# MODELING THE FATE

# OF

# ORGANIC CONTAMINANTS

# IN

# URBAN STORMWATER DETENTION PONDS

by

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## Abstract

A simple quantitative model, based on the fugacity approach, is used to investigate the potential for bioaccumulation of organic contaminants in stormwater detention ponds receiving urban runoff. This is achieved by describing the concentrations and mass distribution of benzene, toluene and hexachlorobenzene in five environmental media within a hypothetical stormwater pond. These media are air, water, sediment, plant and suspended sediment. This is the first use of a multimedia approach to investigate contamination in stormwater ponds. Results indicate that less volatile chemicals tend to be found in higher concentrations in solid phases such as sediment and plant matter. These increased concentrations may result in an increased risk of exposure to biota (e.g. ingestion of plant matter). However, this collection of contaminants in one place facilitates their removal. For more volatile chemicals, a redistribution of mass occurs (e.g. benzene is found primarily in the air), making collection more difficult. Therefore, caution must be exercised when recommending the use of stormwater detention ponds and when considering pollution control measures.

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## 1.0 Introduction

There is a wide range of water-related problems resulting from increased urbanization. This includes increased flooding during storm events, higher surface flows, lower base flows between storm events, and decreased water quality (WRBCR, 1991). Traditionally, urban water management considered only the hydrological impacts of stormwater (Flores-Rodríguez *et al*., 1994) and removing water from a storm event as quickly and efficiently as possible (Ellis, 1986; Andoh, 1994): water quality was not considered a priority. Stormwater is now recognized as a major source of water quality problems to receiving water bodies (Akan, 1992). It can become a threat to public health and affect the recreational and commercial value of these water bodies (Najjar *et al*., 1995).

Rather than efficiently conveying stormwater away from urban areas directly to receiving waters, more attention is now being devoted to reducing stormwater flows and improving stormwater quality. Processes inherent in natural ecological systems are being used to guide treatment and conveyance systems. There are many reported advantages to this approach since some wetlands and ponds may possess hydraulic benefits such as flood attenuation, increasing groundwater recharge, improved water quality, sediment control, nutrient uptake, trapping and degrading contaminants (Taylor, 1992; OMNR, 1993; MMML, 1992). Stormwater ponds are effective at removing large quantities of suspended sediment (MMML, 1992). According to Pries (1994), they can also decrease erosion and significantly reduce concentrations of five day biochemical oxygen demand ($BOD_5$), nutrients and metals. However, stormwater ponds decrease in effectiveness in colder temperatures and contaminant removal rates vary seasonally with the greatest

removal during the growing season and the least during fall and winter during senescence (Novotny, 1995).

Stormwater detention ponds are composed of a permanent pool of water and an overflow storage volume that is designed to temporarily store water from a rainfall event (Finnemore *et al*., 1982; MOEE, 1994). During such a rainfall event, stormwater ponds collect flows of water which can be several orders of magnitude greater than base flows. The collected volume of water is detained for 12 to 24 hours (MOEE, 1994) and then released over an extended period of time. This decreases the rate of flow downstream of the stormwater pond (Taur *et al*., 1987) and prevents flash flooding. Thus, during a rainfall event, the inflow rates of water to these stormwater facilities are greater than the outflow rates.

Although other management practices that control pollution at source exist (e.g., improvement of maintenance practices and development control of land conditions to reduce runoff or pollution potential, Finnemore *et al.*, 1982), stormwater detention ponds are widely used to mitigate the quantity and quality of urban of stormwater from small drainage basins (MMML, 1992; Finnemore *et al.*, 1982; WRBCR, 1991). For example, detention ponds comprise 43 percent of low structural controls used in Montgomery County, Md. for areas between 0.4 to 200 hectares (Finnemore *et al.*, 1982). Additionally, provincial guidelines recommend the use of stormwater quality control facilities for new developments in Ontario (WRBCR, 1991). Using stormwater detention ponds is also increasing in popularity for use as recreation areas and wildlife habitat enhancement (Adams *et al*., 1982).

Unfortunately, there are potential problems with the detention pond approach. For example, urban stormwater runoff contains significant amounts of priority pollutants (Field, 1985). Little research has been done to study the long-term effects and concentrations of organic priority chemicals in stormwater ponds. The Nationwide Urban Runoff Program (NURP), which was conducted from 1979 to 1983, consisted of 28 different run-off studies in the United States that examined organic contaminants in stormwater (MMML, 1992). NURP was commissioned by the US Environmental Protection agency to collect data, evaluate stormwater effects and study control practices (Oltmann and Shulters, 1989). It studied 106 organic chemicals, and was the largest analysis of organic chemicals in stormwater to provide information to water users and decision-makers regarding potentially dangerous contaminants in stormwater in urban areas (Makepeace *et al.*, 1995). NURP stated that wet ponds are effective for mitigation of poor water quality (MMML, 1992).

There are some concerns with the NURP assessment. Ellis (1986) explains that delayed oxygen depletion in benthal deposition was overlooked. Additionally, NURP studied mainly residential areas and few light industrial or commercial areas (Pitt *et al.*, 1995). Furthermore, NURP considered organic contaminants as potential problems if they were found in concentrations in stormwater exceeding health and safety or protection of aquatic life guidelines (Makepeace *et al.*, 1990). It was not considered that, though organic contaminants are found in low concentrations in water, they can accumulate in sediment, have toxic effects, and can bioaccumulate in aquatic organisms and top predators.

There are many sources for these organic contaminants. These include leaking septic tanks, illegal dumping, and automobiles (Novotny, 1995). Chemicals of concern include industrial solvents, fire retardants, fuel from spills and vehicles, pesticides, phenols, and polyaromatic hydrocarbons (Makepeace *et al.*, 1995; Connell and Miller, 1984). Organic compounds from local sources or long range atmospheric transport accumulate on urban surfaces such as roadways and roofs, where they are washed off by rain and incorporated into stormwater runoff (Ellis, 1986; Boxall and Maltby, 1995).

### *1.1 Problem Statement*

The use of stormwater detention ponds to deal with the quality and quantity of urban stormwater flow is increasing in popularity. However, little scientific work has been done to examine the possible negative aspects associated with their use. Stormwater pond design criteria prescribed by MOEE (1994) for water resources protection are defined by consideration of removal of contaminants through particle settling but do not consider organic chemicals or remobilization of contaminants following deposition. Policies promoting the use of stormwater ponds are based on out-moded science because organic contamination is not adequately addressed.

In order to assess potential hazards of organic contaminants, methods of describing their fate are essential (Rodger *et al*., 1983). It is possible that, because of their persistent nature, some organic contaminants may accumulate in various compartments of stormwater ponds. The purpose of this study is to describe the multimedia distribution and concentration of selected organic contaminants that are characteristically found in stormwater detention ponds in order to assess if chemical accumulation in various media

is a potential concern. Additionally, this study identifies the important parameters that are required for this description.

A simple quantitative mathematical model is used to achieve this. Modeling allows researchers to defend conclusions that may be difficult to demonstrate with field experiments that may not be able to account for all changing variables (Southwood et al., 1989). The model developed here is general to stormwater ponds and uses data from the literature. The model is intended to provide order-of-magnitude estimates due to its simple nature: it is not expected to accurately describe actual conditions. This project lays the foundation for future research and assesses future work requirements. It follows from Helfield and Diamond (in Press) who found that the use of artificially constructed wetlands can result in increased contaminant concentration in sediment and wetland vegetation and, therefore, can result in bioconcentration and biomagnification of organic chemicals through the aquatic food web. The next step is to identify knowledge gaps and data requirements, suggesting areas of concern that may need further study, understand mechanisms and relationships which may not be intuitively obvious, and estimate the potential effectiveness of alternative contaminant control strategies such as sediment dredging and plant harvesting.

## 2.0 Methodology

### *2.1 Theoretical Approach*

Using the computer modeling program, *Stella II*, a *Level II* fugacity model approach is used as a tool to consider input flows of chemicals, removal through chemical transformation and advection, and distribution among model compartments (Mackay, 1991). This is the first use of a multimedia approach to study stormwater

detention ponds. The *Level II* model, developed by Don Mackay and co-workers at the University of Toronto, assumes chemical equilibrium among all compartments and steady-state conditions. For detailed descriptions of the fugacity approach refer to Mackay (1991) and Bacci (1994).

The model simplifies the stormwater detention pond environment by considering five compartments: air, plant matter, sediment, suspended sediment, and water. The model estimates chemical concentrations and distribution in each compartment. Benzene, toluene, and hexachlorobenzene (HCB), were selected because they extend over a range of physical-chemical properties (See *Table 2.0*) and are routinely found in stormwater runoff. HCB is present in stormwater runoff since it has been used as a

*Table 2.0: Physical-Chemical Parameters for Each Chemical. Solubility and vapour pressure is given at 25°C and 1°C. $K_{OW}$ is kept constant under both warm and cold regimes.*

| Chemical | Molar Mass (g/mol) | $K_{OW}$ | Solubility ($g/m^3$) at 25°C | Solubility ($g/m^3$) at 1°C | VP (Pa) at 25°C | VP (Pa) at 1°C |
|---|---|---|---|---|---|---|
| **Benzene** | 78.1 [a] | 134.9 [a] | 1780 [a] | 1117.2 [b] | 12700 [a] | 521.8 [b] |
| **Toluene** | 92.1 [a] | 489.8 [a] | 515 [a] | 361.6 [b] | 3800 [a] | 163.7 [b] |
| **HCB** | 284.8 [a] | 316227.8 [a] | 0.005 [a] | $2.81 \times 10^{-5}$ [b] | 0.0023 [a] | $4.2 \times 10^{-7}$ [b] |

*Sources: a. Mackay, 1991 b. Calculated, see Section 2.3*

pesticide as well as being found as an impurity in other pesticides (Licsko *et al*., 1993). Sources of benzene and toluene include fuel spills and fuel combustion. Additional sources of toluene include pesticides, solvents, paints, and inks (Makepeace, 1995).

Introduction of contaminants to the hypothetical system is from background concentrations in stormwater inflow and air (no background air concentrations were available for HCB). The fate of contaminants in the detention pond is modeled under two temperature regimes: “warm” and “cold.” A sensitivity analysis is also done to assess

requirements for input data accuracy and the effectiveness of selected pollution control measures. An explanation of the source of input values follows below.

The following modeling scenarios were completed. For benzene, toluene and HCB, nominal warm and cold scenarios were modeled. The nominal warm scenario involved using a temperature of 25 $^{o}$C with solubility and vapour pressure parameters reported in the literature at this temperature. Faster reaction rates in each media were used in the warm scenario and slower ones were used in the cold scenario. Temperature corrections to chemical parameters for the cold scenario were made for solubility and vapour pressure. All other parameters remained constant. One additional modeling scenario (HCB) was made to compare model predictions and measured data.

### *2.2 Model Description*

#### *2.2.1 Loss and Loading Rates*

D values (mol/Pa.h) are transport parameters that describe the removal of a chemical from the evaluative system either through advection or reaction. For advection, D values are calculated as the product of GZ, where G is the flow of air or water ($m^3$/h), and Z is for the respective medium. For reaction, D is defined as the product of VZk, where V ($m^3$) is the volume and k ($h^{-1}$) is the reaction rate constant for that compartment. Fugacity was calculated by dividing the total input of chemical into the system (mol/h) by the sum of all D values.

Loading via advection in air and water ($N_{input}$) are calculated by multiplying the rate of inflow by concentration of air or water in the inflow, respectively. Loading rates from air inflow were not calculated for HCB since inflow air concentration was assumed to be zero. Loss rates resulting from chemical transformation in each phase are calculated

by multiplying the D value of that phase by the fugacity. This was done for both warm and cold runs. Because of the steady-state assumption, loading of chemical into the stormwater pond system is equal to loss from the stormwater system. Thus, the mass of chemical in the system stays constant.

