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A modeling approach to estimate the solar disinfection of viral indicator organisms in waste stabilization ponds and surface waters

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ABSTRACT

Sunlight is known to be a pertinent factor governing the infectivity of waterborne viruses in the environment. Sunlight inactivates viruses via endogenous inactivation (promoted by absorption of solar light in the UVB range by the virus) and exogenous processes (promoted by adsorption of sunlight by external chromophores, which subsequently generate inactivating reactive species). The extent of inactivation is still difficult to predict, as it depends on multiple parameters including virus characteristics, solution composition, season and geographical location. In this work, we adapted a model typically used to estimate the photodegradation of organic pollutants, APEX, to explore the fate of two commonly used surrogates of human viruses (coliphages MS2 and ϕX174) in waste stabilization pond and natural surface water. Based on experimental data obtained in previous work, we modeled virus inactivation as a function of water depth and composition, as well as season and latitude, and we apportioned the contributions of the different inactivation processes to total inactivation. Model results showed that ϕX174 is inactivated more readily than MS2, except at latitudes >60°. ϕX174 inactivation varies greatly with both season (20-fold) and latitude (10-fold between 0 and 60°), and is dominated by endogenous inactivation under all solution conditions considered. In contrast, exogenous processes contribute significantly to MS2 inactivation. Because exogenous inactivation can be promoted by longer wavelengths, which are less affected by changes in season and latitude, MS2 exhibits smaller fluctuations in inactivation throughout the year (10-fold) and across the globe (3-fold between 0 and 60°) compared to ϕX174. While a full model validation is currently not possible due to the lack of sufficient field data, our estimated inactivation rates corresponded well to those reported in field studies. Overall, this study constitutes a step toward estimating microbial water quality as a function of spatio-temporal information and easy-to-determine solution parameters.

1. Introduction

The discharge of wastewater or untreated human waste into the environment leads to the continuous input of enteric viruses into surface water (Okoh et al., 2010; Simmons and Xagoraraki, 2011). Once in the environment, the infectivity of enteric viruses is compromised by various environmental stressors, including exposure to sunlight, temperature fluctuations, or predation by microorganisms (Fong and Lipp, 2005). Sunlight is known to be particularly effective at reducing virus infectivity, and this property has been exploited for the design of effective natural wastewater treatment systems, such as waste stabilization ponds (WSPs, also known as waste treatment ponds or treatment lagoons) (Davies-Colley et al., 1999, 2000). The processes involved in the solar disinfection, or photoinactivation, of viruses in environmental waters are now fairly well understood (Davies-Colley et al., 1999; Kohn and Nelson, 2007; Mattle et al., 2015; Silverman et al., 2013; Sinton et al., 2002). Yet, we are only just beginning to integrate this information into a quantitative framework that allows the prediction of disinfection efficiencies in WSPs, or of inactivation rates in sunlight-exposed surface waters systems. Such predictive models, however, are instrumental for optimizing the design of natural treatment systems, and assess the water quality of drinking water sources and recreational waters, and to assess risks for water reuse planning (UN, 2015).

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Photoinactivation of viruses occurs by two distinct processes, endogenous (direct or indirect) and exogenous (only indirect) inactivation (Davies-Colley et al., 1999). Endogenous inactivation is mediated by virus-internal chromophores, such as the nucleic acid or aromatic amino acids in the protein coat, which absorb light in the solar range. Upon light excitation, these internal chromophores can degrade and cause the virus to become inactivated. This process is referred to as direct inactivation. Alternatively, endogenous inactivation can occur in an indirect fashion. Hereby, the excited chromophores transfer energy or electrons to dissolved oxygen or other solution constituents, which leads to the formation of a variety of transient reactive species (e.g., singlet oxygen). Along with the excited chromophores themselves, these reactive species can then oxidize surrounding virus constituents and thereby cause inactivation. While direct and indirect endogenous inactivation occur simultaneously, direct sunlight inactivation of viruses (F-DNA phages) has been shown to be efficient, whereas indirect endogenous inactivation was of minor importance (Davies-Colley et al., 1999). It can thus be assumed that endogenous inactivation mainly occurs in a direct manner.

In indirect exogenous inactivation, reactive species are produced by virus-independent chromophores present in solution. In natural waters, they include chromophoric dissolved organic matter (CDOM), nitrate or nitrite, which can contribute to the production of several reactive species ($^{\bullet}OH$, $CO_3^{-\bullet}$, $^1O_2$ and CDOM triplet states, $^3CDOM^*$) (Boule et al., 2005). The efficiency of exogenous inactivation is thus strongly dependent on the characteristics and photoreactivity of the solution (Carratalà et al., submitted; Silverman et al., 2013). In addition, the contribution of the exogenous process to total inactivation depends strongly on the virus under consideration. For example, exogenous inactivation significantly contributed to the photoinactivation of human adenovirus (Silverman et al., 2013), human rotavirus (Romero-Maraccini et al., 2013), human echovirus (Carratalà et al., submitted), phages PRD1 and MS2 (Kohn and Nelson, 2007; Silverman et al., 2013) and native F-RNA phages (Davies-Colley et al., 1999; Sinton et al., 2002). In contrast, its importance was only minor in the solar inactivation of poliovirus (Silverman et al., 2013), porcine rotavirus (Romero et al., 2011; Romero-Maraccini et al., 2013), and native F+ DNA phages (Davies-Colley et al., 1999; Sinton et al., 2002).

