

Advanced Oxidation Process Simulation Software

An Environmental Technologies Design Option ToolTM

AdOx provides design engineers with the capability to evaluate and design advanced oxidation processes for the removal of organic compounds from water.

AdOxTM Features:

- Practical and Easy to Use Advanced Oxidation Model for Organic Contaminants Removal
- Modeling Multiple Target Compounds Destruction
- Variable Operation Mode Options
- Photolysis and Radical Reaction Rate Constants and Photochemical Parameters Database and Estimation Methods
- Comprehensive Mechanism-based Model

AdOxTM Applications:

- Municipal Water Treatment
- Municipal Wastewater Treatment
- Environmental Remediation
- Educational Resource

AdOxTM Capabilities

Advanced oxidation processes are attractive alternatives to traditional non-destructive water treatment processes and are being applied in an increasing number of cases. A successful design of an advanced oxidation process usually requires carefully controlled pilot plant studies. However, these studies can be expensive and time consuming if they are not properly planned.

AdOxTM is capable of simulating the dynamic behavior of the advanced oxidation process and can select the optimum process design so that it provides a complementary approach to laboratory and pilot plant experimentation.

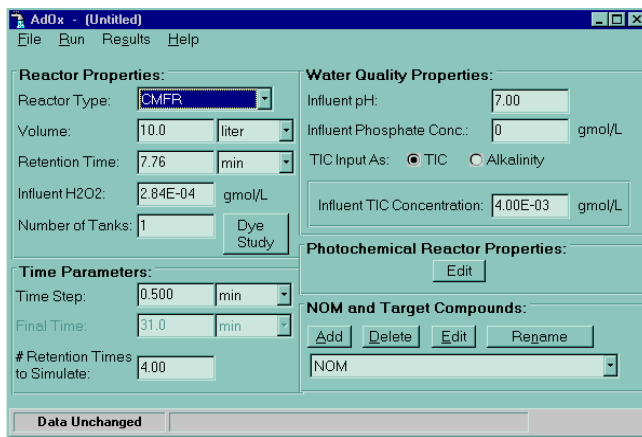


Figure 1. Main window of AdOxTM

The mathematical models contained in AdOxTM can be used to:

- Assess the Preliminary Design and Feasibility of Using Advanced Oxidation Processes
- Plan Pilot Plant Studies and Interpret Their Results
- Provide Key Parameters for Process Design

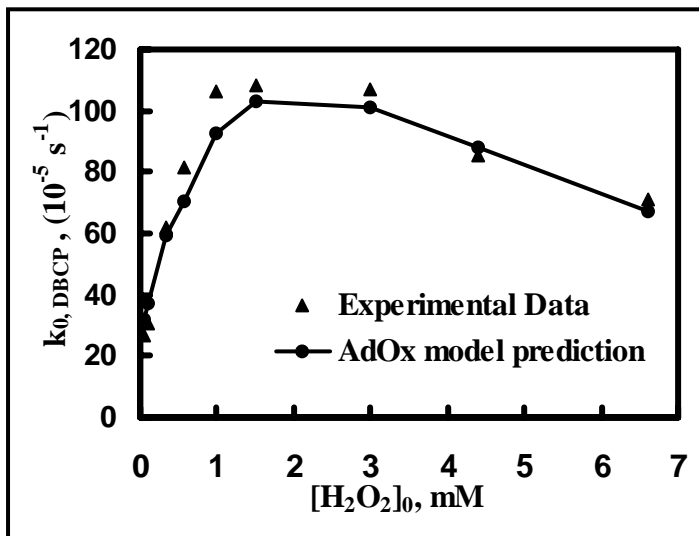


Figure 2. Relationship between Initial Concentration of H₂O₂ and DBCP Degradation Rate (C_T=4mM, I₀=1.04x10⁻⁶Eins./L-s)

AdOx Models

AdOx contains mechanism-based models that can be used to evaluate and design advanced oxidation processes. The current version 1.0 contains H₂O₂/UV process model.

The future version will also include other models:

- H₂O₂/O₃
- UV/O₃

AdOx – Photolysis and Radical Reaction Rate Constants and Photochemical Parameters Database

Advanced oxidation mechanism modeling requires rate constants for the reaction between free radicals and target compounds. UV-induced advanced oxidation process modeling also requires rate constants of direct photolysis reaction of target compounds. In addition, these photochemical and physicochemical properties of the compounds are needed: (1) dissociation constant (pK_a), (2) extinction coefficient and (3) quantum yield of the compounds. Consequently, a database is included in AdOxTM to provide that information.

AdOxTM Model Features

AdOxTM is a dynamic kinetic model for the advanced oxidation process using hydrogen peroxide and ultraviolet irradiation. The model includes the known elementary chemical and photochemical reactions. Photochemical parameters and chemical reaction rate constants reported in the literature are used in this model to predict organic contaminant destruction.