### *2.2.2 Level II Model*

The concentration of chemicals in each compartment ($C_p$; mol/$m^3$) is:

$$C_p = Z_p f \qquad [2.1]$$

where $Z_p$ is the capacity (mol/$m^3$Pa) of the compartment for the chemical (See *Appendix A, Table A2, Section m,* for a detailed description of how Z values are calculated) and f is fugacity (Pa). Fugacity is an equilibrium criterion describing the escaping tendency of a chemical from a phase. In this model, fugacity is calculated by:

$$f = \frac{I}{\Sigma D} \qquad [2.2]$$

where I is the rate on chemical input (mol/h) into the stormwater pond system. This concentration was then converted to values of g/$m^3$ for air, water and plant matter and g/g sed. for sediment and suspended sediment.

Because of the steady-state assumption, the total loading (I) into the stormwater pond system, i.e. the sum of loading through air (Nair) and water (Nwater) advection, is equivalent to the total loss through advection and reaction from all media. Advection or reaction loss in each medium is the product of fugacity and the respective advection or

reaction transport parameter (i.e. D value). Total loss from all media ($N_T$) is the sum of total advection loss and total reaction loss. Total advection loss ($N_{Ta}$) is the sum of air and water advection loss:

$$N_{Ta} = \sum D_a f \qquad [2.3]$$

where $D_a$ is the advection transport parameter for air or water. Total reaction loss ($N_{Trx}$) is the sum of reaction loss from each medium:

$$N_{Trx} = \sum D_{rx} f \qquad [2.4]$$

where $D_{rx}$ is the reaction transport parameter for each medium. Therefore,

$$N_T = (\sum D_a f + \sum D_{rx} f) = f \sum D = I \qquad [2.5]$$

Total loading equals total loss in the stormwater pond system.

The distribution by mass of each chemical in the system is:

$$\frac{n_c}{n_t} \times 100 \qquad [2.6]$$

where $n_c$ is the number of moles of chemical in one compartment and $n_t$ is the total number of moles in the stormwater pond environment.

### *2.2.3 Model Parameters*

An atmospheric height of 500 meters was considered to be the zone of mixing for chemicals above a stormwater pond. Mackay (1991) suggests that the atmospheric height through which mixing can occur can be as much as 1000 meters but can be as little as 10 meters over small ponds. The volume of air in the stormwater system was the product of atmospheric height and pond surface area.

All plant matter is assumed to be submerged macrophytes. Emergent, floating or planktonic plant species are not considered. Also, the entire pond is considered to be littoral zone. Since Royle and King (1991) found dense plant beds to depths of 8 meters (Lake Liddell, New South Wales) it is reasonable to expect that detention ponds with maximum depths of 2 or 3 meters would have dense weed beds. A biomass of 3 kg fresh weight per square meter was used for the pond, based on an approximate median value from a range of 0.041 to 6 kg fresh weight/ $m^2$ for maximum submerged macrophytic biomass values for the littoral zone reported by Duarte and Kalff (1986). This was then used to calculate biomass (by multiplying with sediment surface area) and plant volume (by dividing biomass by density of plant matter). It was assumed that the volume of plant matter remained constant under both temperature regimes.

The density of plant matter in the model is 1 kg/L (fresh weight, Mackay, 1991; Southwood *et al.*, 1989). Tolls and McLachlan (1994) used a similar value of 0.86 kg/L for rye grass. Calamari *et al.* (1987) used a mean density for total terrestrial biomass of 0.8 kg/L in their use of the plant compartment in a fugacity model.

Hydrological parameters (e.g. catchment size, percent imperviousness, rate of water inflow, maximum depth) were modeled after the "Neighbourhood 5D" stormwater pond that services a 62 hectare catchment within the subwatershed of the Little Etobicoke Creek, Mississauga, Ontario (CPWL, 1995). This pond is the first stormwater pond in Mississauga designed according to the guidelines outlined in MOEE (1994). The simulation runs with the assumption that a *Level of Protection* of "2" is required for the operation of the facility. This is the value used for the Neighbourhood 5D development and corresponds to protection of a *Type 2* fishery in the receiving waters (CPWL, 1995). The model is designed so that various protection levels ranging from 1 to 4 can be incorporated into a simulation run by adjusting pond storage volume (See *Table 2.1* for a description of the various levels of protection and the storage volume required).

*Table 2.1: Protection Levels and Storage Volume Required (per hectare of catchment) for Wet Ponds. The volume of storage required for a stormwater detention pond is based on the percent imperviousness of the catchment, the catchment size, and the Level of Protection desired. The Level of Protection considers protection of fish habitat. Only suspended sediment settling is considered for pollution control.*

| **Protection Level** | | **Storage Volume ($m^3$/ha) required for Percentage Imperviousness of Catchment** | | | |
|---|---|---|---|---|---|
| | | **35%** | **55%** | **70%** | **85%** |
| **Level 1** | e.g., fish spawning areas, habitats of endangered or vulnerable species | 140 | 190 | 225 | 250 |
| **Level 2** | fish feeding areas, unspecialized spawning habitat; Level 2 is expected for most areas in Ontario | 90 | 110 | 130 | 150 |
| **Level 3** | habitat with low capacity for production; e.g. municipal drains, highly altered water courses | 60 | 75 | 85 | 95 |
| **Level 4** | for retrofit and redevelopment; lowest level of protection | 60 | 60 | 60 | 65 |

*Source: MOEE (1994)*

Therefore, the storage volume of the hypothetical pond is a function of the protection level, catchment size, and percent imperviousness.

The hypothetical stormwater pond is a rectangular polyhedron with six faces with a length to width ratio of 5:1 based on MOEE (1994). The slope of the sides is 0.25 based on Novotny (1995) and the dimensions of the Neighbourhood 5D stormwater pond in Mississauga (CPWL, 1995). Storage volume, depth, pond surface area, length, width, and sediment surface area are all inter-related so that the researcher can easily change the values of one parameter without needing to recalculate others and without affecting the magnitude of storage volume (See *Appendix A*, *Table A2*, *Sections g*, *h*, and *i*). The mathematical relationships are derived from the Quadratic Formula (Hazewinkel, 1991) and an integration (slice method) of the volume of the polyhedron. The shape of the pond is important in order to calculate the surface area of the sediment, the total volume of sediment, and the volume of plant matter.

Two meters was chosen for the maximum depth of the hypothetical pond similarly to the pond at Neighbourhood 5D (CPWL, 1995). MOEE (1994) states that the average depth of the permanent pool should be in the range of 1 to 2 meters, with a maximum of 3 meters. This is consistent with Taylor (1992) who states that a facility should be deep enough to allow winter flow and part of it should be at least 2 meters deep to allow species to have a winter refugia from ice (Taylor, 1992).

Mackay (1991) stated that the density of sediment and suspended sediment particles is 1.5 kg/L while Southwood *et al.* (1989) use values of 1.3, 1.3, and 1.5 kg/L for their fugacity calculations. Therefore, a value of 1.5 kg/L was chosen for this parameter. The volume of bottom sediment in the evaluative environment corresponds to a depth to which contaminants can exchange with the water column. This ranges from

about 0.02 to 0.05 meters although bioturbation may increase this depth (Mackay *et al.*, 1983; Mackay, 1991). MMML (1992) states that in wet ponds, sediments tend to become stratified, where the first 0.20 meters is contaminated, while sediments deeper than this usually are not. Yousef and Lin (1990) also state that metals and organic chemicals tend to accumulate in the top 0.10 to 0.20 meters below the sediment-water interface. Therefore, the depth of sediment was taken to be 0.10 meters.

Pitt *et al.*, (1995) recorded a mean concentration of suspended sediment of 17 mg/L with a range of 3 to 60 mg/L within a stormwater pond. Measurements of stormwater concentrations of suspended sediment showed a range from 72 to 604 mg/L (Oberts and Osgood, 1991; WRBCR, 1991; Kadlec, 1994; Ellis, 1986). The concentrations in the ponds will be less than this since wet detention ponds are effective at removing large quantities of suspended sediment (MMML, 1992). Therefore, at least some of the incoming suspended solids are deposited from the water column. A value of 50 mg/L for the concentration suspended sediment in pond water was chosen.

Reaction rates in each compartment were calculated from values of half-lives reported in the literature (Howard *et al.*, 1991; Mackay *et al.*, 1992; Paterson *et al.*, 1991)

*Table 2.2: Half-lives of Chemicals in Each Medium. The maximum half-life of the reported range was assumed for the cold scenario and the minimum half-life of the reported range was assumed for the warm scenario.*

| **Chemical** | **$t_{1/2}$ air (h)** | **$t_{1/2}$ water (h)** | **$t_{1/2}$ sed (h)** | **$t_{1/2}$ plants (h)** | **$t_{1/2}$ tsp (h)** |
|---|---|---|---|---|---|
| **Benzene** | 5.1-501[a] | 5.3 - 56.5[a] | 48 - 8760 [a] | 2808 - 16152[a] | 5.3 - 56.5 [a] |
| **Toluene** | 2.4 - 104 [a] | 4.81 - 384 [a] | 48- 528 [a] | No significant degradation [a] | 4.81 - 384 [a] |
| **HCB** | 3753 - 37530[b] | 3753 - 37530[b] | 23256 - 50136 [b] | 200 - 4000 [c] | 23256 - 50136 [b] |

*Sources: a. Mackay* et al.*, 1992 b. Howard* et al.*, 1991 c. Paterson* et al.*, 1991*

(See *Table 2.2*). These half-lives were converted to the first-order reaction rates by:

$$k = \frac{\ln 2}{t_{1/2}} \qquad [2.7]$$

where, k is the reaction rate ($h^{-1}$) and $t_{1/2}$ is the half-life (h) in a given medium. The maximum from a reported range of half-lives was assumed for the cold scenario and a minimum value was assumed for the warm scenario as reaction rates are slower when the temperature is colder (Wania and Mackay, 1993). Sediment reaction rates were estimated from soil half-lives since reaction rates for the sediment compartment were not available. Reaction rates for suspended sediment were estimated from the half-lives for chemicals in water. Reaction rates in plants for HCB were estimated from values reported for the soybean stem and leaf by *Paterson et al.* (1991). Otherwise, for toluene and benzene, rates for plants were assumed to be equal to the aqueous photolysis reaction rate since Paterson *et al.* (1991) suggest chemicals in plants are transformed according to reaction processes such as hydrolysis or photolysis. Also, for these chemicals, hydrolysis is not significant (Mackay *et al.*, 1992; Howard *et al.*, 1991).

It was assumed that air and water advection were the only inputs of contaminants into the system, for both warm and cold scenarios, with no direct emissions. For the nominal warm and cold runs, concentrations of chemicals in water inflow were estimated by using the median value reported in several literature sources (See *Table 2.3*; Makepeace, 1995; Schroeter and Associates, 1992; Maršálek and Ng, 1989; Licsko *et al.*, 1993; and, Struger *et al.*, 1994).

*Table 2.3: Concentrations of Chemicals in Inflow Air and Water. Bracketed values indicate concentrations in inflow air and water used in the model runs to calculate chemical loading rates into the stormwater system.*

| Chemical | Conc. Water ($g/m^3$) | Conc. Air ($g/m^3$) |
|---|---|---|
| **Benzene** | 0.0035-0.013 [a]<br>[$8.25 \times 10^{-3}$] | [$1.28 \times 10^{-5}$] [e] |
| **Toluene** | 0.009-0.012 [a]<br>[0.0105] | [$6.99 \times 10^{-5}$] [e] |
| **HCB** | 0.00000073 [b]<br>0.0000005 [c]<br>0.0000985 [d]<br>0.00000046 [d]<br>0.0000017 [d]<br>0.00002739 [d]<br>[$6.15 \times 10^{-7}$] | [0] |

*a. Makepeace* et al.*, 1995* *b. Schroeter* et al.*, 1992*
*c. Licsko* et al. *1993* *d. Maršálek and Ng., 1989*
*e. City of Toronto, 1993*

For HCB, input concentrations were calculated from measurements reported by Schroeter and Associates (1992) and Licsko *et al.* (1993). Data from Maršálek and Ng (1989) were not used because reported concentrations were up to 3 orders of magnitude greater than the former, more recent sources.

