CHAPTER 3

EXPOSURE ASSESSMENT

Exposure assessment is the process of measuring or estimating the intensity, frequency, and duration of human or other population exposures to risk agents. Exposures may occur in a variety of ways, such as through ingestion (e.g., eating fish contaminated with mercury), dermal contact (e.g., handling toxic substances), or inhalation (e.g., breathing air contaminated by industrial emissions). The appropriate methods and units to be used for exposure assessment depend on the risk agent and pathways for exposure, the level of aggregation adopted for the assessment, and many other factors. For instance, the amount of material ingested is often used as a measure of exposure to toxic contaminants in food, the speed and level of flood water have been used as measures of exposure to dam failure, and the ratio of mosquitoes to human population has been used as a measure of exposure to malaria.

For many risk assessments, exposure assessment is the most difficult task. The reason for this is that exposure assessment often depends on factors that are hard to estimate and for which there are few data. Critical information on the conditions of exposure is often lacking; for example, although industrial manufacturers are generally required to keep records on workers’ exposures to toxic chemicals, the levels of exposure and the particular chemicals involved are often not known or not recorded. Exposures to the general population are even less well-documented due to the limited availability of systems capable of measuring the exposures to specific risk agents actually experienced by people.

A major source of the complexity of exposure assessment is the strong influence that individual personal habits can have on human exposure. In the case of food contaminated with risk agents, food storage practices, food preparation, and dietary habits have a major influence on the amount of the risk agent actually consumed. For example, if raw meats have been contaminated with pathogenic microorganisms, a critical factor in predicting health consequences is whether and to what extent the meat is cooked. As another example, to estimate consumer exposure to a pesticide requires data on pesticide residues, data on how many pesticide-treated food products are consumed by an average person, and data on how many people consume large amounts of the pesticide-treated food products.
If the risk agent is absorbed when a consumer product is used, the patterns of use will affect exposure levels. A solvent whose vapor is potentially toxic, for example, may be used outdoors or in a small, poorly ventilated garage. Thus, for risk assessments associated with consumer products, exposure assessment focuses on understanding how the products may be used and how different use patterns affect exposure levels.

If exposure occurs through the air or water, then exposure assessment must consider how the risk agent moves from its source through the environment and how it is altered over time. Chemical risk agents generally become diluted and may degrade after release. The aim of exposure assessment in this case is to determine the concentration of toxic materials in space and time where they interface with target populations (Travis et al., 1983). With some risk agents, understanding the changes that occur following release is all-important. For example, genetically engineered organisms released to the environment will seek to reproduce, spread, and evolve in ways that are beneficial to their own survival. Exposure assessment for genetic engineering is therefore much concerned with the persistence, establishment, and growth of released organisms (Levin and Strauss, 1991).

Physical risk agents such as mechanical force or heat can also be the subject of an exposure assessment. For example, in automotive safety, exposure assessment is concerned with estimating accident involvement rates for various types of vehicles and with the dynamics and biomechanics of occupant motion during a collision.

Another important aspect of exposure assessment is determining which groups in the population may be exposed to a risk agent; some subgroups may be especially susceptible to adverse health effects. Pregnant women, very young and very old people, and persons with impaired health all may be particularly sensitive to toxic chemicals. Some regulatory laws (such as parts of the Clean Air Act) require explicit consideration of the effect of pollutants on "sensitive or susceptible individuals or groups."

Exposure to multiple risk agents often results in portions of the population becoming more sensitive to single agents. Exposure to risk agents that act synergistically greatly complicates risk assessment because most assessments are conducted on individual risk agents. For example, exposure to both cigarette smoke and asbestos results in a rate of cancer incidence much greater than that indicated by carcinogenicity data for each substance individually (NAS–NRC, 1983a). Synergisms also often necessitate that exposure assessment consider the activities in which the exposed individuals engage. For instance, strenuous activity often increases the magnitude or likelihood of adverse reactions to exposures to many air pollutants. Multiple sources also complicate exposure assessments. An individual can be exposed to a single risk agent from several distinct sources. Exposure to lead, for example, can come from breathing air, eating food, and drinking water.

The same concepts of exposure apply to assessing risks that impact the natural environment. Exposure assessment for environmental risks, however, poses additional difficulties. Unlike humans, who may be regarded as point receptors, a sensitive ecosystem may cover a broad geographical area. Differences in the geographical distribution of risk agents are often crucial given that the environment is inhabited by diverse organisms that have differing sensitivities to impacts.

To be comprehensive, an exposure assessment must describe the levels of exposure and all conditions that might be needed to assess the effects of those exposures, including (1) the magnitude, duration, schedule, and route of exposure; and (2) the size, nature, and sensitive subpopulations of the populations exposed. If environmental effects are of concern, then the exposure assessment might also have to describe the spatial distribution of exposures relative to the distribution and differential sensitivities of exposed elements of the natural environment. In addition, a comprehensive exposure assessment must describe the uncertainties in all of these estimates. Finally, given the variety of pathways by which risk agents can be transmitted, a comprehensive exposure assessment may also have to account for the cumulative effects of simultaneous exposures via distinct environmental media.

This chapter presents and evaluates the various methods used in exposure assessment including monitoring, testing, and modeling methods.

3.1. MONITORING METHODS FOR EXPOSURE ASSESSMENT

Monitoring plays a central role in nearly all exposure assessments. Consider, for example, an assessment of the risks posed by a site at which hazardous wastes have been disposed. Soil, surface water, and groundwater contamination levels at various distances from the site may be monitored using conventional field measurement techniques. Remote techniques, such as aerial photography and multispectral overhead imagery, might be used to delineate waste site releases, and ground-penetrating remote sensing technologies may be used to estimate the subsurface distribution of waste materials (Schweitzer, 1982). Air sampling units may be used to sense airborne releases of respirable particulates or gases from volatile organic compounds. In addition, biological monitoring (Gomerz, 1980) may be used to identify possible food-chain problems, e.g., by measuring chemical residues in the tissues of food crops, livestock, or local fish. Finally, wild animals and indigenous vegetation might be sampled to find indications of local contamination.

Monitoring methods used in exposure assessment can be categorized into direct and indirect approaches. Direct methods are usually practical only for monitoring human exposures. In the direct approach, individual exposures are measured directly by instruments that accompany the individual, such as personal exposure monitors.
(PEMs) (Wallace and Ott, 1982). Depending on the nature of the risk agent and the route by which the individual is exposed, PEMs are designed to measure the concentrations of risk agents in the air, in water, or in food. In the case of water or food, individuals actively test water or food before they consume it. Since it is generally infeasible to provide the entire population of potentially exposed individuals with PEMs, population exposures are usually estimated by obtaining 24-hour exposure profiles from a statistical sample of the population.

An example of the direct approach is provided by an EPA study of carbon monoxide (CO) (Åkland et al., 1985). Several thousand randomly selected individuals were interviewed by telephone and screened to obtain a smaller target sample stratified according to smoking habits, commute times, and other factors likely to influence CO exposures. An interviewer then visited and instructed each individual on the use of a miniaturized personal CO exposure monitor. The monitor was capable of measuring and recording CO concentrations with a time resolution of less than 1 minute. During the next several days, the individuals carried their CO PEMs as they went about their normal daily activities. From the recorded data, it was possible to construct exposure profiles for each person in the sample and to extrapolate the results to the larger populations of the cities in which the people lived. Similar studies have also been conducted to measure exposures to volatile organic compounds (Wallace et al., 1984) and to electric and magnetic fields (EPRJ, 1987). The method is also commonly used to measure exposures of radiation workers, who carry dosimeters, film badges, or other radiation-sensitive devices.

In the indirect approach to exposure monitoring, factors that affect exposure are measured rather than exposure itself. For example, fixed-site monitors are widely used to measure the concentrations of pollutants in media, especially air and water. Site monitoring is often used in situations where risk agents are routinely released or the release occurs over a sufficient period of time to allow a fixed-site monitoring system to be established. Unlike PEMs, fixed-site monitors can be large, heavy, and sophisticated. Commercially available air-sampling devices include sequential samplers that draw air at multiple sampling points according to a programmed sequence and time interval. Samples may be collected in parallel and subjected to different analyses. The most powerful versions continuously complete analyses and record final results (Lioy and Lioy, 1983).

A frequent problem in site monitoring is the spatial and temporal variation of concentrations of a risk agent found in media (especially air and water). Thus, the selection of a particular dose-measurement interval, or more generally, the selection of particular sites or measurements, can have a strong effect on the numerical results. Furthermore, if only site-monitoring data are available, exposures for individuals must be derived indirectly, using additional monitoring data on human activity patterns and models to estimate concentrations of risk agents in unmonitored locations.

Great quantities of data have been generated from studies that monitor pollutants in the air and water. Examples include analyses of the plumes from a power plant to determine the nature of transport and transformation processes occurring from a single-point source of emissions (Schiemer, 1979); studies of air pollution in the city of St. Louis (Strothmann and Schiemer, 1979); monitoring of PCBs and DDT in western Lake Superior (Vieth et al., 1977); and studies of the dispersion of sewage sludge discharged from vessels off the coast of New York (Callaway et al., 1982). Major air quality databases include the National Emissions Data System (NEDS), which contains data on total suspended particulates (TSP), sulfur oxides, nitrogen oxides (NOx), hydrocarbons, and CO; the Sulfate Regional Experiment, which contains data on TSP, sulfur dioxide, sulfates, and NOx; and the Hazardous and Trace Emissions System (HATRAEMS), which contains data on pollutants not regulated by primary ambient air standards (Roth et al., 1984).

