# Integrated dose simulation tool for UV-LED reactors

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## Introduction

Using virtual prototyping for the design of UV-LED reactors can help significantly to reduce the cost and development time. Without the proper simulation tools, the reactor design may need to go through multiple design revisions and prototyping stages without delivering the required dose or LRV at the end. Complete simulation of a reactor's performance requires precise modelling of reactor's hydrodynamics, optics and microbial kinetics, each of which are equally important for an accurate reactor simulation. Hydrodynamic simulation can be quite challenging if not all the parameters are considered or set properly. Mesh quality, fluid flow models including turbulence, and particle tracking setting can all significantly affect the flow simulation and the dose performance, respectively. In addition, optical simulation will equally be important to achieve an accurate prediction of the reactor's performance. Precise simulation of the LED die, package, radiation pattern and wavelength, and modelling of optical surfaces will all influence the accuracy of the simulation tool. Eventually the results of hydrodynamics simulation and optical simulation need to be integrated to measure the overall reactor's performance in terms of dose and LRV. We have used our in-house tool to predict a reactor's performance and the results are compared with bio-assay test results. Results from both tests reveal ±10% variation between the experimental and simulation results.

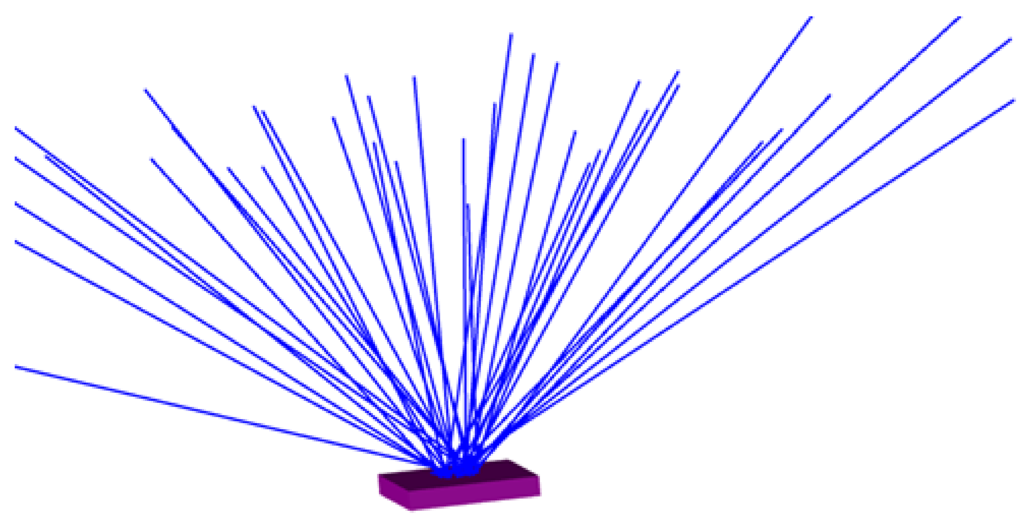
## Optical simulation

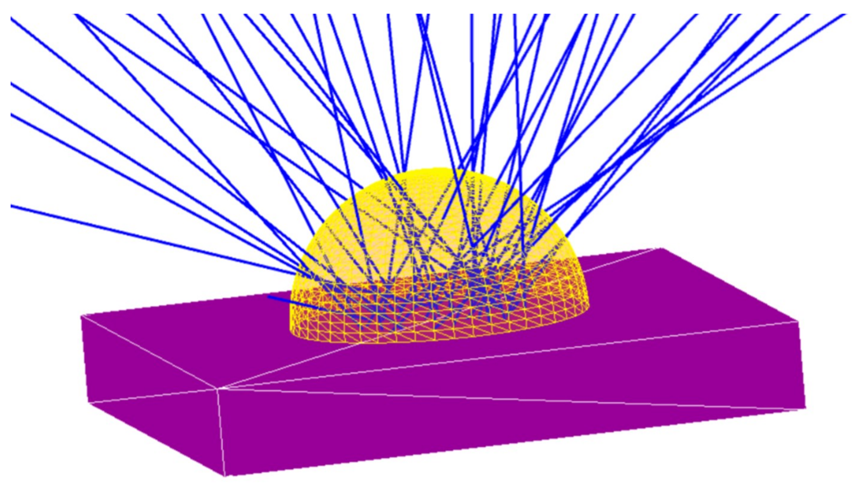
Zemax OpticStudio is used for optical simulation of the LEDs irradiation within the reactor. Non-Sequential ray-tracing mode is used for the simulation of the LED and other optical components within the system. In non-sequential mode, a ray can intersect different objects in varying order and same object multiple times. The main feature in non-sequential mode is the possibility of defining detectors along the ray-tracing path which can provide irradiance data at different spatial and angular data.