### *2.3 The Cold Scenario*

In the cold scenario, all parameters were kept the same with the following exceptions. Temperature was decreased from 298 K (25 $^{o}$C) to 274 K (1 $^{o}$C), which increased $Z_{air}$ and, therefore all other Z values. Thus, the chemical capacities of the media in the stormwater pond environment would be expected to increase (Wania and Mackay, 1992). Additionally, temperature corrections for vapour pressure and solubility were made.

For benzene and toluene, Antoine's Equation (Schwarzenbach *et al*., 1993) was used to calculate the vapour pressure:

$$\log P = A - \frac{B}{(T + C)} \qquad [2.8]$$

where, P is vapour pressure (mmHg), T is temperature ($^{o}$C), and A, B, C are Antoine's Constants (Boublík, *et al*., 1984). Vapour pressure was then converted into Pascals.

Solubility was calculated by:

$$S_{temp} = S_{298K} \times \exp\left\{10000/R \times \left(\frac{1}{T_{298K}} - \frac{1}{T_{ambient}}\right)\right\} \qquad [2.9]$$

For HCB, A, B and C are 10.23, 3874 and 0, respectively and T is expressed in Kelvin (Wania and Mackay, 1995). For solubility,

$$\log S = 0.254 - \frac{1314}{T} \qquad [2.10]$$

where S is solubility (mol/m$^3$) and T is temperature (K) (Wania and Mackay, 1995).

Corrections of state were made for benzene and HCB because they are solids at this temperature. This was achieved by multiplying calculated values for vapour pressure

and solubility by the fugacity ratio ($f_r$):

$$f_r = \exp\left\{6.79\left(1 - \frac{T_m}{T}\right)\right\} \qquad [2.11]$$

where $T_m$ is the melting point of the chemical and T is the ambient temperature.

### *2.4 Comparison with Field Measurements*

Model predictions for concentrations of HCB in sediment were compared with values measured by Struger *et al.* (1994) in the wet detention pond at Fieldstone in the City of Guelph. Model parameters were changed to reflect hydrological parameters associated with reported data for HCB from this site. Catchment size was changed to 14.2 hectares corresponding to the size of the residential development which was serviced by the pond. The flow rate was 314 $m^3$/hr (24.2 mm, 2 hour rainfall event) (Struger *et al.*, 1994). As HCB concentrations in background water inflow were not available for HCB, it was assumed that this value was the same as in the nominal warm HCB run.

### *2.5 Sensitivity Analysis*

A sensitivity analysis was done to determine the effect of modifying selected input parameters on output values, i.e. how much does output change when input changes or, how accurate does input data need to be? Also, the effectiveness of potential control measures was considered in this way. This is also a way to determine the components of the system that require further study or additional data. Parameter values were modified based on the variability in their reported ranges using “SF” factors, or sensitivity factors. These SF factors are multiplication factors which vary by orders of magnitude.

Only one parameter was varied at a time in the sensitivity runs. In warm and cold runs, all SF factors were set equal to 1 so that they did not affect the model output. For the three chemicals, sensitivity runs were completed for five reaction rates (k) using the warm runs only. The respective SF factor for the k value for each compartment was varied from: [0, 0.001, 0.01, 0.1, 1, 10, 100, 1000] (i.e. six orders of magnitude). SF factors affecting the bottom sediment volume, suspended sediment volume, plant volume and the rate of water inflow, were varied between: [0.25, 0.50, 0.75, 1.0, 1.25, 1.5, 1.75, 2.0]. The background concentration in water inflow was varied between [0, 0.01, 0.1, 1, 10, 100].

# 3.0 Results

### *3.1 Concentrations*

For all chemicals, concentrations were greatest in suspended sediment, then sediment, plant matter, water, and air in both warm and cold runs. However, the magnitudes of these concentrations differed according to temperature and each chemical. (See *Table 3.0* for a comparison of concentrations in similar units.)

*Table 3.0: Comparison of Compartments in Similar Units. Units of (g/m3) are used to clearly compare the differences in concentration amongst the media. The greatest concentrations of chemicals are found in the suspended sediment phase, followed by sediment, plant, water and air.*

| Concentration | | | | | |
|---|---|---|---|---|---|
| **Chemical** | **Air** | **Plant** | **Sediment** | **Suspended Sediment** | **Water** |
| | | | | | |
| **Benzene (Warm)** | $7.51 \times 10^{-4}$ | $4.51 \times 10^{-3}$ | $1.39 \times 10^{-2}$ | $4.71 \times 10^{-2}$ | $3.34 \times 10^{-3}$ |
| **Benzene (Cold)** | $1.32 \times 10^{-4}$ | $1.11 \times 10^{-2}$ | $3.41 \times 10^{-2}$ | $1.16 \times 10^{-1}$ | $8.22 \times 10^{-3}$ |
| **Toluene(Warm)** | $6.10 \times 10^{-4}$ | $1.09 \times 10^{-2}$ | $3.35 \times 10^{-2}$ | $1.14 \times 10^{-1}$ | $2.22 \times 10^{-3}$ |
| **Toluene(Cold)** | $1.91 \times 10^{-4}$ | $5.10 \times 10^{-2}$ | $1.57 \times 10^{-1}$ | $5.33 \times 10^{-1}$ | $1.04 \times 10^{-2}$ |
| **HCB (Warm)** | $6.11 \times 10^{-9}$ | $1.93 \times 10^{-3}$ | $5.95 \times 10^{-3}$ | $2.02 \times 10^{-2}$ | $6.11 \times 10^{-7}$ |
| **HCB (Cold)** | $1.16 \times 10^{-9}$ | $1.94 \times 10^{-3}$ | $5.97 \times 10^{-3}$ | $2.03 \times 10^{-2}$ | $6.14 \times 10^{-7}$ |

*Table 3.1* and *Figures 3.0* to *3.2* compare the concentrations for warm and cold runs of chemicals in all compartments. From warm to cold runs, for all chemicals, air

*Table 3.1: Comparison of Concentrations for Warm and Cold Runs. From warm to cold scenarios, concentrations in each media decreased in air and increased in all other phases. All units are $g/m^3$ except for sediment and suspended sediment which are in units of g/g sediment.*

| Concentrations | | | | | |
|---|---|---|---|---|---|
| **Chemical** | **Air** | **Plant** | **Sed.** | **TSP.** | **Water** |
| | ($g/m^3$) | ($g/m^3$) | (g/g) | (g/g) | ($g/m^3$) |
| **Benzene (Warm)** | $7.51 \times 10^{-4}$ | $4.51 \times 10^{-3}$ | $9.24 \times 10^{-9}$ | $3.14 \times 10^{-8}$ | $3.34 \times 10^{-3}$ |
| **Benzene (Cold)** | $1.32 \times 10^{-4}$ | $1.11 \times 10^{-2}$ | $2.27 \times 10^{-8}$ | $7.73 \times 10^{-8}$ | $8.22 \times 10^{-3}$ |
| **Toluene (Warm)** | $6.10 \times 10^{-4}$ | $1.09 \times 10^{-2}$ | $2.23 \times 10^{-8}$ | $7.59 \times 10^{-8}$ | $2.22 \times 10^{-3}$ |
| **Toluene (Cold)** | $1.91 \times 10^{-4}$ | $5.10 \times 10^{-2}$ | $1.05 \times 10^{-7}$ | $3.56 \times 10^{-7}$ | $1.04 \times 10^{-2}$ |
| **HCB (Warm)** | $6.1 \times 10^{-9}$ | $1.93 \times 10^{-3}$ | $3.96 \times 10^{-9}$ | $1.35 \times 10^{-8}$ | $6.11 \times 10^{-7}$ |
| **HCB (Cold)** | $1.16 \times 10^{-9}$ | $1.94 \times 10^{-3}$ | $3.98 \times 10^{-9}$ | $1.35 \times 10^{-8}$ | $6.14 \times 10^{-7}$ |

concentrations decrease and concentrations in all other media increase by less than an order of magnitude. For example, for benzene and toluene, suspended sediment

*Figure 3.0: Benzene: Log(Concentration) Vs. Media. Sediment and suspended sediment concentrations are in g/g sed. All other media are in g/m$^3$. Concentration decreases in the air medium but increases in all other media, going from warm to cold runs.*

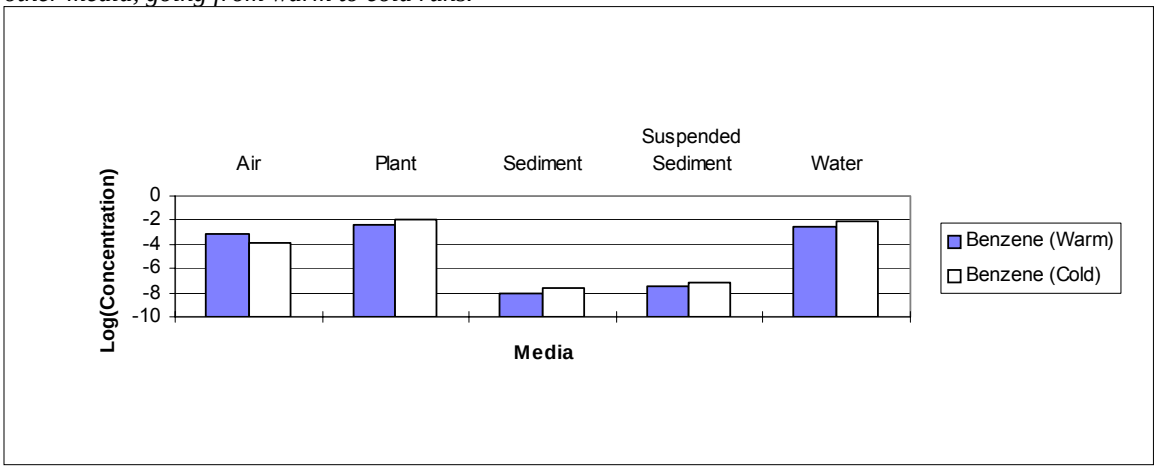



*Figure 3.1: Toluene: Log(Concentration) Vs. Media. Sediment and suspended sediment concentrations are in g/g sed. All other media are in g/m$^3$. Similar to benzene, concentration decreases in the air medium but increases in all other media, going from warm to cold runs*

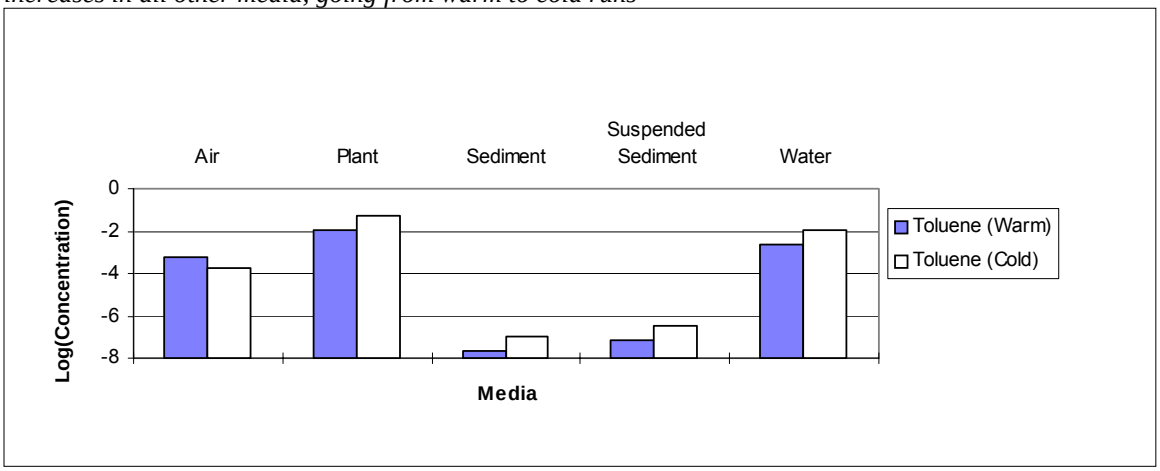
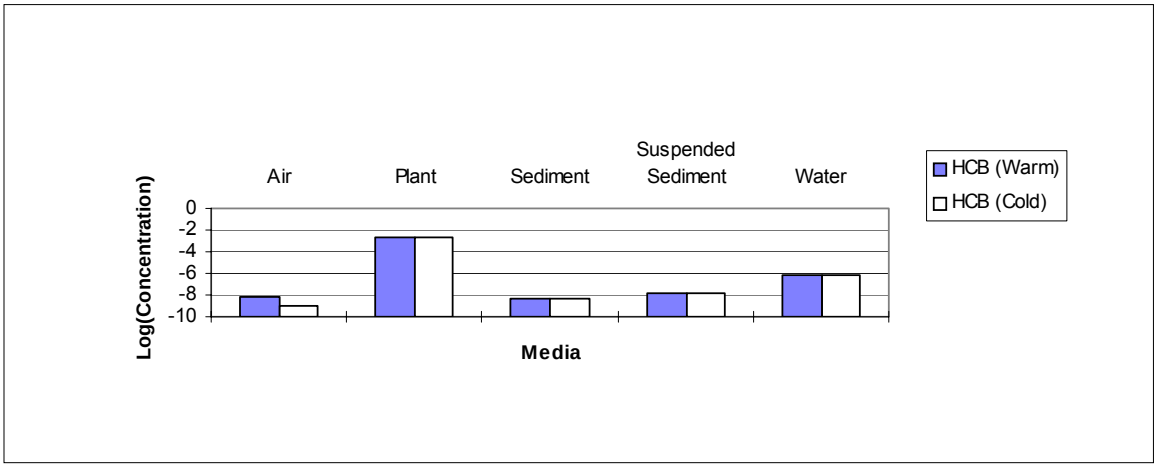


