Evaluation of Drinking Water Contaminants Using Modeling

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Abstract

A wide variety of chemicals are used in manufacturing facilities and transported near water bodies. When preparing emergency response plans for spills of these chemicals, it is important to know where the released chemical may be transported as well as potential concentrations in the water and atmosphere. To help address these needs, the 3D chemical spill model CHEMMAP is used to estimate the fate and concentrations of selected chemicals in water and the atmosphere, as well as the potential human health impacts resulting from a spill into a river. CHEMMAP uses environmental data forcing (currents and wind) and physical-chemical properties to simulate fate processes over time after the release, including: (1) slick spreading, transport, and entrainment of floating materials, (2) transport of dissolved and particulate materials, (3) evaporation and volatilization, (4) dissolution and adsorption, (5) sedimentation and re-suspension, (6) and degradation.

Organic chemicals contained on the Environmental Protection Agency (EPA)'s list of drinking water contaminants are classified into groups based on physical-chemical characteristics and evaluated using CHEMMAP for representative chemicals and release volumes. Based on model outputs, it is possible to select chemicals that would have the highest human health consequences when released via the consumption of water and inhalation pathways. The model results can be used to indicate safe distances for responders using National Institute for Occupational Safety's (NIOSH) thresholds, as well as the volume of water that may be contaminated above EPA's Maximum Contaminant Level (MGL).

Introduction

Thousands of chemicals are transported on a daily basis near water bodies, at any time an accidental release of chemical could occur. When such an accident arises it is imperative to know where the released chemical may be transported as well as potential concentrations in the water and atmosphere.

In this study, we address the potential human health hazards of chemical spills, using chemicals contained on the Environmental Protection Agency (EPA)'s list of drinking water contaminants. The spill represents a hypothetical incident where a chemical truck overturns on a bridge and looses its cargo into the river below the bridge. The hypothetical accident is located on the Benedict Bridge, which crosses the Patuxent River, MD. ASA's chemical spill model, CHEMMAP, was used to predict the fate of a representative sample of chemicals and spill scenarios to identify the degree to which adverse impacts to human health could occur via the consumption of water and inhalation pathways. Each of the specified chemicals is simulated to estimate maximum concentrations in water and atmosphere over time. Water column concentrations are compared to EPA's Maximum Contaminant Level (MGL). A constant wind of 6 m/s, an average wind for the Patuxent River area (NCEP, 2004), and stable atmosphere was used to provide conservatively high estimates of concentrations, as these conditions would result in the slowest dispersion of the chemical. Time-weighted atmospheric concentrations were calculated and compared to US government thresholds for human health effects: the National Institute for Occupational Safety (NIOSH) REL-TWA and Immediately Dangerous to Life or Health concentrations (IDLH) (NIOSH, 2005). Maximum distance exceeding the indicated threshold is calculated. This information describes the expected human hazard, based on calm conditions, for each spill.

CHEMMAP Model Description

The chemical spill model CHEMMAP has been developed over two decades for assessment of physical fate, biological impacts, natural resource damages and ecological and human health risks. While a few chemical spill models exist that can simulate transport and physical fate of single events (Lunel, 1991; Shen et al., 1995; Rusin et al., 1996), CHEMMAP is unique in being able to evaluate biological and human health impacts, and in its interconnection with hydrodynamic models, geographical information systems, and its graphical user interface. This makes the system flexible and applicable to marine and freshwater systems anywhere in the world. The algorithms and assumptions of the chemical spill model have been described previously (French et al. 1996, French McCay and Isaji, 2004; French McCay et al 2004). The fates model processes and database are briefly summarized below.

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 is three-dimensional, separately tracking 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 uses physical-chemical properties to predict the fate of a chemical spill, including density, vapor pressure, water solubility, environmental degradation rates, adsorbed/dissolved partitioning coefficients (K_{ow}, K_{ow}), viscosity, and surface tension. The spilled mass is initialized at the location and depth of the release, in a state dependant upon the physical-chemical properties of the material. In the first hours to days after a spill, when acute effects to water column organisms would occur, the most important properties determining fate are density, vapor pressure, and water solubility. The adsorbed/dissolved partitioning coefficient (K_{oc}), which is used in the model to compute the fraction dissolved versus adsorbed to suspended sediments, is functionally related and highly correlated with solubility. The value of K_{oc} was calculated from K_{ow} (which was obtained from literature compilations) using the regression equation from DiToro et al. (1991).

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). The currents are those provided by the Proudman Oceanographic Laboratory's UK Continental Shelf hydrodynamic model (Proudman, 1999). Wind-driven current (drift) in the surface water layer (down to 5m) is calculated within the fates model, based on hourly wind speed and direction data (Youssef and Spaulding, 1993). 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). Turbulent dispersion is modeled using a random walk scheme (Bear and Verruijt, 1987), with the magnitudes scaled by horizontal and vertical diffusion coefficients (Okubo, 1971). The vertical diffusion coefficient is computed as a function of wind speed in the wave-mixed layer, approximated as 1.5 times wave height, based on Thorpe (1984). Wave height is calculated using the algorithm outlined in CERC (1984).

