; and 2) two multi-objective analyses (i.e. one of which was to maximize the $\log_{10}$ inactivation of *E. coli* ATCC 11229 and minimize the input power). Two additional non-optimal solutions were validated to demonstrate the legitimacy of the predicted inferior solutions. All optimality tests were completed at a flow of 109 mL/min and 92% UVT (based on 254 nm). The numerical solution for the first objective was validated experimentally using biosimetry.

2 METHODS

2.1 REACTOR CONSTRUCTION

The point-of-use reactor was constructed and modeled according to the research performed by Arafin and Ducoste, (2010). The reactor body consisted of one stainless steel box (Figure 1) and a single mid-baffle wall (Supplemental Figure 1). All interior walls were painted black to reduce the contribution of UV irradiance from wall reflection. The reactor was designed to incorporate 30 LEDs oriented in two arrays of 15 on two opposing sides of the reactor. The black arrow in Figure 1 display the direction of entering fluid and red arrow display the direction of fluid exiting the reactor. Additional details related to reactor construction are reported in Jenny et al., 2014.

2.2 NUMERICAL SIMULATIONS

COMSOL Multiphysics (COMSOL Inc., Burlington MA), was used to solve the conservation of mass and momentum equations (Equation 2.1 and 2.22.2, respectively) to predict the flow field and pressure distribution inside the specified domain. The software was used for geometry generation, meshing, physics settings, solving, and post processing. An iterative matrix solver (GMRES) was used to solve the governing equations of fluid dynamics, and convergence was considered to be achieved when relative errors of the numerical solutions were below 1E-06.

The entire flow domain was discretized with 171,893 tetrahedral elements to calculate a flow rate of 109 mL/min. The mesh size provided a grid-independent solution, as refining the mesh further had minimal (~1%) impact on the predicted log inactivation through the system. A 22.56 cm long pipe was modeled at the inlet to obtain a fully developed velocity profile

prior to entrance into the main reactor body. The same length of pipe was also provided at the outlet (Durst et al., 2005). A constant velocity (uniformly distributed over the inlet area), was maintained at the inlet and zero pressure boundary condition was imposed at the outlet. Other closed boundaries were modeled as no slip walls. Calculation of the Reynolds number ($Re = 182$) at the modeled flow rate (109 mL/min) suggests a laminar flow field through the reactor.

Light model (Equation 2.3), which is based on the Multiple Point Source Summation (MPSS) model, was used to calculate the fluence rate inside the computational domain (Liu et al., 2004; Bowker et al., 2011). The model incorporates the term (“UVT”) to account for wavelength-specific transmittance values. In Equation 2.3, the viewing angle $\alpha = 60^\circ$ was used based on the manufacturer specifications (SET, Inc., 2008). Microbial inactivation was calculated using a steady state convective diffusion equation (Equation 2.4) where the model incorporated a microbial fluence response term (R_N). The (R_N) term was dependent on the microorganism. Bacteriophage Q β displays a near log-linear fluence response curve to 260 nm and 275 nm UV-LEDs (as found from collimated beam testing); therefore, the kinetics most accurately follow the Chick-Watson equation (Equation 2.5). Conversely, *E. coli* ATCC 11229 was initially UV-resistant (to both 260 nm and 275 nm light) until it experienced a threshold fluence, after which its inactivation rate increases rapidly. Therefore, the rate of *E. coli* ATCC 11229 degradation was described by the series-event model (Severin et al., 1983) (Equation 2.6). Equations 2.5 and 2.6 account for both wavelengths of light (260 nm and 275 nm). As mentioned previously, the multi-physics of the numerical model were experimentally validated in a prior study (Jenny et al., 2014); therefore, to uphold the reactor

validation results, no significant changes were made to the model. However, researchers have since made minor improvements to modeling such physics, particularly in regards to the light irradiance model. If deemed necessary, readers are encouraged to incorporate notable results (e.g. Simons et al., 2014), to more accurately represent the intensity profile emanating from a flat window UV-LED.