*Figure 3.2: HCB Log(Concentration) Vs. Media. Sediment and suspended sediment concentrations are in g/g sed. All other media concentrations are in g/m$^3$.From warm to cold runs, HCB shows little change in media concentrations.*




concentrations increased from 9.2 x $10^{-9}$ and 2.23 x $10^{-8}$ g/g sed. to 2.27 x $10^{-8}$ and 1.04 x $10^{-7}$ g/g sed., respectively. HCB showed a much smaller increase in suspended solid concentration (e.g. from 1.34 x $10^{-8}$ to 1.35 x $10^{-8}$ g/g sed.).

### *3.2 Relative Mass Distribution*

(See *Table 3.2* and *Figures 3.3* to *3.8.*) For the warm scenario, most of the benzene and toluene in the system is found in air (98.5% and 98.3%), then water (1.2% and 0.98%), respectively. HCB is found mainly in the sediment (94.9%), then in air (3.8%). For the cold runs, the distribution shifted. Most of the benzene is found in the air

*Table 3.2: Comparison of Relative Distribution in the Warm and Cold Runs (Percent). From warm to cold runs, there is a decrease in mass distribution in air for all chemicals, while there was an increase in solid and liquid phase.*

| Mass Distribution | | | | | |
|---|---|---|---|---|---|
| **Chemical** | **Air** | **Plant** | **Sed.** | **TSP.** | **Water** |
| **Benzene (Warm)** | 9.85 x $10^{1}$ | 2.50 x $10^{-3}$ | 2.49 x $10^{-1}$ | 5.64 x $10^{-4}$ | 1.20 |
| **Benzene (Cold)** | 8.29 x $10^{1}$ | 2.95 x $10^{-2}$ | 2.94 | 6.66 x $10^{-3}$ | 1.42 x $10^{1}$ |
| **Toluene (Warm)** | 9.83 x $10^{1}$ | 7.42 x $10^{-3}$ | 7.39 x $10^{-1}$ | 1.67 x $10^{-3}$ | 9.81 x $10^{-1}$ |
| **Toluene (Cold)** | 7.91 x $10^{1}$ | 8.95 x $10^{-2}$ | 8.92 | 2.02 x $10^{-2}$ | 1.18 x $10^{1}$ |
| **HCB (Warm)** | 7.35 x $10^{-1}$ | 9.82 x $10^{-1}$ | 9.79 x $10^{1}$ | 2.22 x $10^{-1}$ | 2.01 x $10^{-1}$ |
| **HCB (Cold)** | 1.40 x $10^{-1}$ | 9.88 x $10^{-1}$ | 9.84 x $10^{1}$ | 2.23 x $10^{-1}$ | 2.02 x $10^{-1}$ |

*Figure 3.3: Relative Distribution of Benzene in the Warm Scenario. Most of the Benzene in the stormwater pond system is found in the air.*

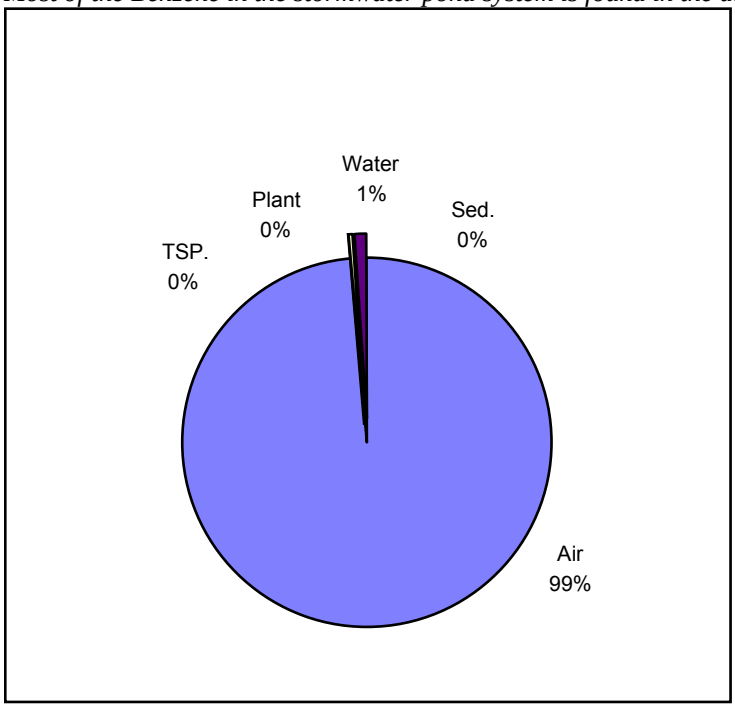



*Figure 3.4: Relative Distribution of Benzene in the Cold Scenario. There is an increase in mass distribution in solid and liquid phases.*

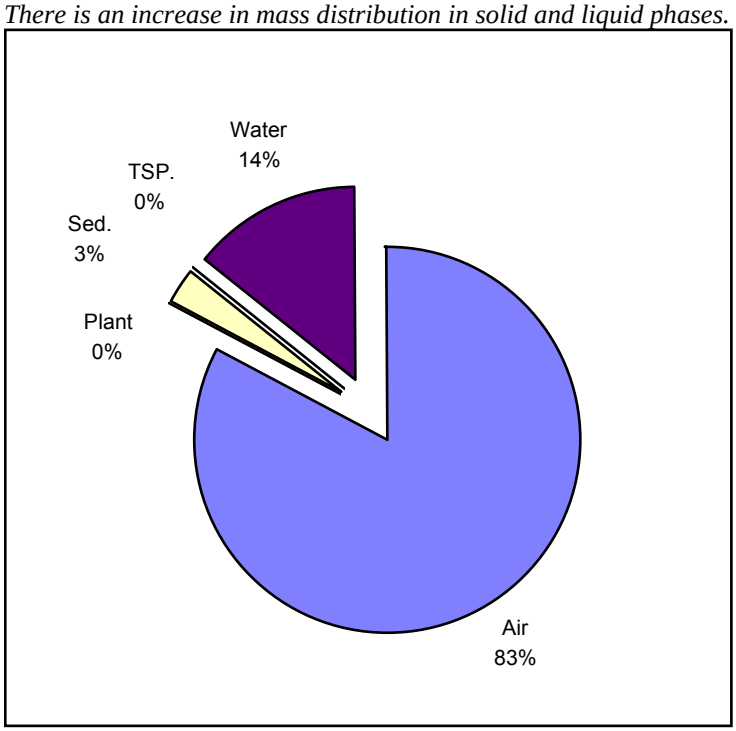


*Table 3.5: Relative Distribution of Toluene in the Warm Scenario.*
*Most of the toluene is found in the air.*

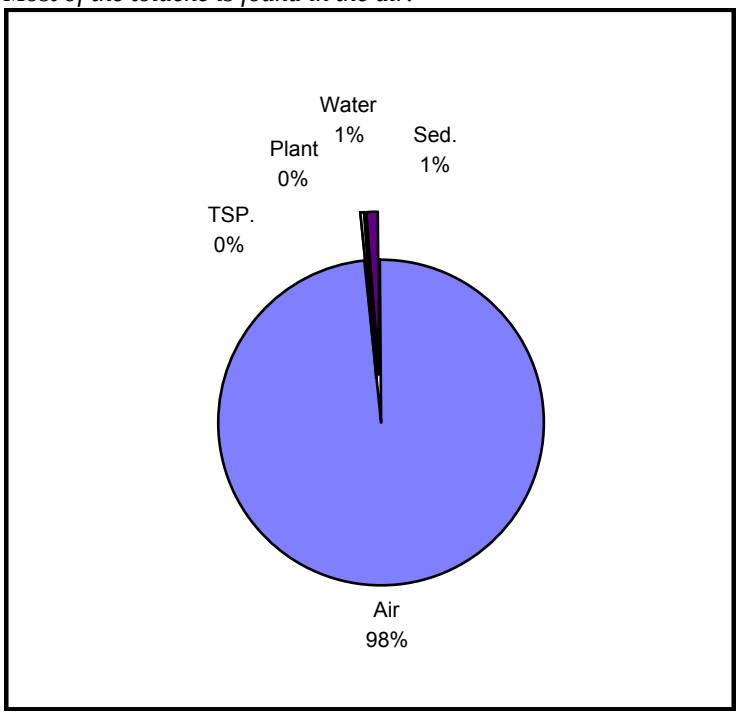



Figure 3.6: Relative Distribution of Toluene in the Cold Scenario.
There is a decrease in concnetration in air and an increase in all other media.

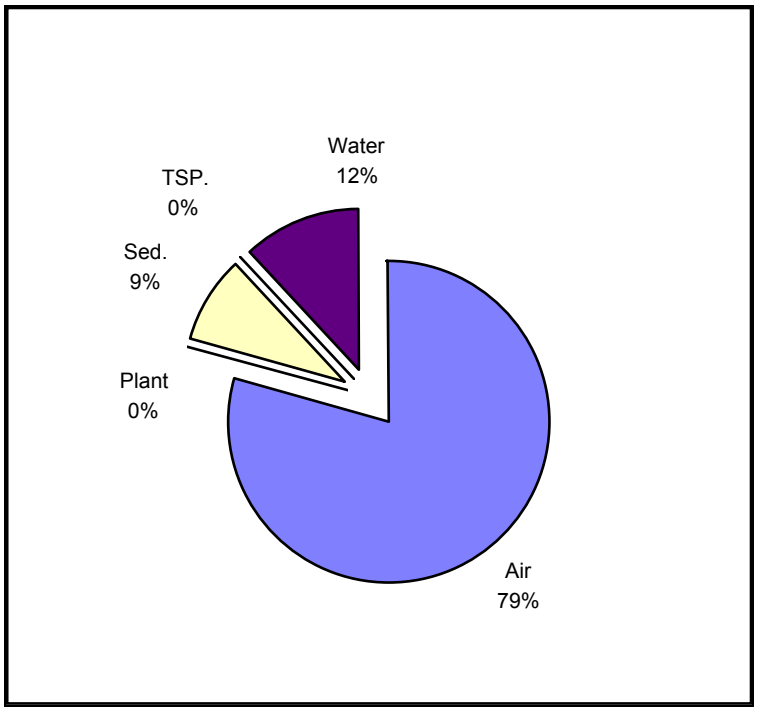


*Figure 3.7: Relative Distribution of HCB in the Warm Scenario. HCB is found primarily in the sediment.*