Evaporation from slicks of 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. Volatilization from the water column is calculated from the chemical's vapor pressure and solubility following the procedure outlined by Lyman et al. (1982). The mass flux to the atmosphere is transported in the air by the wind and degrades at an empirical rate estimated for in air (French et al., 1999, based on Mackay et al. 1992 b,c,d,e). The atmospheric dispersion model provided estimates of air concentrations in the air layer within 2 m of the water and land surface (i.e., within the approximate height of a person who might be exposed). The mass is dispersed horizontally by turbulence following the algorithm from Gifford (1961), as described in Csanady (1973). The model-calculated horizontal dispersion coefficient is a function of wind speed and air stability.

Chemical reactions are not specifically addressed in the model, i.e., the spilled mass is tracked through phase changes and transport, with all reaction products assumed to move together. Loss of chemical by reaction to some other form no longer of concern is included as degradation. Degradation is estimated assuming a constant rate of "decay" specific to the environment where the mass exists (i.e., atmosphere, water column or sediment). It may include biological, chemical or photochemical processes.

Chemicals and Scenarios Examined

Table 1 lists a subset of chemicals contained on EPA's drinking water contaminants list (EPA, 2005) along with their Chemical Abstract System (CAS) registry number, EPA's Maximum Contaminant Level (MCL), the National Institute for Occupational Safety (NIOSH) REL-TWA and Immediately Dangerous to Life or Health concentrations (IDLH) (NIOSH, 2005). MCL is the highest level of a contaminant that is allowed in drinking water and is an enforceable standard. REL-TWA is a 10-hour time-weighted average exposure limit, which should not be exceeded at any time according to NISOH. IDLH concentrations represent the maximum exposure concentration over 30 minutes without experiencing any impairing or irreversible health effects.

The subset of chemicals was then classified into groups based on their physical-chemical characteristics that determine fate: density, water solubility, and vapor pressure (table 2). The chemical quickly disperses in a dissolved state if water solubility is high, or floats or sinks (depending on density) if solubility is low. Adsorption to suspended particulate matter is proportional to degree of insolubility. Volatilization rate is a function of vapor pressure. The classification of chemicals was based on the property ranges in Table 3 (French McCay, 2004). Table 4 lists the physical behavior classes of chemicals and the representative chemical for each class that was modeled in this study. This classification scheme is similar in concept to the standard classification system used in Europe under the Bonn Agreement (http://www.bonnagreement.org/), although the threshold in that system for an "evaporator" is 300 Pa, as compared to 100 Pa used here.

Hypothetical spills representative of each physical behavior class were simulated to estimate maximum concentrations in water and atmosphere over time. The initial state assumed was a likely shipping state for the chemical. A spill size of 500 gallons was simulated, a common spill volume from a chemical truck, and a spill release time of 1 hour was assumed. The chemicals were released from the water surface. The length of the simulation was selected based on preliminary runs and comparison of concentrations to estimated thresholds values (described below). Tables 3 and 4 contain physical – chemical properties assumed in the simulations.

Environmental and Other Input Data for Model Simulations

A geographical database defines water depth and shoreline type in the model. A grid covering the Patuxent River was prepared using World Vector Shoreline 1-100,000 dataset (U.S. Government MIL-W-89012). The cell size in the grid was 45m (W-E) by 70m (N-S. Gridded depth data, of the same dimensions, contained bathymetry from the Hydrographic Survey Data supplied on CD-ROM by the U.S. Department of Commerce, National Oceanic and Atmospheric Administration, National Geophysical Data Center.

Currents have significant influence on the trajectory, and are important data inputs. Tidal currents were manually interpolated from tidal chart vectors in a commercial (digital) tidal data program (Tides & Currents ®). They are assumed rectilinear (in and out equal and opposite) and with two equal high tides per 25 hrs (M2). Downstream freshwater-driven river flow was not included.

The model uses an hourly wind time series specific to the time and location of the spill. This data is more influential to the fate of insoluble floating chemicals than contaminants in the water column. However, wind speed, duration and fetch are used to estimate wave height (CERC, 1984) and vertical dispersion in the surface mixed layer. An average wind direction and speed was used based on data derived from the output of a numerical atmospheric model (the NCEP model reanalysis) provided by the NOAA-CIRES Climate Diagnostics Center in Boulder, Colorado. Other environmental data inputs were assumed as follows, which are mean values for the Patuxent River (NCEP, 2004) salinity, 8 ppt; water temperature 20°C; suspended sediment concentration 10 mg/L.

The spill was assumed to be represent a chemical truck driving east on Maryland State Route 231 over the Benedict Bridge. This truck then overturns and the cargo is released to the Patuxent River on the water surface. The simulations assume that no clean-up or removal actions of the spilled chemical occur. Table 6 lists the spill site latitude and longitude, along with other inputs defining the scenario, environmental conditions, and simulation parameters. For within-spillet concentration distributions, minimum horizontal and vertical diffusion coefficients over the potential range of values were assumed to provide conservative estimates of potential concentrations resulting from spills.

