Modeling and Validation for the Determination of UV Dose in UV Reactors

James R. Bolton

Executive Director
International Ultraviolet Association
President
Bolton Photosciences Inc.

628 Cheriton Cres., NW, Edmonton, AB, Canada T6R 2M5
Tel: 780-439-4709; Fax: 780-439-772
Email: jbolton@boltonuv.com; Web: www.boltonuv.com
Outline

• Introduction
• Some Definitions
• Modeling of UV Reactors
• UV Distribution (UVD) Models
  • Assumptions
  • Mathematical model
  • Model validation
• Computational Fluid Dynamics (CFD) Models
• Interaction of UVD with CFD Programs
Introduction

- Regulators require that UV reactors be ‘validated’ to certify that they will produce a fluence (UV dose) above a ‘critical’ value (usually 400 J/m²)
- Validation must be carried out using ‘biodosimetry’, a process that is complex and expensive
- UV companies need a model that will provide:
  - an accurate estimate of performance before embarking on a biodosimetry test
  - feedback on design changes to optimize the reactor performance

Biodosimetry involves challenging a UV reactor with a non-pathogenic microorganism (e.g., *B. subtilis*) and determining the log inactivation against a laboratory-determined fluence-response curve.
Definitions

• *Irradiance* \((E) \ (W \ m^{-2})^*\) is the total radiant power of all wavelengths incident from *all incident* directions onto an infinitesimally small area \(dA\), divided by \(dA\).

* Sometimes given as mW cm\(^{-2}\) (1 mW cm\(^{-2}\) = 10 W m\(^{-2}\))
Definitions (cont.)

- **Fluence Rate** \((E') (W \, m^{-2})^*\) – the radiant power of all wavelengths incident from all directions onto an infinitesimally small sphere of cross-sectional area \(dA\), divided by \(dA\).

  * Sometimes given as mW cm\(^{-2}\) (1 mW cm\(^{-2}\) = 10 W m\(^{-2}\)) – also (erroneously) referred to as Irradiance
• **Fluence** \((H')\) or **UV Dose** (J m\(^{-2}\))\(^*\) is the total radiant energy of all wavelengths incident from all directions onto an infinitesimally small sphere of cross-sectional area \(dA\) (cm\(^2\)), divided by \(dA\).  

\[ \text{Fluence} = \frac{\text{Total radiant energy}}{dA} \]

\* Sometimes given as mJ cm\(^{-2}\) or mW.s/cm\(^2\) \((1 \text{ mJ cm}^{-2} = 10 \text{ J m}^{-2})\)
Modeling of UV Reactors

- Modeling the performance of UV Reactors requires two distinct models:
  - UV Distribution (UVD) Model
    - describes how the fluence rate (irradiance) varies throughout all volume elements in the reactor
  - Computational Fluid Dynamics (CFD) model
    - Describes the flow and velocity patterns as the water passes through the UV reactor
• **Point Source (PS) Model** – assumes that the fluence rate $E$ falls off spherically from a tiny “point” source as

$$E = \frac{P}{4\pi r^2} 10^{-ar}$$

- $P$ = the radiant power (W) of the source
- $r$ = distance (cm) from the point source
- $a$ = the absorption coefficient (cm$^{-1}$) of the medium

• Not suitable for modeling UV lamps
UVD Models (cont.)

- **Segment Source (SS) Model** – assumes that the fluence rate $E$ falls off from a tiny “cylindrical segment”.

$$E = \frac{P \cos \theta}{4\pi r^2} 10^{-ar}$$

$\theta$ = the angle of an emanating ray to the plane of a cylindrical segment

Tiny cylindrical segment emitting from the exposed surface of the segment.
UVD Models (cont.)

- **Modified Line Source Integration (MLSI) Model** – assumes that the fluence rate $E$ falls off radially from a “line” source as

$$E' = \frac{P}{4\pi Lx} 10^{-ax} \left[ \tan\left(\frac{L/2 + H}{x}\right) + \tan\left(\frac{L/2 - H}{x}\right) \right]$$

$L$ = length of a linear lamp  
$H$ = height above center of lamp  
$x$ = radial distance from lamp
UVD Models (cont.)

- **Multiple Point Source (MPS) Model** – models a linear lamp as a line of multiple “point sources” (about 1000).

