Modelling the Fate and Exposure of Complex Mixtures of Chemicals in the Aquatic Environment

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ABSTRACT

Chemical transport and transformation processes are simulated in many models to estimate concentrations in receiving environments. These processes are examined, in this paper, for potential influence by interactions between chemicals in mixtures. Different approaches to complex mixture modelling are discussed and used to illustrate model results that may occur, depending on the selected approach.

1 INTRODUCTION

Associated with the manufacture, use, and disposal of chemical substances, industry and government need a set of tools to help establish the degree of risk inherent in each chemical that potentially may be discharged into the environment. Models are practical tools for predicting chemical fate and exposure; in this way they can make valuable contributions to risk assessment. Perfect predictions of actual chemical behaviour in the environment are not possible due to the multitude of approximations and assumptions which must be made to model chemical fate. As there will always be some differences between model results and natural occurrences, the extent that the two are in agreement is the extent to which valid assessments can be made (Brown et al., 1982).

Most evaluations of chemical effects on the environment have been done on a chemical basis. However, very few chemicals occur in nature in a pure state. Usually they are found in mixtures with other substances. Air, for example, is a mixture of several different gases. Seawater is an aqueous solution of various salts. Most soils, rocks, and minerals which make up the earth's crust are complex heterogeneous mixtures of many different chemical substances (Masterton and Slowinski, 1977).

Generally, risk assessments of chemical releases to an aquatic environment, for example, ignore factors such as the complex chemistry due to the mixture of the
receiving waters, other chemicals dissolved in the water column, and chemicals sorbed to sediments. Implicitly we know that we are dealing with chemical mixtures; however, for the concentrations of chemicals normally encountered in the environment, we are not uncomfortable with this convenient simplification in which we ignore chemical interactions.

Complex effluents, such as oil spills, synfuels, and chemical manufacturing discharges, pose especially difficult problems for identifying hazardous constituents and predicting their fate in the environment because of the possible chemical interactions within the mixture itself and between the mixture and the environment (Bergman and Meyer, 1982). In the following sections I discuss the chemical transport and transformation processes which may be affected by chemical interactions, and the current approaches used in complex mixture modelling. For simplicity, the following discussion is restricted to chemicals released to the aquatic environment.

2 TRANSPORT AND TRANSFORMATION PROCESSES

The common approach in exposure modelling is to ignore possible chemical interactions, not because they are considered unimportant, but because of the paucity of scientific information necessary to describe these interactions. An important exception to this statement is the work done in developing models of chemical interactions in the atmosphere (ozone modelling). It is widely recognized that complex interactions occur between chemicals in concentrated mixtures. It is highly probable that similar interactions occur in dilute mixtures and that these interactions may change the concentration, distribution, and ultimate fate of chemicals in the environment. The kinetics of such mixtures are probably proportional to the concentrations of the constituent chemicals. In the following discussions, consideration is given to how some chemical fate and transport processes may be affected by dilute mixtures of chemicals.

2.1 Sorption

The extent to which an organic chemical partitions itself between solid and solution phases is determined by several physical and chemical properties of both the chemical and the soil or sediment aqueous solutions. In most cases, however, it is possible to express the tendency of a chemical to be adsorbed or desorbed in terms of the organic carbon partition coefficient ($K_{oc}$) which is largely independent of soil or sediment properties (Lyman et al., 1982). $K_{oc}$ is a chemical-specific adsorption parameter and may be thought of as the ratio of the amount of chemical adsorbed per unit weight of organic carbon (oc) in the soil or sediment to the concentration of the chemical in solution at equilibrium:

$$K_{oc} = \frac{\text{ug adsorbed per g organic carbon}}{\text{ug/ml solution}}$$
Factors which affect measured values of $K_{oc}$ include temperature, pH, salinity, concentration of dissolved oxygen, suspended particulates, and the solids-to-solution ratio. The presence of other chemicals in a complex mixture could alter the activity coefficient of the chemical in the water, the pH of the water, or the solubility of the chemical in water, and, consequently, the sorption of the chemical to soils and sediments. The degree of adsorption will not only affect chemical mobility, it will also affect volatilization, photolysis, hydrolysis, and biodegradation.