Results

The model results indicate that the chemicals would disperse throughout the water column within a few hours after the spill release ends. The areas of water where the vertical average concentration exceeded the MCL at any time after the spill were calculated for each representative chemical for each of the physical behavior class, except for class 8. Physical behavior class 8 contains insoluble chemicals therefore no chemical is dissolved in the water column within the simulated 4 days. Table 7 contains results for the area greater than the MCL for each chemical. Chemicals that were not simulated used the representative chemical from the particular class to determine the area greater than the MCL. Figures 1 and 2 show concentrations resulting from two of the spills simulated (physical behavior class 1, benzene and physical class 3, trichloroethylene, respectively). The areas in Table 7 are areas where there is the potential for contaminated drinking water. Note that contaminated area assumes that no removal actions of spilled chemical are made.

Of the eight physical behavior classes that were evaluated, the class of chemicals presenting the highest contamination based on MCL levels would be those that sink and are highly soluble. As the solubility decreases, for sinking chemicals, the extent of contamination decreases. A floating chemical presents the least contamination based on MCL levels, except for insoluble sinkers, because they are also volatile. The floating chemical will quickly volatilize off the water surface therefore causing smaller amounts of water contamination. Note that the floating chemicals evaluated within this paper were all highly volatile; therefore results may be different if the floating chemical has a low volatility.

After a chemical spill, the immediate concerns are to human health hazards in air. Of the eight physical behavior classes that were evaluated, the class of chemicals presenting the most significant concern for atmospheric concentrations would be chemicals that sink and are soluble followed by highly soluble chemicals. A soluble sinker will create greater time-weighted atmospheric concentrations because there is a more steady flux of chemical into the dissolved state in the water, whereas a highly soluble chemical will immediately dissolve into the water. The sinking chemicals with low volatility have a large distance due to the low IDLH and REL-TWA thresholds. Insoluble sinking chemicals will not have a significant concern because the chemicals immediately sink and have no means to be exposed to the atmosphere. Floating chemicals have short distances from the spill site because the chemical volatilizes very quickly and are moved downwind. There is not a continuous mass flux to the atmosphere as in the sinking chemicals. Note that the floating chemicals evaluated within this paper were all highly volatile; therefore results may be different if the floating chemical has a low volatility.

Table 8 lists the maximum distances from the spill site were the IDLH or REL-TWA are exceeded for each chemical and the time it takes to disperse below the indicated threshold. Chemicals that were not simulated used the representative chemical from the particular class to determine the distance to the IDLH and REL-TWA (table 4 notes the representative chemical). Figures 3 and 4 show ½-hour and 10-hour, respectively, atmospheric time-weighted concentrations resulting from a spill of benzene (physical behavior class 1). Figures 5 and 6 show ½-hour and 10-hour, respectively, atmospheric time-weighted concentrations resulting from a spill of trichloroethylene (physical behavior class 3). Distances in Table 8 for the IDLH (½ hour time-weighted averages) are distances from the spill site that should be immediately evacuated. Distances in Table 8 for the REL-TWA (10 hour time-weighted averages) are distances from the spill site that would require protective equipment if spending more time in the contaminated area than it takes to disperse below the REL-TWA threshold. Note, all distances and times assume that no removal actions of spilled chemical are made.

Conclusions

The chemicals evaluated in this paper that would most likely have the greatest human health consequences via the consumption of water are sinking chemicals that disperse readily (are soluble). As one would expect the least water contamination are chemicals that sink and are insoluble. Chemicals with the greatest human health consequences via inhalation pathways are sinking chemicals that disperse readily (are soluble) and are volatile. Floating chemicals would have the least human health consequence; however the floating chemicals evaluated within this paper were all highly volatile. Therefore results may be different if the floating chemical has a low volatility.

This paper provides an analysis of the subset of chemicals listed on EPA Drinking Water Contaminants list for a scenario representing a chemical truck loosing its cargo into a tidally driven river. The modeling approach provides an objective, quantitative method for determining the consequences of a chemical spill. An improvement to this analysis would be to remove the bias of subjectively choosing the individual model runs to examine the consequence of the chemical spill. To do this one would have to perform stochastic modeling, which would provide a distribution of results with varying environmental parameters that may be statistically described. This type of approach would be important to understand the possible consequences that could occur with varied environmental conditions.

Table 1. Subset of chemicals listed on EPA Drinking Water Contaminants list. MCL values from EPA's website (EPA, 2005), IDLH and REL-TWA are from NIOSH website (NIOSH, 2005).

Chemical	CAS Number	MCL (mg/L)	IDLH (ppm)	REL-TWA (ppm)
1,1,1-Trichloroethane	71-55-6	0.2	700	350
1,1,2-Trichloroethane	79-00-5	0.005	100	10
1,2-Dichloropropane	78-87-5	0.005	400	75
Benzene	71-43-2	0.005	500	0.1
Carbon tetrachloride	56-23-5	0.005	200	10
Chlordane	57-74-9	0.002	0.1	0.0005
Chlorobenzene	108-90-7	0.1	1000	10
Copper	7440-50-8	1.3	0.1	0.01
Dichloromethane	75-09-2	0.005	2300	50
Endrin	72-20-8	0.002	0.002	0.0001
Ethylbenzene	100-41-4	0.7	800	100
Heptachlor	76-44-8	0.0004	0.035	0.0005
Lead	7439-92-1	0.015	0.1	0.00005
Lindane	58-89-9	0.0002	0.05	0.0005
Mercury (inorganic)	7439-97-6	0.002	0.01	0.00005
Pentachlorophenol	87-86-5	0.001	0.0025	0.0005
Selenium	7782-49-2	0.05	0.001	0.0002
Styrene	100-42-5	0.1	700	50
Tetrachloroethylene	127-18-4	0.005	150	25
Toluene	108-88-3	1	500	50
Trichloroethylene	79-01-6	0.005	1000	20
Xylenes (total)	1330-20-7	10	900	100

Table 2. Select EPA Drinking Water Contaminants & MCLs. Physical behavior classes are defined in Tables 3.

