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Evaluating Chemical Spill Risks to Aquatic Biota Using Modeling

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Abstract

Environmental impacts from chemical spills are particularly difficult to address, as they are harder or impossible to visually observe and involve much more contamination of the water column compared to surface oil spills. In addition, there are thousands of chemicals that might be spilled, with a wide variety of physical-chemical properties, causing their fates and modes of action for effects to vary considerably. For example, for aqueous acids and bases which readily disperse in the water, the final pH depends on the buffering capacity of the receiving water body in addition to the volume and concentration of acid or base added, and these factors together determine the degree of effects. Other chemicals, primarily organic substances and some inorganic chemicals, are acutely toxic to aquatic life via narcosis, a general disruption of cellular and tissue function. In addition, impacts may be caused by other modes of action, particularly after longer exposures.

This study provides guidance on the likely risks of consequences from, and the window of sampling opportunity for, spills of acutely toxic chemicals other than acids and bases. The guidance and results to answer these and related questions:

- If there is a chemical spill, what is the potential for impacts to aquatic biota due to acute exposure in the water column?
- Assuming the potential impacts are significant, is it advisable to perform sampling to document impacts, and if so, where and for how long a time interval after the release?

The chemical spill model CHEMMAP was run for chemicals representative of those that are often shipped in bulk. The sizes of the affected volumes above various thresholds of concern were estimated for a standard spill volume; as such, concentrations for other spill volumes may be inferred from the standard case (i.e., the concentrations would be approximately proportional to spill size). Natural dispersion was minimized in the representative cases presented here in order to provide a conservative analysis. In addition, the geography of the spill site was assumed to be a simple open water body of 10-m deep water, simulating a typical diurnal upper mixed layer for stratified waters with a pycnocline beginning at 10 m. Natural dilution would be faster in deeper mixed layers and considerably slower in shallower (<10 m) and more restricted water bodies. Thus, the results should be considered “back-of-the-envelope,” useful as guidance for planning purposes, but not necessarily representative of the particulars for a given spill case.

1 Introduction

Spill response regulations in many jurisdictions require that decisions be made quickly about whether to respond to a spill, and where and when to sample the water column to document contamination or exposure above levels of concern. This project was undertaken to provide guidance on the likely risks of consequences from chemical spills and the window of sampling opportunity to respond to such spills. The guidance and results may be used for planning purposes to answer these and related questions:

- If there is a chemical spill, what is the potential for impacts to aquatic biota?
- Is it advisable to perform sampling, and if so, where and for how long a time interval after the release?

Chemical spills are especially difficult to address, as they are harder or impossible to observe visually and involve much more contamination of the water column than surface oil spills. In addition, there are thousands of chemicals that might be spilled, with a wide variety of physical-chemical properties causing their fates to vary considerably. Thus, our analysis was of necessity technically complex. However, we have produced a set of look-up tables to simplify the problem of determining how extensive the impact of a spill might be given knowledge of the chemical type and volume spilled.

Analysis of chemical spills is also complicated by the fact that there are various causes of toxic effects and impacts. For spills in marine and estuarine waters, most of the impact in the water column results from acute (short-term, i.e., hours to days) exposure to the chemical released. Many chemical spills involve acids and bases, which cause acute effects by pH change. Other chemicals, primarily organic substances and some inorganic chemicals, are toxic to aquatic life via narcosis, a general disruption of cellular and tissue function. In addition, impacts may be caused by other modes of action than these. For modes of action other than those resulting from pH change, toxicity may be directly related to the concentration of the spilled substance and bioassay data measuring effects at different concentrations may be used to identify (minimum) thresholds of concern.

In this study, we evaluated toxic chemicals, i.e., organic and inorganic chemicals that have some mode of toxic effect on marine biota when present in sufficient concentration. We simulated hypothetical spill scenarios for representative toxic chemicals. The purpose of this evaluation was two-fold. First, we developed a methodology for evaluating the physical-chemical behavior of toxic chemicals in the marine environment. Secondly, we provide a practical guide for resource managers to determine the potential risks associated with a particular incident so that they may plan response and impact evaluations.

To develop the guidelines, we utilized ASA's model CHEMMAP (an updated windows version derived from the NRDAM/CME described in French et al. 1996; French McCay, 2001). CHEMMAP was run for spill sizes and chemicals representative of those that are often shipped in bulk. Resulting concentrations and volumes were tabulated to indicate the size of the affected volume (area and plume thickness) above various thresholds of concern. The concentrations were estimated for a representative spill volume; as such, concentrations for other spill volumes may be inferred from the standard case (i.e., the concentrations would be approximately proportional to spill size). A single current condition of zero currents was run, as in a field situation the plume would be similar in volume to that under this condition but would be moved down current at the ambient current speed. The discussion below describes how one can infer the expected size and location of a subsurface chemical plume, given type of chemical, spill volume, and estimated ambient current velocity. The magnitude of the volume above a selected threshold of concern would indicate whether the spill is of significant risk to aquatic biota.

It should be noted at the outset that the model runs performed should be considered representative of relatively conservative conditions. In the model runs, currents are assumed as the worst-case condition where there is no change in current velocities in space and time. In reality, current shear (changes in space) and variability in time will act to disperse a chemical plume. Variable winds can also set up current shear to disperse a chemical. This natural dispersion was minimized in the representative cases presented here in order to provide a conservative analysis. In addition, the geography of the spill site was assumed to be a simple open (such that dilution is not restricted by geography) water body of 10-m deep water. As the diurnal surface mixed layer in stratified waters is often on the order of 10 m in depth, and mixing into deeper waters is considerably slower than within the mixed layer (e.g., French-McCay et al., 2007; Payne et al., 2007a,b), the conditions characterize such surface waters of the worlds oceans and large estuaries. Natural dilution would be considerably slower in shallower (<10 m) and more restricted water bodies. The results should be considered “back-of-the-envelope”, useful as guidance, but not accurate of the particulars for a given spill case.

2 Description of the Model CHEMMAP

The chemical spill model, CHEMMAP, predicts the trajectory and fate of a wide variety of chemical products, including floating, sinking, soluble and insoluble chemicals and product mixtures. Processes simulated include: slick spreading, transport, and entrainment of floating materials; transport of dissolved and droplet/particulate-phase oil in three dimensions; evaporation and volatilization; dissolution and adsorption onto suspended particulate material (SPM); sedimentation and resuspension; and degradation.

The chemical fates model estimates the distribution of chemical (as mass and concentrations) on the water surface, on shorelines, in the water column, and in the sediments. The model incorporates a Lagrangian three-dimensional transport model, separately tracking surface slicks, entrained droplets or particles of pure chemical, chemical adsorbed to suspended particulates, and dissolved chemical.

The model uses physical-chemical properties to predict the fate of a chemical spill. These include density, vapor pressure, water solubility, environmental degradation rates, adsorbed/dissolved partitioning coefficients (K_{OW}, K_{OC}), viscosity, and surface tension. It will run using any of a variety of one- to four-dimensional hydrodynamic data files as inputs. The fates model may be run as a forecast/hindcast of a single event or in stochastic mode to estimate probable contaminant distributions given historical data of environmental conditions. Outputs of the fates model include mass balance information and animated time-varying plots of trajectories and concentrations. The model is described in French McCay (2001). Example applications are discussed in French McCay and Isaji (2004) and French McCay et al. (2007).