Adsorption of organic chemicals will also occur on minerals free of organic matter. It may be significant under certain conditions such as: (1) in clays with very large surface areas; (2) where cation exchange occurs (e.g. for dissociated organic bases); (3) where clay–colloid-induced polymerization occurs; and/or (4) where chemisorption is a factor (Lyman et al., 1982).

### 2.2 Volatilization

Volutilization represents an important loss mechanism in the overall materials balance. The key environmental factors affecting volatilization are the reaeration constant (surface transfer rate of dissolved oxygen per mixed depth of the water body), wind speed, and the mixed depth of the water body (USEPA, 1982). The most significant chemical parameter influencing volatilization is Henry's law constant ($K_H$), an expression which relates the concentration of a chemical dissolved in the aqueous phase to the concentration of the chemical in the gaseous phase when the two phases are in equilibrium. This parameter is a function of temperature, vapour pressure, and solubility.

When evaluating the volatilization of complex mixtures versus single chemicals, it is obvious that only physicochemical properties can be affected differently by mixtures. Thus, only by altering either aqueous solubility or vapour pressure of a chemical by interactions with other chemicals can volatilization rates be altered.

In mixtures at levels well below solubility limits, Henry’s law constant and aqueous diffusivity coefficients of most compounds may be independent of the presence of other contaminants (Herbes, 1982). Mackay and Yeun (1983) measured volatilization rates for 11 organic compounds of varying Henry’s law constants in a 6-metre wind–wave tank. To look for interactions among the compounds, a few runs were conducted using a mixture of compounds for which the individual mass transfer coefficients had been measured. The difference between the two values was within a 10% error, and it was concluded that interactions between compounds at low concentrations are unlikely to occur.

However, the presence of surface-active organic compounds in water increases the amount of colloidal hydrocarbons in the water column. A typical oil, which may be truly soluble to 200 μg/l, may be solubilized to double this concentration by the presence of a few mg/l of dissolved organic surfactant (Mackay and Shiu,
An additional clue to the effect of chemicals on solubility may be found in the common practice of using polar organic solvents to achieve higher aqueous solubilities of some chemicals for toxicity testing.

If the composition of a given mixture were to be known as well as how each compound influenced the solubility of other compounds in that mixture, it would be possible to anticipate that rate of change for volatilization due to chemical interactions. At this time, however, the exact composition of most mixtures remains unknown as well as how the composition may be changing with time. Obviously, it is not possible to estimate the magnitude of rate of change for volatilization due to interactions without further qualification and quantification.

2.3 Hydrolysis

Many organic compounds can be altered by a direct reaction of the chemical with water, known as hydrolysis. In this reaction, a chemical bond is cleaved and two new bonds are formed, each one having either the hydrogen or the hydroxyl component of the water molecule. Typically the hydroxyl replaces another chemical group on the organic molecule (O'Connor and St. John, 1982).

Hydrolysis reactions are usually catalysed by hydrogen or hydroxyl ions. This produces the strong pH dependence often observed. Hydrolysis of some compounds, however, occurs in pH neutral environments (USEPA, 1982).

Sorption to sediments (or to plankton in the water column) generally reduces the rates of hydrolysis for acid- or base-catalysed reactions. Neutral reactions appear to be unaffected by sorption (USEPA, 1982). A number of cases are known of apparently sediment-catalysed transformations. This phenomenon may involve the presence of exoenzymes activated by attachment to sediment particles (USEPA, 1982).

Hydrolysis rates are expressed in terms of the acid-, neutral- and base-catalysed hydrolysis rate constants (USEPA, 1982). It is widely recognized that the hydrolysis of organic compounds is influenced by the composition of the solvent (Lyman et al., 1982). This complex subject is poorly understood, although it has been noted that rate constants may be one to three orders of magnitude higher in water than in organic solvents (Koppel and Palm, 1972; Mabey and Mill, 1978; Wells, 1968).

The introduction of a complex mixture of chemicals into a water body can be expected to produce a significant shift in pH. Consequently it would not be unreasonable to anticipate that hydrolysis would be affected in complex mixtures.