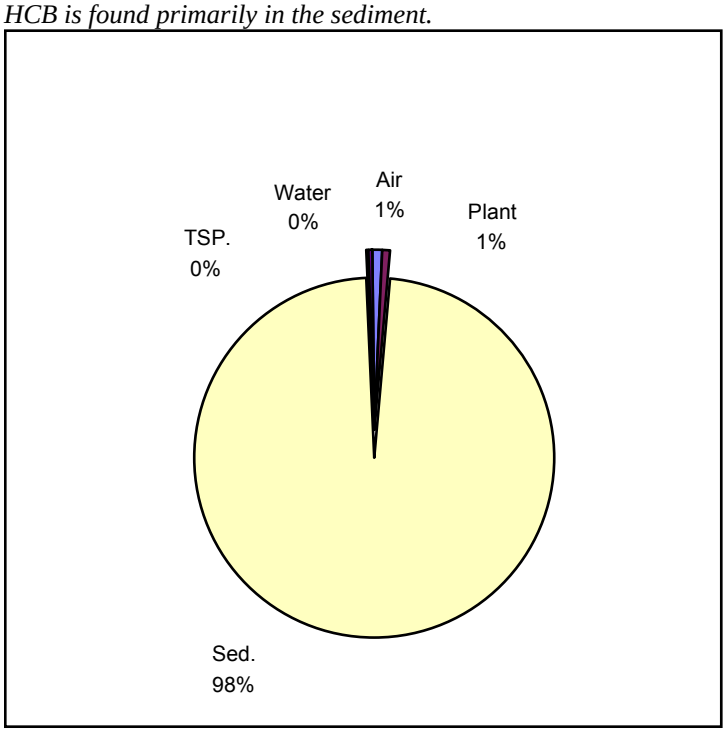
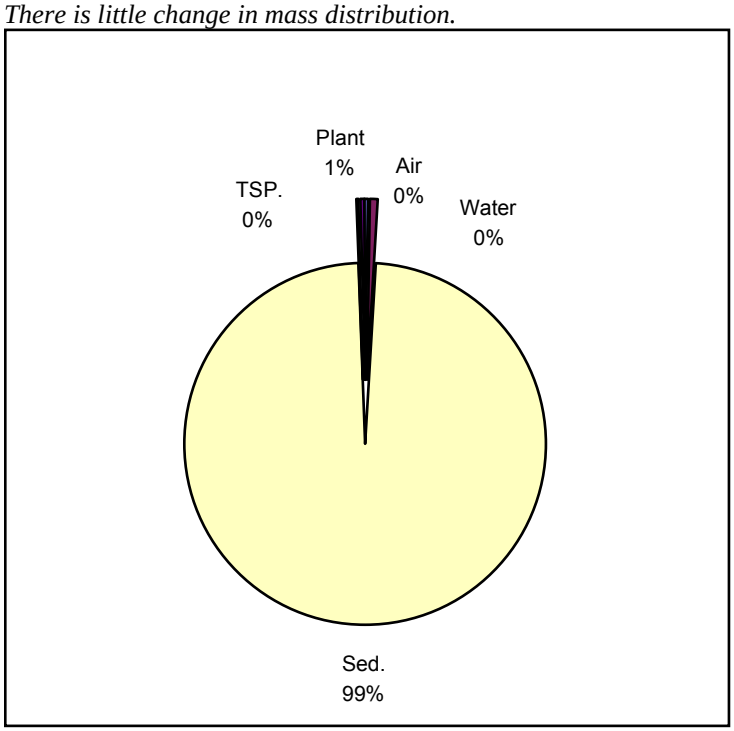



*Figure 3.8: Relative Distribution of HCB in the Cold Scenario. There is little change in mass distribution.*



(82.9%), then the water (14.2%) and sediment (2.9%). Toluene is found mainly in air (79.1%), then water (11.8%) and sediment (8.9%). HCB is found mainly in the sediment (98.4%). There is a change in mass distribution between the warm and cold runs, depending on the chemical. The mass distribution follows the same trend, for all chemicals; however, from warm to cold scenarios, less chemical is found in air and correspondingly more is found in solid or liquid phases. For example, benzene and toluene both show a decreased mass in air and an increased mass in water and sediment in the cold runs.

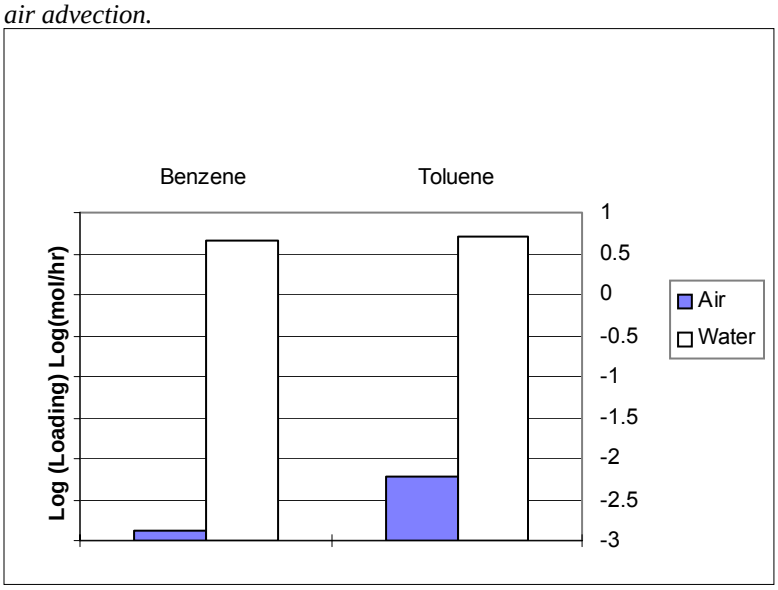
### *3.3 Loss and Loading Rates*

The dominant loading rates are, not surprisingly, via water inflow for all runs (See *Tables 3.3, 3.4* and *Figures 3.9 to 3.12).* For benzene and toluene, loading rates are six

*Table 3.3: Loading Rates of Chemicals (kg/yr.). Loading of contaminants into the stormwater system is primarily through water advection.*

| **Loading** | | | |
|---|---|---|---|
| **Chemical** | **Air Advection** | **Water Advection** | **Total** |
| **Benzene** | $1.30 \times 10^{-3}$ | 4.66 | 4.66 |
| **Toluene** | $6.01 \times 10^{-3}$ | 5.03 | 5.04 |
| **HCB** | 0 | $9.53 \times 10^{-5}$ | $9.53 \times 10^{-5}$ |

*Figure 3.9: Log (Loading Via Advection Vs. Medium of Input). Loading rate through water advection is several orders of magnitude higher than through air advection.*




orders of magnitude greater than loading via air advection. There is no change between warm and cold runs because concentrations and flow rates were kept constant for each chemical. In all model runs, total loading rates equal total loss rates (See *Tables 3.3* and *3.4*).

*Table 3.4: Loss Rates of Chemicals (mol/hr). Loss rates for both advection and reaction are given for warm and cold runs for benzene, toluene and HCB. In all model runs, total loading rates equal total loss rates (See Tables 3.3 for loading rates).*

| **Loss Rates** | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Chemical** | **Air advection** | **Water advection** | **Air reaction** | **Plants reaction** | **Sediment reaction** | **Suspended Sediment reaction** | **Water reaction** | **Total** |
| **Benzene warm** | $7.62 \times 10^{-2}$ | 1.89 | 2.66 | $1.23 \times 10^{-7}$ | $7.15 \times 10^{-4}$ | $1.62 \times 10^{-5}$ | $3.44 \times 10^{-2}$ | 4.66 |
| **Benzene cold** | $1.33 \times 10^{-2}$ | 4.64 | $4.75 \times 10^{-3}$ | $5.25 \times 10^{-8}$ | $9.64 \times 10^{-6}$ | $4.98 \times 10^{-7}$ | $1.06 \times 10^{-3}$ | 4.66 |
| **Toluene warm** | $5.25 \times 10^{-2}$ | 1.07 | 3.90 | 0[a] | $1.47 \times 10^{-3}$ | $3.19 \times 10^{-5}$ | $1.87 \times 10^{-2}$ | 5.04 |
| **Toluene cold** | $1.64 \times 10^{-2}$ | 4.99 | $2.81 \times 10^{-2}$ | 0[a] | $6.24 \times 10^{-4}$ | $1.41 \times 10^{-6}$ | $8.29 \times 10^{-4}$ | 5.04 |
| **HCB warm** | $1.70 \times 10^{-7}$ | $9.48 \times 10^{-5}$ | $8.45 \times 10^{-9}$ | $2.03 \times 10^{-7}$ | $1.74 \times 10^{-7}$ | $3.93 \times 10^{-10}$ | $3.57 \times 10^{-10}$ | $9.53 \times 10^{-5}$ |
| **HCB cold** | $3.22 \times 10^{-8}$ | $9.52 \times 10^{-5}$ | $1.53 \times 10^{-10}$ | $1.02 \times 10^{-8}$ | $8.09 \times 10^{-8}$ | $1.83 \times 10^{-10}$ | $1.66 \times 10^{-10}$ | $9.53 \times 10^{-5}$ |

*Figure 3.10: Benzene, Log (Loss Rate) Vs. Medium. Water advection and air reaction are the predominant loss mechanisms of chemical in the warm scenario. Water advection is the major loss mechanism in the cold scenario.*

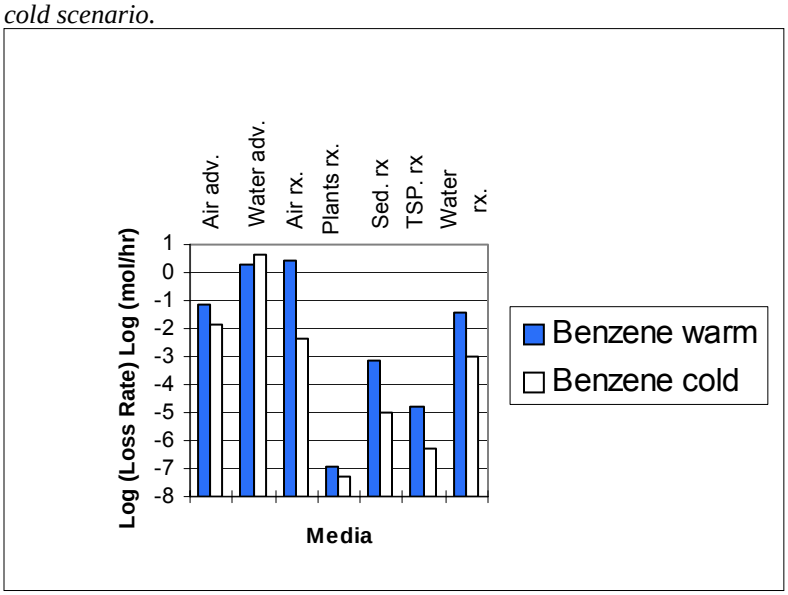
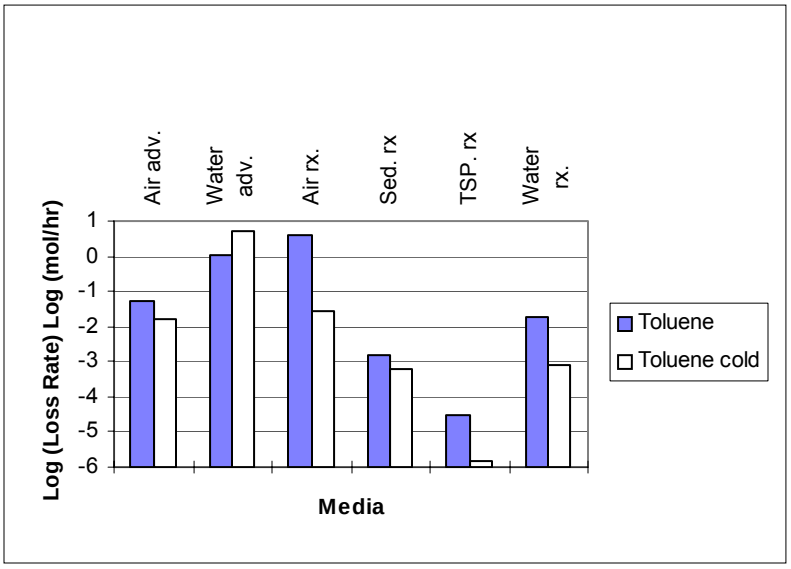
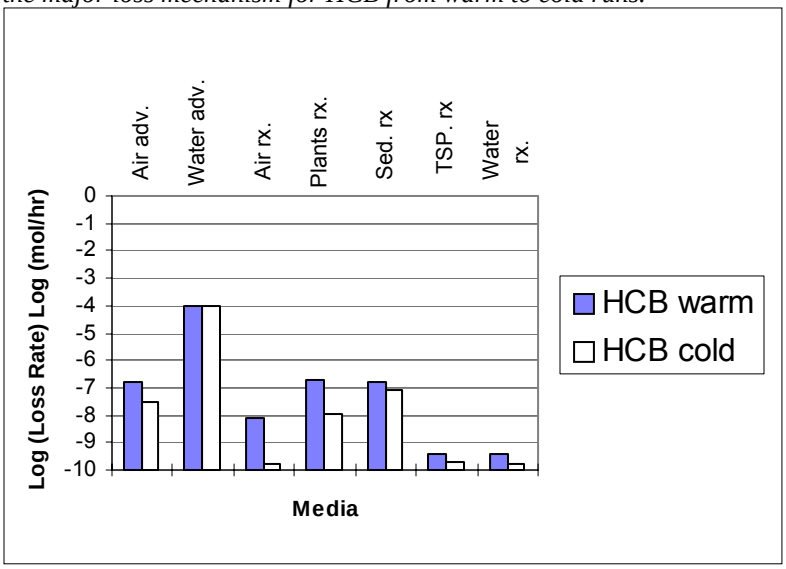