The problem of spatial variation may be addressed in site monitoring through the use of either a random or systematic strategy for locating site monitors. With random sampling, monitoring locations are selected in a random manner such that it is not possible to predict the location of any sampling point based on the location of others. For example, sampling points might be established by choosing a series of pairs of random numbers that can be mapped onto a coordinate system established for the area of concern. Randomly locating sampling locations allows the use of simple statistical methods; average concentrations for the area of concern can be estimated by averaging sample data. Systematic sampling involves laying out a grid of sampling locations that follow a regular pattern, with the initial reference for the grid located randomly. Systematic sampling ensures that the sampling effort across the area of concern is uniform, and it is efficient if the objective is to search for small areas with elevated concentrations. Systematic sampling, however, calls for the use of more complex statistical methods, including the use of special variance calculations to estimate confidence limits on the computed average concentrations (EPA, 1988b).

To address the issue of temporal variations, consideration must be given to the timing of measurements. Repeated samples from a specified location generally produce time-series data whose temporal correlations must be accounted for through the use of statistical methods for analyzing time series. For example, the concentration of a contaminant in an aquifer measured at a given well on a given day will depend in part on what the concentration in the aquifer was on the previous day. If such correlations are ignored and time-series data are treated as a random sample, confidence limits (e.g., for the estimated mean concentration) will be underestimated. Seasonal variations must also be addressed because weather conditions often affect sample composition; heavy rains may result in sediment loading to water bodies, which could increase contamination or affect the concen-
trations of other contaminants through adsorption and settling in the water column. Ideally, monitoring should provide a full annual sampling cycle. If this cannot be accommodated, sampling of water bodies should at least encompass seasonal extremes such as conditions of high water/low water, high recharge/low recharge, windiness/calmness, and high suspended-solids/clear water.

Groundwater contamination has been monitored through the EPA’s National Pesticides in Groundwater Survey, a multiyear monitoring study of 90 organic chemicals and 70 active pesticides and inert ingredients commonly used in agriculture (Poe, 1987). Chemical contaminants in the U.S. food supply are monitored annually through the FDA’s Total Diet Studies, which examine and analyze the purchase of roughly 200 foods sold in grocery stores across the United States. Various data on the kinds and quantities of foods consumed by different population groups have also been collected as part of the U.S. Department of Agriculture’s National Food Consumption Survey and the National Health and Nutrition Examination Survey.

Another means for indirectly determining exposures is biological monitoring focused on biomarkers. Biomarkers are selected biochemical or physiological responses measured in individual organisms that can be used to quantify exposures and levels of sublethal stress. The most direct biomarkers of exposure are chemical residues in tissue, useful for risk agents that bioaccumulate in specific plants or animals and in specific organs. Metals, for example, often accumulate in the liver and kidneys of animals. Methylmercury accumulates in brain tissue and iodine builds up in the thyroid. Human hair obtained from barber shops has been analyzed to monitor for possible exposures to radioactive strontium (Moeller, 1992). Levels of risk agents in tissue can be used to estimate exposures provided there is some understanding of preferential biological absorption and retention process of the risk agent in organs or organisms and some understanding of the physical decay processes of the hazardous substance or material (such as radioactive decay or biodegradation).

Indirect biomarkers of exposure include delta-aminolevulinic acid dehydrase (delta-ALAD) and various cholinesterases. Delta-ALAD is an enzyme that catalyzes a reaction involved in blood synthesis. Because of its sensitivity to inhibition by inorganic lead. Delta-ALAD activity in blood has been used as an index for exposure to inorganic lead in humans and in rats, ducks, pigeons, and fish (EPA, 1989c). Cholinesterases are enzymes that are sensitive to inhibition by organophosphorous and carbamate compounds. Measures of these enzymes, e.g., in the brain tissue of birds, provide an indirect indicator of exposures to the insecticides that contain these compounds (Hayne, 1984).

Sometimes the main advantage of biological monitoring is that the species monitored does the work of collecting samples. For example, since bees cover large areas and collect pollen from a wide range of plants, honey is sometimes monitored as an indicator of arsenic, cadmium, and fluoride contamination. Population effects on sensitive species may give information about exposure levels. For example, certain species of salamanders have proven to be very sensitive to acid rain, leading some researchers to suspect that their decline is a warning of impending widespread damage to forests. Some species may prove to be useful indicators, not because they are harmed by pollutants, but because they thrive in polluted conditions; elevated levels of the coliform bacteria Escherichia coli (E. coli) are often found in waters contaminated with sewage. Other population effects that may be measured for indicator species include altered population distribution, altered population processes (such as survival or productivity) and altered parameters (such as age or sex ratio). On an even broader scale are biological community effects, which include changes in such parameters as species diversity and the ratio of food to consumer organisms.

Accident monitoring also provides a means for indirectly determining exposures. In the area of automobile safety, accident monitoring provides accident exposure rates for different population groups, geographic areas, and vehicles. Two basic accident rates are often monitored. The first is the accident-population rate, which is the number of accidents per unit of population, where the population may be the total number of persons in some driver group (e.g., drivers aged 18 to 21) or the total number of vehicles being studied; the second is the accident-travel rate measured in accidents or collisions per unit of travel (e.g., collisions per 100 million vehicle miles). These two rates are derived from three sets of statistics: the number of vehicles (or persons) in the population being studied, the number of accidents incurred by those vehicles (or persons), and the total amount of travel of the vehicles (or passengers) during the time interval being considered. Other factors that might be monitored to provide additional information useful for accident exposure assessment include the ages of the driver and occupant(s) (because the young can withstand more trauma than older persons) and whether the collision takes place at night or during the day (since post-crash care is typically less efficient and more scarce at night).

3.1.1. Strengths

Exposure monitoring provides estimates of individual and population exposures and helps define the causal connections between the sources of a risk agent and the resulting levels of exposures to human and other populations. Monitoring

When these same concepts are applied to health effects assessment, they are known as epidemiological methods (see Section 4.5). Perezo and Katz (1970) note that with the epidemiological perspective, the accident-population rate can be looked upon as an index of the incidence of the "disease," accidents brought about by motor vehicle use, and the accident-travel rate is an index of the "prevalence" of the disease of motor vehicle use.
is a versatile means for exploring exposure processes. It can encompass surveys of
(a) the uses and misuses of consumer products, (b) exposures of individuals to
accidents involving various activities or technologies, (c) characteristics of the
ambient environment, the human environment, the home, and the workplace,
(d) characteristics of food and water consumed, and (e) doses absorbed and retained
by humans and other populations. In some circumstances, monitoring for exposure
assessment provides direct measures of current exposures, especially in situations
where exposure involves direct contact with the monitored medium (e.g., contact
with chemicals in soil) or where monitoring has occurred directly at an exposure
point (e.g., PEMs or site monitoring of a public water supply). More generally,
monitoring provides data for setting the parameters of exposure models.

3.1.2. Limitations

The most important limitation in monitoring for exposure assessment relates
to the constraints on its ability to provide the basic data needed to apply statistical
methods. The logic of most statistical methods (see Chapter 2) is based on an
assumption of random samples; data are assumed to provide an unbiased
representation of the larger universe of possible observations from which the measure-
ments were taken. In many monitoring systems, however, costs and practicality
demand that sampling be performed at convenient sites and times. Thus, monitoring
often produces an “index,” not an unbiased estimate.

The difficulty of collecting statistically meaningful samples of exposure
measurements is aggravated by the great diversity of environmental media and
exposure pathways. Selecting the right tradeoffs about where, when, and what to
monitor means answering difficult questions. For example, should limited
resources for exposure monitoring focus on a “typical” site or should a location be
selected where environmental stresses are highest, even though the latter would not
provide a representative sample? Should only infrequent, convenient samples be
taken (e.g., sampling during daylight hours, excluding holidays and weekends) or
should more expensive continuous sampling be used to obtain data on the time
correlation among measurements? If the effects of an environmental pollutant
depend on a variety of associated factors (e.g., temperature, humidity, and other
pollutants present), which additional factors must be monitored to ensure that the
collected data prove useful?

Another problem is that the natural variability of the environment over time
and space makes it very difficult to translate measurements obtained from fixed
monitoring stations into actual exposures experienced by people or animals that
move from place to place. To address this issue, field experiments have attempted
to correlate exposures estimated from site monitors with those obtained from
PEMs. The results show that the concentrations experienced by people engaged in
common activities (i.e., driving, walking on sidewalks, shopping in stores, and
working in buildings) do not correlate well with simultaneous readings obtained
from monitoring networks (Cortese and Spengler, 1976; Wallace, 1979; and Ott
and Flachsbart, 1982).

This problem is due in part to the fact that individual behavior has a large
influence on exposure. The problem becomes especially acute when monitoring
exposures to animals, which generally cannot be equipped with PEMs. For example,
the concentration of a chemical in food may not be the concentration actually
taken up by wildlife. The ability to detect and avoid contaminated food is well-
documented for many species. Chemical residue measurements may provide a
means for estimating the exposures of animals that can be subjected to laboratory
analysis. The approach may not be so effective, however, for animals in the wild;
if an animal becomes sick it may seek a secluded location. Thus, biological
monitoring may not provide an accurate assessment of wildlife exposures, due to
the impact of the exposure on the animals' availability for monitoring.