2.4 Photolysis

Photolysis is the degradation process by which chemical bonds are broken as the result of transfer of light (direct photolysis) or radiant energy (indirect photolysis)
to these bonds (O'Connor and St. John, 1982). The rate of photolysis depends upon numerous chemical and environmental factors including the light adsorption properties and reactivity of the chemical, and the intensity of solar radiation (Lyman et al., 1982; USEPA, 1982).

The photochemical mechanism of photolysis is divided into three stages: (1) the adsorption of light which excites electrons in the molecule; (2) the primary photochemical processes which transform or de-excite the excited molecule; and (3) the secondary ('dark') thermal reactions which transform the intermediates produced in step (2) (Turro, 1978).

Direct photolysis occurs when the reacting molecule directly absorbs radiant energy. Only light—which is absorbed can contribute to photolysis. Near the earth’s surface, the radiation spectrum of interest is between 290 and 750 nm wavelength (Harris, 1982).

Before photolysis can occur, the photochemically excited state must be deactivated. One deactivation pathway involves a radiative process, fluorescence, in which a quantum of light is emitted during the transition to ground electronic state and some residual vibrational excitation is rapidly lost via collision processes. This process is the inverse of the absorption process (Kan, 1966). Other photophysical deactivation processes include quenching, radiationless conversion to ground state and phosphorescence.

Quenching of a photochemical process occurs when the excitation energy in the target organic molecule is transferred to some other chemical species in solution. This process results in net deactivation of the organic substance of concern via energy transfer. Energy can be transferred to any chemical species with a lower triplet energy. A very important and effective quencher (acceptor) is molecular oxygen (Harris, 1982). Presumably other chemicals in a complex mixture could act as acceptors and thereby reduce the photolytic degradation rate of a given compound to below that expected.

Indirect photolysis or sensitized photolysis occurs when the light energy captured (absorbed) by one molecule is transferred to the organic molecule of concern. The donor species (the sensitizer) undergoes no net reaction in the process but has an essentially catalytic effect (Harris, 1982).

Numerous substances can sensitize photochemical reactions including humic acids, titanium dioxide and synthetic organic compounds (USEPA, 1982). Most potential sensitizers, however, occur at such low environmental concentrations that they have negligible effects on photolysis rates (USEPA, 1982). Humic acids, however, frequently occur in concentrations of 1–10 mg/l. They absorb sunlight wavelengths shorter than 500 nm and effectively catalyse the photolysis of many compounds. The probability of a sensitized molecule donating its energy to an acceptor molecule is proportional to the concentration of both chemical species. Complex mixtures may, in some cases, produce enhancement of photolysis rates of individual constituents through sensitized reactions (Herbes, 1982).
2.5 Bioconcentration

The bioconcentration factor (BCF) indicates the degree to which a chemical may accumulate in fish (and other aquatic animals, such as mussels, etc.) by transport across the gills or other membranes, excluding feeding. Bioconcentration is distinct from food-chain transport, bioaccumulation or biomagnification. The BCF is a constant of proportionality between the chemical concentration in fish and water. It is a steady-state ratio of the rate of uptake (absorption across the gills) to the rate of depuration (metabolism and elimination).

Antagonistic interactions have been observed with chemical mixtures and bioconcentration. Matsumura (1977) reported an antagonistic effect of PCB (polychlorinated biphenyl) on DDT accumulation in fathead minnows; DDT accumulation decreased with increasing PCB concentrations. Reinert et al. (1974) reported a similar relationship between DDT and dieldrin with reduced accumulation of dieldrin in yearling lake trout when the fish were exposed simultaneously to DDT.

Synergistic interactions are also possible as enzyme systems can be induced or inhibited by different compounds (Bergman and Meyer, 1982). Cytochrome P-450 and mixed function oxidase systems can be induced by one organic compound resulting in enhanced metabolism of a second organic compound (Gillette, 1979). Conversely, other organic compounds and some heavy metals can inhibit these same enzyme systems (Bergman and Meyer, 1982).