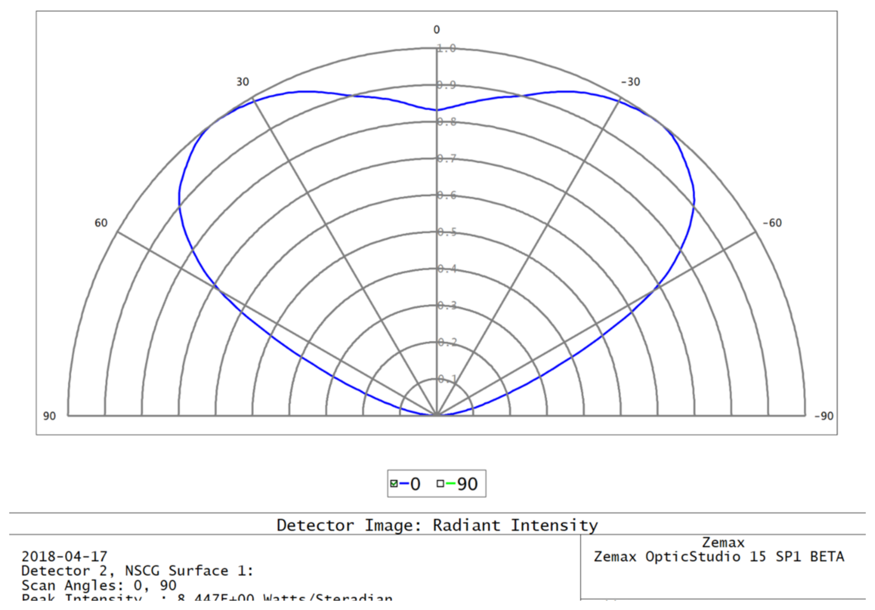
- **LED modelling**

The key for a successful optical simulation is the proper modelling of the LED. The following parameters should be considered in Zemax while modelling the LED's irradiation.

- View angle and radiation pattern
- Irradiation wavelength spectrum
- Die modelling including the size, position and the pattern
- Package modelling including the window size and transparency








## Hydrodynamic Simulation

Ansys-Fluent software is used for flow simulation within the reactor. Using User Defined Functions (UDF), the irradiance data are imported from Zemax OpticStudio and is used to determine the inactivation rate along with the flow data. Two different techniques are used for the hydrodynamic simulation of the reactor

- **Eulerian Method [1]**

1- Solving another partial differential equation which gives the distribution of inactivation ratio throughout the field

$$\frac{\partial R}{\partial t} + \nabla\cdot(\vec{V}R) = D_{eff}\nabla^2 R + S$$

$$S = -\ln(10)\,ER\,\frac{df}{dD}$$

2- Calculating the amount of inactivation by averaging $R$ over the outlet

$N/N_0 = 1/A_o \int R(x,y,z)dA$

- **Langrangian Method [2,3]**

1- Injecting enough particles distributed uniformly over the inlet in the field

2- Calculating the trajectory of each particle

3- Calculating the amount of dose received by each particle from inlet to outlet $D = \int_0^t E dt$

4- Computing the inactivation ratio for each particle, $(N/N_0)_i = f(D_i)$, from the inactivation curve

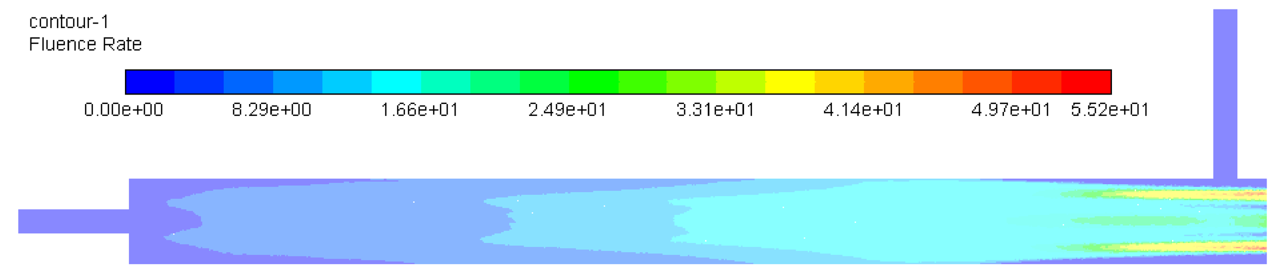
5- Evaluating the overall performance by averaging over all particles

