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Optical fluence modelling for ultraviolet light emitting diode-based water treatment systems

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ABSTRACT

This work presents a validated optical fluence rate model optimised for ultraviolet light-emitting diodes (UV-LEDs), which allow a very wide range of emission wavelengths and source geometries to be used in water treatment units. The model is based on a *Monte Carlo* approach, in which an incremental ray-tracing algorithm is used to calculate the local volumetric rate of energy absorption and subsequently convert it to the local fluence rate distribution for an UV-LED water treatment chamber of arbitrary design. The model includes contributions from optical reflections and scattering by treatment chamber walls and from scattering due to particulates and/or microorganisms. The model successfully predicts optical fluence rates in point-of-use water treatment units, as verified using biodosimetry with MS-2 bacteriophage at a UV-LED emission wavelength of 254 nm. The effects of chamber geometry are also modelled effectively and are consistent with the inactivation data for *E. coli* at 254 nm. The data indicate that this model is suitable for application in the design and optimisation of UV-LED-based water treatment systems.

1. Introduction

Ultraviolet light emitting diodes (UV-LEDs) are of growing interest in the field of water treatment. They offer significant advantages compared to conventional mercury vapour lamps for point-of-use water treatment applications, including low power requirements, mechanical robustness, small form factors and long lifetimes. Although further technological development is still required, UV-LEDs have the potential to show very high electrical efficiencies (Khan et al., 2008; Kneissl et al., 2011). Furthermore, the spatial distribution of light emission from UV-LEDs can be controlled through design of the device packaging, while the emission wavelength can be tuned by varying the composition of the active semiconducting light-emitting regions of the device. This versatility offers great promise for achieving higher disinfection efficiencies at wavelengths other than the conventional 254 nm line emitted by low pressure UV lamps (Linden and Thurston, 2007; Coohill and Sagripanti, 2009; Chen et al., 2009).

However, differences in UV wavelength will affect the UV disinfection efficiency (Setlow and Boyce, 1960; Gates, 1929; Linden et al., 2001). Optical fluence modelling across different UV wavelengths is therefore important for disinfection system testing and validation, as fluence determination by current biodosimetry methods is validated only for 254 nm (Bolton and Linden, 2003; Kuo et al., 2003; National Water Research Institution, 2012). The spatial non-uniformity of the UV fluence will also affect the UV disinfection efficiency (Sommer et al., 1996). Optical fluence modelling is therefore

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also important for the design of UV disinfection systems, in which the UV fluence non-uniformity should be minimised to maximise disinfection efficiency. Other fluence determination methods are not yet adequate in the case of significant fluence non-uniformity: for example, the average fluence determined using actinometry can differ significantly depending on the chemical species and on the degree of fluence non-uniformity, even when used in combination with mathematical modelling, probably due to uncertainty in the wavelength and fluence dependence of the quantum yield values (Jin et al., 2006).

Furthermore, fluence modelling is required for basic microbiological studies using UV-LEDs, in which the UV fluence must be related accurately to the microbiological inactivation rates. Unfortunately, the protocol established previously for mercury lamps (Bolton and Linden, 2003) assumes that the UV fluence is uniform and equivalent to the irradiance. This assumption is valid for a collimated UV lamp, but not for UV-LEDs. Although collimation of light from UV-LEDs has been attempted (Bowker et al., 2011), the relatively low output powers of the UV-LEDs meant that they had to be placed close to the sample using a relatively wide collimating tube in order to provide enough power for the experiments. These limitations meant that collimation could not truly be achieved. Therefore, in the case of UV-LEDs, optical modelling is needed to calculate the fluence delivered accurately.

Different optical fluence models have already been developed in response to these concerns, which are also relevant to existing UV lamp technologies. For example, Liu et al. (2004) reviewed fluence calculation models, based on the solution to the radiation transfer equation (RTE) at each point within a treatment chamber. These models usually neglect the contributions from light reflected or scattered by the chamber walls (Sozzi and Taghipour, 2006; Wols et al., 2010; Bohrerova et al. 2006). Diffuse scattering can be modelled within the RTE method, as described by Bo Yu et al. (2008), though this assumes either a cylindrical chamber with a single lamp emitting normal to the plane of the wall, or assumes that the walls are purely diffuse reflectors. Li et al. (2012), amongst others (Sommer et al., 1996), have highlighted the importance of accurate modelling of reflections by internal chamber walls, which should be taken into account by an effective optical fluence model.