It is possible, for many organic chemicals, to estimate the BCF from the octanol-water partition coefficients ($K_{ow}$). The empirical relationships between $K_{ow}$ and BCF have been developed on a chemical-by-chemical basis. No data exist to evaluate the influence of complex mixtures on BCF.

2.6 Biodegradation

Biodegradation is one of the most important environmental processes that cause the breakdown of organic compounds (Scow, 1982) and, for some compounds, may be the only process by which decomposition may occur. In the presence of microbially-produced biological enzymes, chemical reactions may proceed at rates up to 11 orders of magnitude faster than without.

Some microorganisms can utilize some organic chemicals as food sources to provide energy and carbon for growth and cell maintenance of the microbial population. This is known as growth metabolism. Some organic chemicals may be transformed by microbes without the microbial population being able to derive energy from the chemical reactions. This is termed co-metabolism.

Growth metabolism, the use of the pollutant as a food source, requires that the microbial community adapt to the chemical. Usually a lag phase is associated with this adaptation during which the microbial population develops sufficiently large numbers to be effective in rapidly degrading the chemical. The time required for
adaptation depends upon prior exposure of the community to the pollutant (Spain et al., 1980), the initial numbers of a suitable species (Ward and Brock, 1976), the presence of more easily degraded carbon sources (Ward and Brock, 1976), and the concentration of the pollutant in the water (Spain et al., 1980; Tabak et al., 1981). Growth metabolism frequently results in complete mineralization of the pollutant.

Co-metabolism, the degradation of compounds that cannot be used as growth substances, is believed to occur when some microbially produced enzymes alter the compound to form products which other enzymes cannot utilize. The resulting metabolites are structurally similar to the parent molecule and frequently retain their toxicity. In some instances, the metabolites may be more toxic than the parent compounds. Frequently these metabolites accumulate in the environment (Alexander, 1980); however, they may occasionally be used as food sources by other organisms.

Several environmental conditions, many of which may be modified by the presence of other chemicals in solution, have been shown to influence biodegradation rates. Important parameters include temperature, nutrient availability, sorption to substrates, solubility, pH, and dissolved oxygen.

Microbial degradation has been shown to be a major source of uncertainty for complex mixture fate prediction (Herbes, 1982). At the present time, it is not possible to predict chemical interactions affecting biodegradation rates. Microcosms may prove to be particularly effective tools for investigating this area.

3 CURRENT APPROACHES TO COMPLEX MIXTURE MODELLING

When compared with the exposure modelling efforts for single compounds, very few mathematical models have been used with complex mixtures. The few attempts that have been made can be divided into four classes:

1. one compound at a time;
2. bulk properties;
3. representative chemical classes; and
4. chemical fractions.

Any one of these approaches is amenable to the use of currently existing models.

3.1 Model One Compound at a Time

Perhaps the most common approach is to model the fate and exposure of one compound at a time. Individual model runs are conducted for each identified constituent and the results of all the runs are used to assess the mixture. Ideally, it is desirable to identify and quantify each constituent chemical in the mixture; however, it is highly unlikely that the identity of each constituent can be determined.
Contemporary wisdom suggests that it is neither technically practical nor economically prudent to conduct exhaustive analytical characterizations on all effluent components (Stubblefield and Maki, 1982). Bergman and Meyer (1982) also state that it may be impractical to determine, by testing, the rate constants for processes such as volatilization, hydrolysis, photolysis, and biodegradation for each chemical. They suggest the use of structure-activity relations to estimate chemical properties where data are non-existent and the use of microcosms to investigate transformation rates of mixtures.

3.2 Model Bulk Properties of the Mixture

Conceptually, this approach is the same as that used with the single component models. However, rather than determining properties for each chemical in the mixture, chemical properties, fate processes, and rates are determined for the mixture. A single run of the model provides the estimate of chemical concentration and distribution in the environment.

Although laboratory support requirements are lessened with this approach, laboratory determinations of process rates will probably reflect only those components that are most volatile, sorptive, degradable, etc., and the remaining mixture will differ greatly in composition and properties.

3.3 Model by (Representative) Chemical Classes

Where the constituent identity of a waste stream is known, it should be relatively straightforward to model the fate and exposure by representative chemical classes. The investigator can select and quantify the more important classes of chemicals in the mixture. Compounds are then selected from each class and their properties are taken as representative of the class.

