Fate and Transport of Organic Chemicals in the Environment: A Practical Guide 3rd Ed

FATE *and* TRANSPORT *of* ORGANIC CHEMICALS *in the* ENVIRONMENT

A Practical Guide

Third Edition

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Preface

Would you like to be able to predict potential exposure to a toxic chemical? Of course you would. Would you like to be able to prevent your exposure to a toxic chemical. Of course you would, if possible. This book will help you predict and prevent your exposure to toxic chemicals through tracking the fate and transport of chemicals in the environment.

Chapter 1 demonstrates what the book is about the use of techniques to predict the fate and transport of a chemical in the environment. Definitions are given in terms simple enough for any reader of the book to understand them. Chapters 2 and 3 present predictive techniques and ways of using them. Tables are given in which users can insert data to make the predictions. Chapter 4 ties together the material of the previous chapters, showing how data and predictive techniques may be combined to assess the route of exposure. Chapter 5 gives examples of specific chemicals, showing different types of data, and guides the user, as if hands on, through a step-by-step prediction procedure. The reader will learn how to use and interpret pertinent data and how to predict the fate and transport of a chemical, as well as to predict exposure routes.

Chapter 6 begins to focus on pesticides. This half of the book, which comprises the second edition, presents predictive methods and provides a unique tool to help you predict the potential for exposure to toxic chemicals, mainly pesticides.

Chapter 7 presents general discussions on chemicals in different environments so that the reader will be cognizant of his or her environment and the environment of others.

Chapters 8 through 12 discuss mechanisms of prediction, techniques for using the mechanisms, and practice in making assessments on potential exposure. Exercises and answers are also given to help the reader practice using these mechanisms.

Chapter 13 discusses pesticide dosage and safety predictions moving towards acceptable pesticide use patterns.

Chapter 14 discusses the use of chemical structure to predict adverse effects.

Chapter 15 discusses dissipation in soil.

Chapter 16 presents a hypothetical method to prevent environmental aquatic kills.

Chapter 17 presents discussions on chemicals in different environments so the reader will be cognizant of his or her environment and the environments of others.

Chapter 18 presents equations for predicting the the fate and transport of chemicals other than pesticides, although pesticides fit into some of the presented equations.

The entire book will enable you to assess whether a chemical will bioaccumulate in animals. If bioaccumulation does occur, there is a good possibility that the chemical can be passed on the future generations through sperm, ovum, blood, and milk.

The book is intended for use by either laypersons or scientists. It will enable real estate agents and appraisers, lending institutes, developers, waste managers, chemical manufacturers and users, environmentalists, educators, government officials, environmental assessors, private citizens, and others to predict potential routes of exposure to chemicals.

As you read the book, I hope you will learn the fate and transport of organic chemicals in the environment and become able to predict your potential exposure to a toxic chemical.

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Contents

Chapter 1
Fundamentals

FATE AND TRANSPORT

Many questions must be considered when we attempt to determine what happens to a chemical and its breakdown products (i.e., degradates, biodegradates, metabolites, transformation products, dissociation products, hydrolytic products) in the environment. After we obtain data about such chemicals, it can be quite difficult to interpret them. The intention of this book is to present an overview of the data that are obtainable and of their interpretation.

We will: (1) discuss a chemical as the parent chemical because almost any organic chemical, parent or breakdown product, will fit the examples given; (2) present discussions on what could happen to a chemical in an environmental compartment; (3) show how to make predictions on chemical fate in the environment; and (4) demonstrate how, in most cases, to determine and predict the fate of an organic chemical in a particular environmental compartment when few or no data are available. The overall purpose of this book is that it should offer insight and understanding, as well as be a guide to predicting the fate and transport of chemicals (mostly organic chemicals) in the environment.

There are many questions to answer in the assessment of the fate of a chemical in environmental compartments. Six are considered here.

1. *What are the mechanisms that break down a chemical to a toxic, nontoxic, or naturally occurring chemical(s)* [1]? These mechanisms include the following:

a. Photolysis. If a chemical can sorb sunlight, the chemical can be transformed in media (i.e., air, water, and soil) or on media (i.e., water, soil, plants, and animals) to produce transformation products.

b. Biodegradation in all environmental compartments to produce biodegradates, if microbes are present.
c. Metabolism in plants and animals to produce metabolites.
d. Hydrolysis in all environmental compartments to produce hydrolytic products.
e. Dissociation in all environmental compartments to produce dissociated products.
f. Sorption in all environmental compartments.
g. Bioaccumulation in plants and animals.