2.1 Chemical Property Data

The physical-chemical properties required by the model to simulate the transport and fate of the spilled material were compiled from published literature sources. CHEMMAP uses a variety of text and numeric descriptors (names, synonyms, registry numbers, etc.) to identify and characterize the spilled chemical or mixture. The model simulates spills of pure chemicals, chemicals in aqueous or hydrophobic solutions, or chemicals in emulsions (i.e., mixtures of particulate material suspended in an aqueous carrier or solvent). Thus, the model inputs also include characteristics that define these mixtures and solutions.

CHEMMAP uses either the Chemical Abstract System (CAS) registry number or the UN number to index the chemical. In addition, the chemical state under spill conditions is defined as one of the following:

- Pure chemical
    - Solid, powder
    - Solid, pellets or granular crystals
    - Solid, block
    - Liquid
    - Gas
- Suspended and/or dissolved in a bulk liquid
    - Dissolved in an aqueous solution
    - Particulate (solid) suspended in aqueous solution (an emulsion)
    - Dissolved in a hydrophobic solvent
    - Dissolved in or adsorbed to hydrophobic material that is suspended as an emulsion in an aqueous solution
    - Both dissolved in an aqueous solution and adsorbed to hydrophobic particulate material that is suspended as an emulsion in the aqueous solution

Several properties vary with temperature. Thus, the model input values are for a standardized temperature of 25^{o}C. The model corrects these parameters to the ambient temperature for a spill incident. The algorithms for changing viscosity and vapor pressure to ambient temperature are taken from French et al. (1996), who developed a regression using the data in Gambill (1959). For pure chemical processes, the increase per 10 degrees Celsius is assumed a factor of 2. For biological processes (e.g., degradation rates), the increase in rate per increase of 10 degrees Celsius is assumed a factor of 3.

2.2 Chemical Fates Model

The chemical fates model estimates the distribution of chemical (as mass and concentrations) on the water surface, on shorelines, in the water column and in the sediments over time. The model separately tracks surface floating chemical, entrained droplets or suspended particles of pure chemical, chemical adsorbed to suspended particulates, and dissolved chemical. Processes that are simulated are spreading (floating liquids), transport, dispersion, evaporation-volatilization, entrainment (liquids), dissolution, partitioning, sedimentation, and degradation.

The model is initialized with the spilled mass at the location and depth of the release, in a state dependant upon the physical-chemical properties of the material. The state (i.e., the categories described above) and solubility are the primary properties influencing the initialization. If the chemical is highly soluble in water, and is either a pure chemical or dissolved in water (before it is spilled), the chemical mass is initialized in the water column in the dissolved state and in a user-defined initial volume. If chemical is an insoluble or semi-soluble liquid, its density is less than or equal to that of water, and the release is defined as at the water surface, the model initializes the material as floating on the water surface. For insoluble or semi-soluble solids, liquids and gases released underwater, the spilled mass is initialized in the water column at the release depth in a user-defined plume volume, as particles, droplets or bubbles, respectively. The median particle size is characterized by a user-defined diameter.

If the chemical is a particulate in an aqueous emulsion or dissolved in a hydrophobic solvent, the spilled mass is initialized as particles (droplets) in the water column at the release depth. The particle size is typically based on product specification data. The initial plume volume is assumed that of the bulk liquid volume spilled. Insoluble solids in large pelletized or block state when spilled are also initialized in this manner. For the state where the chemical of interest is both adsorbed to particles and dissolved (to a limited extent) in the water phase of the bulk liquid, dissolved mass is also initialized in the initial plume volume. The mass of chemical spilled is corrected from the bulk spill volume using appropriate density and concentration data input to the model.

Chemical mass is transported in three-dimensional space and time, by surface wind drift, eddy mixing, currents, and vertical movement in accordance with buoyancy and dispersion. The model simulates adsorption onto suspended sediment, resulting in sedimentation of material. Stoke’s Law is used to compute the vertical velocity of pure chemical particles or suspended sediment with adsorbed chemical. If rise or settling velocity overcomes turbulent mixing, the particles are assumed to float or settle to the bottom. Settled particles may later resuspend (assumed to occur above 20 cm/sec current speed). However, if the chemical is specified as “sticky in water,” resuspension will not occur. (Thus, the “stickiness” is a parameterization of poorly understood processes at the sediment and shoreline interface, where chemical may be specified to remain permanently after contact.)

Wind-driven current (drift) in the surface water layer is calculated within the fates model, based on hourly wind speed and direction data. Surface wind drift of oil has been observed in the field to be 1-6% of wind speed in a direction 0-30 degrees to the right (in the northern hemisphere) of the down-wind direction (Youssef and Spaulding, 1993, 1994). The algorithm developed by Youssef and Spaulding (1993, 1994) is used for wind transport in the surface wave-mixed layer.

The horizontal turbulent diffusion (randomized mixing) coefficient normally ranges from 0.1-10 m^2/sec for modeling turbulent dispersion in coastal and marine waters (Okubo and Ozmidov, 1970; Okubo (1971). The vertical turbulent diffusion (randomized mixing) coefficient is computed as a function of wind speed in the wave-mixed layer, based on Thorpe (1984). In deeper water below the wave-mixed layer, the vertical turbulent diffusion coefficient is typically 0.0001-0.001 m^2/sec.

The diffusion coefficients (other than the vertical in the wave-mixed layer) are model inputs.

For surface floating liquids, the model estimates surface spreading, transport, and entrainment into the water column, to determine trajectory and fate at the surface. Spreading is simulated using the algorithm of Fay (1971). Entrainment is modeled as for oil, using data in Delvigne and Sweeney (1988). Surface floating chemicals interact with shorelines, depositing and releasing material according to shoreline type and whether the material is assumed "sticky." The algorithms used are those developed for oil spills, as described in French McCay (2004).

Dissolution of the chemical of interest from an insoluble solvent (such as naphtha) is modeled using algorithms previously developed for oil (French et al., 1996). The model developed by Mackay and Leinonen (1977) is used for dissolution from a surface slick. The slick (spillet) is treated as a flat plate, with a mass flux (Hines and Maddox, 1985) related to solubility and temperature. A well-mixed layer is assumed, with most of the resistance to mass transfer lying in a hypothetical stagnant region close to the slick.

For subsurface solvent droplets, dissolution of the chemical of interest is treated as a mass flux across the surface area of a droplet (treated as a sphere) in a calculation analogous to the Mackay and Leinonen (1977) algorithm. Dissolution rate of pure chemicals is a function of solubility using a first-order constant rate equation. Dissolved chemical in the water column is assumed to adsorb to particulate matter according to equilibrium partitioning theory, where partitioning between dissolved and adsorbed is in constant proportions (using a partition coefficient related to the octanol-water partition coefficient, DiToro et al, 1991).