Chemical	State	Density of Pure Chemical (g/cm3)	Solubility (in pure water, mg/L)	Vapor Pressure (kPa, at 25oC)	Physical Behavior Class #
1,1,1-Trichloroethane	Liquid	1.3 [a]	1495 [g]	1.650E+01 [f]	3
1,1,2-Trichloroethane	Liquid	1.442 [a]	4394 [g]	3.220E+00 [f]	3
1,2-Dichloropropane	Liquid	1.159 [a]	2800 [g]	6.620E+00 [f]	3
Benzene	Liquid	0.877 [a]	1780 [e]	1.270E+01 [c]	1
Carbon tetrachloride	Liquid	1.594 [a]	800 [g]	1.525E+01 [f]	4
Chlordane	Solid	1.67 [a]	1.85 [a]	1.333E-06 [a]	6
Chlorobenzene	Liquid	1.107 [a]	484 [e]	1.580E+00 [c]	4
Copper	Solid	8.94 [i]	0.2 [c]	0.000E+00 [i]	8
Dichloromethane	Liquid	1.33 [a]	13200 [g]	2.622E+01 [f]	3
Endrin	Solid	1.65 [a]	0.25 [g]	1.333E-07 [f]	8
Ethylbenzene	Liquid	0.865 [h]	152 [e]	1.270E+00 [c]	2
Heptachlor	Solid	1.58 [a]	0.056 [c]	3.999E-05 [a]	8
Lead	Solid	11.34 [a]	1.00E-06 [c]	0.000E+00 [a]	8
Lindane	Solid	1.87 [a]	10 [a]	3.999E-03 [a]	5
Mercury (inorganic)	Liquid	13.59 [a]	0.025 [h]	2.667E-04 [a]	7
Pentachlorophenol	Solid	1.978 [a]	14 [e]	1.466E-05 [c]	6
Selenium	Solid	4.81 [a]	1.00E-06 [a]	0.000E+00 [a]	8
Styrene	Liquid	0.906 [h]	300 [g]	8.800E-01 [f]	2
Tetrachloroethylene	Liquid	1.623 [a]	150 [g]	2.415E+00 [f]	4
Toluene	Liquid	0.8669 [h]	515 [e]	3.800E+00 [c]	2
Trichloroethylene	Liquid	1.465 [a]	1100 [g]	9.900E+00 [f]	3
Xylenes (total)	Liquid	0.869667 [a]	198.33 [e]	1.147E+00 [c]	2

[a] "Oil and Hazardous Materials Technical Assistance Data System" (OHMTADS) NIH/EPA, 1983

[b] "Quantitative Structure Activity Relationship Data Base (QSAR) - U.S. EPA, Duluth, MN, 1986

[c] Environment Canada, "Manual for Spills of Hazardous Materials", Environmental Protection Service, Environment Canada, Ottawa, Ontario, 1984

[d] EnvironTIPS, Environment Canada, 1985

[e] Mackay, D., W.Y. Shiu and D.C. Ma; Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume I Monoaromatic Hydrocarbons, Chlorobenzenes and PCBs. Lewis Publishers, Inc. Chelsea, Michigan; 1992

[f] Mackay, D., W.Y. Shiu and D.C. Ma; Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume III Volatile Organic Chemicals. Lewis Publishers, Inc. Chelsea, Michigan; 1992

[g] Mackay, D., W.Y. Shiu and D.C. Ma; Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume III Volatile Organic Chemicals. Lewis Publishers, Inc. Chelsea, Michigan; 1992 (Did not state if solubility was

[h] Mackay, D., W.Y. Shiu and D.C. Ma; Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume IV Oxygen, Nitrogen, and Sulfur containing compounds. Lewis Publishers, Inc. Chelsea, Michigan; 1992 (Did not s

[i] Fob.com company (2000). MSDSonline leading source for MSDS information. MSDSonline. http://www.msdsonline.com

Table 3. Classification of physical behavior.

Buoyancy Relative to Water	Solubility Behavior	Volatility
Floater: density < 1.0 g/cm^3	Highly soluble: solubility > 1000 mg/L	Highly volatile: vapor pressure > 0.1 kPa
Neutral: density 1.01-1.03 g/cm^3	Soluble: solubility 100 - 1000 mg/L	Semi-volatile: vapor pressure 10^{-5}- 0.1 kPa
Sinker: density > 1.03 g/cm^3	Semi-soluble: solubility 1 - 100 mg/L	Low-volatile: vapor pressure < 10^{-5} kPa
	Insoluble: solubility < 1 mg/L	

Table 4. Classification of chemicals by physical behavior and representative chemical for each physical behavior class.