Continuity equation:

$$\nabla \cdot \mathbf{u} = 0$$

2.1

Conservation of momentum equation:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \mu \nabla^2 \mathbf{u} + \rho \mathbf{g}$$

2.2

Light model:

$$I = \frac{P}{2 * \pi * r^2 * (1 - \cos \alpha)} * UV T^{(r/0.02)}$$

2.3

Microbial inactivation:

$$\nabla \cdot (-D \nabla N) = R_N - \mathbf{u} \cdot \nabla N$$

2.4

Chick-Watson model:

$$R_N = -(k_{260} I_{260} + k_{275} I_{275}) N$$

2.5

Series-Event model:

$$R_{N_i} = (k_{260}I_{260} + k_{275}I_{275})N_{i-1} - (k_{260}I_{260} + k_{275}I_{275})N_i$$

2.6

2.3 UV FLUENCE DISTRIBUTION CHARACTERIZATION

The fluence distribution within the reactor was numerically determined using a Lagrangian approach described in Ducoste et al., (2005), to which the reader is directed for the equations describing particle position, velocity, and interactions with turbulent eddies. Generating the UV fluence distribution data was also completed in an identical manner as reported in Jenny et al., (2014).

2.4 MICROBIAL INACTIVATION CHARACTERIZATION

Microbial inactivation data for the reactor was generated using bacteriophage Q β and the bacterium *E. coli* ATCC 11229. A standard collimated beam procedure was followed to characterize the kinetics of each respective microorganism (Bolton and Linden, 2003). For the continuous flow experimental tests, a peristaltic pump (Ocaton PC 2700 Master flex L/S Drives, Cole-Parmer, Court Vernon Hills, Illinois) propelled the testing solution through the reactor at a flow rate of 109 mL/min. Flow-through experimental tests were completed at 92% or 80% UV-Transmittance (UVT). To maintain consistency with the literature, the UVT values presented throughout this research are in reference to a 254 nm UV emission wavelength. As discussed in the Numerical Simulations section, the higher UV transmittance resulting from 260 nm (93% UVT) and 275 nm (94% UVT) wavelengths are used in the light irradiance model. Collimated beam and continuous flow samples were collected in sterile dark tubes and promptly assayed. Additional details describing microbial enumeration, propagation, and sampling methods are described in the supplementary section.

2.5 OPTIMIZATION ROUTINE

ModeFrontier, a multi-objective optimization software, was coupled with COMSOL Multiphysics, a commercial CFD program, to determine optimal UV-LED configurations in the small-scale water disinfection reactor. MS DOS batch scripts and Matlab code were used to link ModeFrontier with COMSOL, using the LiveLink for Matlab module in COMSOL 4.3a.

Two multi-objective and one single objective function were developed, where all three functions were constrained by the number of activated UV-LEDs (30 or fewer) and the emission wavelengths (260 nm or 275 nm). Each analysis characterized the degradation of *E. coli* ATCC 11229 and was performed under 109 mL/min flow conditions at 92% UVT (UVT based on 254 nm UV). The two multi-objective functions are as follows: 1) Maximize the $\log_{10}$ inactivation and minimize the system supply power; 2) Minimize the $\log_{10}$ inactivation and maximize the system supply power. The second multi-objective criterion was performed to find the worst case design alternatives and to provide a lower bound to the solution space. The third function was a single-objective analysis, where the goal was to minimize the supply power by maintaining at least 2.0 $\log_{10}$ inactivation of the microorganism. The multi-objective analyses provide a set of optimal designs, referred to as the Pareto front. The single objective function presents one optimal solution.

In ModeFrontier, the MOGA-II algorithm was chosen as the evolutionary algorithm to determine the optimal three-dimensional design. MOGA-II is a multi-search elitism algorithm that maintains potentially optimal solutions without pre-mature convergence on local optimal

solutions (Poles 2003). The total number of design evaluations is defined as the initial population size multiplied by the number of generations. In this study, the initial population consisted of 100 “design options”, where each design option can represent a specific UV-LED placement location, number of LEDs, and emission wavelength. Ten of the 100 design options were user-defined inputs, and represented previously simulated configurations (e.g. 30 260 nm UV-LEDs activated, 30 275 nm UV-LEDs activated, 15 260 nm UV-LEDs activated, 15 275 nm UV-LEDs activated). The remaining 90 were determined by the SOBOL sampling algorithm, which attempts to uniformly distribute the input variables across the decision space (ModeFrontier Manual, 2013). The genetic algorithm performed 100 generations, providing a total of 10,000 simulations for a given multi-objective problem.