Evaporation from floating chemicals is modeled following the approach in Mackay and Matsugu (1973) where the rate of mass flux to the atmosphere increases with vapor pressure, temperature, wind speed, and surface area. Conceptually, this model assumes that the transfer of mass from liquid to the air is limited by molecular diffusion across a stagnant boundary layer in the air just above the chemical's surface.

Volatilization from the water column is calculated from the chemical's vapor pressure (a strong function of temperature) and solubility. The procedure outlined by Lyman et al. (1982), based on Henry's Law and mass flux (Hines and Maddox, 1985), is followed in the model. The volatilization depth for dissolved substances in the water column is limited to the maximum of one half the wave height. Wave height is computed from the wind speed (CERC, 1984).

Degradation is estimated assuming a constant rate of "decay" specific to the environment where the mass exists (i.e., atmosphere, water column, or sediment). This degradation rate accounts for biological and chemical changes to another chemical form, assumed not to be toxic and/or to be no longer tracked in the simulation.

The spilled chemical is modeled using the Lagrangian approach, where multiple sublots, called spillets, of the entire mass (or volume) spilled are tracked as they move in three-dimensional space over time (by addition of the transport vectors due to wind, currents, and buoyancy). At each time step, phase transfer rates (evaporation, dissolution, volatilization, and entrainment) are calculated and a proportionate percentage of the spillets are transferred to the new phase. Thus, thousands of particles (10,000-40,000) were used in the simulations. The fates model computes, in space and time, the following:

- Water surface:
    - area covered by surface floating chemical
    - radius and thickness of surface floating chemical
- Water column:
    - total chemical concentration
    - pure chemical droplet or particulate concentration
    - dissolved chemical concentration
    - chemical concentration adsorbed to suspended sediments
- Sediments:
    - total mass in sediments
    - pure chemical droplet or particulate concentration in the bioturbated layer (assumed 10 cm)
    - dissolved concentration in interstitial water (bioturbated layer)
    - chemical concentration adsorbed to sediments (bioturbated layer)
- Shorelines:
    - area and length contaminated
    - mass of chemical per unit area

CHEMMAP has a Graphical User Interface (GUI), so the user can visualize individual time steps of the model integration and export complete animations of the scenario. The model also calculates and outputs area, plume thickness, and volume of exposure above a range of thresholds.

3 Approach and Methods

3.1 Representative Chemicals, Classification and Model Runs

Chemicals typically shipped in bulk would be those most likely to be spilled in significant quantities. The U.S. Coast Guard has proposed regulations mandated under the 1990 Oil Pollution Act that require response plans for marine transportation-related facilities (US CFR Vol.65, No. 63, March 31, 2000) and tank vessels (US CFR Vol.64, No. 54, March 22, 1999) carrying hazardous substances. The list of hazardous substances carried in bulk and included in the proposed regulations are those (1) containing at least 10% by weight of a chemical covered by the Clean Water Act and (2) transferred to/from or shipped in a vessel in bulk quantities.

For toxic chemicals, i.e., for which acute toxicity is a direct function of concentration in the receiving water body, we established eight classifications based on physical-chemical properties to represent the range of compounds that are typically shipped in bulk. Since the fates of the compounds within each class are similar, hypothetical spills representative of each class were simulated to estimate maximum exposure concentrations around the spill site at any time after the spill. Thus, the results of the representative chemical may be used to estimate concentrations for spills of other chemicals in that class. Concentrations may be compared to ecological effects endpoints to determine volumes of potential ecological impact. An endpoint is a threshold defining a hazardous condition, such as an exposure level (e.g., dose) or pollutant concentration.

The physical behavior classes were defined as in Tables 1 and 2. The reasons for using the properties density, water solubility, and vapor pressure to classify chemicals are as follows. For a pure chemical with moderate or low solubility in water, density relative to water determines whether it initially floats or sinks. If water solubility is high, the chemical quickly dissolves (before floating or sinking) and is diluted in the water column. Likewise, if it is already dissolved in water before it is spilled, it is neutrally buoyant and dilutes as the spilled volume is mixed into the surrounding water. Also, adsorption to suspended particulate matter is proportional to the chemical's degree of insolubility. This is important to (1) the fate of the chemical as the particulate matter may subsequently settle and (2) bioavailability as most organisms are exposed to dissolved rather than particle-bound chemicals (with the exception of filter-feeders). Thus, solubility is a key property determining both fate and toxicity. Volatilization, which can be a significant loss from water after a spill, is a function of vapor pressure. Thus, it influences fate and concentrations. The property ranges were selected to correspond with critical values where the fate of the chemical varies (e.g., for density) or to divide the range for the universe of chemicals into a reasonable number of bins.

Table 1. Classification of physical behavior.

Buoyancy in Water	Solubility Behavior	Volatility
Floater: density < 1.0 g/cm^3	Highly soluble: solubility > 1000 ppm	Highly volatile: vapor pressure > 10^{-3} atm
Neutral: density 1.01-1.03 g/cm^3	Soluble: solubility 100 - 1000 ppm	Semi-volatile: vapor pressure 10^{-7} - 10^{-3} atm
Sinker: density > 1.03 g/cm^3	Semi-soluble: solubility 1 - 100 ppm	Non-volatile: vapor pressure < 10^{-7} atm
	Insoluble: solubility < 1 ppm	

Table 2. Physical behavior classes (code number, behavior) and example chemicals modeled.

Code #	Buoyancy in Water	Solubility Behavior	Volatility	Example Chemical(s) Modeled
1	floater	highly soluble	highly volatile	Benzene Methyl Ethyl Ketone (MEK)
2	floater	semi-soluble	highly volatile	Styrene
3	sinker	highly soluble	highly volatile	Trichloroethylene (TCE)
4	sinker	highly soluble	semi-volatile	Ethylene Glycol
5	sinker	soluble	highly volatile	Carbon Tetrachloride
6	sinker	semi-soluble	semi-volatile	Naphthalene
7	sinker	highly	non-volatile	
8	Neutrally buoyant	(assumed soluble)	(assumed zero)	Conservative Chemical, 10% Aqueous Solution

Note that the physical properties and behavior of the chemicals depends not only on the pure chemical's properties but the state and characteristics of the chemical as it enters the water. Whereas, for example, a soluble chemical may be denser than the ambient water if the chemical is in its pure form, it may already be dissolved in an aqueous solution and so behave as a neutrally buoyant chemical.

Table 3 lists representative chemicals carried in bulk, based on the U.S. Coast Guard list and reported incidents, along with our classification to a behavior class based on density, water solubility, and vapor pressure. Table 4 lists the physical behavior class assignments of these representative chemicals next to a characterization of the key properties based on the property ranges in Table 1.

Hypothetical spills representative of each physical behavior class were simulated to estimate maximum concentrations in water at any time after a spill. Table 2 lists the example chemicals that were selected for use in the analysis. Table 5 contains additional chemical properties for these compounds that are necessary to perform the simulations. It is assumed that the chemicals are not reactive, but they will adsorb onto suspended particulate matter (in accordance with K_{ow}) and degrade at the rates given in Table 5.

