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Project Summary

Water Treatment Model for Pollutant Exposure Assessment: System Documentation and Users Manual

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A mathematical model of potable water treatment to remove toxic substances has been developed for use in exposure assessment modeling. Treatment processes modeled include sedimentation, coagulation-flocculation, filtration, aeration, chemical oxidation, and granular activated carbon adsorption. Besides describing the use of the program, this users manual presents example runs of the model.

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The Toxic Substances Control Act requires that the potential hazard to human health or to the environment be evaluated before new chemicals are marketed. An effective technique in the process of assessing hazard is the use of mathematical models that predict the transport and transformation of toxic substances in the environment. These models can predict concentrations in air, water, and food on the basis of the characteristics of the toxic substance and of the environment through which it passes.

One important exposure route for humans is the ingestion of chemicals in drinking water. Before reaching humans, these chemicals must pass through municipal water plants where various treatment processes can change the pollutant concentration. An understanding of the transformations and the removal processes in the treatment plant linked to information on the transport and transformation of toxic substances in its source waters allows the development of mathematical models that can predict the concentration of a given chemical in drinking water at the tap. If the number and distribution of the population at risk is known and human health and toxicological data are available, then the potential hazard of exposure to the chemical can be estimated.

This users manual documents and describes the use of a model of municipal water treatment processes for predicting the degree of removal of a toxic substance. Removal processes and transformation algorithms for this Water Treatment Processes (WTP) Model are, wherever possible, the same as those used in another EPA model (*Environmental Pathways of Selected Chemicals in Freshwater Systems, Part I. Background and Experimental Procedures,* EPA-600/7-77-113; *Part II. Laboratory Studies,* EPA-600/7-78-074). Predictions of ambient chemical concentrations may be used as input to the WTP Model.

The objective of this effort was to develop a model of water treatment processes that predicts the quantity of a toxicant in the finished water. When such a model is linked to an aquatic fate and transport model, a source identification and loading model, and a model for estimating the population at risk, the amount of toxicant reaching a population for consumption in their drinking water can be predicted. An aquatic fate and transport computer model and supporting laboratory procedures had been developed to measure the sorption partition coefficient and the rate constants for volatilization, oxidation, hydrolysis, photolysis, and microbial

transformations, under conditions that were extrapolatable to environmental conditions. These procedures were applied to 11 toxic chemicals of environmental concern, and the results were used with an aquatic fate and transport model to predict the pathways for these chemicals in ponds, lakes and rivers. The descriptions, coefficients and constants from that earlier work were used whenever possible as input to the WTP Model.

Results and Discussion

Table 1 shows the partition coefficients and rate constants for volatilization, photodegradation, and oxidation used for the 11 toxic chemicals modeled. As an example, if the WTP Model is run using the water treatment process train shown in Figure 1 and the partition coefficients and rate constants from the earlier work, the removals shown in Table 2 are obtained for these 11 compounds.

These results illustrate the effect that the partition coefficient of a toxicant has upon its mechanism of removal in water treatment. Toxic chemicals that have a high partition coefficient will be removed by those processes that tend to remove particulate matter. Hence, a chemical such as mirex, which is almost completely sorbed to particulates, will be removed at or near the same rate as the particulates. Processes such as sedimentation, coagulation-flocculation, and filtration will be effective in removing a chemical from the product water. A chemical that has a low partition coefficient such as quinoline, however, will be essentially unaffected by those processes that remove particulate material. Consequently, chemicals that do not readily sorb to particulates are not removed unless they undergo some other transformation, in which case, aeration, chemical oxidation, or carbon adsorption may be effective in reducing the toxicant's concentration in the finished water. The detention time of water in a water treatment system is on the order of one day. Therefore, it should be noted that compounds that have halflives significantly greater than the detention time of the system will not be degraded or volatilized. In general for significant degradation to occur, the halflife must be on the order of one third of the system detention time.

Thus, if the influent to the water treatment plant diagrammed in Figure 1 contained 60 μg/l of mirex and 6 g/l of quinoline (the approximate solubility limits), then it would be predicted by the WTP Model that the effluent concentrations would be 3.5 μg/l and 5.4 g/l, respectively.