3 RESULTS AND DISCUSSION

3.1 BACTERIOPHAGE KINETIC RESPONSE

Bacteriophage Q β was exposed to three different UV light sources (254 nm mercury vapor LP, 260 nm UV LED, and 275 nm UV LED) under batch conditions to determine the UV response rate to each light source. The kinetic data was modeled and incorporated in the steady-state convective diffusion transport equation. When comparing each of the wavelengths, Q β had the greatest UV inactivation rate when exposed to the 260 nm UV-LEDs. The faster degradation kinetics was attributed to the peak RNA UV absorbance at 260 nm. Results and additional discussion of the collimated beam Q β data is provided in the supplementary section (Supplemental Figure 2).

3.2 BIODOSIMETRY: BACTERIOPHAGE Q β

Upon collection of the Q β kinetic data, biodosimetry was performed to characterize the accuracy of the numerical model. Initial Q β phage biodosimetry tests were completed with four different operating conditions; each consisted of a 109 mL/min fluid flow rate, and all available (30) UV-LEDs activated. The initial tests were completed at 92% and 80% UVT (based on 254 nm), with each experiment involving only one UV wavelength (260 nm or 275 nm). Figure 2 compares the experimental and numerical biodosimetry results from these tests.

The numerical predictions show good agreement (less than 7% deviation) with experimental results for both UVT values and wavelengths. The model predicts the slight decrease in log inactivation with decreasing UVT, which is caused by the fraction of light that is absorbed by the super-hume, as opposed to the microorganisms. The model also follows experimental results showing a decrease in log inactivation as wavelength of light shortens from 275 nm to 260 nm. The decreased log inactivation appears counter-intuitive, as the data from the collimated beam study showed the 260 nm UV-LEDs were more fluence-efficient. However, the 275 nm UV-LEDs used in this research emit nearly twice the radiant output power (with a 1:1 input power ratio) than the 260 nm lights (0.89 mW LED⁻¹ versus 0.5 mW LED⁻¹, respectively) and do not produce significantly lower degradation kinetics compared to the 260 nm wavelength. Therefore, with respect to Q β phage, the 275 nm source currently generates greater germicidal intensity when provided the same input power. However, it should be reiterated that the 275 nm source currently has a higher germicidal efficacy in a continuous flow system because of the current state of UV-LED technology. In comparing watt-for-watt output power, it is expected that a 260

nm UV-LED reactor would outperform a 275 nm UV-LED reactor, due to the average peak DNA absorption spectrum near 260-265 nm.

3.3 FLUENCE DISTRIBUTION DATA

The previous section (Section 3.2) provided insight into the efficiency of each respective UV-LED wavelength, but provides no information on the hydraulic and light distribution efficacy of the device. Understanding the hydraulic and light distribution within a UV reactor is vital for the design and optimization of such a system. A detailed hydraulic analysis has been performed with this reactor in a previous study (Jenny et al., 2014). The UV fluence distribution data is used to understand reactor performance, and was used in the present research to provide confidence in the optimization results. It was hypothesized that a numerically generated UV fluence distribution will provide insight to the efficiency of specific sub-regions (influent and effluent sides) within the UV-LED reactor. In turn, the general UV-LED spatial orientation could be hypothesized (for an optimal design).

The fluence distribution curves were numerically generated using the Lagrangian particle tracking approach. The disinfection system was solved using four different operating conditions, each with 15 UV-LEDs of a common wavelength: 275 nm Influent (275I), 275 nm Effluent (275E), 260 nm Influent (260I), and 260 nm Effluent (260E). Figure 3 displays the numerical UV fluence distribution curves for the 275I and 275E reactor configurations. The fluence distribution data for the 260 nm wavelength is provided in the supplementary section (Supplemental Figure 3).

303 The fluence distribution data predicts that the 275 nm light source results in greater average
304 fluence than the 260 nm source on both the influent and effluent sides of the reactor,
305 respectively. The higher average fluence for the 275 nm lights was expected due to their ability
306 to emit nearly twice the radiant output power than the shorter wavelength. Additionally, the
307 model predicts an increase in average UV fluence exposure (regardless of wavelength emission)
308 as microorganism's progress to the effluent side of the reactor. Jenny et al., (2014) showed that a
309 high velocity fluid jet enters the UV-LED reactor body as fluid exits the small-diameter inlet
310 piping (Supplemental Figure 4). Following progression around the mid-baffle wall, the fluid
311 then travels in a more uniform manner, at a lower average velocity, until exiting the system.
312 Therefore, the hydraulics suggest that the average microorganism spends more time on the
313 effluent side of the reactor, is exposed to more light, and receives a greater average UV fluence
314 than when progressing through the influent side, regardless of wavelength emission.