2. *What is the rate of dissipation or half-life ($t_{1/2}$) of a chemical in environmental compartments* [1]? The rate of dissipation or the half-life is the time that it takes for the chemical to be reduced by one-half of its original amount, measured from the time of its introduction into an environmental compartment (i.e., when 50%) of the chemical has vanished and only 50% of it remains. The lost 50% could be in the form of a breakdown product(s), either toxic, nontoxic, or naturally occurring. This is why in real situations breakdown products must be identified and studied in the same way that the parent chemical is studied. The dissipation of a chemical may be real, resulting in the breakdown of the parent chemical (usually organic chemicals), or not real, due to adsorption or movement of the chemical from contaminated areas to noncontaminated areas. There are ways to predict this, even when no or few data are available, as will be discussed later. In any event, these aspects should be determined by sorption or mobility studies. One must always remember that the fact that a chemical cannot be found does not mean it is not there. Good testing will establish its whereabouts.

3. *How is a chemical moved in the environment by natural means* [1]? These means include:

a. Volatilization: A chemical that is volatile can move into the air; and once in the air, the chemical can be transformed, hydrolyzed, dissociated, biodegraded, or sorbed to dust particles. The chemical also can be released from air to contaminate soil, water, plants, and animals via dust particle fallout or by precipitation.
b. Leaching: A chemical may be transported through soil by solvents (water, etc.) or with soil movement. Any chemical that leaches can contaminate groundwater, an action that in turn may result in the contamination of air, soil, other waters, plants, and animals.

c. Runoff: A chemical may move across a surface with a solvent or with soil movement to contaminate air, water, soil, plants, and animals.
d. Food-chain contamination: A chemical that is passed from one environment can be passed on to water, air, soil, plants, or animals and on up the food chain. For example:
   (1) A chemical that gets into the aquatic environment can be taken up by microscopic organisms, which are eaten by fish, which are eaten by wildlife and humans.
   (2) A chemical in water could reach crops via irrigation, and the crops could be eaten by wildlife and humans.

4. *What happens to a chemical adsorbed or absorbed in soil or in plants or animals* [1]? We will only discuss sorption in soil; because sorption in plants and animals is beyond the scope of this book although it will be discussed in general, in terms of bioaccumulation. These are the possibilities in soil:

a. Absorption: A chemical that is absorbed in soil can be released in any environment (like water being released from a sponge).
b. Adsorption: A chemical that is adsorbed to soil particles is unlikely to be leached by water. An adsorbed chemical may be leached with other solvents (if they get into soil), by soil movement, or by water if soil sorption sites have been filled or taken up by another chemical. Another cause of leaching is saturation; that is, leaching occurs as the starting chemical is continuously added to the soil, thus saturating the soil sites. (Consider the analogy of a parking lot that is full; where do the cars park?) A plant can release soil-bound residues via its root system and translocate the chemical throughout the plant. Likewise, animals that ingest soil can release the chemical residues adsorbed in the soil and translocate them throughout their bodies. These residues could be absorbed in the fat tissue or by protein in the animals [2].

5. *How does food-chain contamination occur* [1]? This type of contamination occurs when one environment is contaminated by a chemical, and that chemical is released into another environment, the end result being that animals ingest the chemical. For example:

a. A chemical that gets into air can be released onto soil, water, plants, and animals, and then noncontaminated animals may eat, drink, or breathe the contamination.
b. Fish may bioaccumulate the chemical in their tissue, and when other animals eat the fish, they in turn also will become contaminated. Thus food-chain contamination has occurred, followed by bioaccumulation up the food-chain ladder.

6. *What are accumulation and bioaccumulation?* These terms refer to the condition in which a chemical builds up and does not dissipate; in soil it is called accumulation, and in plants or animals it is called bioaccumulation. The chemical is not broken down in an environmental compartment. In mammals another problem exists—the potential for residues to be passed on into mothers' milk, then to nursing infants.

REFERENCES

[1] Ney, Ronald E., Jr., "Regulatory Aspects of Bound Residues," Workshop V-C, 4th International Congress of Pesticide Chemistry, International Union of Pure and Applied Chemistry, Zurich, Switzerland, Unpublished paper, 1978.
[2] Yip, George and Ronald E. Ney, Jr., "Analysis of 2,4-D Residues in Milk and Forage," *Weeds, Journal of the Weed Society of America,* vol. 14, pp. 167-170, April 1966.

