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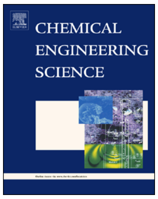

Modeling a continuous flow ultraviolet Light Emitting Diode reactor using computational fluid dynamics

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HIGHLIGHTS

- A CFD model of a UV-LED disinfection reactor was experimentally validated.
- Hydraulics, biodosimetry, and chemical actinometry showed good agreement with model.
- UV-LED reactor demonstrates high efficiency as a point of use disinfection device.

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ABSTRACT

The use of ultraviolet (UV) light for water treatment disinfection has become increasingly popular due to its ability to inactivate chlorine-resistant microorganisms without the production of known disinfection by-products. Currently, mercury-based lamps are the most commonly used UV disinfection source; however, these lamps are toxic if broken during installation or by foreign object strike during normal operation. In addition, disposal of degraded, hazardous mercury lamps can be challenging in rural and developing countries for point-of-use (POU) drinking water disinfection applications. UV Light Emitting Diodes (LEDs) offer an alternative, non-toxic UV source that will provide design flexibility due to their small size, longer operating life, and fewer auxiliary electronics than traditional mercury-based lamps. Modeling of UV reactor performance has been a significant approach to the engineering of UV reactors in drinking water treatment. Yet, no research has been performed on the experimental and modeling of a continuous flow UV-LED reactor. A research study was performed to validate a numerical computational fluid dynamics (CFD) model of a continuous flow UV-LED water disinfection process. Reactor validation consisted of the following: (1) hydraulic analysis using tracer tests, (2) characterization of the average light distribution using chemical actinometry, and (3) microbial dose–response and inactivation using biodosimetry. Results showed good agreement between numerical simulations and experimental testing. Accuracy of fluid velocity profile increased as flow rate increased from 109 mL/min to 190 mL/min, whereas chemical actinometry saw better agreement at the low flow rate. Biodosimetry testing was compared only at the low flow rate and saw good agreement for log inactivation of bacteriophage Qβ and MS-2 at 92% and 80% UV transmittance (UVT). The results from this research can potentially be used for the design of alternative point-of-use drinking water disinfection reactors in developing countries using UV LEDs.

1. Introduction

The use of ultraviolet (UV) light for water treatment disinfection has become increasingly popular due to the ability of UV to inactivate the chlorine-resistant protozoa *Cryptosporidium* and *Giardia*. Other advantages of UV light include no known disinfection by-product (DBP) formation, no resulting taste/odor issues, and over-dosing will not compromise public health (Chatterley and Linden, 2010).

Presently, the majority of UV light technologies used for water treatment are generated by mercury-based lamps. The three most common mercury-based UV sources are low-pressure (LP), low-pressure high output (LPHO), and medium-pressure (MP) lamps. LP and LPHO lamps emit monochromatically at 253.7 nm, at approximately 10^{-4} pounds per square inch (psi), and generate

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low to medium power outputs. Conversely, MP lamps emit polychromatic light (200–400 nm) and operate at much higher temperature, pressure, and intensity than LP and LPHO lamps. Although MP lamps emit higher output energy than LP and LPHO lamps, the broadened wavelengths emitting from the MP lamp reduces its germicidal efficiency (USEPA, 2006).

Recent technological advances has allowed for the use of small Light Emitting Diodes (LEDs) between 5 and 9 mm in diameter that generate light in the germicidal range (Chatterley and Linden, 2010; Bowker et al., 2011). Currently, UV-LEDs operate in the range of 247–365 nm (Gaska et al., 2011). LEDs can be manufactured to produce a desired wavelength of light, which can offer a significant increase in design flexibility over traditional lamp technologies (Shur and Gaska, 2008). The additional design flexibility offered by UV-LEDs provides an opportunity to engineer a more efficient disinfection process. Further drawbacks to traditional UV lamps include its toxic components. Mercury is hazardous to both human health and the environment, and if the lamps are broken during installation, maintenance, disposal, or by foreign-object strike, mercury vapor may enter the drinking water supply or may expose plant personnel (USEPA, 2006). Replacement and disposal of hazardous LP lamps can be especially difficult in developing countries where energy-saving POU disinfection processes are desired. In these rural and undeveloped regions, it is critical to implement systems that provide energy savings, long light replacement intervals, and components that are safe to handle and dispose. LEDs provide these benefits, as they have been recognized as a system that saves energy (input power is in range of mW), lowers maintenance cost, lengthens replacement intervals, and are non-toxic (Chatterley and Linden, 2010). In addition, LEDs are compact in size, shape, durable in transit and handling, easily reconfigurable, require less auxiliary electronics than mercury based lamps, and ensure robust construction (Chatterley and Linden, 2010). For all these reasons, LEDs have the potential (assuming wall plug efficiency continues to improve) to replace fluorescent lamps for point-of-use drinking water disinfection systems in developing countries.