315 The spread of the UV fluence distribution curves is another important way to characterize reactor
316 efficiency, as it is beneficial to understand the likelihood that a given microorganism will
317 experience the average fluence within the reactor. The dimensionless variance (calculated using
318 a non-linear regression technique, Haas et al., 1997) was used to characterize the width of the
319 UV fluence distribution. A dimensionless variance of 0.033 and 0.036 was calculated for the
320 light configuration of 275 nm and 260 nm LEDs on the effluent side of the reactor, respectively,
321 while the dimensionless variance was 0.137 and 0.129 for the 275 nm and 260 nm LED
322 configuration on the influent side of the reactor, respectively. The smaller dimensionless
323 variance values on the effluent side are a function of the amount of dispersion in that section.
324 The high influent velocity causes fluid mixing in the influent side, particularly around the mid-
325 baffle wall. The same level of dispersion is not present on the effluent side.

Ultimately, the results from the UV fluence distribution data suggest that the effluent side of this particular reactor contributes to the increased disinfection efficiency of this UV LED reactor, regardless of wavelength analyzed. Biodosimetry tests experimentally validated the trends found in the numerical UV fluence distribution data, and the results are discussed in the following section.

3.4 ALTERNATING WAVELENGTH EXPERIMENTS: BIODOSIMETRY

Two operating conditions were experimentally tested to validate the trends found from the numerical UV fluence distribution curves. The tests compared the impact of implementing 30 total UV-LEDs; 15 260 nm UV-LEDs were on the influent side of the reactor and 15 275 nm UV-LEDs were on the effluent side (260I/275E). Following the initial tests, the configuration was flipped (275I/260E), ensuring that 30 total UV-LEDs were activated. This arrangement of tests will hereafter be referred to as the “Alternating Wavelength” experiments. The benefit of the Alternating Wavelength experiments is two-fold: 1) it validates the models’ ability to predict the log inactivation using multiple wavelengths; 2) it can provide insight to the influent/effluent reactor efficacy. Figure 4 displays the comparison between experimental and numerical results for the Alternating Wavelength trials.

The numerical model displayed good agreement in predicting the log inactivation of Q β phage under both operating conditions (Figure 4). Under the hypothetical situation in which the 260I/275E and 275I/260E operating conditions produced similar log inactivation, the conclusion could be drawn that both sides of the reactor have similar fluid mixing and light distribution efficiency. However, the results in Figure 4 do not support that prediction; rather, the 260I/275E

outperformed the 275I/260E configuration. Given that the $(k_{275}I_{275})$ term is larger than the $(k_{260}I_{260})$ term for a given location within the reactor (as demonstrated in Section 3.2), it can be said that the most photo-chemically efficient side is the one which takes greatest advantage of the most germicidal intense light. The results in Figure 4 shows a higher Q β phage inactivation when fifteen 275 nm UV-LEDs are located on the effluent side; therefore, the effluent side of the reactor has greater UV disinfection efficiency than the influent side. The identical conclusion was drawn from the numerically-generated UV fluence distribution curves.

The results in Sections 3.1-3.4 lead us to two hypotheses: 1) the optimal lights are expected to emit at 275 nm; and 2) the optimization routine will preferentially place the majority of the lights on the effluent side of this specific reactor system. It is important to remember that the objective of the work completed in Sections 3.1-3.4 was to explain the general trends relating to the optimal design of this specific UV LED reactor. The results from these sections should not be generalized to suggest all UV-LED reactors should position 275 nm UV-LEDs on the effluent side of a reactor.

3.5 *E. COLI* ATCC 11229 KINETIC RESPONSE

Current UV-LED technology is only capable of supplying sufficient UV-LED output power suitable for low flow, point-of-use reactor applications. In that regard, the relatively high Q β UV-resistance combined with the low output power of UV-LEDs in the biodosimetry results made it challenging to explore the optimal design configurations using Q β . Therefore, *E. coli* strain ATCC 11229 was chosen as a non-pathogenic testing microorganism to display the proof-of-concept model for an optimized UV-LED continuous flow point-of-use disinfecting device, due to its higher UV sensitivity. The results of the *E. coli* ATCC 11229 batch biodosimetry

experiments and the series-event degradation model can be reviewed in the supplemental portion of the manuscript.