ENVIRONMENTAL COMPARTMENTS

Five environmental compartments are considered herein. Many chemical, physical, and living reactions can occur in these compartments; and before any data can be discussed, we must know what the compartments are, and what could occur in each one. We now consider relevant features of each compartment.

Compartment Air

- *Contamination:* Air contamination occurs when a volatile chemical or airborne particulate matter (dust) containing a chemical gets into the air as a result of a spill, evaporation, or any release.
- *Reactions:* A chemical can be phototransformed in air, or it can be sorbed to particulate matter and be biodegraded, dissociated, hydrolyzed, or phototransformed.
- *Mobility:* Chemicals can be moved throughout air, by air or precipitation, or can move as fallout with precipitation or with particulate matter to contaminate other environmental compartments.
- *Exposure:* Airborne chemicals could result in chemical exposure of all environmental compartments [1].

Compartment Water

- *Contamination:* Water contamination occurs by fallout from air, from spills, from substances directly applied or intentionally put into water, with runoff, or from leaching into water.
- *Reactions:* Depending on the water (i.e., streams, lakes, ponds, groundwater, ocean, etc.), reactions may include dissociation, hydrolysis, phototransformation, biodegradation, or sorption to particulate matter.
- *Mobility:* Movement may occur with volatilization, water movement, evaporation, irrigation with well water, or animals, resulting in environmental contamination.
- *Exposure:* Chemicals in this compartment could result in the chemical exposure of all environmental compartments [1].

Compartment Soil

- *Contamination:* Soil contamination occurs by spills, fallout from air, or substances directly or indirectly applied to or put into or on soils.
- *Reactions:* Hydrolysis, dissociation, sorption, biodegradation, and photolysis reactions are possible.
- *Mobility:* Volatilization, runoff, leaching, or plant and animal uptake resulting in food-chain contamination may occur.

- *Exposure:* Soil contamination could result in the chemical exposure of all environmental compartments [1].

Compartment Plants

- *Contamination:* Plant contamination may result from fallout, spills, substances indirectly or directly applied to soils, irrigation, and materials in manure and in compost.