The assumptions in Table 6 were used for all model simulations (i.e., for both conservative and non-conservative chemicals). A spill size of 100 m^3 (26,400 gal) of (pure) chemical was used, based on likely spill volumes developed by Boehm et al. (2001) in their evaluation of storage and handling data for chemicals used in the offshore oil and gas industry, many of which are typically transported in bulk. Note that results for other spill sizes are proportional to the mass of chemical spilled. Thus, the concentrations from the simulated spills are representative of that class of chemicals, for the spill size (100 m^3), and conditions listed. The results may be used to infer the magnitude of water volume that would be contaminated after a spill of these or other chemicals of similar properties.

Table 3. Chemicals carried in bulk and evaluated in this study. Physical behavior classes are defined in Table 1.

Chemical Name	CAS Number	State	Density of Pure Chemical (g/cm^3)	Solubility (in pure water, mg/L)	Vapor Pressure (atm, at 25^{o}C)	Physical Behavior Class #
Acetaldehyde	75-07-0	Liquid	0.453[d]	1,000,000[d]	1.197E+00[d]	1
Ammonia	7664-41-7	Gas or Liquid	0.680[g]	346,000[f]	1.000E+01[e]	1
Benzene	71-43-2	Liquid	0.877[e]	1,780[a]	1.253E-01[a]	1
Carbon Tetrachloride	56-23-5	Liquid	1.594[e]	800[c]	1.505E-01[c]	5
Chlorobenzene	108-90-7	Liquid	1.107[e]	484[a]	1.559E-02[a]	5
Chloroform	67-66-3	Liquid	1.483[e]	8,200[c]	2.590E-01[c]	3
Cyclohexane	110-82-7	Liquid	0.778[e]	55[c]	1.253E-01[c]	2
Ethylbenzene	100-41-4	Liquid	0.865[f]	152[a]	1.253E-02[a]	2
Ethylene Glycol	107-21-1	Liquid	1.140[f]	1,000,000[d]	1.184E-04[d]	4
Ethylenediamine	107-15-3	Liquid	0.900[e]	1,000,000[e]	1.410E-02[e]	1
Furfural	98-01-1	Liquid	1.160[e]	79,400[d]	3.059E-03[d]	3
Formaldehyde	50-00-0	Liquid	0.652[d]	1,000,000[d]	6.000E-02[f]	1
Hydrochloric Acid[j]	7647-01-0	Liquid	1.160[f]	1,000,000[e]	3.200E-02[f]	3
Isopropanol	67-63-0	Liquid	0.785[e]	1,000,000[d]	5.625E-02[d]	1
Methanol	67-56-1	Gas or Liquid	0.791[e]	1,000,000[d]	1.600E-01[d]	1
Methyl Ethyl Ketone	78-93-3	Liquid	0.805[e]	240,000[d]	1.194E-01[d]	1
Naphthalene	91-20-3	Solid	1.162[e]	31[b]	1.026E-04[b]	6
Phenol	108-95-2	Solid	1.132[f]	88,360[d]	4.639E-04[d]	4
Sodium Hydroxide[j]	1310-73-2	Liquid	2.130[e]	521,500[f]	0.000E+00[h]	7
Styrene	100-42-5	Liquid	0.906[f]	300[c]	8.685E-03[c]	2
Tetraethyl Lead	78-00-2	Liquid	1.659[e]	2[f]	3.600E-04[f]	6
Toluene	108-88-3	Liquid	0.867[f]	515[a]	3.750E-02[a]	2
Trichloroethylene	79-01-6	Liquid	1.4650[e]	1,100[c]	9.771E-02[c]	3
Triethylamine	121-44-8	Liquid	0.7290[e]	12,300[e]	7.543E-02[e]	1
Xylene (mixed isomers)	1330-20-7	Liquid	0.8697[a]	198[a]	1.132E-02[a]	2

[a] Mackay et al. (1992a); [b] Mackay et al. (1992b); [c] Mackay et al. (1992c); [d] Mackay et al. (1992d)
[e] French et al. (1996)
[f] EnvironTIPS, Environment Canada (1985, as reported in French et al., 1996)
[g] Environment Canada (1984)
[h] CambridgeSoft Corporation (2000)
[i] U.S. Coast Guard (1999)
[j] as pure chemical

Table 4. Classification of chemicals by physical behavior.

Chemical Name	Buoyancy Relative to Water	Solubility Behavior	Volatility	Physical Behavior Class #
Acetaldehyde*	floater	highly	highly	1 or 8
Ammonia	floater	highly	highly	1
Benzene	floater	highly	highly	1
Ethylenediamine*	floater	highly	highly	1 or 8
Formaldehyde*	floater	highly	highly	1
Isopropanol*	floater	highly	highly	1 or 8
Methanol*	floater	highly	highly	1 or 8
Methyl Ethyl Ketone	floater	highly	highly	1
Triethylamine	floater	highly	highly	1
Cyclohexane	floater	semi-soluble	highly	2
Ethylbenzene	floater	soluble	highly	2
Styrene	floater	soluble	highly	2
Toluene	floater	soluble	highly	2
Xylene (mixed isomers)	floater	soluble	highly	2
Chloroform	sinker	highly	highly	3
Furfural	sinker	highly	highly	3
Hydrochloric Acid **	sinker	highly	highly	3 or 8
Trichloroethylene	sinker	highly	highly	3
Ethylene Glycol*	sinker	highly	semi-volatile	4 or 8
Phenol	sinker	highly	semi-volatile	4
Carbon Tetrachloride	sinker	soluble	highly	5
Chlorobenzene	sinker	soluble	highly	5
Naphthalene	sinker	semi-soluble	semi-volatile	6
Tetraethyl Lead	sinker	semi-soluble	semi-volatile	6
Sodium Hydroxide**	sinker	highly	non-volatile	7 or 8
Dissolved conservative chemical	Neutrally buoyant	(assumed soluble)	(assumed zero)	8

* These density differences are for the pure chemical. In actual fact, the identified chemicals are 100% miscible with water, and as such, they will rapidly mix/dissolve into the water column. Some of the chemical may briefly float (and evaporate) or sink, but the majority of the spilled mass will act like neutrally buoyant chemicals, i.e., class 8. The smaller the spill volume, the more the chemical will behave as class 8. Thus, the indicated density-based class applies for relatively large spills under low turbulence conditions or in restricted water bodies, and class 8 applies for small spills, particularly in turbulent open water. Class 8 is the most conservative and worst-case in terms of water concentrations.

** The considerations above apply to pure acid or base. However, pre-dissolved acid or base would be neutrally buoyant, class 8. Correction of concentration to pH is required in order to evaluate potential impacts (not addressed in this paper).

Table 5. Modeled chemicals and additional physical properties used in simulations (n/a = not applicable).