Subsequent to characterizing the *E. coli* ATCC 11229 batch kinetic data, microbial inactivation predictions from two reactor designs were experimentally validated. The validation steps were completed to ensure the numerical model accurately captures the multi-hit degradation kinetics. The numerical predictions showed good agreement with the experimental measurements. Details of the *E. coli* ATCC 11229 biodosimetry results are also provided in the supplemental section.

3.6 OPTIMIZED UV-LED REACTOR

The potentially optimal design chosen for experimental validation testing was extracted from the single-objective analysis, where COMSOL and Mode-Frontier were coupled to solve for the minimum electrical input power while achieving at least 2.0 log inactivation. The single-objective analysis was used to experimentally validate the numerically-predicted optimal design. A multi-objective analysis was subsequently incorporated to generate a set of potentially optimal solutions, by simultaneously solving for the maximum log inactivation and minimum electrical power to the reactor. A second multi-objective optimality criterion was performed that minimized the log inactivation and maximized the input supply power to produce the worst-case (lower-bound) conceivable UV-LED reactor designs. The results from the single-objective analysis can be found in the supplementary section (Supplemental Figure 8) of the manuscript. Both multi-objective analyses are combined and plotted in Figure 5 to show the breadth of conceivable reactor designs for the system, for a given microorganism, flow rate (109 mL/min), and UVT (92%).

The possible reactor configurations are striated along power values, as the individual input UV-LED power is constant, regardless of emission wavelength. As expected, Figure 5 shows that increasing the supply power will lead to increasing log inactivation. The inherent nature of multi-objective analyses provides insight to the trade-off between the objective functions, where the set of optimal solutions is located along the Pareto front (green line). Any solution on the Pareto front represents optimality, where one objective function can theoretically no longer be improved without compromising the other objective. Additionally, the least efficient solutions (lower bound, worst-case) are also plotted in Figure 5 (marked by the red line). Although the two multi-objective plots are effective at representing the wide range in potential reactor configurations, the

plot is not exhaustive. Figure 5 encompasses nearly 20,000 possible reactor configurations; however, additional arrangements (within the Pareto front and lower bound) are conceivable.

Three (one potentially optimal, two suboptimal) reactor configurations were extracted from the single-objective analysis and experimentally validated. Two of the data points revolved around the optimal solution, where the reactor was designed to achieve 2.0 $\log_{10}$ inactivation of *E. coli* ATCC 11229 by minimizing the input power. The data points are reproduced on Figure 5 for visual understanding. Non-Optimal solution #1 represents a potential design that achieves 2.0 $\log$ inactivation, but requires more UV-LEDs than what is theoretically necessary. Conversely, Non-Optimal #2 represents a design that uses the same input power as the optimal design, but poorly distributes the UV-LEDs and results in near 1.0 $\log_{10}$ inactivation. The optimal solution as determined using the single-objective analysis will be discussed initially, where Figure 6 (a and b) display the influent and effluent side light configurations, respectively, for this solution.

The optimal configuration consists of seven UV-LEDs (all emitting 275 nm) with five of the seven lights located on the effluent side of the reactor. The design agrees well with the hypothesis developed earlier, where it was predicted that the ideal configuration will consist of 275 nm lights, the majority of which will be placed on the effluent side of the reactor. Although the placement of the UV-LEDs was hypothesized based on preliminary experiments and modeling, the number of UV-LEDs and the exact location of each UV-LED were not as intuitive. The configuration has five of the seven UV-LEDs arranged along the center columns (two on influent; three on effluent), with the remaining two lights placed along each side wall on the effluent section. UV-LED placement along the center line of fluid flow is logical, as the

microbial concentration and light intensity is high compared to the side walls, and the microbial degradation rate depends on both concentration and light intensity.

The results suggest that including two UV-LEDs on the influent side is more beneficial than moving these lights to the effluent side. Although it was hypothesized that the majority of UV-LEDs would be located on the higher efficiency effluent side, it is not surprising that some UV-LEDs are located along the influent section, as the dispersion on the influent is low (Jenny et al., 2014) and only minimally decreases efficiency. It is possible that the influent lights are acting to minimize the negative impact the impinging jet has on the system (Supplemental Figure 4). Although the spacing of five of the seven UV-LEDs can be at least partially explained, the two UV-LEDs located along the effluent side walls are not well understood.