Random variability also creates problems by making it difficult to distinguish
a risk-signaling trend from random variations. For example, although even a small
reduction in the earth’s stratospheric ozone would cause a discernable increase in
ultraviolet radiation reaching the earth’s surface, day-to-day, month-to-month, and
year-to-year variabilities in stratospheric ozone make it difficult to detect long-term
trends. Pintock (1974) has estimated that a sudden 2 percent depletion of ozone
would require an additional 10 years of observation before the event could be
identified through statistical methods with 95 percent confidence.

As is the case with monitoring for release assessment, monitoring for
exposure assessment may be limited by legal, natural, or technological barriers; for
instance, agencies may not have the authority to monitor indoor air pollutants at a
factory. Concentrations of toxic chemicals in a food source might be monitored,
but not how much is eaten, and how often. The deposition of an airborne pollutant
can be measured directly using filter instruments, but monitoring the transmission
of the deposited pollutant through soil and groundwater systems is much more
difficult.

For some media pollutants, concentrations measured in parts per million or
parts per billion may be sufficient to cause significant effects. Such minute levels
may be extremely difficult or impossible to measure given the current sensitivity
of monitoring technology. With antimony, the lowest level that can be accurately
and reproducibly measured is well above reference concentrations suspected of
producing cancer risk (EPA, 1989a). Even when low levels of a risk agent can be
measured, they may be masked by background levels. With radioactivity, regula-
tions limit exposures near nuclear power plants to about 0.05 mSv per year,
however, the average external dose rate from naturally occurring cosmic and
terrestrial radiation is 0.6 to 0.7 mSv per year (Moeller, 1992).
3.2. TESTING METHODS FOR EXPOSURE ASSESSMENT

Since it is generally difficult to conduct controlled tests in large environmental systems under artificial conditions, most of the data relevant to exposure assessment are collected under natural conditions. Thus, monitoring plays a larger role in exposure assessment than the closely related methods of testing and controlled experimentation. Nevertheless, laboratory tests and controlled experiments do play a limited but important role in exposure assessment.

One productive application of testing to exposure assessment is in the study of microcosms. Microcosms attempt to recreate portions of the environment, e.g., a marine ecosystem, in a laboratory setting. Ideally, a microcosm faithfully mimics the processes occurring in nature. Experiments that could not be conducted in the real environment, such as the introduction of specific chemicals, can be performed in the microcosm in a controlled way. Using a microcosm, the partitioning of a chemical among the various components of the environment, together with the associated chemical and biological conversions, can be studied in a single integrated experiment. Performance testing of microcosms has been applied to marine, freshwater, terrestrial, subsurface, and atmospheric microcosms (OSTP, 1984). The method has also been applied to help predict indoor exposures to air pollutants (Duan, 1981).

Microcosms need not be full-scale re-creations to be useful. Scale models sometimes provide an adequate means of simulating exposure processes. For example, a detailed scale model of an urban area has been constructed for the purpose of accounting for the effect of terrain on pollution concentrations caused by emissions from truck and automobile traffic (Murphy and Davies, 1988). Mobile source emissions were represented by a continuous line source simulator, which was built into the model. The entire model was placed in a wind tunnel, with the dispersion of vehicle exhaust simulated by imposing properly scaled meteorological conditions (wind speed and direction) on the model. The impact of the source was then assessed by measuring concentrations at strategically placed receptors.

In general, laboratory tests are useful whenever conditions relevant to exposure can be replicated and more easily studied in the laboratory setting than in the real world. Depending on what exposure processes are being studied, a vast array of such methods may be available. Finkel and Covello (1986), classify methods for quantifying the potential of pathogenic organisms to survive, grow, and become dispersed in an environment. These include (1) methods that involve the growth of microorganisms on or in a cultivation medium or host, (2) methods that measure biochemical activity in dilution-to-extinction media (most-probable-number methods), and (3) methods that measure directly by microscopic observation.

Not all test methods are laboratory-based. Performance testing conducted in the field can often help clarify exposure processes. For example, a nontoxic tracer dye might be introduced into a water system to improve understanding of the transport of pollutants. An example of how large-scale field tests can be used for exposure assessment is a planned Department of Energy facility in Nevada designed to explore how winds and gravity affect large-scale releases of cryogenic or pressurized flammable fluids, toxic substances, and heavy gas. A system of sensors and data collection equipment would monitor release characteristics, including rate, volume, temperature, and pressure. An additional system of sensors would acquire data on meteorological parameters, downwind gas concentrations and aerosol characteristics, and blast and fire effects (DOE, undated).

In the case of exposures to accidents, performance testing has been used to study the dynamics and biomechanics of various types of accidents, including automobile-pedestrian collisions (Schneider and Beier, 1974). One technique utilizes anthropometric dummies in full-scale collision experiments. The experiments are designed to collect data on the relative frequency with which various parts of the body are impacted and the resulting accelerations and forces that collisions produce.

3.2.1. Strengths

Testing provides a means for experimentally studying processes that influence exposures to risk agents. By creating special conditions that occur infrequently or that are difficult to study in nature, the researcher can isolate key factors and improve understanding. Data that are collected can be used to provide the necessary inputs for exposure models and to help calibrate these models to faithfully replicate real conditions relevant to the risk assessment.

3.2.2. Limitations

As in other applications of testing and laboratory methods, the principal question regarding their use for exposure assessment is how well such tests are able to replicate the real world. In the case of microcosms, for example, portions of the environment that are omitted from the laboratory re-creation may mask or alter processes critical to determining real-world response. Similarly, anthropometric dummies used to study the impacts and violent forces to which people are subjected in accidents cannot fully account for the infinite variability of both individual characteristics and accident conditions. Validating laboratory test conditions is often extremely difficult and yet is of critical importance to judging the significance of tests.

The complexity of processes relevant to exposure assessment also creates problems of data collection and test design. In the case of microcosms, comparing results of different tests is difficult due to the wide diversity of testing methods currently in use, each with a narrow sphere of applicability. Distinguishing signifi-
3.3. MODELS FOR EXPOSURE ASSESSMENT

As applied to exposure assessment, a "model" is a mathematical expression representing a simplified version of the essential elements of exposure processes. Its purpose is to provide a means by which diverse data on relevant factors can be combined to predict levels of human or other exposures in the absence of complete or adequate monitoring or testing data.

In general, an exposure model must account for the intensity, routes, and conditions of exposure, the frequency and duration of exposure, and the segments of the population exposed. The models are often developed by generalizing a physical relationship or phenomenon observed in the laboratory or derived empirically from field measurements. For example, the air monitoring data from St. Louis and the power plant plume studies cited previously have been used to construct models for predicting population exposures to air pollution (OSTP, 1984).

Hundreds of exposure models have been developed for a diversity of risk sources, risk agents, and routes of exposure. These models range from "back of the envelope" calculations to large, user-friendly models implemented on mainframe computers. In recent years, there has been a rapid increase in the number of microcomputer-based exposure models.

Some exposure models address physical risk agents, such as acoustic energy and vibration. For example, models have been developed to represent the transmission of ground motion from the source of an earthquake to a given site, taking into account the magnitude of the earthquake, local soil conditions, and the distance from the epicenter to urban areas or a facility at risk, such as a dam (Patwardhan et al., 1980). Models have also been developed to approximate the dynamics and biomechanics of exposures to mechanical energies that occur during accidents involving consumer products or specific technologies. For instance, based on the collision tests with dummies, models have been developed to study the factors that are most important in determining the accelerations and points of impact that occur during automobile–pedestrian collisions (Schneider and Beier, 1974).

Within the general class of exposure models, the largest category of well-developed models consists of specialized models for describing the transport and transformation of specific pollutants released into the environment. Often referred to as pollutant transport and fate models, their objective is to determine the average concentrations of a pollutant for a particular time frame and population group for one or more exposure pathways. The pollutant might be a chemical or biological risk agent, such as a toxic chemical or genetically engineered microorganisms, or it might be a form of energy, such as heated water released by an electric power plant or the ionizing energy of radionuclides released by a nuclear power plant.

The temporal resolution of these models varies from seconds to years, and the exposure pathways considered may include ingestion, inhalation, and dermal absorption. Pollutant transport and fate models are among the most computationally complex of existing exposure models because the processes by which pollutants are dispersed, transformed, and removed from air, water, and other environmental media are extremely complex.

Most pollutant transport and fate models have been developed for specific applications such as estimating radionuclide exposures at locations surrounding a nuclear power plant or estimating exposures from pesticides used in agriculture. The models vary in their data requirements, costs, difficulty of use, types of output, accuracy, and ability to interface with other models. Although a model designed for one application (e.g., radionuclide transport) can seldom be directly applied to another (e.g., genetically engineered microorganisms), it can often be adapted without great difficulty.

Fiksel and Skow (1983) list seven factors that differentiate various pollutant transport and fate models: (1) environmental transport media (e.g., air, surface water, soil, groundwater, or biota), (2) geographic scale (e.g., global, national, regional, or local), (3) pollutant source characteristics (e.g., continuous or instantaneous releases from industrial, residential, and commercial point or area sources), (4) risk agents (e.g., a specific compound or a class of related substances), (5) receptor populations (e.g., humans, animals, plants, microorganisms, and habitats, as well as specific subpopulations exposed to high pollutant levels or particularly sensitive to exposure), (6) exposure routes (e.g., ingestion, dermal contact), and (7) time frame (e.g., retrospective, current, or prospective assessment). Several other general reviews of pollutant fate and transport models have been published, including those by Hoffman et al. (1977), Miller (1978), and Bolton et al. (1985). The subsections below provide brief summaries of the various types of exposure models, organized by transport medium.