Chemical Name	Molecular Weight (g/mole)	Viscosity (at 25°C, cp)	Octanol/Water Partition Coefficient as log(K_{ow})	Sorption Coefficient for Organic Carbon as log(K_{oc})	Degradation Rate in Surface Waters (instantaneous, per day)
Benzene	78.1[a]	0.602[e]	2.13[a]	2.09[j]	0.0978[a]
Methyl Ethyl Ketone (MEK)	72.1[d]	0.477[g]	0.29[d]	0.29[j]	0.302[d]
Styrene	104.1[c]	0.703[e]	3.05[c]	3.00	0.0978[c]
Trichloroethylene	131.4[c]	n/a	2.53[c]	2.49[j]	0.0302[c]
Ethylene Glycol	62.1[d]	n/a	-1.36[d]	-1.34[j]	0.302[d]
Carbon Tetrachloride	153.8[c]	n/a	2.65[c]	2.61[j]	0.00978[c]
Naphthalene	128.2[b]	n/a	3.37[b]	3.31[j]	0.0978[b]
Conservative Chemical	100	n/a	0[k]	0.00028[j]	0[k]

[a] Mackay et al. (1992a); [b] Mackay et al. (1992b); [c] Mackay et al. (1992c); [d] Mackay et al. (1992d)

[e] French et al. (1996)

[g] Lyman et al. (1982)

[h] U.S. Secretary of Commerce (2000) – NIST

[i] Syracuse Research Center (2000)

[j] Calculated using regression of log(K_{oc}) on log(K_{ow}) from DiToro et al. (1991)

[k] Assumed to be conservative.

Table 6. Assumed inputs for model simulations.

Model Input	Light Wind Conditions	Strong Wind Conditions
Release duration	Instantaneous	Instantaneous
Release depth	Water surface	Water surface
Wind speed	5 kts	15 kts
Temperature	15°C	15°C
Salinity	32 ppt	32 ppt
Suspended sediment concentration	10 mg/L	10 mg/L
Horizontal diffusion coefficient[a]	1 m^2/sec	10 m^2/sec
Vertical diffusion coefficient (below the surface wave-mixed layer)	0.0001 m^2/sec	0.001 m^2/sec
Simulation time step and run duration	15 min for 7 days	15 min for 7 days

[a] Typical values based on Okubo (1971) and Okubo and Ozmidov (1970)

3.2 Thresholds of Concern

For most aquatic biota, only the dissolved chemical is bioavailable (i.e., where there is exposure via uptake through the organism's surface, gills or gut). However, filter-feeding organisms may be exposed to chemical dissolved from particles (either of the chemical or of suspended sediments with adsorbed chemical) taken into their tissues via feeding. Uptake via gills is another potential exposure route. In the model output fields, we have used dissolved concentrations to determine potential for impact. However, given the assumption of 10 mg/L of suspended sediments in the model runs (a typical coastal value, with lower concentrations typical offshore), most of the chemical is in dissolved rather than particulate form. Thus, the particulate exposure pathway is not significant for the scenarios examined.

To determine if the resulting concentrations from a spill of a potentially toxic chemical are of concern, a toxicity threshold must be identified. We have assembled some example thresholds based on two sources: (1) the analysis of the toxicity of aromatic hydrocarbons by French McCay (2002) or (2) acute toxicity bioassay data compiled by the US EPA (2002). French McCay (2002) compiled LC50 (lethal concentration to 50% of exposed organisms) data for aromatic hydrocarbons from bioassay data reported in the literature and estimated the mean and standard deviation of LC50s for a range of species sensitivities. The LC50 for 95% of species falls within the range of the mean plus or minus two standard deviations. The published literature indicates that the ratio of the sublethal threshold for effects to LC50 is 0.10 (i.e., 10%, Geisy and Graney, 1989). Thus, 10% of the LC50 for the mean minus two standard deviations, which is protective against impacts to 97.5% of species, is taken as the threshold of concern.

For the other chemicals, bioassay data were taken from the AQUIRE database compiled by US EPA (2002). The endpoints used were the LC50, EC50 (effects concentration for a 50% reduction in a measured rate of growth or other function, and LOEC (lowest observable effects concentration). The threshold value was assumed equivalent to the minimum of the following values: (1) 10% of the minimum LC50 for any species test, (2) the minimum EC50 for any species test, or (3) the minimum LOEC reported in the US EPA database. Bioassay results for fish and invertebrates in either freshwater or saltwater were included.

Table 7 lists the threshold values estimated for the chemicals included in Table 1. These estimated threshold values are the lowest concentrations where a sublethal effect has been observed in at least one bioassay test. The durations of exposure for those tests are also listed in Table 7. In the spill model simulations, the duration of exposure is typically less than in these bioassay tests. Because toxicity increases (threshold concentration for effects decreases) as duration of exposure increases, and the concentration for the most sensitive species is assumed, the estimated thresholds are conservative indicating *potential* for impact on sensitive, but not necessarily all, species.

Table 7. Estimated effects threshold values (mg/m^3 = μg/L = ppb), based on the analysis in French McCay (2002, source noted as FM) or from data obtained from US EPA (2002, source noted as EPA), where the threshold is assumed to be the minimum endpoint for any aquatic animal species of: (1) 10% of the minimum LC50, (2) the minimum EC50, or (3) the minimum LOEC.

Chemical Name	Threshold (mg/m^3)	Source and Endpoint	Species (Latin name) or Reference	Species: English name	Duration of Exposure (hrs)
Acetaldehyde	210	EPA(1)	*Lepomis macrochirus*	Bluegill	96
Ammonia	72	EPA (2)	*Strongylocentrotus purpuratus*	Purple sea urchin	48-120
Benzene	351	FM(1)	(2.5th percentile species)		
Carbon Tetrachloride	20	EPA (1)	*Dugesia japonica*	Flatworm	7
Chlorobenzene	2	EPA (1)	*Leuciscus idus melanotus*	Carp	48
Chloroform	52	EPA (2)	*Daphnia magna*	Water flea	48
Cyclohexane	240	EPA (1)	*Crangon franciscorum*	Bay shrimp	96
Ethylbenzene	39	FM(1)	(2.5th percentile species)		
Ethylene Glycol	10,000	EPA (1)	*Crangon crangon*	Common shrimp, sand shrimp	48
Ethylenediamine	1,400	EPA (1)	*Artemia salina*	Brine shrimp	96
Furfural	1,057	EPA (1)	*Americamysis bahia*	Opossum shrimp	96
Formaldehyde	4	EPA (1)	*Ictalurus punctatus*	Channel catfish	96
Isopropanol	2,128	EPA (1)	*Spirostomum ambiguum*	Protozoa	24
Methanol	3,702	EPA (1)	*Anodonta imbecillis*	Mussel	96
Methyl Ethyl Ketone	40,000	EPA (1)	*Cyprinodon variegatus*	Sheepshead minnow	24-96
Naphthalene	26	FM(1)	(2.5th percentile species)		
Phenol	1	EPA (2)	*Daphnia magna*	Water flea	24
Styrene	47	FM(1)	(2.5th percentile species)		
Tetraethyl Lead	2	EPA (1)	*Crangon crangon*	Common shrimp, sand shrimp	96
Toluene	102	FM(1)	(2.5th percentile species)		
Trichloroethylene	170	EPA (1)	*Dugesia japonica*	Flatworm	7
Triethylamine	3,200	EPA (3)	*Oncorhynchus mykiss*	Rainbow trout, Donaldson trout	60
Xylene (mixed isomers)	34.7	FM(1)	(2.5th percentile species)		

4 Results

4.1 Volumes Exceeding Thresholds of Concern Over Time

The spilled chemical dilutes and disperses into the water over time. Figure 1 shows the volume exceeding effects thresholds between 1-100 ppm over time for a 100-m^3 spill of a conservative (class 8) chemical. The volume at a given threshold increases for some period as the initially high and localized concentration dilutes, and then decreases as the lower concentrations away from the plume source dilute to below the threshold. For a 100-m^3 spill, in less than 24 hours concentrations fall below 10 ppm under all wind conditions and below 1 ppm in strong wind conditions. In light winds concentrations remain above 1 ppm for 6 days. If the spill were of 10 times the volume (1,000 m^3), in less than 24 hours concentrations would fall below 100 ppm under all wind conditions and below 10 ppm in strong wind conditions. This type of scaling can be used to apply the results in Figure 1 to any spill volume.