Interestingly, upon examination of the multi-objective solutions, the optimal design (for 2.0 log inactivation) deviated slightly in spatial UV-LED arrangement from the solution formulated with the single-objective analysis. The improvements are that the two effluent side-wall UV-LEDs were relocated to the center locations on the effluent side of the reactor (Supplemental Figure 9). As for the influent lights, the UV-LED toward the back-end of the reactor was moved from the center of the fourth row to the center of the most downstream row (fifth) on the influent side. The design change for this specific reactor resulted in minimal efficiency improvements, predicting an increase in the $\log_{10}$ inactivation by 5% from 2.0 to 2.1.

The minor change in the multi-objective-generated optimal result brings about a few realizations: 1) the multi-objective heuristic predicts a more-optimal reactor design than the single-objective

analysis, which suggests the single-objective solution converged on a local optimal and requires additional design iterations; 2) the improved solution found using the multi-objective analysis supports our intuition that the UV-LEDs are best served in the center of the reactor; 3) the reactor design is not proven to be globally optimal, as the heuristic procedure did not perform an exhaustive search. For that reason, a second multi-objective iteration process, using a reduced decision space, may be performed to determine if further improvements exist. Although it can be conceded that the algorithm is not proven to converge on a global optimal solution, it was quite effective at significantly reducing the decision space, and can still be considered a powerful tool in aiding the design engineer to develop a potentially-optimal UV-LED reactor design.

Until this point, the discussion has focused on the first optimized design and the validation results defending the spatial arrangement and emission wavelength of the optimal reactor configuration. However, no discussion has been made regarding the number of activated UV-LEDs required to achieve the target log inactivation. Predicting the number of UV-LEDs necessary to produce a target inactivation in a continuous flow UV-LED reactor is complex (i.e., due to spatial mixing, light distribution, UV sensitivity of microorganism). An increase in the number of activated UV-LEDs may not lead to a significant increase in the log inactivation if the lights are not appropriately distributed spatially. As a result, predicting the number of UV-LEDs to achieve a target log inactivation will likely be solved using a trial-and-error approach. Clearly, this approach is time-consuming and inefficient. Moreover, even if the designer has a thorough understanding of the hydraulics and light distribution in the reactor, it remains exceedingly challenging to predict the number of UV-LEDs necessary to achieve a target inactivation. This discussion leads nicely to the next set of experimental tests, where a non-

optimal solution (Non-Optimal #1) was experimentally validated to show that incorrectly designing the reactor can still provide 2.0 log₁₀ inactivation of *E. coli* ATCC 11229, but at an increased energy cost (1.5x) compared to the optimal configuration.

The Non-Optimal #1 light distribution results (Supplemental Figure 9) show a distribution of lights that are nearly symmetrical about the center column on both influent and effluent sides, 6 of the 11 lights are on the effluent side, and 6 of the 11 lights emit at 275 nm. Overall, the light configuration is well distributed throughout the reactor, with a near-equal use of both wavelengths of light. For these reasons, it appears to be a practical UV-LED design for an engineer who does not have thorough background information on the particular system. However, given the validation data that has been collected, it is clear that this particular design is not optimal, even though it achieves 2.0 log₁₀ inactivation of *E. coli* ATCC 11229 under 109 mL/min and 92% UVT conditions.

The second non-optimal design was analyzed to demonstrate that even in situations where the reactor provides adequate light power, the spatial light distribution, and emission wavelength have a profound impact on the efficiency of the system. Non-Optimal #2 was extracted from the multi-objective solutions plot, where the number of UV-LEDs (seven; input power: 1.61W) was held constant in relation to the optimal solution. The light distribution from Non-Optimal #2 is shown in the supplemental section (Supplemental Figure 10).

Assuming a practicing engineer has not accumulated the validation (both wavelength and reactor sub-regions) data, the influent side of Non-Optimal #2 is a conceivable arrangement

incorporating three UV-LEDs along the center channel to inactivate a high concentration of microorganisms. Given the peak DNA germicidal effectiveness of the 260 nm UV-LEDs, it is reasonable for a designer to select the shorter wavelength to provide an initial high disinfection efficiency. Similarly, an engineer may theorize that arranging the 275 nm UV-LEDs on the effluent side may inhibit enzymatic dimer repair activity within the cell (Kalisvaart, 2004). However, the validation testing performed in this research showed that the 275 nm UV-LEDs currently have higher disinfection efficiency (due to significantly higher optical output power) and the reactor's effluent side has a higher hydraulic efficiency. For these reasons, it is clear to see why Non-Optimal #2 is not an ideal design.