- **Multiple Segment Source (MSS) Model** – models a linear lamp as a line of multiple cylindrical “segments” (about 1000).
An Example of a UVD Model*

- Published by Bolton in 2000
- Originally a “Multiple Point Source” Model.*
- Incorporates refraction and reflection at the air/quartz/water sleeve interface.
- Later modified to a “Multiple Segment Source” Model as a result of validation experiments (see below).
- Uses 1001 “Segments” to approximate a linear lamp.

An Example of a UVD Model (cont.)

[Diagram showing UV Lamp, Quartz Sleeve, irradiated volume, symbols and equations]

- \( s \sin \theta_1 \)
- \( \theta_1 \)
- \( \theta_3 \)
- \( A_1 \)
- \( A_3 \)
- \( I \)
- \( x \)
- \( S \)
- \( H \)
- \( H' \)
- \( h \)
- \( m \)
- \( L \)

Irradiated volume
UV Distribution in an Annular UV Reactor

Fluence Rate Distribution (95 %T)
1 kW lamp, 25% UVC Effic., 8 cm long, quartz radius = 2.0 cm

Fluence Rate (W/m²)

1.6
3.2
4.8
6.4

Radial Distance (cm)

Longitudinal Distance (cm)

quartz sleeve

one half of UV lamp
Multiple Lamps

- One first calculates the annular fluence rate distribution in high resolution around a single UV lamp. This is then stored as a ‘lookup’ table.
- From a given volume element, the radial and longitudinal distances to the center of each lamp in the array are calculated.
- One then ‘Looks Up” the fluence rate for each lamp.
- The total fluence rate is then the sum of the fluence rate contributions from all of the lamps.
UV Distribution in a Multiple Lamp UV Reactor

24 Lamp UV Reactor

Fluence Rate (W/m²)

X (cm)  Y (cm)
UV Distribution in a Multiple Lamp UV Reactor (cont.)

%T = 65%
UV Distribution in a Multiple Lamp UV Reactor (cont.)

% $T = 50\%$
UV Distribution in a Multiple Lamp UV Reactor (cont.)

\[ \% T = 35\% \]
An Example of a UVD Model (cont.)

Broadband Lamps

• Some UV lamps (e.g., medium pressure lamps) emit over a broad range of wavelengths. The ‘germicidal’ wavelength range is considered to be 200 – 300 nm.

• Divide the 200 – 300 wavelength range into twenty 5 nm bands and assume monochromatic behavior in each band.
An Example of a UVD Model (cont.)

Broadband Lamps

• For each band one requires:
  • the $\% T$ (1 cm path length) of the water.
  • the relative spectral emittance of the lamp.
  • the quartz transmittance
  • germicidal factor

• One carries out twenty calculations and then weights each fluence rate by the product of the relative spectral emittance and the germicidal factor to determine the ‘germicidal’ single lamp fluence rate distribution.
Validation* of UVD Models

• Used quartz ‘spherical actinometers’ filled with a KI/KIO₃ solution to experimentally measure the fluence rate.
• Arranged 34 quartz spheres (1 cm OD) on a scaffold around a single UV lamp in an annular UV reactor.
• Determined the fluence rate distribution for %T = 70% and 100%.

Validation* of UVD Models (cont.)

- Studied both a low pressure (monochromatic at 254 nm) and a medium pressure UV lamp.

- The results of agreed with the experimental results very well, but only when the model was modified from a MPS to a MSS model.
Spherical Actinometry
UV Reactor
Fluid Dynamics Modeling

- Various models have been developed to take into account the laws of fluid dynamics as the water passes through a UV reactor.
- These models are generally called ‘Computational Fluid Dynamics’ (CFD) models.
- They provide for the UV reactor:
  - velocity distributions
  - flow rate patterns
  - fluence (UV dose) distributions (this requires a UV light distribution).
Coupling of UVD Models with CFD Programs

- The CFD Program produces a file containing the coordinates of all the volume elements it needs to carry out the CFD analysis.
- This file is read into the UVD model, which then calculates the fluence rate for each volume element in the reactor.
- The UVD program then generates the same input file but with the fluence rate appended for each volume element.
- This ‘output’ file then goes back to the CFD program so that it can determine the fluence for each particle that passes through the reactor.
An Example of UV Reactor Modeling

Comparison of Reduction Equivalent Doses (REDs) from biodosimetry with predicted REDS from a CFD analysis for a 36 inch (0.91 m) diameter 6-lamp UV reactor with the lamps perpendicular to flow;

Source – Keith Bircher, Calgon Carbon Corporation
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(IUVA)

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