Chemical	Buoyancy Relative to Water	Solubility Behavior	Volatility	Physical Behavior Class #	Representative Chemical for Class
1,1,1-Trichloroethane	Sinker	Highly soluble	Highly volatile	3	
1,1,2-Trichloroethane	Sinker	Highly soluble	Highly volatile	3	
1,2-Dichloropropane	Sinker	Highly soluble	Highly volatile	3	
Benzene	Floater	Highly soluble	Highly volatile	1	*
Carbon tetrachloride	Sinker	Soluble	Highly volatile	4	*
Chlordane	Sinker	Semi-soluble	Low-volatile	6	*
Chlorobenzene	Sinker	Soluble	Highly volatile	4	
Copper	Sinker	Insoluble	Low-volatile	8	
Dichloromethane	Sinker	Highly soluble	Highly volatile	3	

Endrin	Sinker	Insoluble	Low-volatile	8	
Ethylbenzene	Floater	Soluble	Highly volatile	2	
Heptachlor	Sinker	Insoluble	Low-volatile	8	
Lead	Sinker	Insoluble	Low-volatile	8	
Lindane	Sinker	Semi-soluble	Semi-volatile	5	*
Mercury (inorganic)	Sinker	Insoluble	Semi-volatile	7	*
Pentachlorophenol	Sinker	Semi-soluble	Low-volatile	6	
Selenium	Sinker	Insoluble	Low-volatile	8	
Styrene	Floater	Soluble	Highly volatile	2	*
Tetrachloroethylene	Sinker	Soluble	Highly volatile	4	
Toluene	Floater	Soluble	Highly volatile	2	
Trichloroethylene	Sinker	Highly soluble	Highly volatile	3	*
Xylenes (total)	Floater	Soluble	Highly volatile	2	

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

Chemical	Molecular Weight (g/mole)	Viscosity (at 25oC, cp)	Octanol/Water Partition Coefficient as log(Kow)	Sorption Coefficient for Organic Carbon as log(Koc)	Degradation Rate in Surface Waters (instantaneous, per day)
1,1,1-Trichloroethane	133.41[h]	0.7709[b]	2.49[h]	2.44795[b]	1.36E-02[k]
1,1,2-Trichloroethane	133.41[h]	0.7243[g]	2.38[h]	2.33982[b]	1.09E-03[k]
1,2-Dichloropropane	112.99[h]	0.8133[b]	2[h]	1.96628[b]	9.78E-03[h]
Benzene	78.11[g]	0.6022[b]	2.13[g]	2.09407[b]	9.78E-02[g]
Carbon tetrachloride	153.82[h]	0.9073[b]	2.65[h]	2.60523[b]	9.78E-03[h]
Chlordane	409.78[a]	NA[k]	4.0688[b]	3.9999[k]	1.09E-03[k]
Chlorobenzene	112.6[g]	0.7524[b]	2.8[g]	2.75268[b]	9.78E-03[g]
Copper	63.54[k]	NA[k]	-0.571[j]	-0.561[b]	9.49E-06[k]
Dichloromethane	84.94[h]	0.3274[g]	1.25[h]	1.22903[b]	9.78E-03[h]
Endrin	380.91[a]	NA[k]	4.024[b]	3.9559[k]	1.09E-03[k]
Ethylbenzene	106.2[g]	0.6382[b]	3.13[g]	3.07707[b]	3.02E-02[g]
Heptachlor	373.32[a]	NA[k]	4.6632[b]	4.5842[k]	1.09E-03[k]
Lead	207.2[a]	NA[k]	5.0542[b]	4.9685[k]	6.95E-04[k]
Lindane	290.83[a]	NA[k]	3.4382[b]	3.38[k]	1.09E-03[k]
Mercury (inorganic)	200.59[a]	1.519[b]	2.4726[b]	2.4309[k]	9.49E-06[k]
Pentachlorophenol	266.34[i]	NA[k]	5.05[i]	4.96443[b]	3.02E-02[i]
Selenium	78.96[a]	NA[k]	5.0542[b]	4.9685[k]	9.49E-06[k]
Styrene	104.14[h]	0.7033[b]	3.05[h]	2.99843[b]	9.78E-02[h]
Tetrachloroethylene	165.83[h]	0.841[b]	2.88[h]	2.83132[b]	3.02E-02[h]

Toluene	92.13 [g]	0.5546 [b]	2.69 [g]	2.64455 [b]	3.02E-02 [g]
Trichloroethylene	131.39 [h]	0.5563 [b]	2.53 [h]	2.48727 [b]	3.02E-02 [h]
Xylenes (total)	106.2 [g]	0.647833 [b]	3.17667 [g]	3.2101 [b]	3.02E-02 [g]

[a] "Oil and Hazardous Materials Technical Assistance Data System" (OHMTADS) NIH/EPA, 1983

[b] "Chemical Hazardous Response Information System" (CHRIS) U.S. Coast Guard

[c] "Quantitative Structure Activity Relationship Data Base (QSAR) - U.S. EPA, Duluth, MN, 1986

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[f] Calculated using regression of log(Koc) on log(Kow) from DiToro, D., C.S. Zarba, D.J. Hansen, W.J. Berg, R.C. Swartz, C. E. Cowan, S.P. Parlou, H.E. Allen, N.A. Thomas, and P.R. Paquin, 1991. Technical basis for esta

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[k] Fob.com company (2000). MSDSonline leading source for MSDS information. MSDSonline. http://www.msdsonline.com (20 March 2001) (using manufacture EM Science)

Table 6. Assumed model input parameters for all modeled chemicals.