Until now, only limited research has been performed on UV-LED disinfection. Hamamoto et al. (2007) developed a new UV-LED device incorporating 8 LEDs of 365 nm wavelength. The study focused on the primary inactivation method of various bacterial strains in the UV-A range. Vilhunen et al. (2009) tested *E. coli* (K12) in two batch reactors using an array of 10 LED lights (269 nm and 276 nm). Their study revealed greater inactivation efficiencies using the 269 nm lights; possibly because of a peak DNA absorbance near 260 nm. Chatterley and Linden (2010) found slightly higher inactivation of *E. coli* K12 for 265 nm collimated beam LEDs than for a 254 nm collimated beam LP lamp; this may also be related to the peak DNA absorbance near 260 nm. Bowker et al. (2011) determined the response kinetics of MS2, T7, and *E. coli* 11229 by conducting bench scale collimated beam experiments with a LP mercury lamp and two different arrays of LEDs (255 nm and 275 nm). The study revealed that MS-2 and T7 displayed similar response kinetics for all of the sources with few exceptions, where MS-2 showed a slightly higher inactivation rate with the LP mercury lamp and T7 displayed a lower inactivation with the 255 nm UV-LEDs compared to other sources. Gaska et al. (2011) tested the efficiency of a point-of-use deep UV-LED (DUV) disinfection system on the inactivation of bacteriophage MS-2 using 272–273 nm wavelengths. Their research found 1.6 log inactivation of MS2 at 0.5 l/min flow rate (34 mW input power).

Although a steadily increasing amount of experimental research has been performed using UV-LEDs, only limited research has combined the results from a computational fluid dynamics (CFD) model and experimentally validated the numerical results (Wang et al., 2012). In their work, Wang et al. (2012) performed a CFD model of a photo-catalytic process for odor removal in a continuous flow reactor. The limited validation research is largely due to the current state of UV-LED technology, where UV-LEDs are at the initial stage of development and therefore have limited commercial point-of-use applicability to date. Nonetheless, CFD is still considered a powerful and well-established tool for UV reactor modeling and design (Liu et al., 2007; Wols et al., 2010). Several authors used CFD calculations to validate reactor hydraulics, and in most of the cases, a relatively good agreement was established (Ducoste et al., 2005; Sozzi and Taghipour 2006; Zhao et al., 2009; Wols et al., 2010). Knowledge of the reactor hydraulics, irradiance, and microbial response of the reactor is necessary for validation for a variety of reasons. The hydraulic validation provides comprehensive information about the flow field, pressure distribution, and mixing behavior of the fluid inside a reactor (Wols et al., 2010). Chemical actinometry is vital to understanding the average irradiance inside the reactor at various operating conditions (flow rate, water transmittance, and lamp power output). For a given set of reactor operating conditions, the hydraulics and average irradiance can provide information about the average dose within the reactor. The final validation component involves the prediction of the microbial log inactivation. These validation approaches, although performed separately, are combined to provide important understanding of the model performance to predict the UV reactor behavior. In this study, the CFD-predicted numerical solutions were validated by a NaCl step input tracer test (hydraulic validation), iodide/iodate chemical actinometry (average irradiance), and biodosimetry (microbial inactivation).

2. Methods

2.1. Hydraulic characterization

The hydraulic characteristics of a UV reactor is generally determined by a tracer test, where a non-reactive tracer is injected at the inlet under steady state flow conditions, and time dependent tracer concentration is measured at the outlet. In this study, a positive step tracer test was conducted where a NaCl (127 μS/m) (Certified ACS Crystalline S271-1, Fischer Scientific Pittsburg PA) solution was used as a non-reactive tracer. NaCl solution was injected as a continuous input at the inlet and samples were collected at the outlet at an interval of 5% of theoretical residence time. Conductivity of all the samples were measured with a digital conductivity meter (PH/CON 2700 MTR W/PROBE, Cole-Parmer, Court Vernon Hills, Illinois) and normalized to the initial conductivity of the salt solution. These normalized values were plotted against elapsed time to get the cumulative residence time distribution curve $F(t)$. Tracer simulations were performed using COMSOL Multiphysics (version 4.3a, COMSOL, Inc., Burlington, MA). The transport of the tracer chemical was performed using the flow field (as calculated using the continuity and Navier–Stokes equations) and the scalar convective-diffusion transport equations (Liu et al., 2007). The back ground fluid transport was performed at steady state while the tracer transport simulation was performed under transient conditions to replicate the experimental conditions.

2.2. Fluence rate characterization

The fluence rate characterization was performed using chemical actinometry. Standard actinometry solution was created using potassium iodide, potassium iodate, and borax. The concentrations of iodide, iodate, and borax used were 0.6 M, 0.1 M and 0.01 M, respectively. When the iodate and iodide are exposed to UV light, the chemical species react to form triiodide. The triiodide