Grapperhaus et al. (2007) used an alternative approach, using a commercial ray tracing program (OptiCAD™) to model fluence in a quasi-collimated beam apparatus, accounting for ray attenuation by the water plus absorption, scattering or reflection by chamber walls. The software modelled the total light absorption within the sample, but did not provide information on fluence uniformity, which is essential for the design of effective UV-LED chambers.

Related optical modelling approaches have also been used in other fields. For example, the local volumetric rate of energy absorption (LVREA) has been used to assess the efficiency of surface catalytic processes in photocatalytic reactors, using the discrete ordinate (DO) and finite volume (FV) approaches, alongside *Monte Carlo* (MC) methods (Pareek et al., 2008). Recently Valades-Pelayo et al. (2014), also presented a MC method capable of accurately modelling a heterogeneous medium in a chamber of arbitrary design. However, in this approach the LVREA was calculated, rather than the local fluence rate (LFR) distribution which is needed to assess fluence uniformity within a chamber.

To address the limitations of current modelling approaches, we have therefore developed an MC-type model in which an incremental ray-tracing algorithm is used to calculate the LVREA and subsequently convert it to the LFR distribution for an UV-LED water treatment chamber of arbitrary design. The model also incorporates all contributions from chamber wall reflections and scattering. This work employs a ray-tracing method in which the rate of radiation absorption is calculated and converted to local fluence rates. The model has been validated against MS-2 biodosimetry data as well as for the *E. coli* suspensions used in microbiological studies in which considerable optical scattering occurs. The primary purpose of the model is to assist the design and development of small-scale point of use water treatment systems using UV-LEDs. The model is open source and is freely available online at http://nitrides.net/research/fluence_rate_project/.

2. Model design

In this model, multiple UV rays are incrementally propagated through a chamber of specified dimensions and their power attenuated according to the Beer–Lambert equation; incremental losses being recorded stepwise at each voxel within a Cartesian grid bounded by the chamber walls. A 3-dimensional grid of LVREA values is recorded as a result. Multiple rays are generated by a spatially uniform Monte Carlo algorithm, with each ray's power weighted to reproduce the spatial emission profile of a UV-LED. Then the rays are propagated along different paths, undergoing reflection or scattering events, until convergence is observed in the resulting LVREA distribution, where convergence is defined as a variation of <0.1% in the value of each voxel on each iteration. This iterative process is illustrated in Fig. 1.

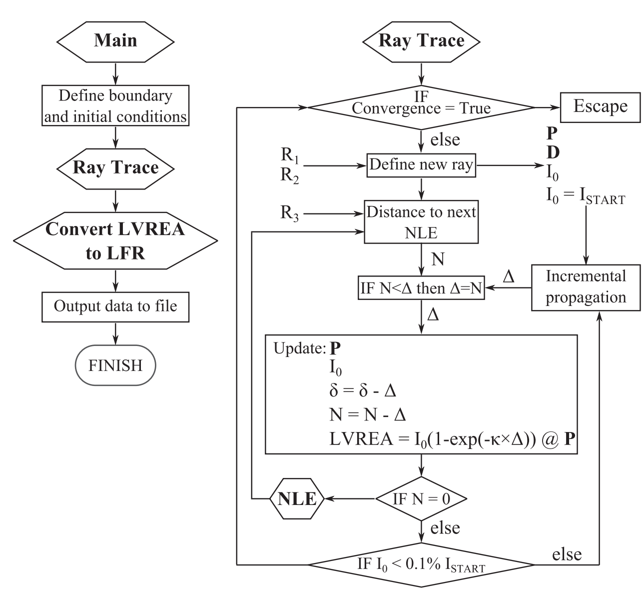

Fig. 1 – Flow chart showing the main processes in the model, including details of the ray tracing algorithm.