*Figure 3.11: Toluene, Log (Loss Rate) Vs. Medium. Water advection and air reaction are the predominant loss mechanisms of chemical in the warm scenario. Water advection is the major loss mechanism in the cold scenario. Relative loss rates are similar to benzene.*




Reaction in air is the dominant loss mechanism for benzene and toluene for the warm runs (2.66 and 3.90 mol/h, respectively ). For the cold runs, the dominant loss rates for benzene and toluene are through water advection (4.64 and 4.99 mol/h, respectively). Water advection is the dominant loss mechanism for HCB for both warm and cold runs ($9.48 \times 10^{-5}$ and $9.52 \times 10^{-5}$ mol/h). For all chemicals, there is an increased loss via water

*Figure 3.12: HCB, Log (Loss Rate) Vs. Medium. Water advection remains the major loss mechanism for HCB from warm to cold runs.*




advection but decreased losses from all other media from warm to cold runs. This occurs because, in the cold runs, the mass of chemical decreases in air (where reaction and advection rates are greatest) and there is an increase in the solid and liquid phases resulting in a greater advective loss from water. As expected, loss via reaction decreases in all media from warm to cold as it is assumed that the rates of all reaction mechanisms are temperature dependent.

### *3.4 Comparison with Field Measurements*

Predicted concentration of HCB in sediment of a stormwater detention wet pond is $2.87 \times 10^{-9}$ g/g sed. and measurements by Struger *et al*. (1994) are $1.000 \times 10^{-9}$ g/g sed. Predicted values were 3 times greater but within the same order of magnitude as measured values. This is only a partial validation of the model. Almost all the HCB introduced to the stormwater pond environment partitions directly into the sediment phase. It does not volatilize and degradation is very slow in all phases, including in

sediment. Very little partitions into the other media (e.g., water) where it can be removed rapidly. Therefore, this comparison does not consider all media or removal rates and cannot be used to test how well the model describes partitioning into other media or the loss rates of benzene and toluene.

### *3.5 Sensitivity Analysis Results*

The following trends were observed from the sensitivity analysis. Increasing the reaction rate in any medium resulted in a minimal decrease in chemical concentration in all media. This effect is greater if there is a greater relative mass distribution of chemical found in the media whose reaction rate is being affected (See *Figures 3.13* to *3.17*). If

*Figure 3.13: Change in Concentration in All Media Vs. Fraction of Air Reaction Rate. The fraction of the concentration of the base case is compared to 0.001 and 1000 times the base case air reaction rate. increasing air reaction rate decreases concentration of chemical in all media.*

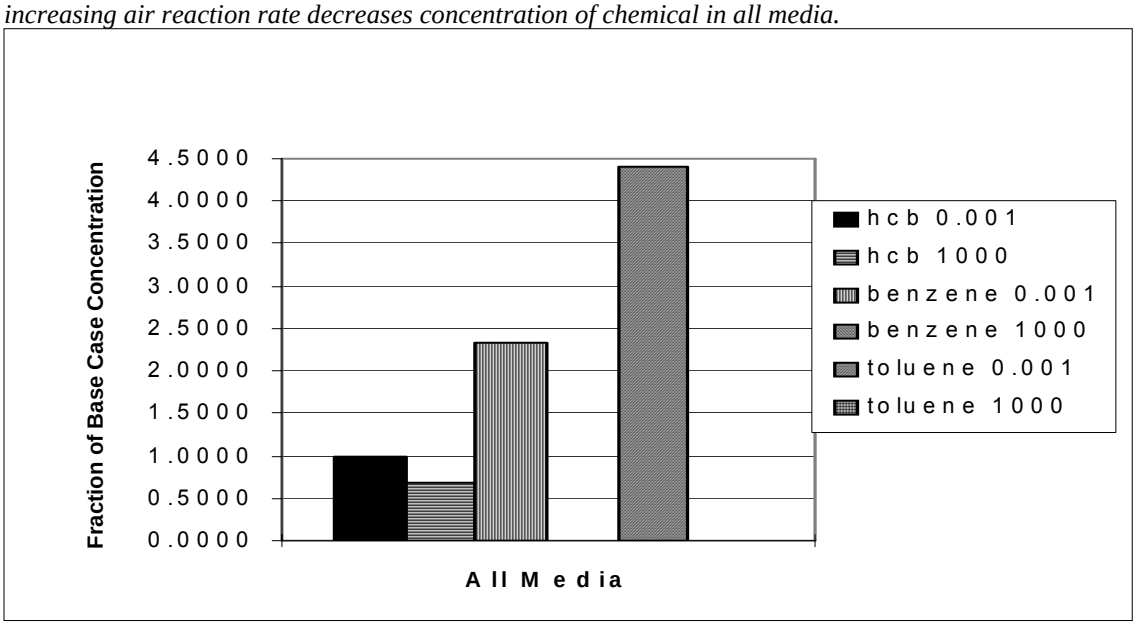



*Figure 3.14 Change in Concentration in All Media Vs. Fraction of Plant Reaction Rate. The fraction of the concentration of the base case is compared to 0.001 and 1000 times the base case plant reaction rate. Increasing plant reaction rate decreases concentration of HCB but does not significantly affect benzene or toluene.*

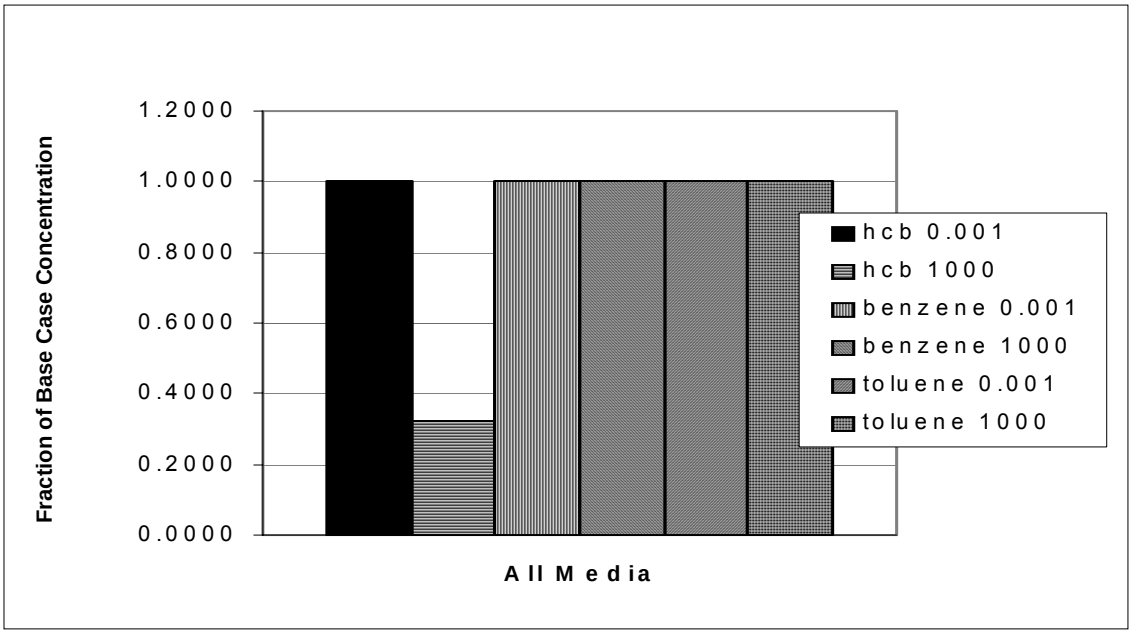
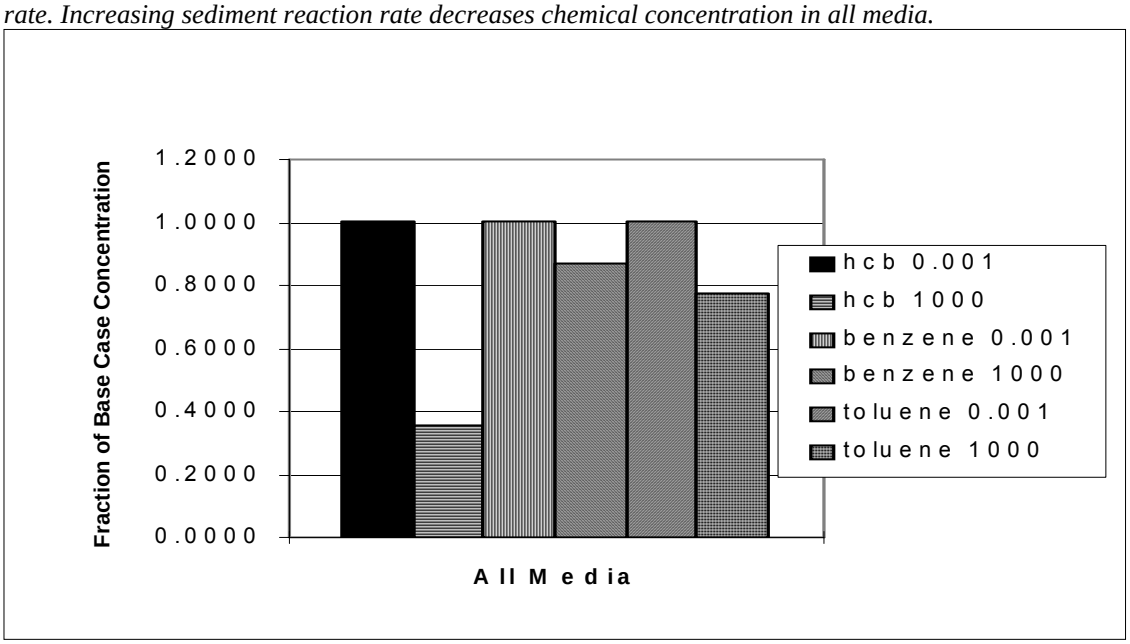



*Figure 3.15: Change in Concentration in All Media Vs. Fraction of Sediment Reaction Rate. The fraction of the concentration of the base case is compared to 0.001 and 1000 times the base case sediment reaction rate. Increasing sediment reaction rate decreases chemical concentration in all media.*




there is very little chemical in the affected medium (e.g. plants and suspended sediment) then the change in chemical concentration is not significant. Increasing the reaction rate

*Figure 3.16: Change in Concentration in All Media Vs. Fraction of Suspended Sediment Reaction Rate. The fraction of the concentration of the base case is compared to 0.001 and 1000 times the base case suspended sediment reaction rate. There is no significant change in concentration of chemical in any medium with variation of suspended sediment reaction rate.*