The thresholds of concern and of analytical detection determine if and how soon sampling would be indicated for a chemical spill. Assuming a 100-m^3 spill, and a toxic threshold of 10 ppm, a certain volume of water would be impacted. For a 1,000-m^3 spill and a toxic threshold of 100 ppm, that same volume of water would be impacted (and so on). Thus, the spill volume and toxicity of the chemical are the key data needed to determine the likely impact volume.

4.2 Maximum Volumes Exceeding Thresholds of Concern for the Simulated Chemicals

Based on the model results for all runs (representing the high turnover and mixing of water in the thin mixed layer), chemicals entering the water would disperse throughout the 10-m water column within an hour under strong winds and by 14 hours under light winds. Thus, the volumes of water where the vertical average concentration exceeds a range of thresholds any time after the spill were calculated. The area exceeding the threshold was multiplied by 10 m to estimate volume affected at that concentration. (Thus, in light winds and before one day after the spill the volumes affected are slightly overestimated to the degree that the plume has not yet reached the 10 m depth.) Table 8 contains the potential volume impacted by a 100-m^3 spill for the toxic chemicals considered herein at their indicated effects threshold.

From the data in Table 8, it may be seen that:

1) The results vary by physical behavior class because of differences in physical-chemical behavior.
2) Within a physical behavior class, the lower the effects threshold, the larger the water volume impacted.
3) Stronger winds dilute the chemical faster, such that the volumes affected at high concentrations are smaller but the volumes with low concentrations are larger.

During light wind conditions, the total volume of water that is affected by a chemical release is less than for strong wind conditions. However, for light winds the concentrations are higher within the smaller plume volume. During strong wind conditions the chemical is more rapidly dispersed in the water column (i.e. more quickly diluted). The worst wind conditions for a chemical release could be either light wind or strong wind, depending on what threshold would cause a sublethal or lethal effect relative to the volume spilled (i.e., if the threshold is higher, more chemical needs to be spilled to contaminate the same water volume).

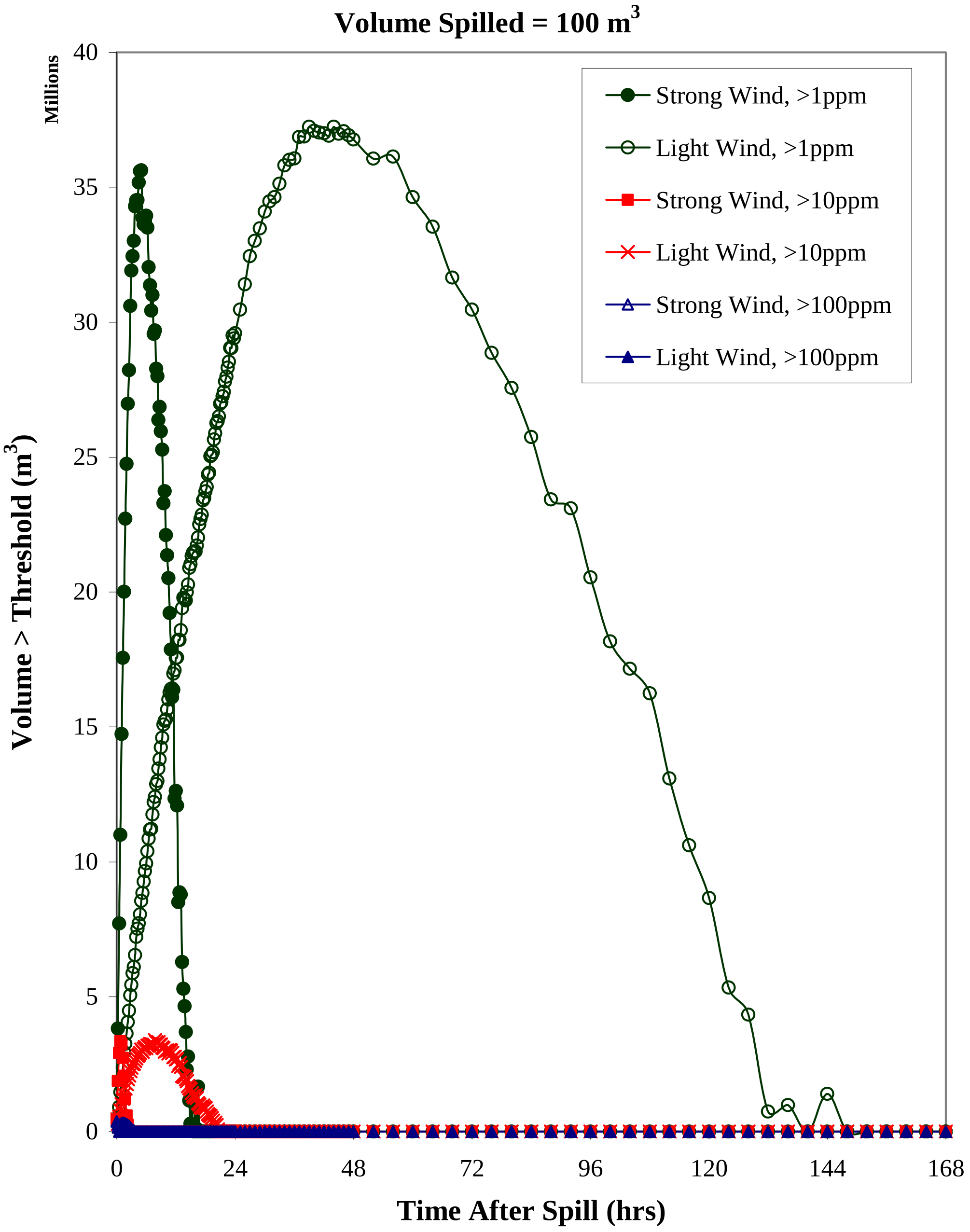

Figure 1. Volumes (millions of m^3) exceeding thresholds of 1-100 ppm over time for a 100-m^3 spill of a conservative (class 8) chemical.

Table 8. Estimated volume (million m^3) where dissolved chemical concentrations in the water column exceed indicated toxicity threshold at some time after a 100-m^3 spill.