$N/N_0 = 1/n_p\,(N/N_0)_i$

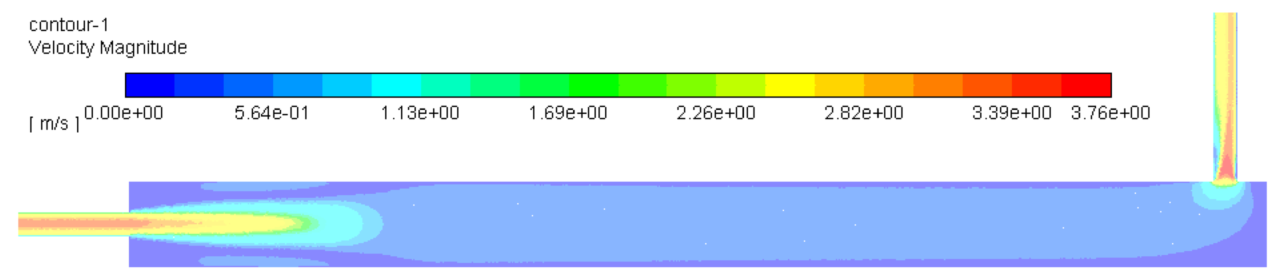
## Integrated Dose Simulation

Once the optical and flow simulations are performed, the in-house integrated dose simulation tool will be used to determine the LRV and dose. There are important parameters during the simulation which can influence the results including the turbulence model, number of particles for the Langrangian model.

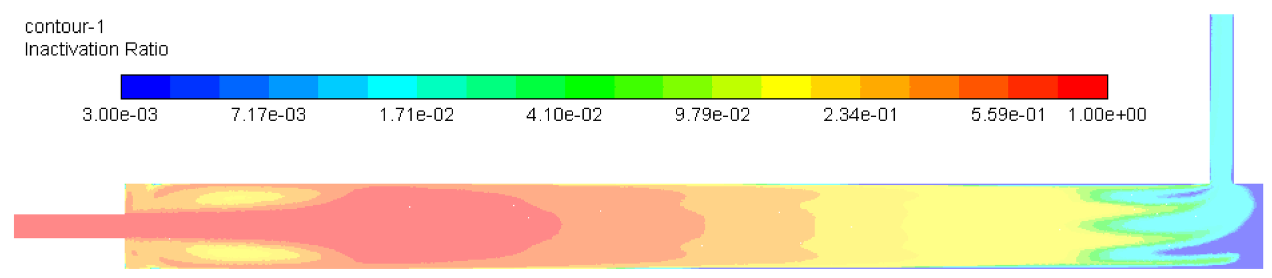
**Fluence Rate**



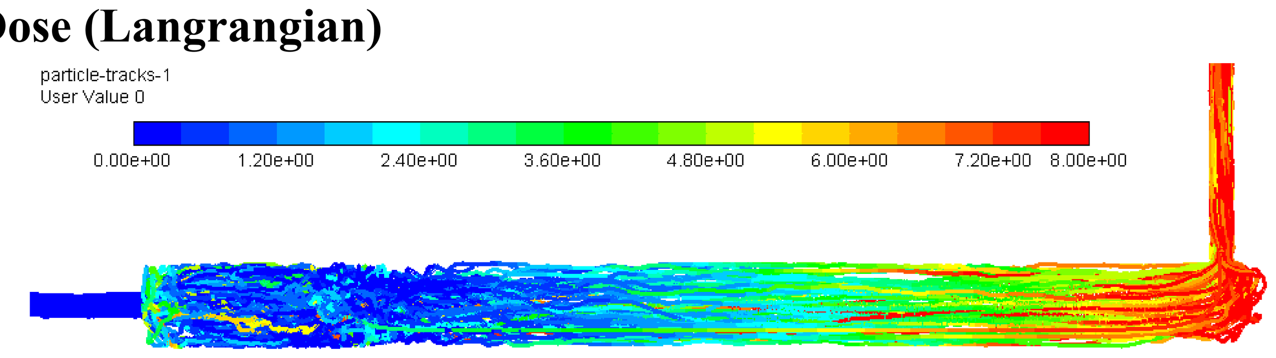

**Velocity Magnitude**




**Inactivation (Eulerian)**




**Dose (Langrangian)**




| Flow Rate (lpm) | Bacteria | LRV (Eulerian) | LRV (Langrangian) | LRV (Experiments) |
|---|---|---|---|---|
| 2 | E-Coli (8739) | 2.0 | 2.1 | 2.2 |
| 1.5 | E-Coli (8739 | 3.2 | 3.3 | 3.5 |

## References

1-Elyasi S, Taghipour F. Simulation of UV photoreactor for water disinfection in Eulerian framework. Chemical Engineering Science. 2006 Jul 1;61(14):4741-9.

2- Sozzi DA, Taghipour F. UV reactor performance modeling by Eulerian and Lagrangian methods. Environmental science & technology. 2006 Mar 1;40(5):1609-15.

3-Munoz A, Craik S, Kresta S. Computational fluid dynamics for predicting performance of ultraviolet disinfection sensitivity to particle tracking inputs. Journal of Environmental Engineering and Science. 2007 May 1;6(3):285-301.