Name	Description	Value(s)
Spill Latitude	Latitude of the spill site	38° 30.76′ N
Spill Longitude	Longitude of the spill site	76° 40.07′ W
Depth of release	Water surface (release depth)	0 m
Model time step	Time step used for model calculations	0.25 hour
Number of Lagrangian particles	Number of Lagrangian elements used to simulate spilled mass	1,000
Salinity	Surface water salinity	8 ppt
Temperature	Water temperature	20°C
Suspended sediment concentration	Average suspended sediment concentration during spill period	10 mg/l
Horizontal turbulent diffusion coefficient	Randomized turbulent mixing parameter in x & y, for concentration distribution within a spillet	1 m^2/sec
Vertical turbulent diffusion coefficient	Randomized turbulent mixing parameter in z, below the wave mixed layer	0.001 m^2/sec

Table 7. Area (km^2) where water concentrations exceed MCL; maximum distance (km) from spill site to IDLH and REL-TWA for air concentration within the lower 2 m of the atmosphere; and time to disperse below IDLH and REL-TWA for air concentration within the lower 2 m of the atmosphere.

Chemical	Physical Behavior Class #	Area greater than MCL (km2)	Distance to IDLH (km)	Time to disperse below IDLH (hrs)	Distance to REL-TWA (km)	Time to disperse below REL-TWA (hrs)
Benzene*	1	1.63311	0.4	2	7.6	> 96
Ethylbenzene	2	0.003128562	<0.1	1	NA[2]	3
Styrene*	2	0.36291	0.23	1.5	0.2	36
Toluene	2	0	0.26	2	0.200	36
Xylenes (total)	2	0	<0.1	0.5	NA[2]	3
1,1,1-Trichloroethane	3	1.22014	NA[1]	< 0.5	NA[2]	0.5
1,1,2-Trichloroethane	3	12.23268	3	> 96	3	> 96
1,2-Dichloropropane	3	12.23268	2.75	0.5	<0.1	> 96
Dichloromethane	3	12.23268	NA[1]	< 0.5	0.75	> 96
Trichloroethylene*	3	12.23268	NA[1]	< 0.5	2.7	> 96
Carbon tetrachloride	4	11.96049	4.5	36	4.5	> 96
Chlorobenzene	4	2.20251	NA[1]	< 0.5	4.5	> 96
Tetrachloroethylene	4	11.96049	4.6	> 96	<0.1	> 96
Lindane*	5	6.70451	4.4	> 96	4.5	> 96
Chlordane*	6	7.35525	4.6	> 96	4.7	> 96
Pentachlorophenol	6	7.79638	4.6	> 96	4.7	> 96
Mercury (inorganic)*	7	7.35525	(no volatilization)	(no volatilization)	(no volatilization)	(no volatilization)

Copper	8	(no dissolved)	(no volatilization)	(no volatilization)	(no volatilization)	(no volatilization)
Endrin	8	(no dissolved)	(no volatilization)	(no volatilization)	(no volatilization)	(no volatilization)
Heptachlor	8	(no dissolved)	(no volatilization)	(no volatilization)	(no volatilization)	(no volatilization)
Lead	8	(no dissolved)	(no volatilization)	(no volatilization)	(no volatilization)	(no volatilization)
Selenium	8	(no dissolved)	(no volatilization)	(no volatilization)	(no volatilization)	(no volatilization)

* representative chemical for the physical behavior group
NA[1] - concentrations are below IDLH threshold within a ½ hour
NA[2] - concentrations are below REL-TWA threshold within 10 hours

Tables and Figures:

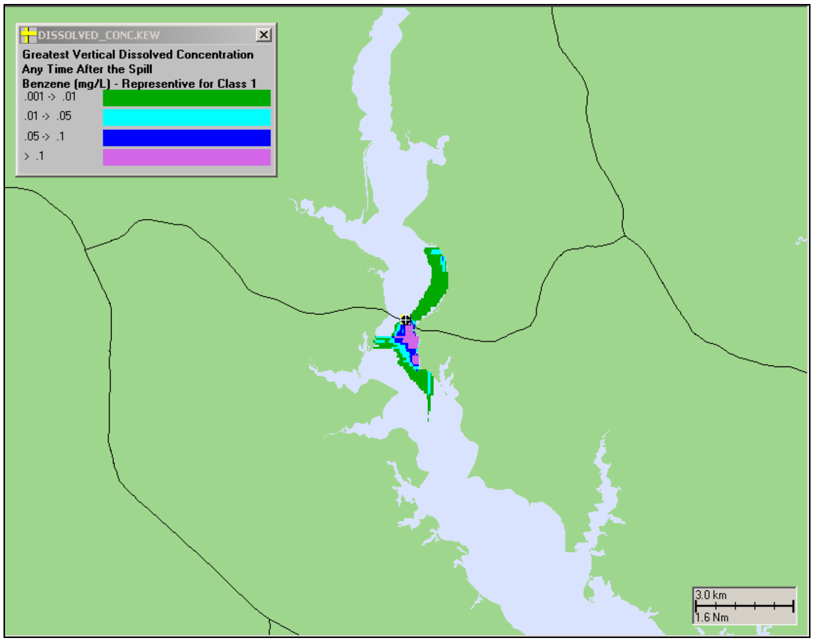

Figure 1. Aerial view of maximum dissolved concentration (mg/L) after a 500 gallon spill of benzene (representative chemical for physical behavior class 1). The map displays the highest vertically-averaged concentration at any time over 4 days.