Physical Behavior Class #	Chemical Name	Threshold (mg/m^3)	Volume (million m^3)	
			Light Wind Conditions	Strong Wind Conditions
1	Formaldehyde	4	658	3,396
1	Ammonia	72	267	568
1	Acetaldehyde	210	161	200
1	Benzene	351	117	136
1	Ethylenediamine	1,400	25	5
1	Isopropanol	2,128	20	4
1	Triethylamine	3,200	15	3
1	Methanol	3,702	14	2
1	Methyl Ethyl Ketone	40,000	1	0
2	Xylene (mixed isomers)	35	339	964
2	Ethylbenzene	39	324	863
2	Styrene	47	301	702
2	Toluene	102	203	49
2	Cyclohexane	240	130	31
3	Chloroform	52	404	1,315
3	Trichloroethylene	170	260	441
3	Furfural	1,057	55	35
4	Phenol	1	784	5,024
4	Ethylene Glycol	10,000	4	1
5	Chlorobenzene	2	658	4,560
5	Carbon Tetrachloride	20	442	2,110
6	Tetraethyl Lead	2	451	2,340
6	Naphthalene	26	211	561

4.3 Inferred Maximum Volumes Exceeding Thresholds of Concern

The expected fate and concentrations of equal sized spills of chemicals with similar physical-chemical properties would be approximately the same. Thus, the results of the representative chemicals can be used to estimate concentrations for spills of other chemicals in that physical behavior class (see Table 2). The results in Table 8 were based on runs for the representative chemical in the class (e.g., benzene for class 1). Thus, it is assumed, for the purposes of this guidance that other chemicals in the class behave as the representative chemical, a simplification.

Appendix A contains the model results for each representative chemical for a range of potential thresholds that might be used to evaluate spills of other chemicals in the respective physical classes. Results for other thresholds of concern may be estimated by interpolation of the data in Tables A.1 to A.7.

These impact volumes are for a 100-m^3 spill. If the spill volume were ten times higher, the volume impacted would be approximately ten times higher, i.e., the results are approximately proportionate to spill volume. Note that this rule of thumb does not consider the change in concentrations gradients resulting from larger amounts of spill mass. However, the model results are useful for scaling the problem at hand.

For different size spill volumes, the volume of water where the vertical average concentration of dissolved chemical exceeds a particular threshold can be determined using Tables A.1 to A.7 by adjusting the threshold levels in the tables. If the volume spilled is larger than the modeled volume, scale the thresholds up by the ratio of the new volume to the modeled volume. If the spilled volume is smaller than the modeled volume, scale the thresholds down by the ratio of the new volume to the modeled volume. For example, if 1000 m^3 of benzene is spilled, the scaling ratio would be 1000m^3/100m^3, which is a factor of 10. The volume of water exceeding the particular threshold can then be determined by scaling the thresholds up by the factor of 10 (also see guidance summary in Section 5).

5 Guidance for Spills of Any Toxic Chemical or Volume

The representative spills were run for a single volume and uniform environmental conditions to provide an indication of dilution and resulting concentrations that might be expected after a chemical spill. To use this information to determine the volume of potential impact for a spill of a chemical X, follow these steps:

1. Based on the properties of chemical X, use Tables 2 and 3 to determine the chemical class. Select the results in Tables A.1 to A.7 for the chemical class most closely related to chemical X. If the chemical is already dissolved in water or extremely soluble and sufficiently conservative (losses are minimal for the period of interest, i.e. the first week after the spill), use the conservative chemical (Physical Behavior Class 8) results.
2. Determine a threshold of concern, from Table 7 or bioassay data (e.g., US EPA's AQUIRE database and other on-line sources).
3. Determine the correction ratio for the *mass* spilled relative to 100 m^3 (26,400 gal.) of pure chemical. Note that if it is a mixture or solution of less than 100% of the chemical of interest, you will need to correct for both the spill volume and percentage of the chemical in the mixture.
4. From the correct table, and correcting (proportionately) for the mass ratio spilled relative to 100 m^3 of pure chemical, determine the water volume exceeding the threshold of concern.

When applying these results to a spill, one should first determine the closest physical behavior class for the chemical spilled. Note that if the chemical is in a form that is neutrally buoyant, such as in a dissolved state or a fine particle (on the order of microns in diameter), it will behave more like those in class 8 than the class defined by density of the chemical. However, class 8 is defined as a conservative neutrally buoyant chemical that does not degrade or volatilize. Thus, to the extent that a chemical is non-conservative, use of the class 8 results will over-estimate the concentrations. In addition, some chemicals are so soluble that they are 100% miscible with water, and as such, they will rapidly mix/dissolve into the water column. Some of the chemical may briefly float (and evaporate) or sink, but the majority of the spilled mass will act like neutrally buoyant chemicals, i.e., class 8. The smaller the spill volume, the more the chemical will behave as class 8. Thus, the density-based class applies for relatively large spills under low turbulence conditions or in restricted water bodies, and class 8 applies for small spills, particularly in turbulent open water. Class 8 is the most conservative and worst-case in terms of water concentrations.

In the situation where currents are near zero, the location of the plume would be centered on the spill site. However, if there are currents, the plume center will move down-current at the speed of the current. Wind transport of floating hydrocarbons is about 3-4% of wind speed, which would normally be in addition to ambient currents. Wind also drives surface currents that extend below the very surface of the water. Thus, the location of the center of the plume can be calculated by adding the wind (3.5%, if a floater) and current vectors over time. This is in fact what a transport model does. Sampling locations can be planned using a transport model.

6 Discussion and Conclusions

The model results for toxic chemicals (other than acids and bases) may be summarized by the following:

1) The results vary by physical behavior class because of differences in physical-chemical behavior.
2) Within a physical behavior class, the lower the threshold, the larger the water volume impacted.
3) Stronger winds dilute the chemical faster, such that the volumes at high concentrations are smaller but the volumes at low concentrations are higher.
4) Interpretation of the volume affected requires consideration of the threshold for effects, as well as spill volume and chemical characteristics.

Based on the model results, neutrally buoyant and dissolved chemicals would disperse throughout a 10-m water column within an hour under strong winds and by 14 hours under light winds.

Note again that the model runs performed should be considered representative of relatively conservative conditions. In the model runs, currents are assumed the worst-case condition where there is no change in current velocities in space and time. In addition, the geography of the spill site was assumed to be a simple open water body of 10-m deep water. As the diurnal surface mixed layer in stratified waters is often on the order of 10 m in depth, and mixing into deeper waters is considerably slower than within the mixed layer, the conditions characterize typical surface waters of such waters. Natural dilution would be considerably slower in shallower (<10 m) and more restricted water bodies. Thus, the results should be considered “back-of-the-envelope”, useful as guidance, but not accurate in the particulars for a given spill case.

The threshold of concern should be considered to determine if sampling would be indicated for a chemical spill. Assuming a 100-m^3 (26,400 gal) spill, and a toxic threshold of 10 ppm, a certain volume of water would be impacted. For a 1000-m^3 spill and a toxic threshold of 100 ppm, that same volume of water would be impacted (and so on). Thus, the spill volume and toxicity of the chemical are the key data needed to determine the likely impact volume.