3.3.1. Atmospheric Models

Air pollutant transport-and-fate modeling has reached a relatively high degree of sophistication. In general, atmospheric models address the processes of pollutant transport, diffusion, and deposition. Transport refers to the movement of a suspended pollutant through air currents. Air currents typically cause emissions from a point source to follow a zigzag course initially, and then to veer off to one side in an arc. Diffusion refers to the motion of individual particles and molecules that tends to spread and dilute the pollutant. Diffusion is the same process that causes smoke particles from a cigarette in a still room to spread out slowly to all
parts of the room. Deposition is the transfer of particulate matter to the ground, water bodies, and vegetation. Deposition is caused by gravity, as individual particles fall to the ground (dry deposition) or as pollutants contained in falling raindrops or snowflakes reach the ground (wet deposition). Models distinguish between wet and dry deposition because the rate of deposition is generally much higher during rain or snow than it is otherwise.

Transport, diffusion, and deposition occur through complex processes. One important consideration is atmospheric stability, that is, conditions that tend to resist or enhance the vertical motion of air. At most times and in most places, the atmosphere gets steadily colder with greater altitude. Since warm air rises, this produces a general upwelling of warm air; however, if for some reason the temperature at the surface becomes cooler than the temperature above, then the dense, cooler air near the surface cannot get enough lift to rise. In this case, an atmospheric inversion occurs, and upwelling stops. Without upwelling, any pollutant injected into the atmosphere at the surface from chimneys and tailpipes builds up in the air near the surface. For emissions into the air from industrial exhaust stacks, momentum and buoyancy usually cause emissions to rise to a considerable distance. The height to which emissions will rise depends on the conditions of the release (e.g., velocity, temperature, and stack height) and on atmospheric stability. Atmospheric stability is particularly important for estimating atmospheric concentrations near the ground, because it determines where the plume will first reach ground level.

The primary outputs of atmospheric models are (1) atmospheric concentrations of the pollutant, and (2) deposition rates, both wet and dry. Atmospheric concentrations determine human exposure through direct inhalation. Deposition rates determine how much of the pollutant emitted to the atmosphere reaches the soil, surface water, and groundwater.

Most models simplify the process of computing atmospheric concentrations and deposition by dividing the dispersion process into two phases: initial plume rise and subsequent dispersion and deposition. Plume rise is generally assumed to occur without significant dispersion. For industrial exhaust stacks, the amount of rise is added to the actual stack height to determine the effective stack height. Briggs (1975) has developed equations to describe plume rise under different atmospheric stability conditions, using atmospheric stability and Pasquill stability classes described by Martin (1979) and Hanna et al. (1982).

Since so many variables affect the diffusion process, no rigorous mathematical solution has been found. Instead, the most common modeling approach, called the Gaussian plume model, is statistical in nature. The model assumes that the plume from an emission source spreads laterally and vertically in accordance with a Gaussian distribution. Gaussian models often assume that wind is distributed uniformly whenever it is within a specific angular sector. Consequently, the estimated pollutant concentration varies according to the downwind distance from the source but is constant in the crosswind direction within each angular sector. To apply the Gaussian approximation, one must assume a distribution of mean wind speeds and directions as a function of atmospheric stability class. The long-term concentration for a particular angular sector is then computed as the sum of the concentrations over all stability classes.

Gaussian models have limited applicability when the terrain is complex or uneven and when release rates are highly variable. They are fairly accurate, however, for predicting ground-level concentrations where reasonably flat terrain exists and where an average, fairly stable release rate can be assumed (Travis et al., 1983). Validation studies have concluded that Gaussian plume models can predict within a factor of two the annual average atmospheric concentrations at distances of 10 kilometers or less over relatively flat terrain (Hoffman et al., 1978). Predictions over time scales of a few hours or days, however, tend to be less accurate.

The Gaussian plume model is widely used for representing the aerial dispersal of particulates. It has also been used to represent the aerial dispersal of microorganisms. For example, Lighthart and Frisch (1976) developed a modified Gaussian plume model to estimate ground-level concentrations of airborne microorganisms dispersed from a cooling tower, sewage treatment plant, or other point source. The model actually superimposes many Gaussian plumes, one for each droplet size category. Lighthart and Mohr (1987) further refined the model by taking into account the survival rate of microorganisms as a function of weather, including temperature, relative humidity, solar radiation, and time in the aerosol.

Another, more computationally demanding class of atmospheric models attempts to compute the trajectory that a pollutant might follow. Trajectories are typically composed of a connected sequence of trajectory segments estimated for fixed intervals of time and based on historical wind data. Running the models requires solving complex systems of equations that represent continuity of motion and conservation of mass. Trajectory models are most often used for long-range predictions of atmospheric concentrations. Short-term concentrations are assumed to follow some specified frequency distribution. Distributions often used include lognormal, gamma, and Weibull distributions. The approach typically consists of (1) selecting a frequency distribution to represent short-term concentrations, (2) using a Gaussian or trajectory model to estimate how releases might alter the parameters of the distribution (e.g., mean and variance) from historically observed values, and (3) inferring values for short-term concentrations and probabilities from the revised frequency distribution produced by the estimated parameter values.

To handle cases where the terrain is not flat and clearly has an effect on transport and dispersion, complex terrain models have been developed. In addition to accounting for plume rise, atmospheric stability, dispersion, and deposition, such models account for plume interaction with terrain, including plume deflection
around obstacles, plume lifting over terrain, plume impingement on terrain, and terrain contours (Strimatis et al., 1987).

To represent rapid, short-duration emissions, such as might result from explosions, "puff" transport models have been developed. Puff transport models frequently adopt the simplifying assumption that transport and dispersion of a pollutant in the crosswind and vertical directions are uncoupled from the downwind direction. Typically, dispersion in the crosswind and vertical directions is assumed to have a Gaussian distribution. Pollution distribution in the downwind direction is most simply represented as "plug flow," wherein it is assumed that the pollutant is carried by the wind with no dispersion in the downwind direction and no change in the size of the puff. More complicated models account for downwind dispersion and growth of the puff (Overcamp, 1988).

Models for short-term or transient releases that are neither puffs nor continuous plumes have also been developed. One approach is to assume that the short-term release behaves like a succession of puffs. In this case, the results of repeated runs of a puff model are numerically integrated to obtain the desired concentrations. Another approach is to assume a mathematically convenient form for the short-term release that leads to a mathematically convenient form for the concentration as a function of space and time. For example, models have been developed that assume that the release rate of the pollutant from the source decreases exponentially, often a reasonable assumption for a gas leaking from a tank (Wilson, 1979).

Atmospheric models have also been developed for the indoor air environment (OSTP, 1984). Indoor emissions may occur in various ways, including transport of outdoor-generated dust or vapors indoors, or as a result of volatilization of chemicals indoors during use of contaminated water (e.g., during showering, cooking, washing). Accounting for differences in indoor and outdoor concentrations can be crucial. Levels of some pollutants are typically much lower indoors than outdoors (e.g., ozone), while the reverse is true for other pollutants (e.g., styrene). Few models are available for estimating indoor air concentrations originating from outside sources. As a result, most applications make simple assumptions; for instance, indoor concentrations of dust are usually assumed to be some fraction of those outdoors. For vapor transport originating outdoors, concentrations indoors and outdoors are often assumed to be equivalent.

For representing vapor concentrations from indoor emissions, such as where subsurface soil gas or groundwater seepage are entering indoors, compartmental models have been developed. Compartmental models account for the multiple sources and sinks of pollutants and the ventilation rates among discrete volumes of air within a building (NAS-NRC, 1982). Such models can be either steady-state or time-segmented to account for dynamics. Indoor models can be as complex as or more complex than outdoor models. For example, even a model of a single room can become quite complex if it incorporates the effects of air filter efficiencies, particulate aggregation, nonplanting out, nonspecific heterogeneous decay of reactive pollutants, multiple sources and sinks, and varying source strengths (OSTP, 1984).

In addition to transport and dispersion, many atmospheric models account for transformations of airborne risk agents (e.g., photochemical transformations of chemicals or the survival of microorganisms). Such models are necessary in situations where transformation products may pose greater or less hazard than the parent pollutant. The formation of acid rain is one example. Sulfuric acid and nitric acid, the two acids that make up acid rain, are formed in the atmosphere from the gaseous pollutants sulfur dioxide and nitrogen oxides, which are emitted when coal or oil is burned. The formation of these acids in the atmosphere occurs during the chemical reaction of oxidation. Chemical transformation processes and changes in the populations of microorganisms are often approximated by first-order rate reactions. A simple rate model that does not account for the growth of microorganisms (Levin and Strauss, 1991). The Monod equation assumes that population growth continues until the available nutrient source is depleted.