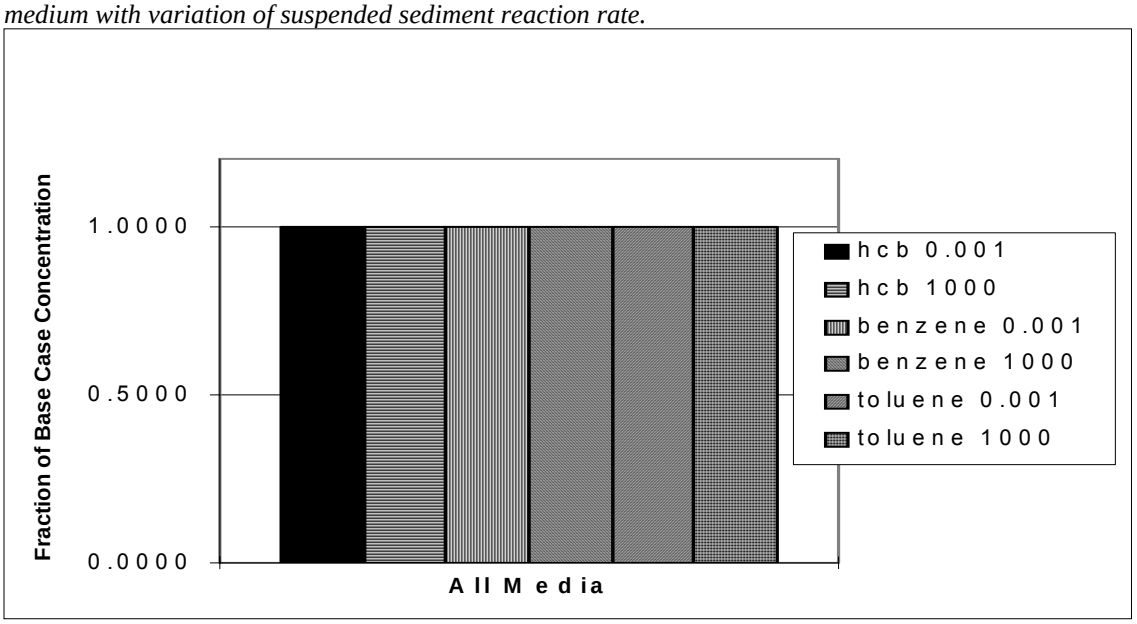
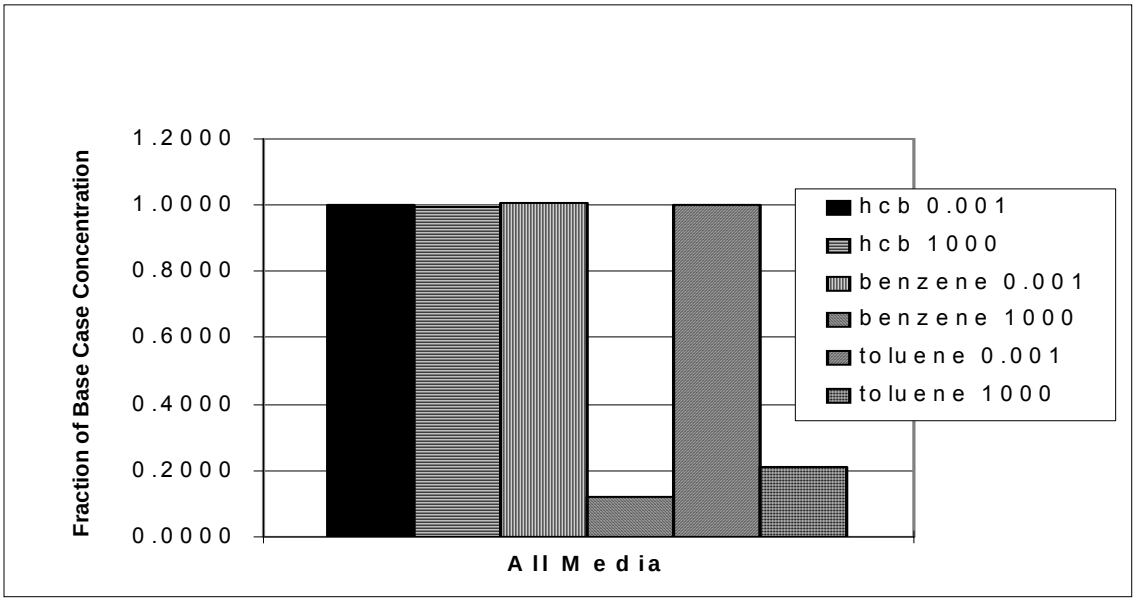



*Figure 3.17: Change in Concentration in All Media Vs. Fraction of Water Reaction Rate. The fraction of the concentration of the base case is compared to 0.001 and 1000 times the base case water reaction rate. HCB shows little decrease in concentration. Benzene and Toluene show much greater decreases in chemical concentrations in all media.*




in a given medium decreases the total amount of chemical in the system being distributed. Therefore, concentrations decrease in all media by the same proportion fraction and, so, the relative mass distribution does not vary with reaction rate.

Increasing the volume of a medium causes a minimal decrease in the concentration of chemical in all media. This is a dilution effect. As expected, there is a greater decrease in concentration if the medium being affected has a higher mass distribution of chemical. Therefore, more of the chemical in the pond system would be distributed into a larger volume. For example, as sediment volume increases, the concentration of HCB in sediment decreases. This effect is minimal for toluene and benzene (See *Figure 3.18*) because their masses are predominantly distributed in air. An increase in the volume of a medium results in an increase in the mass distribution in

*Figure 3.18: Change in Concentration in All Media Vs. Fraction of Sediment Volume. The fraction of the concentration of the base case is compared to 0.5 and 2 times the base case sediment volume. Increasing sediment volume results in a decrease in concentration for chemicals in all media.*

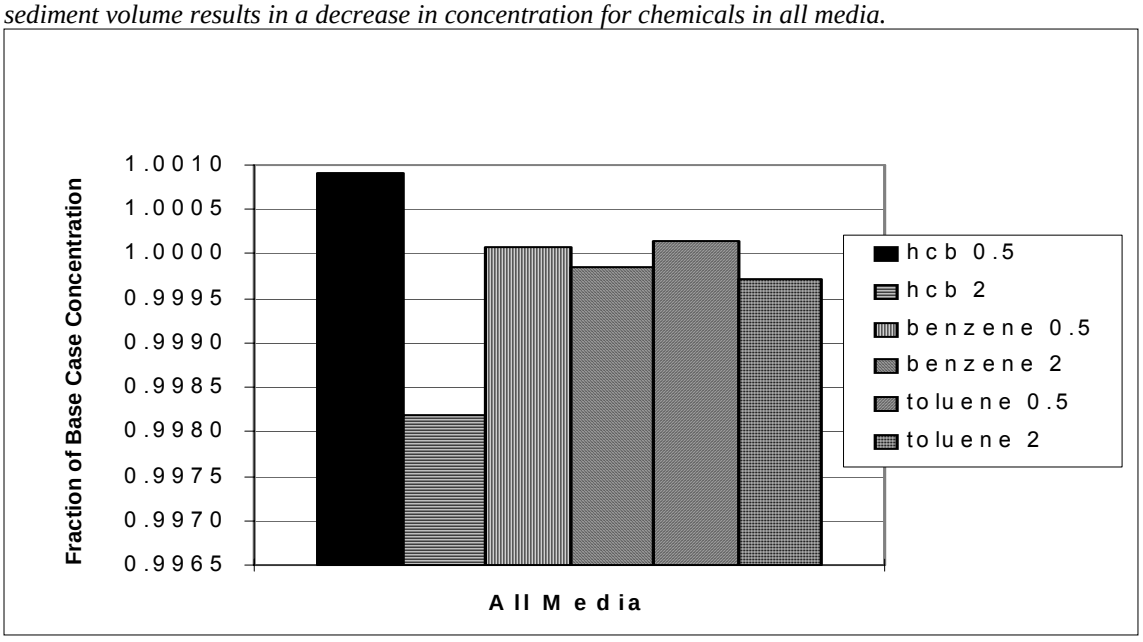


*Figure 3.19: Change in Concentration in All Media Vs. Fraction of Plant Volume. The fraction of the concentration of the base case is compared to 0.5 and 2 times the base case plant volume. Only HCB shows a decrease in concentration in all media.*

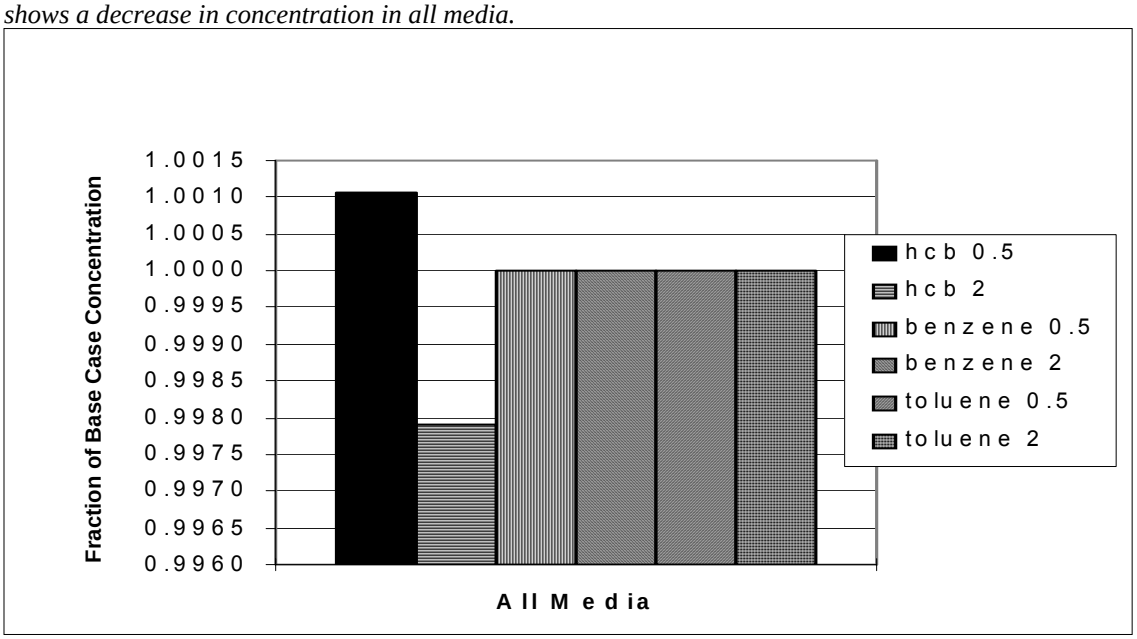



*Figure 3.20: Change in Concentration in All Media Vs. Fraction of Suspended Sediment Volume. The fraction of the concentration of the base case is compared to 0.5 and 2 times the base case suspended sediment volume. Concentration is not sensitive to suspended sediment volume changes.*