The window of opportunity for sampling and detecting the chemical depends on the wind conditions (turbulence, and so dilution rate), the volume spilled, the threshold of concern (background or based on toxicity) and the analytical methods. The results of this study give an indication of the time and spatial scales involved. The location of the plume would be down current from the release site, moving at the velocity of the current.

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Appendix A. Volumes Exceeding Thresholds For Modeled Scenarios

Table A.1. Estimated volume of water (million m^3) where the dissolved chemical concentration exceeds the indicated threshold at some time after a 100 m^3 spill. Thresholds and associated volumes (summarized in Table 8) for the chemicals included in this study are indicated. The model was run for benzene – a floating, highly soluble and highly volatile chemical (Physical Behavior Class 1).

Physical Behavior Class 1

	Volume (million m^3)	
Threshold (ppb)	**Light Wind Conditions**	**Strong Wind Conditions**
< 0.01	1,204	10,544
< 0.1	1,173	7,782
< 1	849	5,174
< 4 (Formaldehyde)	658	3,396
< 10	532	2,221
< 72 (Ammonia)	267	568
< 100	223	293
< 210 (Acetaldehyde)	161	200
< 351 (Benzene)	117	136
< 1000	29	6
< 1400 (Ethylenediamine)	25	5
< 2128 (Isopropanol)	20	4
<3200 (Triethylamine)	15	3
< 3702 (Methanol)	14	2
< 10000	2	0
< 40000 (Methyl Ethyl Ketone)	1	0
< 100000	0	0
< 1000000	0	0

Table A.2. Estimated volume of water (million m^3) where the dissolved chemical concentration exceeds the indicated threshold at some time after a 100 m^3 spill. Thresholds and associated volumes (summarized in Table 8) for the chemicals included in this study are indicated. The model was run for styrene – a floating, soluble and highly volatile chemical (Physical Behavior Class 2).

Physical Behavior Class 2

	Volume (million m^3)	
Threshold (ppb)	**Light Wind Conditions**	**Strong Wind Conditions**
< 0.01	1,077	10,330
< 0.1	1,051	7,963
< 1	795	5,051
< 10	497	2,038
< 34.7 (Xylene)	339	964
< 39 (Ethylbenzene)	324	863
< 47 (Styrene)	301	702
< 100	205	50
< 102 (Toluene)	203	49
< 240 (Cyclohexane)	130	31
< 1000	6	0
< 10000	0	0
< 100000	0	0
< 1000000	0	0

Table A.3. Estimated volume of water (million m^3) where the dissolved chemical concentration exceeds the indicated threshold at some time after a 100 m^3 spill. Thresholds and associated volumes (summarized in Table 8) for the chemicals included in this study are indicated. The model was run for trichloroethylene – a sinking, highly soluble and highly volatile chemical (Physical Behavior Class 3).

Physical Behavior Class 3

Threshold (ppb)	**Volume (million m^3)**	
	Light Wind Conditions	**Strong Wind Conditions**
< 0.01	1,100	10,638
< 0.1	1,084	8,929
< 1	897	6,122
< 10	615	3,211
< 52 (Chloroform)	404	1,315
< 100	321	563
< 170 (Trichloroethylene)	260	441
< 1000	56	36
< 1057 (Furfural)	55	35
< 10000	4	0
< 100000	0	0
< 1000000	0	0

Table A.4. Estimated volume of water (million m^3) where the dissolved chemical concentration exceeds the indicated threshold at some time after a 100 m^3 spill. Thresholds and associated volumes (summarized in Table 8) for the chemicals included in this study are indicated. The model was run for ethylene glycol – a sinking, highly soluble (actually miscible) and semi-volatile chemical (Physical Behavior Class 4).

Physical Behavior Class 4

Threshold (ppb)	**Volume (million m^3)**	
	Light Wind Conditions	**Strong Wind Conditions**
< 0.01	1,084	10,767
< 0.1	1,055	7,778
< 1 (Phenol)	784	5,024
< 10	505	2,099
< 100	210	372
< 1000	37	41
< 10000 (Ethylene Glycol)	4	1
< 100000	0	0
< 1000000	0	0

Table A.5. Estimated volume of water (million m^3) where the dissolved chemical concentration exceeds the indicated threshold at some time after a 100 m^3 spill. Thresholds and associated volumes (summarized in Table 8) for the chemicals included in this study are indicated. The model was run for carbon tetrachloride – a sinking, highly soluble and highly volatile chemical (Physical Behavior Class 5).

Physical Behavior Class 5

Threshold (ppb)	**Volume (million m^3)**	
	Light Wind Conditions	**Strong Wind Conditions**
< 0.01	887	9,516
< 0.1	873	7,932
< 1	721	5,307
< 2 (Chlorobenzene)	658	4,560
< 10	512	2,825
< 20 (Carbon Tetrachloride)	442	2,110
< 100	279	449
< 1000	45	0
< 10000	0	0
< 100000	0	0
< 1000000	0	0

Table A.6. Estimated volume of water (million m^3) where the dissolved chemical concentration exceeds the indicated threshold at some time after a 100 m^3 spill. Thresholds and associated volumes (summarized in Table 8) for the chemicals included in this study are indicated. The model was run for naphthalene – a sinking, semi-soluble and semi-volatile chemical (Physical Behavior Class 6).

Physical Behavior Class 6

	Volume (million m^3)	
Threshold (ppb)	**Light Wind Conditions**	**Strong Wind Conditions**
< 0.01	678	7,042
< 0.1	664	5,290
< 1	519	2,938
< 2 (Tetraethyl Lead)	451	2,340
< 10	293	951
< 26 (Naphthalene)	211	561
< 100	95	11
< 1000	2	0
< 10000	0	0
< 100000	0	0
< 1000000	0	0

Table A.7. Estimated volume of water (million m^3) where the dissolved chemical concentration exceeds the indicated threshold at some time after a 100 m^3 spill. The model was run for a conservative (non-reactive, non-volatile, non-degrading) chemical (Physical Behavior Class 8), pre-dissolved as a 10% solution in 1,000 m^3. These results would apply to any dissolved or neutrally-buoyant substance where losses by volatilization and degradation are low.

Physical Behavior Class 8

	Volume (million m^3)	
Threshold (ppb)	**Light Wind Conditions**	**Strong Wind Conditions**
< 0.01	1,120	10,761
< 0.1	1,104	8,548
< 1	860	5,523
< 10	559	2,798
< 100	282	393
< 1,000	38.7	40.3
< 1,775	21.7	23.8
< 1,805	21.5	22.9
< 2,425	17.3	14.7
< 2,480	16.6	14.7
< 10,000	5.93	1.83
< 17,750	3.78	0.00
< 18,050	3.78	0.00
< 24,250	3.47	0.00
< 24,800	3.27	0.00
< 100,000	1.02	0.00
< 177,500	0.00	0.00
< 180,500	0.00	0.00
< 242,500	0.00	0.00
< 248,000	0.00	0.00
< 334,000	0.00	0.00
< 612,000	0.00	0.00
< 1,000,000	0.00	0.00