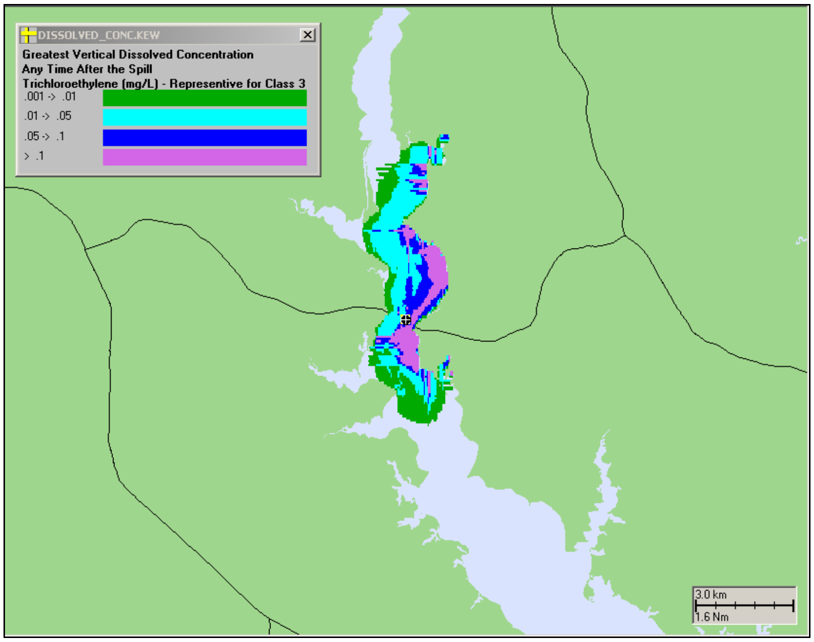

Figure 2. Aerial view of maximum dissolved concentration (mg/L) after a 500 gallon spill of trichloroethylene (representative chemical for physical behavior class 3). The map displays the highest vertically-averaged concentration at any time over 4 days.

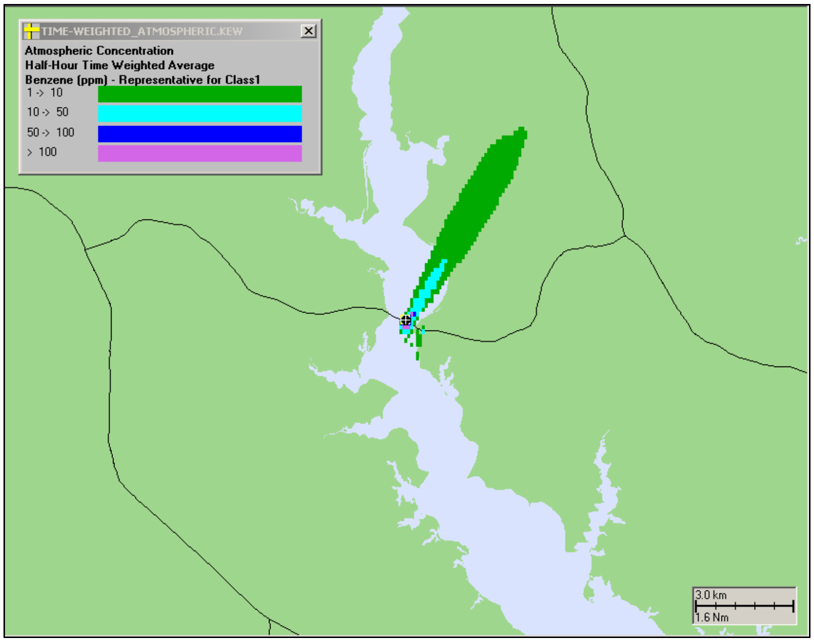

Figure 3. Maximum ½ hour time-weighted average concentration in the atmosphere just above the water surface, benzene (representative chemical for physical behavior class 1). Concentration comparison with IDLH.