The users manual describes a digital computer program that can be used to compute the quasi-steady-state concentration of a toxic substance in a typical water treatment process train. This program is written in FORTRAN and is designed to be run interactively. The program presently consists of a main executive program and nine process subroutines; each subroutine computes the transformation of a toxic substance undergoing a single water treatment process. Three other subroutines are also provided. The first, entitled PER, simply calculates the amount of removal of the toxic substance in each process as percent removed from the water, with the sediment, and total for that process. The second subroutine, entitled PN1, calculates the equilibrium concentration of the toxic substance on the sediment in milligrams of toxic substance per gram of sediment. The third subroutine, entitled PRINT, simply prints all pertinent data. The nine processes presently included in the program together with the subroutine names are listed below:

Process Name	Subroutine Name
Primary sedimentation	SED1
Aeration	AER2
Chemical oxidation	COX3
Coagulation	COAG4
Filtration	FIL5
Granular activated carbon column adsorption	GAC6
Chlorination	THM7
Mixing	MIX
Steam splitting	SPLIT

Table 1. *Rate Constants[a] of 11 Selected Chemicals*

Chemical	CP ($X10^{-3}$)	KV ($X10^{4}$ hr^{-1})	KPD ($X10^{2}$ hr^{-1})	KOX ($X10^{6}$ hr^{-1})
p-Cresol	0.01	40	0.05	7
Quinoline	0.01	1	0.06	7
Methyl Parathion	0.05	0.02	0.2	0.35
Benzothiophene	0.05	150	0.06	0.70
9H-Carbazole	0.2	0.07	11	290
Benzoquinoline	1.4	0.08	25	0.01
Dibenzotniophene	1.4	50	0.18	0.70
7H-Dibenzocarbazole	20	0.47	69	100
Benzoanthracene	25	0.07	3.4	1800
Benzopyrene	50	50	23	200
Mirex	300	14	0.009	7

[a] *Partition coefficient (CP), volatilization (KV), photodegradation (KPD), and oxidation (KOX).*

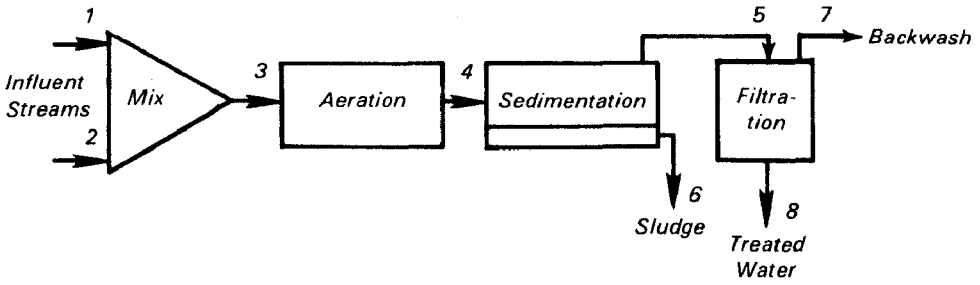

Figure 1. *Example water treatment process train.*

Table 2. *Predicted Removals Using WTP Model for 11 Selected Chemicals*

CP ($X10^{-3}$)	% Removal With Sediment	K's ($X10^{2}$ hr^{-1})	% Removal in Water Phase	% Removal (Total)
0.01	0.1	0.05	9.1	9.2
0.01	0.1	0.077	9.2	9.3
0.05	0.7	0.2	10.1	10.8
0.05	0.7	1.5	11.8	12.5
0.2	2.9	11	58.4	61.3
1.4	16.7	25	31.8	48.5
1.4	49.6	0.68	3.9	53.5
20	63.0	70	17.0	80.0
25	67.2	5.2	2.6	69.8
50	76.4	24	2.7	79.1
300	80.9	0.14	0.2	81.1

Summary

The WTP Model calls subroutines for each of the treatment processes being modeled, an output subroutine and several other supporting subroutines. The process subroutines presently include sedimentation, coagulation-flocculation (two versions), filtration, aeration (two versions), chemical oxidation and granular activated carbon adsorption. The chlorination subroutine needs more experimental data upon which to base the modeling effort, and in all probability chemicals will need to be modeled on an individual basis. Any specific process can be similarly added for which enough experimental information is available upon which to construct a model algorithm. The WTP Model provides a means of predicting the quantity of a toxic in tap water following treatment. When linked with an aquatic fate and transport model, a source identification and loading model, and a model for estimating the population at risk, the WTP Model can be used to predict the amount of a toxicant actually reaching a population for consumption in the drinking water.

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The complete report, entitled "Water Treatment Model for Pollutant Exposure Assessment: System Documentation and Users Manual," (Order No. PB 84-158 328; Cost: $10.00, subject to change) will be available only from:

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
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