The features of the AdOxTM are:

- Considers all of the most important elementary reactions involved in the H₂O₂/UV process.
- Provides steady state solution for flow reactors and fully dynamic solution for both batch and flowing systems.
- Predicts the change in pH.
- Considers the influence of hydroxyl radical scavenging.
- Simulates fates of multiple compounds in both batch and flow reactors
- Considers the attenuation of UV light due to background compounds in the water matrix

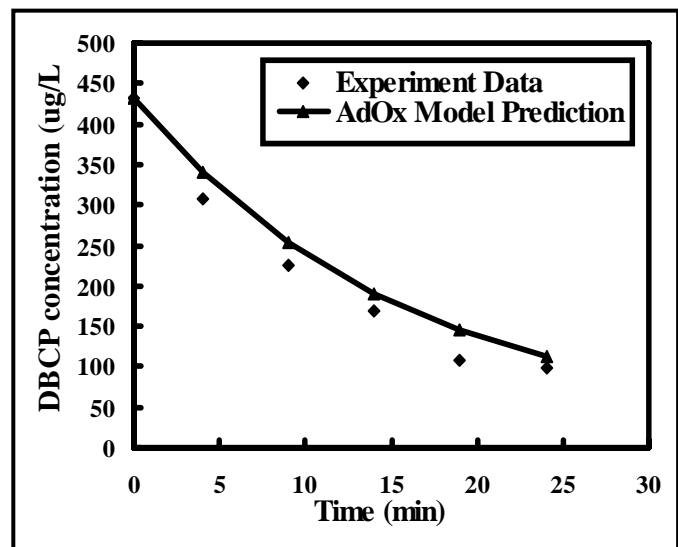


Figure 3. Modeling of DBCP Degradation in CMBR (I₀=1.04x10⁻⁶Eins./L-s, C_T=4mM, [H₂O₂]₀ = 1.00 mM, [DBCP]₀ = 1.83 mM)

AdOx™ can be used both for design and for analysis and improvement of an existing system by simulating process performance for various designs or operating variables. AdOx™ can analyze a dye study to obtain the fluid residence time distribution and determine the most appropriate reactor model, which simulates the observed non-ideal mixing in the reactor.

Dye Study Model

The dye study model contained in AdOx™ can analyze a pulse dye study data and determine the appropriate number of tanks in series that are required to describe the mixing conditions in the reactor. This in turn can be used to select the appropriate number of tanks for designing the photochemical reactor.

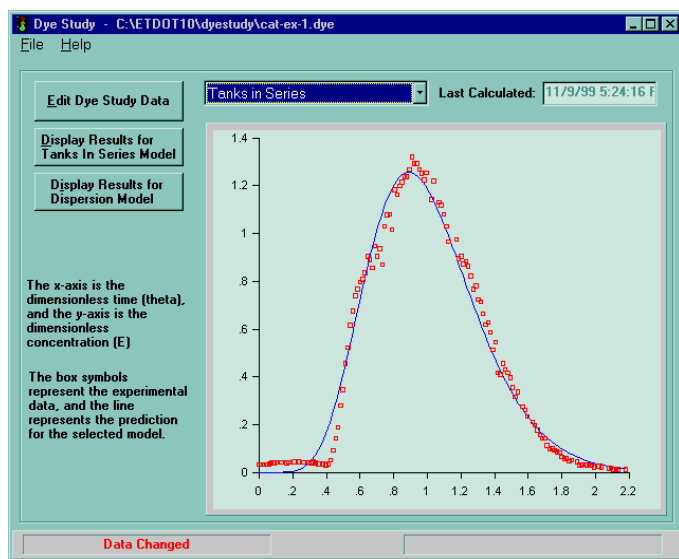


Figure 4. Fit of Catalytic Oxidation Reactor Experimental Data With Tanks In Series Model

Other AdOx Options

- Choice of English or System International Units of Expression
- Flexible Printing Options

Graphical User Interface

AdOx™ is designed for the Microsoft Windows environment with a graphical user interface (GUI) to maximize user-friendliness. Making use of the Microsoft Windows interface, with its built-in file and hardware control features, AdOx™ frees the engineer from concerns over printer drivers and other "machine" issues and allows more attention to the computational algorithms. The GUI consists of a Microsoft Visual Basic front-end shell that calls FORTRAN subroutines to perform the calculations.

System Requirements

The minimum ETDOT system requirements are as follows:

- English-language version of Microsoft Windows 95, Microsoft Windows 98, or Microsoft Windows NT 4.0; in the case of Microsoft Windows NT 4.0, Service Pack 3 or more recent is required
- 50 MB of hard disk space
- 32 MB of RAM is recommended
- A Pentium or more recent processor is recommended
- A graphic VGA or more recent video display
- A mouse or other pointing device is recommended

Product Information

For additional information on product sales and technical support contact:

David W. Hand, Ph.D.
National Center for Clean Industrial and
Treatment Technologies (CenCITT)
Michigan Technological University
1400 Townsend Drive
Houghton, MI 49931

Phone: (906) 487-2777
E-mail: dwhand@mtu.edu

References:

Crittenden, John C., Shumin Hu, David W. Hand, and Sarah A. Green, "A Kinetic Model for H₂O₂/UV Process in a Completely Mixed Batch Reactor," *Water Research*, **33**(10), 2315-2328 (1999).