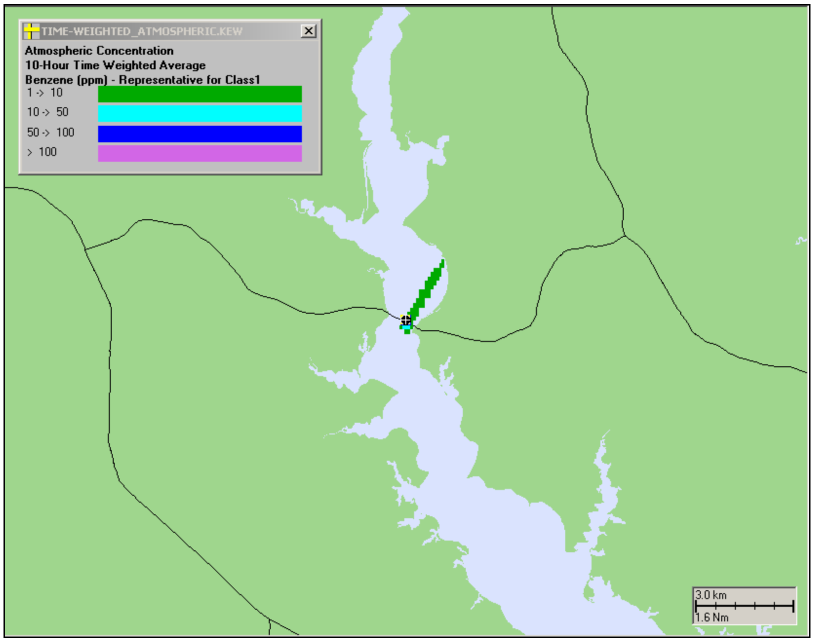

Figure 4. Maximum 10 hour time-weighted average concentration in the atmosphere just above the water surface, benzene (representative chemical for physical behavior class 1). Concentration comparison with IDLH.

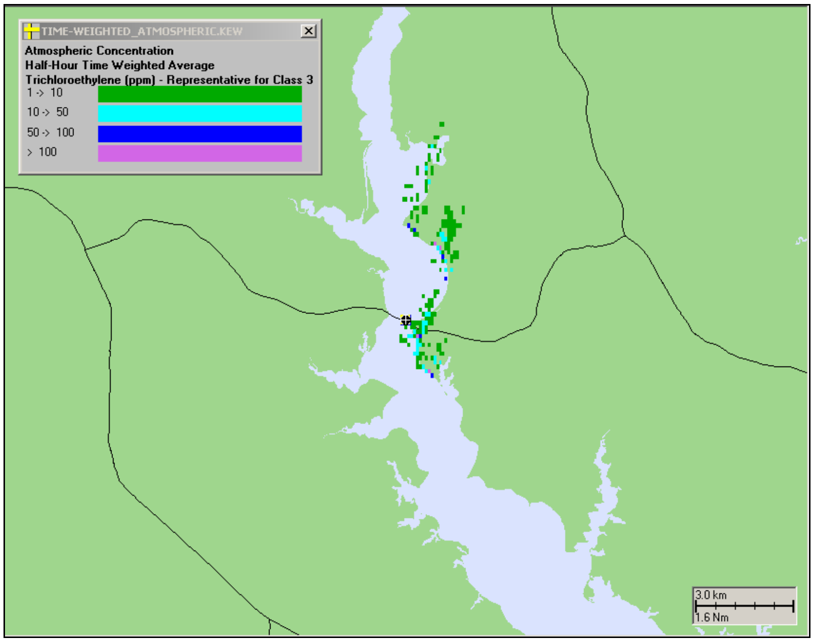

Figure 5. Maximum ½ hour time-weighted average concentration in the atmosphere just above the water surface, trichloroethylene (representative chemical for physical behavior class 3). Concentration comparison with IDLH.

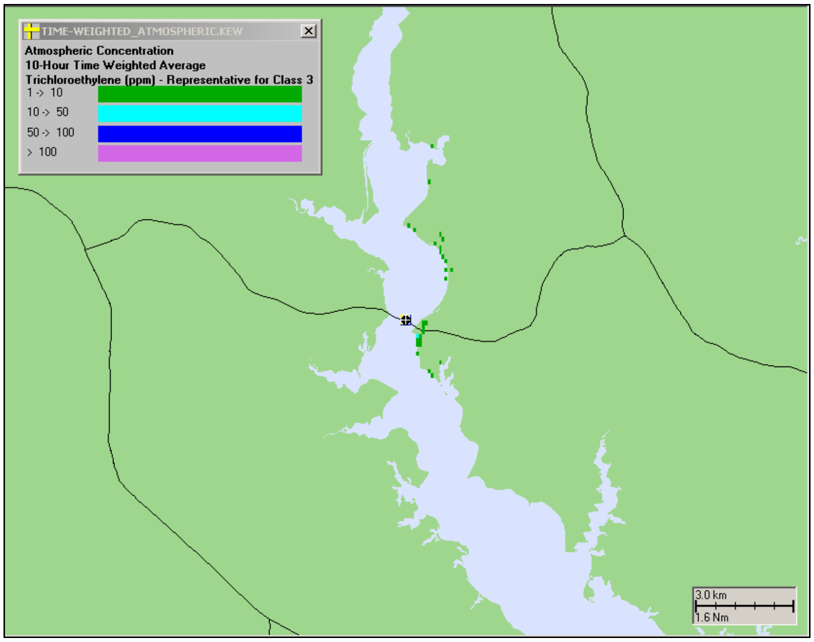

Figure 6. Maximum 10 hour time-weighted average concentration in the atmosphere just above the water surface, benzene trichloroethylene (representative chemical for physical behavior class 3). Concentration comparison with IDLH.

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