To account for more complicated transformation processes, researchers have developed more sophisticated models. For example, Storløkken and Isaksen (1986) have used a two-dimensional atmospheric chemistry model to estimate changes in stratospheric ozone concentrations as a function of atmospheric concentrations of chlorofluorocarbons (CFCs) and other gases. Their model accounts for the following processes: (1) migration of CFCs to the stratosphere, (2) breakdown of CFCs and release of chlorine as a result of ultraviolet radiation, (3) chemical reactions in which chlorine acts as a catalyst to convert two molecules of ozone to three molecules of oxygen, and (4) the return of the chlorine atom to the troposphere, where it is rained out as hydrochloric acid.

3.3.2. Surface-Water Models

Surface-water transport and fate models are similar in several respects to atmospheric transport and fate models. Pollutants in surface water can originate from point sources (e.g., toxic industrial wastes or heated discharges from cooling technologies) or from nonpoint sources (e.g., seepage from groundwater, direct deposition from air, or normal or storm rainfall runoff of pollutants deposited on land). As with atmospheric models, the concentrations produced by surface water depend on the flow and mixing characteristics of the water body and any physical, chemical, radiological, or biological transformations that may occur.

There are, however, certain key differences between surface water and atmospheric models. Pollutants released to water may dissolve (as acids do) or float on the surface (as petroleum products usually do). Volatile pollutants (i.e., benzene and toluene) will tend to escape from water by turning to vapor. Pollutants in dissolved form may be adsorbed from solution onto sediments, or removed by
aquatic organisms. Pollutants in the form of particulate matter may settle, or precipitate, to the bottom (as metals often do). Adsorption and precipitation tend to reduce the concentrations in surface water, but create deposits that become long-term pollutant sources through desorption or resuspension processes.

The characteristics of the water body that determine mixing also differ from those important in the atmosphere. Pollutants entering surface water are initially dispersed by currents and local turbulence; subsequent concentrations depend on flushing characteristics. In a lake, for example, the rate at which new water enters from incoming streams and leaves by an outlet stream are important. A shallow lake will tend to be well stirred because wind keeps the waters mixed. In contrast, a deep lake may have a well-stirred surface layer and an unmixed deeper layer. Such lakes are called stratified (i.e., layered). Lake stratification is particularly common in summer when the top 10 feet or so of a lake warms in the sun and floats above the colder, deeper water. Thermal stratification can trap and partition pollutants in the various water layers, causing large concentration gradients and temporarily high concentrations.

Chemical processes can be very important in water. Ionization occurs when water molecules, in effect, pull apart the molecules of the contaminant. The resulting ions are reactive, and readily combine with other ions to create different chemicals that may be more or less toxic, dissolvable, volatile, or likely to bioconcentrate. The rates at which such chemical processes occur often depend on water temperature, oxygen levels, and the acidity of the water. With metals, the less oxygen combined with the metal and the more acidic the water, the more dissolvable the metal. Dissolved metals are more likely to be taken up by plants and ingested by animals. Warmer water typically causes reactions to speed up.

Surface-water models must account for such effects. The objective of most surface-water models is to predict the movement, dilution, partitioning, and degradation of contaminants in surface water. Typical applications include (a) estimating the position and size of plumes and/or mixing zones for point-source discharges; (b) estimating the downstream movement rate, dispersion, and fate of contaminants following spills or other pulse discharge events; and (c) estimating average concentrations as a function of distance for continuous point-source or nonpoint-source discharges. The models are generally designed for specific types of water bodies such as streams, rivers, estuaries, coastal waters, impoundments, reservoirs, or lakes.

Descriptions of the basic principles and uses of dynamic surface-water models can be found in engineering textbooks (e.g., Thomann, 1972); however, implementing these principles can be complicated. Representation of the physical processes responsible for transporting pollutants in water bodies presents many challenges. Models for stratified or partially mixed reservoirs and estuaries can be especially complex. Even calculating the time variation of flow in simple streams can be computationally demanding. Silts and clays are often important pollutant-carrying media, but modeling their deposition and sedimentation processes is difficult. Estuaries also present a particularly difficult case, combining conditions of unsteady flow, uncertain residual circulation, and variable salinity (SETAC, 1987).

Underlying most surface-water models is a set of partial differential equations that describe the movement of water, sediments, and contaminants as defined by the physical laws of conservation of mass and momentum. For example, the concentration of a chemical in a water body might be represented by the mass-balance equation. The mass-balance equation states that the rate of change in the concentration $c$ of a chemical in a volume of water $V$ must equal the total inputs of the chemical to the volume minus the total outputs of the chemical from the volume:

$$\frac{dc}{dt} = \text{Inputs} - \text{Outputs}$$

The various terms that appear in such equations represent specific aspects of relevant phenomena. For example, inputs and outputs would include chemical inflows to and outflows from the water volume from external sources, as well as formations and decay within the volume that are associated with chemical reactions and other processes.

Simpler surface-water models often assume steady-state conditions, complete vertical and lateral mixing, and constant decay rates. The steady-state assumption implies that conditions do not change over time but only over distance along the waterway. The assumption of complete mixing implies that pollutant concentrations are constant across the entire waterway at all depths and locations. If an assumption of complete mixing is unrealistic, surface-water models often represent the water body as a series of completely mixed, interconnected compartments. Each compartment is then described by a mass-balance equation, with the inputs and outputs for each equation including transfers from other compartments.

For example, a complicated waterway may be divided into reaches, each of which is assumed to be uniform in character (i.e., velocity, depth, etc.). The mass-balance equations are then solved to calculate pollutant concentrations within each reach as a function of distance downstream from the beginning of the reach. The concentrations and flow information at the end of each reach provide the boundary conditions for the next reach and are combined with the appropriate source and flow information for that reach.

Dynamic models have been developed for use in situations where the goal is to simulate contaminant distributions in space and time. The physical and chemical processes represented in these models are the same as in steady-state models; however, dynamic models can simulate the effects of time-varying contaminant inputs and hydrological parameters on contaminant concentrations. Examples include effluent plume models for calculating contaminant concentration or term-
temperature distributions in the vicinity of time-varying point sources (Koh and Fan, 1970), and the various water quality simulation models described by Basta and Bower (1982) and Boutwell and Roberts (1983).

Reviews and evaluations of available surface-water models are presented in the following: Grimes et al. (1976), Hoffman et al. (1977), EPA (1979), Smith et al. (1977), Mills et al. (1982), Onishi et al. (1980; 1981), and Boutwell et al. (1986). The models differ according to (a) whether they are steady-state or time-dependent, (b) the types of water bodies to which they apply (c) the number and kinds of pollutants addressed, (d) how transformation and decay processes are treated, and (e) whether they emphasize sediment processes, water quality, or other processes. The review by Onishi et al. (1981) groups available models into three categories: (1) water quality models, which primarily address the interaction of waste substances and life forms present in water systems, (2) radionuclide models, which are designed to track releases of radioactive elements from nuclear power plants, and (3) sediment models, which address the movement of sediment through water systems.

3.3.3. Groundwater Models

Groundwater models are used to estimate the fate of contaminants that enter groundwater. Most groundwater models have been developed to analyze the transport of chemicals released from hazardous waste disposal sites.

Once a contaminant enters the groundwater flow system, its motion is determined largely by underground water-flow patterns. These patterns depend on local geohydrological features such as the location of aquifers, saturated layers in the soil and rock that are generally more permeable than the geological units directly below them, natural water recharge, infiltration and withdrawal rates, and factors that influence the density of the liquid (such as temperature and brine concentration). Whether or not groundwater flow is present, contaminants can be transported by dispersion through molecular diffusion. In many cases, however, a large proportion of contaminants in groundwater are absorbed into the soil, thus greatly retarding their movement relative to that of the groundwater. In addition, as in other media, contaminants in groundwater can be transformed through chemical reactions or biological breakdown.

The objective of most groundwater models is to calculate the distribution of contaminants in the unsaturated soil around the sources of leached pollutants (such as disposal sites) and in the saturated soil of aquifers. One output of primary concern in risk assessment is the concentration of pollutants in groundwater used for irrigation and drinking. Groundwater models are often complex, due to the many physical and chemical processes that may affect transport and transformation in groundwater. The important mechanisms that may have to be addressed include contaminants leaching from the surface, advection (including infiltration, flow through the unsaturated zone, and flow with groundwater), dispersion, sorption (including adsorption, desorption, and ion exchange), and transformation (including biological degradation, hydrolysis, oxidation, reduction, complexation, dissolution, and precipitation). The fact that not all chemicals may be dissolved in water means that groundwater models may have to represent chemicals that float on top of groundwater or sink to the bottom of the aquifer.

Groundwater transport and fate models typically include two components: a model for groundwater flow and a model for contaminant transport. Groundwater flow models define the convective flow field and provide estimates of water velocities or flow paths and travel times. The basic equations underlying flow models are based on theories of groundwater hydrology. For example, the equation used to describe an aquifer system is either one defining a fluid flow continuum in porous media, or one defining a porous media equivalent flow for a fracture flow dominated system (Bolton et al., 1983). Based on the results of the groundwater flow model, the contaminant transport model estimates the migration of contaminants, taking into account dispersion and retention. The contaminant transport model also may account for degradation and transformation of the pollutants.

Since groundwater systems are interconnected over vast geographic distances, appropriate limits must be placed on the geographical scale of the groundwater model. This is typically accomplished through the specification of boundary conditions, which describe flow and transport conditions along the perimeter of the modeled area. Boundary conditions can include the specification of fluid and concentration fluxes across the boundary and water-table elevation and contaminant concentrations at the boundary. For example, boundary conditions would include the locations of streams, lakes, and pumping wells and their contribution to discharge and recharge of groundwater, the locations of impermeable geological features across which no-flow conditions occur, the quantity of rainfall infiltrating the subsurface, and the concentrations of source contaminants.