This modelling approach may be especially good where one or more component fractions can be pinpointed as being of biological significance and where chemical data exist on these fractions. Frequently, however, chemicals are selected because their properties have been determined, not because they, in any objective way, are representative of a class of chemicals.

3.4 Model by Chemical Fractions

An approach that is especially applicable to synfuels is to chemically fractionate the mixture. In this way the mixture can be divided physically into several fractions, each containing chemicals of greater similarity (Parkhurst, 1982). Each chemical fraction is further analysed to determine properties such as water solubility, volatility, degradability, etc., and these property values are used in the modelling analysis. This modelling approach is conceptually similar to modelling
by chemical classes and there may be greater similarity between chemicals within a fraction than between chemicals in a designated class.

Any fractions that are determined to be significantly toxic can be further fractionated and tested to determine their chemical properties and even the specific chemical identities of problem compounds.

4 DISCUSSION

The theoretical and technical challenges to exposure modelling of complex mixtures are not appreciably different from those challenges posed by complex mixtures for toxicity assessment. Experimental methods which may be devised to establish the toxicity of complex mixtures, and their major components, will probably be similar to methods devised to evaluate chemical fate processes. If, for instance, it is decided to evaluate toxicity of the mixture by chemical fractions, the transport and transformation processes will be determined for these same chemical fractions.

Significant differences in model requirements exist between the research laboratory and the regulatory agency. Research scientists view models as tools which can be used to integrate knowledge and to direct research efforts into scientifically deficient subject areas. These models tend to be site specific and to require detailed environmental parameterization. Frequently, they also require parameters which are difficult to obtain and which may have to be measured for the chemical(s) of concern. Consequently, models developed for research purposes may be unsuitable for use by regulatory agencies.

Within the regulatory agencies, many of the estimates of chemical concentrations in the environment, chemical transport within and between environmental media, and chemical transformations are made for generic situations or for situations in which site-specific data are not well developed. Consequently, the more sophisticated (complex) models are less frequently used than are the screening level models.

Mills and Porcella (1983) discuss the use of screening level models in helping to identify and prioritize problems associated with environmental contamination from synfuel activities. A particular advantage of the screening level approach is that a multitude of conditions can be rapidly and inexpensively analysed. The screening model is reapplied as many times as desired with input parameters perturbed within a range dictated by variability or uncertainty. Once situations have been analysed, they can be screened and prioritized for more detailed study. This approach is particularly useful for complex mixtures where there is a variety of constituents, contaminants, and environmental settings as well as uncertainty in fate processes.

To illustrate some of the differences that might occur when each component of a chemical mixture is modelled versus when one chemical is taken as representative of a group (class, mixture, fraction, etc.), the following exercise was conducted.
Five phthalate esters were chosen to constitute a class of chemicals which could conceivably be found together in a mixture. This small class of chemicals certainly does not represent the range of parameter values that might be found in a complex mixture. Nevertheless, it serves to provide an interesting look at how the results of a modelling exercise depend upon the approach taken.

The Exposure Analysis Modeling System (Burns et al., 1982) was used to model the fate and exposure of individual phthalate esters in a river. The simulated river had a volume flow of 1000 cubic feet per second. The mean residence time (for chemicals in the water column) of the segment of the river being simulated was 8.8 hours (with the exception that a fraction of the biodegradation occurs in sediments for which the residence time is considerably longer).

The broad differences in behaviour, persistence, distribution, and estimated concentrations of the five phthalates emphasize the significance of identifying the important components of the mixture and modelling each component. Rates of transformation and intermedia transport processes range over two orders of magnitude between the individual chemicals. Similar ranges were estimated for distribution and persistence. Concentrations of phthalates in the water column and in sediments ranged over three orders of magnitude. If any one of these chemicals were selected to represent this chemical class, as might be done when modelling by chemical classes, a two to three order of magnitude error would result.