In recent work, we have demonstrated that the total photoinactivation of two commonly used surrogates of human viruses, phages MS2 and ϕX174, can be estimated by simply summing up the contributions of endogenous and exogenous inactivation (Mattle et al., 2015). Specifically, we formulated the following model:

$$\frac{dC_{virus}}{dt} = -k^0_{virus}C_{virus} = -P_a^{virus}\Phi_{virus} - \sum_x k_{virus,x}C_{ss,x}C_{virus} \qquad (1a)$$

$$C_{virus} = C_{virus,0}e^{-k^0_{virus}t} \qquad (1b)$$

Hereby the subscript “virus” is a placeholder for “MS2” or “ϕX174”. C_{virus} and $C_{virus,0}$ are the infective virus concentrations at times t and 0 respectively, and k^o_{virus} is the first-order photoinactivation rate constant. The term $-P_a^{virus}\Phi_{virus}$ quantifies the direct endogenous inactivation($= -k^0{}_{endo}C_{virus}$), with Φ_{virus} being the virus-dependent photoinactivation quantum yield (number of viruses inactivated/number of photons absorbed by the virus), and P_a the photon flux absorbed by the virus. The second term of eq. (1a) describes the contribution of exogenous inactivation, whereby four relevant reactive species x were considered: singlet oxygen ($^1O_2$), hydroxyl radical ($^{\bullet}OH$), carbonate radical ($CO_3^{-\bullet}$) and excited (triplet state) chromophoric dissolved organic matter ($^3CDOM^*$). It was found that virus inactivation by these reactive species can be described by apparent second-order kinetics, where $k_{virus,x}$ is the second-order inactivation rate constant, and $C_{ss,x}$ is the steady-state concentration of the reactive species under consideration. The experimental methods used to obtain the model parameters are described elsewhere (Mattle et al., 2015). This approach successfully predicted the inactivation of MS2 and ϕX174 in laboratory experiments using WSP water and a solar simulator. In contrast, the inactivation of human adenovirus was less accurate, and was underestimated two-fold.

Silverman et al. (2015) pursued a similar approach. This group also considered total solar inactivation as the sum of endogenous and exogenous processes. However, the approach proposed by Silverman et al. differed from ours in two aspects: first, instead of a virus-dependent quantum yield, they used a virus- and wavelength-dependent sensitivity coefficient to describe endogenous inactivation. Second, rather than considering different reactive species individually, they considered inactivation by singlet oxygen as a proxy for all exogenous processes. Using these assumptions, they were able to estimate the inactivation of MS2 observed in lab experiments and an open-water wetland.

A limitation of the models used thus far is that they focused on the context of a specific solution, water body, and geographic location. Here, we exploit our model to expand our predictions of photoinactivation rates to a range of conditions. Specifically, we model the inactivation of MS2 and ϕX174 as a function of water depth, geographic setting (in terms of latitude), season, and water characteristics. The combination of these two viruses is ideally suited to explore the boundaries of photoinactivation, as they exhibit opposite sensitivities to endogenous and exogenous processes: MS2 is sensitive to exogenous inactivation but not too sensitive to endogenous inactivation, whereas ϕX174 is very sensitive to endogenous inactivation but resistant to exogenous inactivation (Mattle et al., 2015; Sommer et al., 2001). Finally, we compare our model output to published data on solar disinfection, to demonstrate our model's general applicability.

2. Methods

2.1. Photochemical modeling

The model assessment of virus photoinactivation was carried out with the APEX software (Aqueous Photochemistry of Environmentally-occurring Xenobiotics; available for free download as Electronic Supplementary Information of Bodrato and Vione, 2014), which predicts photochemical reaction kinetics from photoreactivity parameters (quantum yields and second-order reaction rate constants with reactive species) and from data of water chemistry and depth (Bodrato and Vione, 2014; Vione, 2014). APEX is based on a photochemical model, validated by comparison with field data of phototransformation kinetics in surface freshwaters (De Laurentiis et al., 2013; Maddigapu et al., 2011; Marchetti et al., 2013).

The absorption of radiation by the photosensitizers (CDOM, nitrate and nitrite) and the studied substrates is computed by taking into account competition for sunlight irradiance in a Lambert–Beer approach (Bodrato and Vione, 2014; Braslavsky, 2007). APEX applies to well-mixed waters and its results are average values over the water column. Therefore, they include the contributions of the well-illuminated surface layer and of darker water at the lower depths (Loiselle et al., 2008).

The solar spectrum was obtained for fair-weather conditions. For summer and seasonal data at mid-latitude, we used the standard APEX spectra that are taken from Frank and Klöpffer (1988). Data as a function of latitude were obtained with the NCAR-TUV