Distinct types of models using different assumptions are usually required to describe groundwater flow and contaminant transport in the unsaturated and saturated zones. The unsaturated zone normally extends down from the surface to the groundwater table; the saturated zone includes the volume below the water table. Flow and transport in the unsaturated zone are typically dominated by vertical movement. Water in an aquifer, however, tends to flow in horizontal directions along the bedding plane of the more permeable geological formation because the resistance to flow is less. The less-permeable (aquitards) or impermeable (aquiclude) layers below, and sometimes above, the aquifer tend to retard or completely block the vertical flow. As a result, one-dimensional models are often adequate for describing groundwater flow in saturated zones.

Due to their independence, some physical transport mechanisms (i.e., filtration and diffusion) can be treated separately for each contaminant. Other processes,
generally chemical in nature (e.g., ion exchange reactions and precipitation), must be modeled simultaneously for all contaminants present in the water, as these mechanisms can interact or compete with each other. Basic retention phenomena, however, are usually not specifically distinguished in groundwater models. Their total effects are typically represented by a constant ratio between the amount of contaminant retained on rocks or soil and the amount in solution. These linear distribution coefficients are defined either per unit mass of the soil or rock or by unit area of fractures. The linear assumption implies that each element migrates independently in a unique chemical form and that retention is instantaneous and reversible.

Hundreds of different groundwater models have been described in the literature, and many have been reviewed, summarized, and tabulated by different authors including: Bachmat et al. (1978), Knox and Canter (1980), Lappala (1980), Moiser et al. (1980), Science Applications, Inc. (1981); Kones (1982); Nelson (1982); Onishi et al. (1982), Oster (1982), Kincaid et al. (1983), Boutwell et al. (1986), and the EPA (1988c). Each model has its own specific assumptions and limitations. The proper selection and application of groundwater models requires a thorough understanding of the physical, chemical, and hydrogeologic characteristics of the site. The EPA has published various guidance documents for the selection of groundwater models (e.g., EPA, 1988d).

3.3.4 Watershed Runoff Models

Many of the pollutants deposited on plants, rocks, and soil end up largely in lakes and streams. Pesticides and other soluble pollutants, for example, are typically flushed out by rain into water bodies. Even pollutants that adhere tightly to soil particles eventually find their way to water bodies; for instance, heavy metals adhering to soil particles can be transported through soil erosion. Watershed runoff models focus on surface transport of contaminants—transport driven by rainfall, overland water flow (runoff), and erosion. These models are generally designed to estimate nonpoint-source pollutant delivery to streams and other surface-water bodies and pollutant infiltration through the soil into the groundwater. Substance-specific factors such as sorption characteristics, solubility (which may depend on soil pH), degradation such as biodegradation by soil microorganisms, and volatility (which depends on meteorological conditions) affect rates of removal and delivery to surface water. Thus, watershed models must account for the chemical characteristics of the watershed as well as the basic hydrologic characteristics. The number of soil chemical phenomena included and the sophistication of simulated chemical processes vary widely among available models.

Despite this diversity of components, most available watershed models incorporate the same or very similar mathematics. A simple approach is to base the model on mass-balance equations that consider all important sources and sinks for the pollutant, including atmospheric deposition, deposition in irrigation water, uptake by plants, leaching into subsurface soil, runoff into surface water, and accumulation in surface soil. The model may represent the drainage basin as a whole, without accounting for the spatial distribution of contaminants within the basin, or it may represent the region under study on a grid or map that accounts for variations in hydrologic processes and contamination distributions from point to point throughout the basin. These grid-type models generally divide the area under study into subregions within which the mass-balance equations are applied. For example, the quantity of pollutant in a volume of surface soil at the end of a particular time period might be determined by the background pollutant concentration in the soil at the beginning of the period, the deposition rate, and the rate at which the pollutant leaves the soil volume. Pollutants can leave through runoff, plant uptake, or infiltration into deeper soil layers and groundwater (Bolton et al., 1985).

Processes controlling runoff, soil erosion, and overland contaminant transport are essentially continuous. Thus, watershed runoff models are often continuous simulation models that describe runoff flow and runoff quality within a drainage basin over an extended period (e.g., 1 year). The bulk of contaminant migration over an extended period, however, is often concentrated in a few storm events that produce runoff. Thus, discrete storm event models that describe response to a single storm (perhaps in storm-averaged form) tend to be more widely used than continuous simulation models.

Many models of overland contaminant transport are basically modified versions of erosion models. Erosion involves two steps: detachment of soil particles from the land surface, and transport of these particles by overland flow. Soil detachment is dependent upon a number of factors, such as particle cohesiveness, organic-matter content of the soil profile, rainfall intensity, vegetative cover, slope gradient, slope length, and soil cultural practices (Wischmeier and Smith, 1978). Thus, erosion models calculate erosion as a function of rainfall, soil characteristics, slope, and vegetative cover. Modifying the models to reflect overland transport of contaminants entails accounting for the properties of the contaminants themselves (e.g., solubility and degradability), simple partition coefficients and first-order rate constants are generally used. For example, Mills et al. (1982) describe a model for the overland transport of pesticides based on the universal soil loss equation (Wischmeier and Smith, 1965) but modified to account for pesticide degradation and volatilization. More complex models of runoff and erosion are also available (see Domigan, 1981; Basta and Bower, 1982; Crawford, 1982). In these models the universal soil loss equation is replaced by mechanistic descriptions of hydrologic processes such as interception, evapotranspiration, infiltration, percolation, and interflow. Several summaries of overland models have been prepared, including ones developed by EPA (1976), Bolton et al. (1983), and Bolton et al. (1985).
3.3.5. Food-Chain Models

Small amounts of persistent substances (i.e., substances not metabolized or biodegraded) can reach large environmental concentrations if they are captured by plants and animals and then transferred to other animals and microorganisms in a stepwise fashion through the food chain. This process is known as bioconcentration or bioaccumulation. Persistent substances include organochlorine insecticides (e.g., dieldrin, and PCBs), heavy metals (e.g., mercury and lead), and radioactive materials (e.g., strontium-90, cesium-137, and iodine-131). Risk assessments often employ food-chain models to account for exposure to such substances.

Bioaccumulation of persistent substances occurs in aquatic organisms as well as in other animals and in certain plants. In the case of aquatic organisms, the accumulation and concentration of toxic materials can occur through processes of absorption and adsorption as well as through metabolic mechanisms. These processes and mechanisms vary according to species characteristics, feeding habits, and environmental variables such as water temperature and salinity (Moghissi et al., 1980). In the case of nonaquatic animals, pollutants may be concentrated within animal organs or products as a result of the animal's consuming contaminated vegetation, drinking contaminated water, or inhaling pollutants. In the case of plants, pollutants may reach the plant via deposition from the atmosphere, irrigation, application of pesticides, or uptake from groundwater. Once in the plant, pollutants behave in different ways. Some elements (e.g., arsenic, beryllium, chromium, lead, nickel, and vanadium) accumulate normally in the roots, whereas others (e.g., cadmium, copper, and zinc) move freely to leaves and other edible portions of the plant (Kabata-Pendias and Pendias, 1984).

In general, the transfer of toxic pollutants through food chains is poorly understood. Consequently, most food-chain models use a simplified approach based on empirically derived concentration or bioaccumulation factors and on estimates of consumption rates for the contaminated food product. For example, estimates of exposures from a contaminated aquatic species are generally based on bioaccumulation factors that relate the pollutant concentration in the organisms to that of the surrounding water. These factors may be derived from experimental data for the pollutant of interest or inferred from data obtained for materials that are expected to behave similarly. When no bioaccumulation factor is available from direct measurement, it is often estimated based on parameters called octanol-water partition coefficients, denoted K_{ow}. This coefficient measures the tendency of a chemical to remain in water versus partition to octanol, which is used as a surrogate for lipids (fat). Through a regression equation, the K_{ow} value may be used to predict bioconcentration in aquatic organisms.

Likewise, the concentration of a pollutant in animal products such as meat, milk, or eggs is often calculated from the animal's feed and water consumption rates, the pollutant concentration in the animal's feed and water, and the transfer coefficients that give the fractional transfer of contaminants between food and water and the animal's products. To translate estimated pollutant concentrations in animals and plants to the concentrations in the food products that people actually ingest, food-chain models must account for any changes in concentration that occur during processing of the product by the producer or preparation by the consumer.

3.3.6. Multimedia Models

If the transport of a pollutant through the environment involves significant transfers and interactions among various media (e.g., air to land to groundwater), the pollutant transport and fate model may require coupling individual media models. Solvents buried in landfills, for example, often move from soil to the air or from soil to groundwater and surface water. Multimedia models simulate the transport and transformation of chemicals or other pollutants in multiple environmental media.
An example of a multimedia transport model is that described by McKone and Layton (1986). As illustrated in Fig. 17, this model views the environment as composed of eight interacting compartments. The compartments represent major components of the environmental system (including air, water, and soil) that exchange physical quantities such as thermal energy, chemical contaminants, or nutrients. Each compartment contains matter in one of three phases: solid, liquid, or gas. A chemical is assumed to be in chemical equilibrium among the phases of a single compartment; however, there is no requirement for equilibrium between adjacent compartments. Physicochemical and transfer properties are used to estimate the interphase transport rates, and a computer program is used to obtain the transient mass balance of a chemical contaminant in the multicompartment environment.