The experimental and numerical data from the optimal (as predicted using the single-objective analysis) and the sub-optimal configurations are displayed in Figure 7. The numerical predictions agree well with experimental results, slightly over-predicting the experimental data in each reactor configuration. The slight deviation may be due to the minor over-prediction of the kinetic degradation rate in the intermediate fluence range (2-4 mJ cm⁻²) by the series-event *E. coli* ATCC 11229 kinetics (Supplemental Figure 6). The experimental validation of the numerical optimization results suggest that the approach used in this study could help design engineers develop an efficient, potentially optimal, UV disinfection system using LEDs, in spite of the increased level of design degree of freedom.

4 CONCLUSIONS

In this study, a numerical optimization routine was coupled with CFD to optimize a point-of-use continuous flow UV-LED disinfecting reactor. Optimal designs were generated at a flow rate of

109 mL/min and 92% UVT using the *E. coli* ATCC 11229 batch response kinetics. The multi-objective analysis improved the design predicted using the single-objective results, which suggests that the single-objective solution converged on a local optimal. A second round of iterations, using a reduced decision space, is a potential technique to improve confidence in the predicted optimal solution, if desired. Regardless, using a defined reactor shape and partially constraining the spatial UV-LED arrangement, the coupled numerical method (CFD linked with an optimization program) was effective at significantly decreasing the design decision space and finding a potentially near-optimal UV-LED reactor solution.

The optimal design required to achieve the $2.0 \log_{10}$ inactivation of the microorganism contained some non-intuitive features, including the spatial UV-LED arrangement and the requisite number of UV-LEDs. The non-intuitiveness is particularly in reference to the seven total UV-LEDs required to achieve the target $\log_{10}$ inactivation, and the exact location of two of the seven UV-LEDs placed along the influent center column. Although the experimental validation tests provided support for the general spatial light arrangement (majority on the effluent side) and the emission wavelength (275 nm), it could not explain every optimal design characteristic. In practical applications, it is conceivable that engineers would not have an equivalent degree of background data, and may therefore design the system sub-optimally. For example, the 260 nm source would appear to be the ideal emission wavelength (given its high germicidal effectiveness). Additionally, it is reasonable that an approximately equal spacing of UV-LEDs should be distributed throughout the reactor system (to minimize the locations absent of light penetration). Two suboptimal designs were experimentally validated to highlight the challenge that stems from designing UV-LED reactors.

544

545 The Non-Optimal #1 design was primarily used to portray the added energy costs that are
546 associated with poorly designing a UV-LED reactor; however, it also supports the idea that the
547 multi-objective analysis presents design alternatives for the engineer. In addition to there being a
548 series of alternative optimal designs existing entirely along the Pareto front, Non-Optimal #1 can
549 also represent an idea for designing reactors that exist in the inferior, but feasible objective
550 space. It is possible that design engineers have restrictions (beyond the modeled constraints)
551 inhibiting the actual design of a UV-LED reactor that lies along the Pareto front. Limitations
552 may include construction difficulties, ease of maintenance, installation, and repair, among others;
553 some of which may be difficult to describe in a numerical model. The additional constraints may
554 force practicing engineers to examine a set of alternative designs meeting a target log
555 inactivation, but are slightly less than optimal, in terms of energy costs.

556

557 Ultimately, the results provide evidence for the need to use CFD and optimization algorithms to
558 design efficient UV-LED disinfection reactors. The challenge with achieving an efficient reactor
559 design is due to the inherent nature of UV-LEDs, which are small point-sources of light capable
560 of being spatially organized in a nearly infinite number of ways. As technology improves and
561 UV-LEDs become more efficient, designs will become even more challenging. The use of 260
562 nm UV LED light sources will become more realistic, meaning that coupling the high kinetic
563 efficiency of 260 nm light with 275-280 nm UV-LEDs will require numerical models to
564 delineate between wavelength, number, spatial orientation of light, and reactor shape. The
565 research reported herein is the first to tackle this design paradigm, and was predictive in
566 generating an optimal design for what is likely to be a key future UV disinfection approach.

5 ACKNOWLEDGEMENTS

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Heuristic Optimization of a Continuous Flow Point-of-Use UV-LED Disinfection Reactor using Computational Fluid Dynamics

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