Development of a CFD Based Simulator for Design Optimization of Photo-Reactors

Fariborz Taghipour*

Chemical & Biological Engineering Department
University of British Columbia
2357 Main Mall, Vancouver, B.C. V6T 1Z4, Canada

Key words: Design Optimization.

CFD-based models that integrate reactor hydraulics, kinetics, and optics were developed in order to simulate the performance of photo-reactors for fluid treatment. The flow paths of chemical contaminants were computed from the CFD generated velocity profiles, using a particle-tracking algorithm. The path of each chemical species was integrated with the intensity and kinetic models to calculate the overall conversion of the target compound in the reactor. The models were applied to design optimization of photo-reactors.

Introduction

The presence of toxic organic compounds in water supplies and in the discharge of wastewater is of great environmental concern. The majority of these contaminants can be destroyed completely by photolysis (direct absorption of ultraviolet –UV– light) or photo-oxidation (activation of strong oxidants such as hydrogen peroxide or ozone by UV to form oxidative hydroxyl radicals). In the past few years, there has been considerable research and commercial interest in UV-oxidation/photolysis processes for the removal of toxic organic compounds in water.

Despite a growing number of studies on the photolysis/photo-oxidation of chemical pollutants, little is known about the process optimization of these technologies. As a result, their industrial application to water treatment has been limited and commercial systems, in general, have met with only limited success. Efficient design of the system is required to make these technologies successful, reliable, and cost effective.

Simulation of UV reactors for design optimization is required before this technology can be applied as an efficient fluid treatment process. This is due to the complexity of the UV systems and interaction of many parameters including hydraulics, optics, and kinetics. Development of a reactor model for UV oxidation allows for design optimization, process scale-up, and determination of process limitations. Such a model can also be the basis of developing novel devices for the on-line monitoring of photo-reactor performance; a highly desired capability that currently does not exist for any photo-oxidation reactor. On-line monitoring can be used to determine changes in reactor performance (based on input data from on-line sensors for UV intensity, flow rate, etc.) that result from any process/system variations.

In this research, CFD-based models that integrate reactor hydraulics, kinetics, and related physical phenomena (i.e. irradiation distribution) were developed in order to predict reactor performance. The models were applied to design optimization of photo-reactors.

Background

A number of modeling techniques has been employed to simulate UV reactor performance for water disinfection (e.g. Scheible 1987, Darby *et al.* 1995, Chiu *et al.* 1999). Recently, CFD has been used for simulating flow fields in UV reactors (e.g. Bass 1996; Do-

*E-mail: fariborz@chml.ubc.ca

Quang *et al.* 1997; Lyn *et al.* 1999, Lawryshyn and Lu, 1999, Buffle *et al.*, 2000). Inactivation kinetics and radiation intensity have been combined with CFD generated turbulent flow field to predict reactor performance. Despite some work on the modeling of UV reactors for fluid disinfection, UV reactor modeling for fluid treatment (removing chemical contaminants) has received little attention.

CFD-based model for UV reactor performance simulation

A state-of-the-art model for simulating UV reactor performance was developed, taking into account relevant parameters such as hydraulics, kinetics, and intensity fields within the reactor. Hydrodynamics is the main component of these models that was integrated with kinetics and optics. Because of the high non-homogeneity of the intensity field in UV reactors, the hydrodynamic behavior of UV systems can significantly impact their performance. The combination of complex hydrodynamics and irregular UV intensity results in a broad distribution of UV doses/oxidation, which is impossible to calculate or measure using conventional methods.

In this research program, the fluid flow patterns and turbulence within UV reactors were characterized through CFD analysis. Sensitivity analysis showed that the choice of the appropriate turbulence model algorithm and boundary condition assumptions are very important to obtain precise results. Detailed information on the path taken by chemical contaminants and particles through a photo-reactor is critical to design optimization. Therefore, along with the computation of the entire flow field, a particle-tracking algorithm was calculated. The flow paths of chemical contaminants were computed from the CFD generated velocity profiles, using a Lagrangian particle-tracking algorithm. For a direct photolysis process, the path of each chemical species was integrated with the intensity model to determine its cumulative dose. For photo-oxidation processes a similar approach was adopted, taking into account hydroxyl radical concentration (a function of intensity and hydrogen peroxide concentration) along the path of the organic contaminants. By considering thousands of such flow paths through the reactor, dose distribution data was generated. Using statistical analysis tools, the dose distribution data was integrated into the kinetic models to calculate the overall conversion (degradation) of the target compound in the reactor.

The model, which was developed through this study, provided a new insight into UV reactor performance. The models were effectively applied to the conceptual design of photo-reactors and optimization of reactor parameters. Various design concepts for UV reactors were investigated. The effect of varying geometric parameters (e.g. inlet/outlet positions, lamp configurations, placement of static mixers, etc.) on the reactor flow distribution was also examined.

References

1. Bass, M.M. (1996) Latest Advances in UV Disinfection Hydrodynamic Simulation and Relation to Practical Experiences, *Proceedings AQUATECH*, Amsterdam
2. Buffle, M.O., Chiu, K., Taghipour, F. (2000) UV Reactor Conceptualization and Performance Optimization with Computer Modeling, *Disinfection of Wastes in new Millennium Conference*, New Orleans
3. Chiu, K., Lyn, D.A., Savoye, P., Blatchley, E.R. (1999) Integrated UV Disinfection Model Based on Particle Tracking, *J. Env. Eng. ASCE*, 125:459-466
4. Darby, J. L., Heath, M., Jacangelo, J., Loge, F., Swaim, P., Tchobanoglous, G. (1995) Comparison of UV Irradiation to Chlorination: Guidance for Achieving Optimal UV performance. *Project Report for WERF, Project 91-WWD-1*, WERF, Alexandria, VA
5. Do-Quang, Z., Djebbar, R., Blatchley, E., Lain, J-M. (1997) Computational Fluid Dynamics Modeling of Ultra-Violet Disinfection Reactor Performances: Optimization of Flow in Vertical Lamp Open Channel, *ASCE-CSCE Environmental Engineering Conference*, Edmonton

6. Lawryshyn, Y. and Lu, D. (1999) UV Reactor Design, It's More than Putting a Lamp in a Pipe, *J. WCPM* 41:106-109
7. Lyn, D.A., Chiu, K., Blatchley, E.R. (1999) Numerical Modeling of Flow and Disinfection in UV Disinfection Channels, *J. Env. Eng*. ASCE, 125:17-23
8. Scheible, O.K. (1987) Development of a Rationally Based Design Protocol for Ultraviolet Light Disinfection Process, J. WPCF 59:1-4