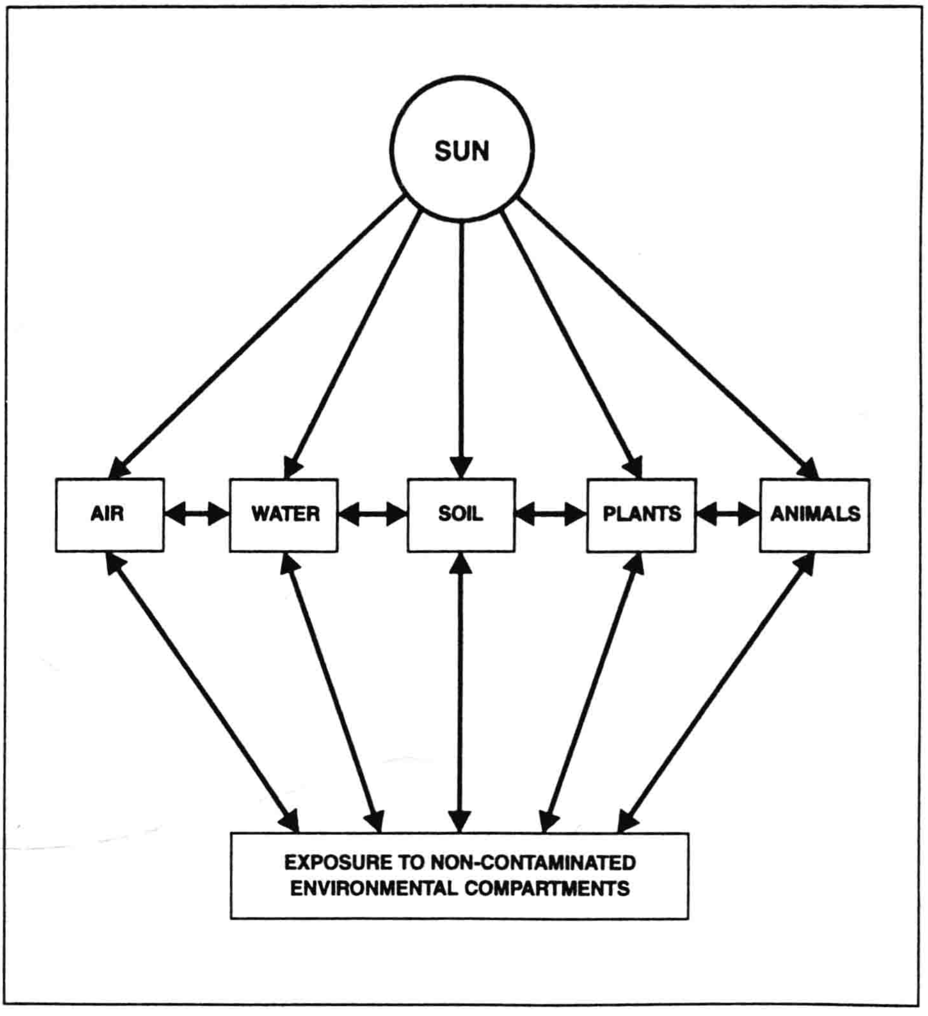

Figure 1-1. Environmental compartments. A never ending circle, from self-contamination to contamination of noncontaminated compartments and back again.

- *Reactions:* Metabolism, hydrolysis, dissociation, photolysis on the plant surface, or sorption may occur.
- *Mobility:* Movement may be occur by release into the air, into the soil via the root system, into the air if the plant is burned, or into the food-chain if the plant is eaten.
- *Exposure:* Plant contamination could result in the chemical exposure of all environments [1].

Compartment Animals

- *Contamination:* Animal contamination may occur by fallout, substances directly or indirectly applied to or on animals, eating other plants or animals, drinking water, or breathing.
- *Reactions:* Metabolism, hydrolysis, dissociation, bioaccumulation, and phototransformation on surfaces are possible.
- *Mobility:* Respiration, excretion, and release if the substance is burned or eaten are means of movement.
- *Exposure:* Animal contamination could result in exposure of all environmental compartments [1].

Thus we have seen: how environmental compartments are contaminated; reactions that could occur to chemicals in those compartments; mobility in and out of the compartments, and how one compartment can contaminate other noncontaminated compartments; and the exposure possibilities (see Figure 1-1 and Table 1-1).

Table 1-1. Reactions in Environmental Compartments.

REACTIONS	AIR	WATER	SOIL	PLANTS	ANIMALS
Hydrolysis	X	X	X	X	X
Phototransformation	X	X	X	X	X
Dissociation	X	X	X	X	X
Solubility	X	X	X	X	X
Sorption	X	X	X	X	X
Biodegradation	X	X	X	X	X
Metabolism				X	X
Accumulation			X		
Bioaccumulation				X	X
Volatilization	X	X	X		
Respiration				X	X
Excretion					X

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[1] Ney, Ronald E., Jr., "Exposure Assessment Considerations and Problems," Exposure Assessment Workshop, U.S. Environmental Protection Agency, UP, 1982.

Chapter 2
Physical and Chemical Processes

WATER SOLUBILITY

Water solubility is perhaps the most important chemical characteristic, used to assess (1) chemical mobility, (2) chemical stability or breakdown, (3) chemical accumulation, (4) chemical bioaccumulation, and (5) chemical sorption in any environmental compartment. Water solubility should be one of the easiest chemical test methods; however, if you were to look up the solubility of DDT, you would find a long list of solubilities. Luckily those values are presented in a range that enables one to make some kind of assessment or prediction; and that is the purpose of our discussions.

What can water solubility be used for? Remember these key points:

1. The higher the water solubility of a chemical, the more likely it is to be mobile, and the less likely it is to be accumulative, bioaccumulative, volatile, and persistent; and a highly soluble chemical is prone to biodegradation and metabolism that may detoxify the parent chemical.
2. The lower the water solubility of a chemical, the more likely it is that it will be immobilized via adsorption, and thus it is less mobile, more accumulative or bioaccumulative, persistent in environmental compartments, and slightly prone to biodegradation, and it may be metabolized in plants and animals.
3. The in-between range of high and low water solubilities indicates chemicals whose behavior could go either way, as discussed in 1 and 2 above.

The above generalities are meaningless unless we have values or ranges on which to base predictions. Thus, to discern the fate of chemi-