If a mixture composed of these five phthalate esters were analysed to determine its general properties, the mixture would probably be characterized to reflect the most volatile, most soluble, most degradable constituents. Results of a simulation based on this premise are presented as ‘bulk properties’ mixture in Table 1. As might be expected, the results suggest rapid hydrolysis, rapid biodegradation, low water column concentrations, and high sediment concentrations. These results do not provide a satisfactory alternative to modelling one compound at a time.

Also presented in Table 1 are the results of a simulation in which the mixture is characterized by the mean values of the properties of constituent chemicals. Geometric means were used in this analysis to better represent chemical property values that range over several orders of magnitude. The results of this simulation suggest very little hydrolysis and volatilization, no biodegradation, low water column concentrations, and high sediment concentrations. Even with this relatively uniform mixture of chemicals, the widely divergent results between individual chemicals and the mean value representation argue for modelling one compound at a time.

5 SUMMARY

The scientist or reviewer attempting to evaluate environmental fate and exposure of complex mixtures is presented with at least four possible alternative
Table 1  Estimated fate, persistence and exposure concentrations in five phthalate esters in a river system

<table>
<thead>
<tr>
<th></th>
<th>Dimethyl</th>
<th>Diethyl</th>
<th>Di-n-butyl</th>
<th>Di-n-octyl</th>
<th>Di (2-ethylhexyl)</th>
<th>'Bulk properties' mixture</th>
<th>Mean value mixture</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrolysis (%)</td>
<td>0.23</td>
<td>0.15</td>
<td>20.64</td>
<td>28.80</td>
<td>0.26</td>
<td>17.85</td>
<td>0.01</td>
</tr>
<tr>
<td>Biodegradation (%)</td>
<td>4.29</td>
<td>0</td>
<td>0.06</td>
<td>0</td>
<td>0</td>
<td>44.08</td>
<td>0</td>
</tr>
<tr>
<td>Volatilization (%)</td>
<td>0.05</td>
<td>0.26</td>
<td>6.06</td>
<td>0</td>
<td>0.02</td>
<td>0</td>
<td>0.66</td>
</tr>
<tr>
<td>Water column</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(distribution, %)</td>
<td>92.90</td>
<td>47.91</td>
<td>1.35</td>
<td>0.15</td>
<td>0.14</td>
<td>0.17</td>
<td>0.45</td>
</tr>
<tr>
<td>(concentration, mg/l)</td>
<td>9.66E-3</td>
<td>9.78E-3</td>
<td>7.96E-3</td>
<td>6.79E-6</td>
<td>2.38E-5</td>
<td>5.65E-6</td>
<td>7.10E-4</td>
</tr>
<tr>
<td>Sediment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(distribution, %)</td>
<td>7.10</td>
<td>52.09</td>
<td>98.65</td>
<td>99.85</td>
<td>99.86</td>
<td>99.83</td>
<td>99.5</td>
</tr>
<tr>
<td>(concentration, mg/kg)</td>
<td>4.22E-2</td>
<td>6.4E-1</td>
<td>3.3E-1</td>
<td>3.3E+1</td>
<td>4.7E+2</td>
<td>1.79E+2</td>
<td>1.4E+1</td>
</tr>
<tr>
<td>Self-purification time (months)</td>
<td>0.3</td>
<td>2</td>
<td>4</td>
<td>19</td>
<td>24</td>
<td>13</td>
<td>4</td>
</tr>
</tbody>
</table>
approaches. The relative merit and limitations of each approach have not been
fully explored at this time.

In none of the approaches used with complex mixture exposure modelling has
any attempt been made to incorporate, or to account for, interactions between
chemicals in the mixture. The modelling of chemical kinetics awaits development
of scientific understanding. Other limitations shared by each of these approaches
include the extensive and costly analytical support required for chemical
characterization of the mixtures and the probability that the composition of the
mixture (as released from the source) will change with time.

Based on analyses presented above, it is suggested that:

(1) Many transport and transformation processes may be influenced by the
presence of other chemicals in a mixture.
(2) Modelling chemical interactions in a mixture must await the development of
scientific understanding.
(3) Attempts to model the fate and exposure of complex mixtures using bulk
property or representative chemical class approaches will increase the
uncertainty of the predictions while providing few compensating benefits.

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