In general, multimedia models can be based on a fully coupled approach in which submodels for each media pathway are fully integrated as shown in Fig. 17, or on a composite approach wherein appropriate models are selected and loosely combined by transferring the output files of one pathway model to the input files of the next (Bolton et al., 1983). The development of fully coupled, computerized multimedia models is a considerable undertaking that generally requires a large amount of input data, computer core size, and run time; however, interconnecting existing media models to produce a composite is also difficult because most individual environmental models are not designed for interaction with other models. (Basic issues of model coupling are discussed in detail in Chapter 5.)

3.3.7. Exposure-Route Models

Exposure-route models are used to address a basic problem in risk assessment: how to convert the output of pollutant transport and fate models into the doses actually received by individuals. The measures and scales by which such models represent exposure depend on the route of exposure, which might be inhalation, ingestion, or dermal contact. For example, inhalation exposure is often expressed in terms of an average inhaled concentration over a given time period. Ingestion exposure is often expressed as an average pollutant concentration in total food consumption. Dermal exposure, a less standard measure, might be expressed in terms of pollutant concentration in the contact medium averaged for continuous, whole-body exposure.

In general, exposure-route models estimate an individual's pollutant intake by multiplying the pollutant concentration in the medium (providing by a pollutant transport and fate model) by an estimated intake rate for that medium times the duration or period over which the individual is exposed to the contaminated medium. Table 12 lists the units typically used to express pollutant concentrations in various media. Table 13 presents the general equation used for computing an intake rate for chronic exposures to chemicals, and Table 14 provides some adaptions and specific values.

### TABLE 12. Measures and Units Typically Used for Expressing Pollutant Concentrations in Various Media

<table>
<thead>
<tr>
<th>Medium</th>
<th>Measures</th>
<th>Typical units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>Weight of pollutant per unit volume or</td>
<td>µg/m³—micrograms per</td>
</tr>
<tr>
<td></td>
<td>mass of air</td>
<td>cubic meter</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ppm—parts per million</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(by weight)</td>
</tr>
<tr>
<td>Air</td>
<td>Volume of pollutant per unit volume of</td>
<td>µg/m³—micrograms per</td>
</tr>
<tr>
<td></td>
<td>air</td>
<td>cubic meter</td>
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<tr>
<td></td>
<td></td>
<td>ppm—parts per million</td>
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<tr>
<td></td>
<td></td>
<td>(by volume)</td>
</tr>
<tr>
<td>Water</td>
<td>Weight of pollutant per unit volume or</td>
<td>µg/l—milligrams per</td>
</tr>
<tr>
<td></td>
<td>mass of water</td>
<td>liter</td>
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<tr>
<td></td>
<td></td>
<td>ppm—parts per million</td>
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<tr>
<td></td>
<td></td>
<td>(by weight)</td>
</tr>
<tr>
<td>Food</td>
<td>Weight of pollutant per unit weight of</td>
<td>µg/kg—milligrams per</td>
</tr>
<tr>
<td></td>
<td>food</td>
<td>kilogram</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ppm—parts per million</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(by weight)</td>
</tr>
<tr>
<td>Soil</td>
<td>Weight of pollutant per unit weight of</td>
<td>µg/kg—milligrams per</td>
</tr>
<tr>
<td></td>
<td>soil</td>
<td>kilogram</td>
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<td></td>
<td></td>
<td>ppm—parts per million</td>
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<tr>
<td></td>
<td></td>
<td>(by weight)</td>
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</tbody>
</table>

### TABLE 13. General Equation for Estimating Chemical Intake

\[ I = \frac{C \times CR \times EF \times EP}{BW} \]

- **I** = Intake (mg/kg-body weight)
- **C** = Average concentration in the media during the exposure period
- **CR** = Contact rate, the amount of contaminated medium contacted per unit time or event
- **EF** = Exposure frequency (days/year)
- **EP** = Exposure period (years)
- **BW** = Body weight, the average body weight over the exposure period (kg)

*Adapted from EPA (1988).*  
*Typical values for exposure period (EP) are 70 years for lifetime exposures and 10 years at one residence.*  
*Typical body weight (BW) values are 70 kg for adults, 60 kg for men, 50 kg for women, and 30 kg for children (10 kg for children under 6 years). Situation-specific values should be used in actual risk assessments.

It is not always clear when a given model dealing with aspects of pollutant intake should be regarded as an exposure-route model (and therefore part of an overall exposure model) or as part of a dose-response model (and therefore part of an overall consequence model). The choice depends in part on whether the exposed entity is an individual, or a target organ (e.g., the lung or liver). In applying the toxicologic framework for categorizing risk assessment methods described in Chapter 1, we have chosen to treat the individual as the exposed entity. Therefore, models describing the activities of pollutants once they have entered the body are discussed in terms of consequence assessment (see Chapter 4). In some situations (see below) it may be more convenient to treat the target organ as the exposed entity and include aspects of pollutant transport through the body as part of an exposure-route model.
<table>
<thead>
<tr>
<th>Pathway</th>
<th>Concentration Type</th>
<th>Equation</th>
<th>Assumptions</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ingestion of drinking water</td>
<td>Chemical in drinking water (mg/liter)</td>
<td>$CR = IR \times SD$</td>
<td>$IR = \text{Ingestion rate} = 0.5 \text{ l/hr}$</td>
<td>365 days/yr</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$SD = \text{Swim duration} = 2.6 \text{ hr/swim}$</td>
<td></td>
</tr>
<tr>
<td>Ingestion of surface water while swimming</td>
<td>Chemical in recreational surface water (mg/liter)</td>
<td>$CR = SA \times PC \times SD \times CF$</td>
<td>$SA = \text{Skin surface area} = 1.8 \text{ m}^2 \text{ (adult)}, 1.94 \text{ m}^2 \text{ (man), 1.69 m}^2 \text{ (woman)}$</td>
<td>7 swim/yr</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$PC = \text{Chemical dermal permeability constant (e.g.,}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$8.4 \times 10^{-5} \text{ mol/m}^2 \text{ hr for water}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$SD = \text{Swim duration} = 2.6 \text{ hr/swim}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$CF = \text{Conversion factor} 1000 \text{ liter/m}^2$</td>
<td></td>
</tr>
<tr>
<td>Ingestion of chemicals in soil</td>
<td>Chemical in soil (mg/kg)</td>
<td>$CR = IR \times CF$</td>
<td>$IR = \text{Ingestion rate} = 200 \text{ mg/day \text{ (child \leq 6 yrs)}}$</td>
<td>Depends on context (days/yr)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$CF = \text{Conversion factor} 10^{-5} \text{ kg/mg}$</td>
<td></td>
</tr>
</tbody>
</table>
| Dermal absorption through contact with soil | Chemical in soil (mg/kg) | $CR = SA \times AF \times ABS \times CF$ | $SA = \text{Exposed skin surface area \text{ m}^2/\text{contact}}$ | Depends on context children: 3
|                                    |                    |          | $= \text{Adults \text{ arms} = 23, hands = 0.82}$ | contact/s, during school yr. 5
|                                    |                    |          | $= \text{Children \text{ (5-6 yrs), arms} = 11,}$ | contact/s, summer
|                                    |                    |          | $= \text{hands} = 0.41, \text{ legs} = 24$ |           |
|                                    |                    |          | $AF = \text{Soil adherence factor} = 1.45 \text{ mg/cm}^2 \text{ spotting soil} = 2.77 \text{ mg/cm}^2 \text{ (clay)}$ |           |
|                                    |                    |          | $ABS = \text{Chemical absorption factor \text{ (unsplashed)}}$ |           |
|                                    |                    |          | $CF = \text{Conversion factor} 10^{-5} \text{ kg/mg} \times 10^6 \text{ cm}^{-2}$ |           |
| Inhalation of airborne vapor phase chemicals | Contaminant in air (mg/m$^3$) | Inhalation rate = 20 m$^3$/day (adult), 15 m$^3$/day (child), 0.7 m$^3$/shower | Depends on context
|                                    |                    |          | 365 days/yr, 365 showers/yr |           |
| Ingestion of fish and shellfish | Contaminant in fish (mg/kg) | $CR = IR \times F1$ | $IR = \text{Ingestion rate} = 113 \text{ kg/meat (fish, shellfish)}$ | 48 meals/year |
|                                    |                    |          | $F1 = \text{Fraction ingested from contaminated source}$ |           |
| Ingestion of contaminated fruits and vegetables | Contaminant in food (mg/kg) | $CR = IR \times F1$ | $IR = \text{Ingestion rate} \text{ (kg/meat) depends on fruit and vegetable types}$ | Depends on context
|                                    |                    |          | $F1 = \text{Fraction ingested from contaminated source}$ |           |
|                                    |                    |          | $= \text{homegrown fruit} = 20, \text{ homegrown vegetables} = 25$ |           |

*Adapted from ICRP (1975), EPA (1989a)
common numeric assumptions. As indicated, intake is typically expressed per unit of time and per unit of exposed individual body weight. Thus, in the case of exposures through the food chain, the basic elements of the model for ingestion are the concentration of the contaminant in each item of the diet (obtained from a food-chain model), the amount consumed (portion size) of each item that contains the contaminant, the frequency with which each item is consumed, and the average body weight over the exposure period.

