ABSTRACT

Ahmed, Yousra M.H.I.H. PhD., Purdue University, April 2017. Stochastic Evaluation of Disinfection Performance in Large-Scale, Open-Channel UV Photoreactors. Major Professor: Ernest R. Blatchley III.

Ultraviolet (UV) irradiation is an effective disinfection method for inactivating waterborne microbial pathogens and/or indicator organisms in wastewater or drinking water treatment. The performance of UV disinfection reactors depends strongly on several design and operation parameters. Design guidelines for UV disinfection systems generally require compliance with inactivation standards based on indicator organisms (e.g. *E. coli*, fecal coliforms…etc) or validation of delivery of a nominal UV dose requirement defined as the "average" dose or Reduction Equivalent Dose (RED). Biodosimetery is the default method for experimental validation for UV reactors. However, conventional validation tests oftentimes are impractical and costly to apply for large-scale UV system; moreover, they are inadequate for describing the actual variability attributes of the UV disinfection system and may also induce biased estimates for UV reactor performance which can be associated with over-design and increases in capital and/or operating costs. The development of alternative methods for characterizing photoreactor performance, such as numerical simulation techniques, may facilitate photoreactor design optimization for UV disinfection process based on detailed knowledge of the flow field, the fluence rate distribution, and the dose distribution that characterize these systems.

The objective of the research described herein was to apply combinations of computational fluid dynamics and irradiance field models (aka, CFD-I models) to simulate the performance of full-scale UV disinfection systems, including variability. The central hypothesis of this research was that CFD-I models (which are essentially deterministic, by nature) can be applied via a non-deterministic (stochastic) approach to simulate process performance including variability, by allowing appropriate variations in input variables. As such, this approach has the potential to yield numerical simulation results that can be used to refine reactor design and tailor operating conditions, so as to improve reactor performance and efficiency.

Combined application of CFD simulations and ray tracing was employed to model the flow field (with the embedded particle tracking models) and fluence rate field, respectively, for the

existing UV disinfection system at the Belmont WWTP in Indianapolis, IN, which comprises 7 channels with 384 high-output, low-pressure mercury amalgam UV lamps in each channel parallel to the flow, and two full-scale UV disinfection test channels, Aquaray® HiCAP, and LIT MLV-24A, which are designed for wastewater disinfection and water reuse applications, which use vertically oriented LP-HO mercury lamps.

Ray tracing has been widely used for modeling of optical (visible) lighting systems, which include visible light, LED, and solar light sources. Ray tracing simulates the spatial distribution of electromagnetic radiation from one or more sources by tracking a large number of rays that are assumed to emanate from the source(s) in a probabilistic manner. This approach allows rigorous simulation of optical behavior, including refraction, reflection, absorbance, and shadowing. By simulating the behavior of a large population of rays, it is possible to accurately describe the distribution of radiant energy within the system. In this study, fluence rate calculations were performed using commercial ray-tracing software (Photopia, LTI Optics, Westminster, CO). The practical application of ray-tracing was evaluated and validated through comparisons with experimental methods and other numerical models for small scale and large scale UV reactors. The ability of the ray tracing approach to accurately simulate fluence rate fields in UV photo-reactors was demonstrated, as were challenges and limitations related to ray tracing analysis implementation. For larger, more complex systems where physical measurements are more challenging, the implications of the simulation results are discussed.

Monte Carlo simulations based on a CFD-I modeling approach were applied to predict variability in UV disinfection performance under the influence of the observed variability in the input parameters (including dose response behavior of *E. coli* and MS2, initial bacterial count) for different reactors and operating conditions. The input parameters of the systems were measured using standardized experimental methods and on-site measuring devices. The results showed that variability in *E. coli* dose-response parameters (K_A K_B, c) and N_o plays an important role in the variability in predictions of effluent *E. coli* (N) and RED. However, MS2 dose-response parameters caused insignificant variation in the predictions of RED.

The stochastic CFD-I approach was used to simulate the behavior of the Belmont system for seven operating conditions that span the range of common use of this system. These simulations indicated that the likelihood of violating the regulatory permits for *E. coli* inactivation was essentially zero for some operating conditions, which indicated that it may be possible to reduce the amount of UV power applied in treatment; by extension, this implies the potential to reduce input electrical power, while retaining compliance with treatment objectives.

On the other hand, simulation of a hypothetical worst-case scenario at the Belmont UV system, based on peak flow rate, 60% lamp power and UVT 60%, and is operating by only one bank of lamps in each channel, resulted in 16% probability that N will exceed permit limitations for *E. coli*, which suggests that these operating conditions might be not sufficient to achieve reliable compliance with treatment objectives and permit limitations, given the observed variability of the inputs.

Sensitivity analysis between the remaining viable *E. coli* in the effluent stream (N) and the variable inputs, including UV dose-response parameters (DRP) and the initial concentration of *E. coli* (N_o), using Spearman's rank test revealed the presence of associations between the variable output N and the variable inputs of the DRP and N_o; the degree and the ranks of this correlation appeared to be dependent on the operating conditions applied. Uncertainties in the CFD-I numerical simulations results, such as those that are attributed to selection of the turbulence model, the number of particle trajectories, and the number of simulated rays were also addressed in this work.

The results suggested that using the deterministic numerical approach based on single-valued input parameters is unrealistic and can be misleading in the assessment of reactor performance. The main benefit of using the stochastic (non-deterministic) approach for the numerical predictions of the UV disinfection process is the comprehensive description of the system performance under the influence of variability. Moreover, quantifying variability in UV disinfection design by application of Monte Carlo methods offers the possibility to optimize the operating conditions and costs based on the estimated likelihood margins of disinfection (inactivation) rate.

A challenge to the application of this approach is the computational requirements of the CFD-I simulations to determine the dose distribution of the UV reactor for the range of relevant operating conditions. Thus, part of this study focused on developing interpolation and scaling methods that allows estimating unknown reactor UV dose distributions under various operating conditions with a reduced number of CFD-I simulations; this method was constructed based on the dependence relationships between UV doses and the operating parameters (i.e. flow rate, UVT, and lamp power).

Lastly, a software tool was developed to facilitate programming of the stochastic Monte Carlo calculations for predicting the UV system performance (*i.e.*, fractional inactivation, effluent microbial concentration, and RED) in accordance with the variability in dose-response parameters and N_o. The tool also includes a programmed algorithm which can be used to find optimum operating conditions for the UV disinfection process This object-oriented program was constructed using MATLAB app design features.