Average consumption rates are generally used in estimating food intake. For example, market basket analysis typically produces an average or representative intake. Estimates of per capita food intake are typically calculated by dividing the sum of annual production plus imports of a given food item by the number of people in the country. Bolton et al. (1983) provide default consumption rates for various regional population groups for a number of animal and vegetable products, aquatic organisms, and drinking water. To obtain intake estimates for special groups with high intake rates, analysts often rely on dietary surveys in which consumers are asked to recall what foods they ate with what frequency and in what amounts over a defined period of time (Food Safety Council, 1980).

In the case of dermal contact, "intake" is estimated through an analogous process. For example, if the concern is dermal exposure at a polluted water recreational facility, exposure rates would be calculated using data on the length of the exposure period, the concentration of the pollutant in the recreational water, and the fraction of the body area exposed (which would depend on the recreational activity). If the concern is dermal contact through domestic water supplies, on the other hand, the efficiency of domestic water treatment processes would have to be accounted for by the model because such processes can remove significant fractions of dissolved and suspended pollutants. If the concern is dermal exposure to radiation, the body is typically regarded as being "immersed" in a radioactive field.

As described in Chapter 2, the standard units of exposure measurement are the sievert and the rem.

If the pollutant is present in multiple media or if multiple exposure routes exist, each must be modeled separately. For example, to obtain the total dose originating from the concentration of a substance in water, it may be necessary to estimate the dose due to (1) direct ingestion through drinking, (2) skin absorption from water during washing and bathing, (3) inhalation from contaminants in the air resulting from showering, bathing, and other uses of water, (4) ingestion of plants and animals exposed to the water, and (5) skin absorption from contact with soil exposed to the water. It may be appropriate to sum the doses received by each individual route; however, this is seldom the case, since the toxic effects of many substances depend on the route of exposure. For example, inhaled chromium is carcinogenic to the lung, but it appears that ingested chromium is not. The extent to which exposures from different routes must be dealt with separately depends on how the pollutant behaves once it enters the body, a subject that is addressed more thoroughly in Chapter 4.

3.8. Population Models

For a model to estimate populations at risk from a given pathway of exposure, at least two aspects of the exposed populations must be accounted for: demographics and activity. Other characteristics of the population such as the presence of hypersensitive individuals may also need to be considered. For example, to estimate human populations at risk, one must determine who works or lives at various sites and who breathes the air, drinks the water, eats the food, or uses the products affected by a particular risk source. Population models provide this information by describing the population at risk.

Typically, population models disaggregate the exposed population into distinct population groups based on characteristics that increase the probability or severity of health effects occurring to members of the group. The characteristics used to define population groups are called risk factors and fall into two basic categories: lifestyle and genetic. Lifestyle risk factors include age, socioeconomic status, and behavioral traits or factors influencing exposure levels. Genetic risk factors are inherited characteristics, such as sex, that determine an individual's ability to deal with environmental insults. Hypersusceptible groups might be identified on the basis of capacity for enzymatic detoxification or elimination of harmful chemicals, immunologic competence, and developmental or metabolic abnormalities and predispositions to specific diseases. For example, the populations most susceptible to microorganisms are those whose immune systems have been compromised or are less effective, such as persons undergoing drug therapy for cancer, those with nutritional deficiencies, and those with diseases such as AIDS.

In its simplest form, a population model computes an integrated exposure for an individual within a population group by summing the products of the concentrations encountered by the individual in each microenvironment and the time spent in that microenvironment. Average exposures for any averaging period can be computed by dividing the integrated exposure by the time duration of the average period. At a minimum, a population model must include data on the distinct microenvironments visited by a representative individual from each population group, the concentration of the risk agent in each of those microenvironments, and the average time spent in each microenvironment. Population models typically include submodels for the population distribution within a geographic area surrounding the source of risk (e.g., road, power plant, aircraft flight path), submodels of the age distribution of a given population over time, and submodels of mobility and activity patterns of sensitive population groups.
An example of a detailed population model is the National Ambient Air Quality Standard Exposure Model, which is designed for estimating exposures of urban populations to carbon monoxide (Johnson and Paul, 1982). The model generates data on hour-by-hour movements of representative population groups through districts of a city and through selected microenvironments within each district over a period of one year. Another example, the Simulation of Human Air Pollution Exposures (SHAPE) model, combines data on activity patterns of the population with statistical descriptions of pollutant concentrations in specified microenvironments (Ott, 1984). SHAPE uses fourteen microenvironments, and exposures are computed on a person-by-person basis with a time resolution of one minute. The resulting 24-hour exposure profile is then computed for each person, and the frequency distribution of exposures for the population is generated.

If the entities of concern are plants and wildlife rather than humans, population models are needed to estimate the numbers and characteristics of the species that may be exposed. The difficulties associated with human population models are also present here, as well as several additional complicating factors. Most significantly, aquatic and terrestrial wildlife are composed of numerous species with different sensitivities and habits. At a minimum, this complication means that the population model must account individually for each important species or ecosystem exposed. In some cases, this is relatively straightforward. Population models for exposures of many types of aquatic species, for example, are a case in point. When pollutants are fairly evenly distributed in water, there is little need to account for the movement of aquatic species from location to location. With most wildlife, however, modeling the geographical location and behavior of each species is often critical. A population model for a critical species may need to account for feeding behavior, range patterns, and the extent to which individuals of the species are attracted to or repelled by a risk agent. As is the case with humans, some individuals within an animal population may be exposed to greater amounts of a risk agent than the average because of group status, habitat choice, specialized feeding habits, or other factors. Variations may also be related to sex and age, or to individual differences within a sex or age class.

The basic input for most population models is detailed, current demographic data. Compiling such data is often difficult but usually straightforward. Important sources for demographic data include census data, atlases, and environmental or safety reports. Data necessary for characterizing sensitive populations are particularly important, yet often difficult to obtain. Examples include the numbers and characteristics of people living in areas served by a particular drinking water supply, participating in specific recreational activities (e.g., swimmers, fishermen, joggers, and boaters), having particular dietary habits (consumers of seafood or home garden produce), or living in specific subregions (e.g., near sources). Sensitive subpopulations that might be identified include those that are particularly suscep-

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of the dry deposition rates of particulate matter, which in turn affect estimates of the average level of pollution at various distances from an emissions source. Similarly, major uncertainties also surround estimates of the wet deposition caused by rainfall, which in turn may affect the low-probability, high-consequence tails of the distributions of exposures.

In the case of food-chain models, some pathways by which chemicals enter the food chain are often omitted due to a lack of knowledge. For instance, foliar uptake may be omitted from the model but may nonetheless be as crucial as root uptake in the transport of volatile chemicals deposited on soil. Similarly, metabolic transformation of chemicals by plants and their subsequent incorporation into the food chain may be difficult to estimate due to lack of knowledge and the complexity of the processes involved. The regression equation approach to estimating bioaccumulation factors based on octanol/water partition coefficients can overstate concentrations in fish tissue depending upon the chemical of concern and the studies used to develop the regression equations. For example, polycyclic aromatic hydrocarbons (PAHs), found in mixtures in fossil fuels and by-products of fossil fuels, can cause cancer in humans. PAHs with high molecular weights and high $K_{ow}$ values, such as benzo(a)pyrene, lead to the prediction of high fish-tissue residues; however, PAHs are rapidly metabolized and do not appear to accumulate significantly in fish. Regression equations using $K_{ow}$ cannot take into account such pharmacokinetics, and thus may overestimate bioconcentration (EPA, 1989a).

In the case of aquatic transport models, major uncertainties often surround estimates of groundwater transport and sedimentation in rivers. Even if the transport portion of a fate-and-transport model is appropriate for a risk assessment, the fate portion may not be. In the case of surface water models, the effects of biodegradation and the removal of pollutants from soils, sediments, and muds are often poorly represented. For example, the effect of temperature on biodegradation is not well understood. More generally, very little is known about how enzymes break down molecules or about structural characteristics of molecules that inhibit breakdown (SETAC, 1987). The problems are particularly significant if the risk agent is a microorganism. In exposure assessments of microorganisms, a common practice is to couple a transport model developed for particles to a simple fate-model describing the growth or death of the organisms; however, simple fate-models such as a first-order rate equation or the Monad equation represent steady-state conditions only and fail to account for transient conditions likely to be found after a microorganism is introduced into a new environmental setting. Also, if the microorganism is a genetically engineered organism in which DNA has been introduced, then the fate of the DNA rather than the organisms is what is important. As noted in Chapter 2, DNA may remain in the introduced microorganism, be lost from the introduced microorganism and degraded, and/or be transferred from the introduced microorganism into other microbes. Furthermore, because both the DNA and microorganism can replicate, conservation of mass, which lies at the heart of the transport equation, may not necessarily hold.

Exposure-route modeling can also be highly uncertain. Even when ample information is available for computing average exposure rates, the use of such averages can obscure population variations. For example, to estimate ingestion of contaminants in drinking water, risk assessors often assume a lifetime average ingestion rate of 0.03 liters of drinking water per kilogram of body weight. Some sensitive population groups may, however, have a much higher (or lower) intake rate. Formula-fed infants and young children, for instance, have average intake rates that are as much as eight times greater than those of average adults (Cotner et al., 1986).