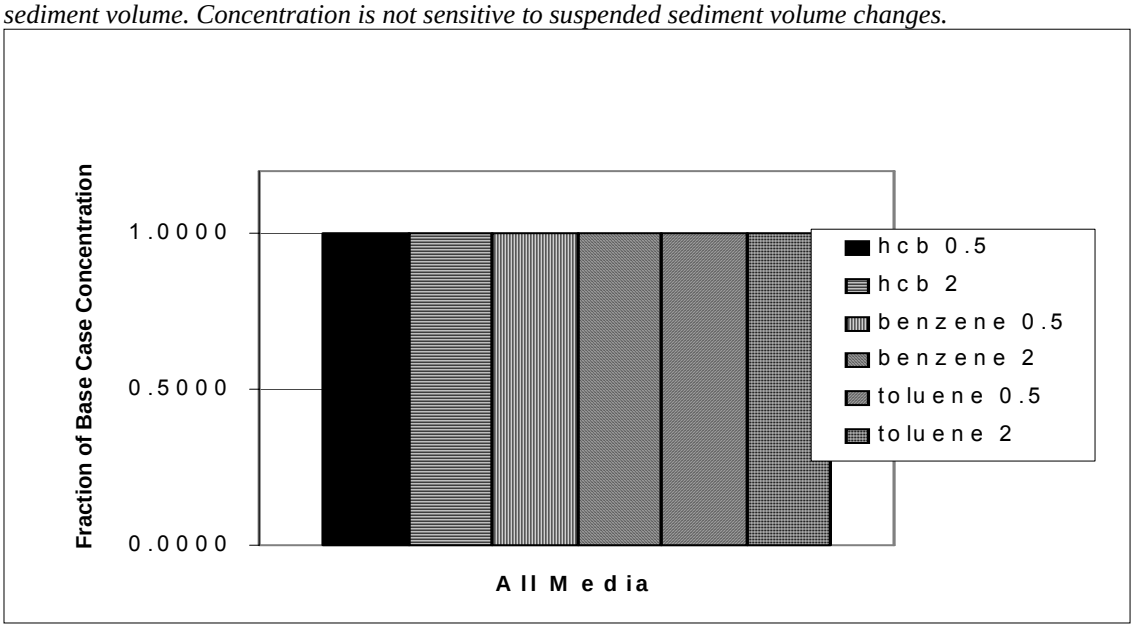


*Figure 3.21: Change in Mass Distribution Vs. Fraction of Sediment Volume. The fraction of the mass distribution of the base case is compared to 0.5 and 2 times the base case sediment volume. Increasing the sediment volume results in a decrease in the mass distribution in all other media, especially in HCB. This also results in a greater mass of chemical being distributed into the sediment medium.*

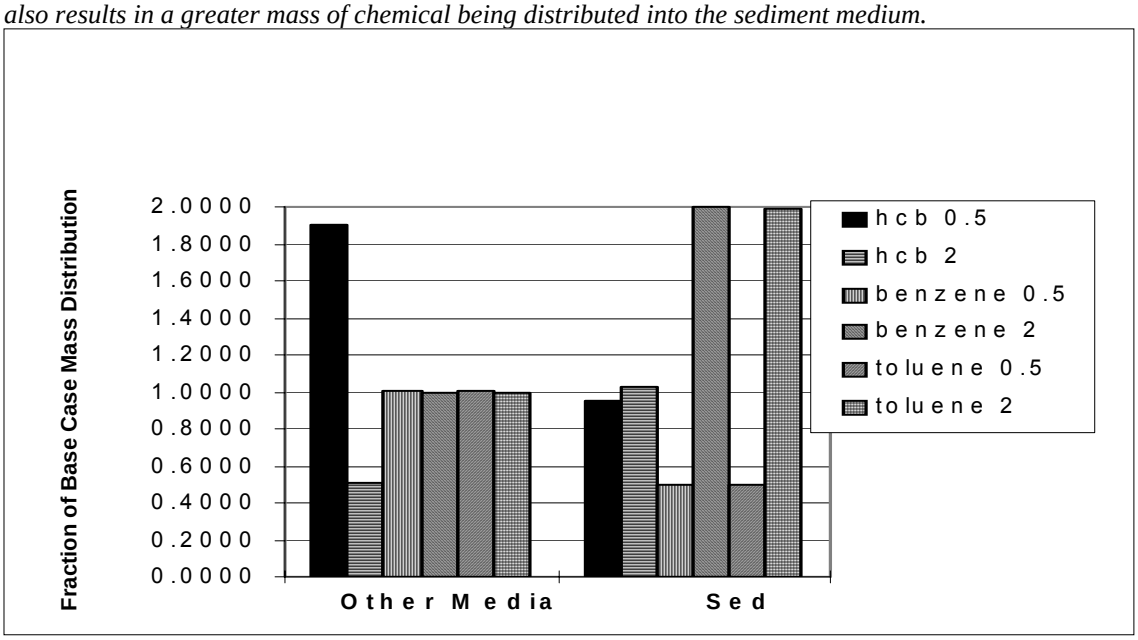



*Figure 3.22: Change in Mass Distribution Vs. Fraction of Plant Volume. The fraction of the mass distribution of the base case is compared to 0.5 and 2 times the base case plant volume. Increasing plant volume increases the mass distribution of chemical in the plant medium. There is a minimal decrease in mass distribution in the other media.*

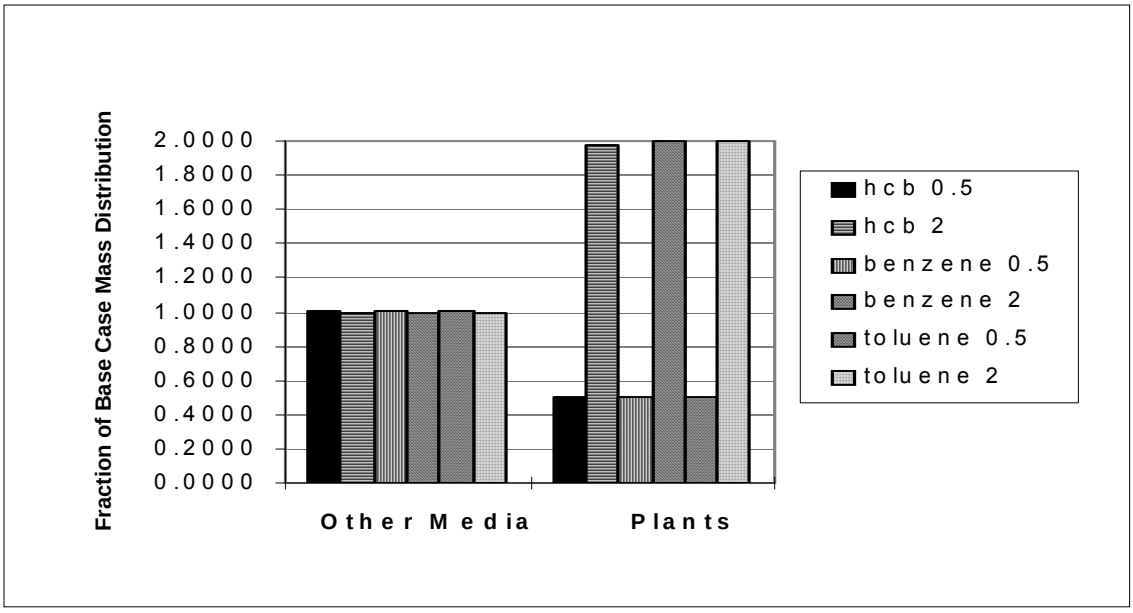
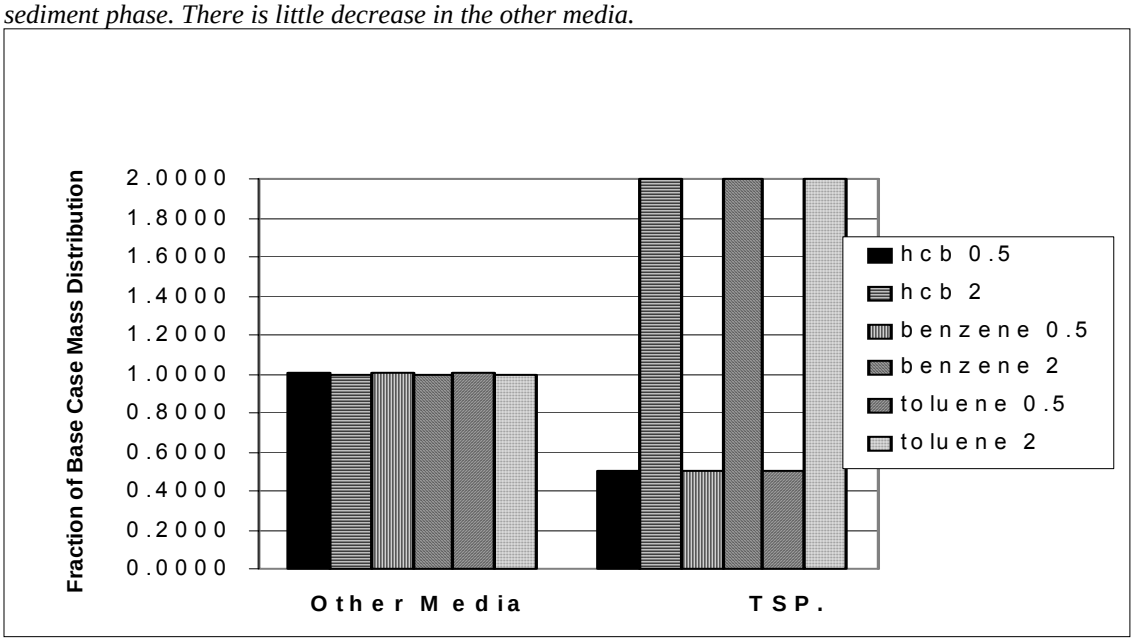


*Figure 3.23: Change in Mass Distribution Vs. Suspended Sediment Volume. The fraction of the mass distribution of the base case is compared to 0.5 and 2 times the base case suspended sediment volume. Increasing suspended sediment volume results in an increase in mass distribution in the suspended sediment phase. There is little decrease in the other media.*




that medium. However, if there is a large distribution of chemical in a given media (e.g. HCB in sediment) then there will be a smaller percentage increase of chemical in the affected medium.

Increasing the rate of water inflow and the chemical concentration in water inflow increases the concentrations in all media (*Figures 3.24* and *3.25*) because this results in a higher loading rate of chemical into the system through water advection. Increasing the flow rate also results in increasing the loss rate of chemical from the stormwater pond system. Therefore, the resulting increase in media concentration is less than from increasing the inflow concentration. There were no changes in the mass distribution.

*Figure 3.24: Change in Concentration in All Media Vs. Fraction of Rate of Water Inflow. The fraction of concentration of the base case is compared to 0.5 and 2 times the base case water inflow rate. Increasing inflow rate results in an increase in the concentrations of chemical in all media..*

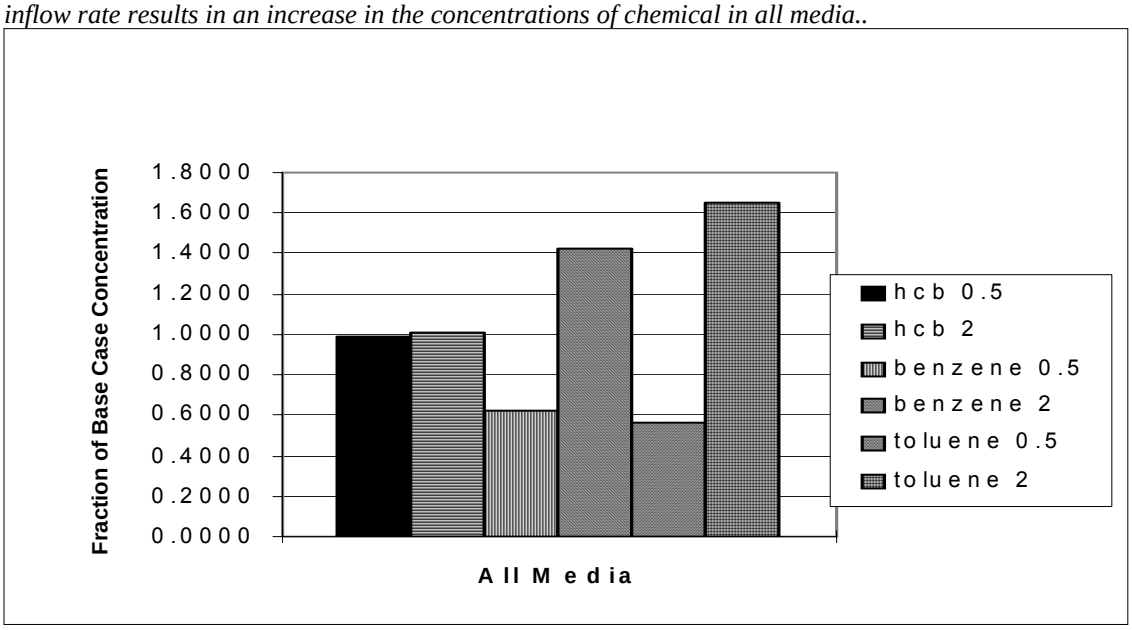
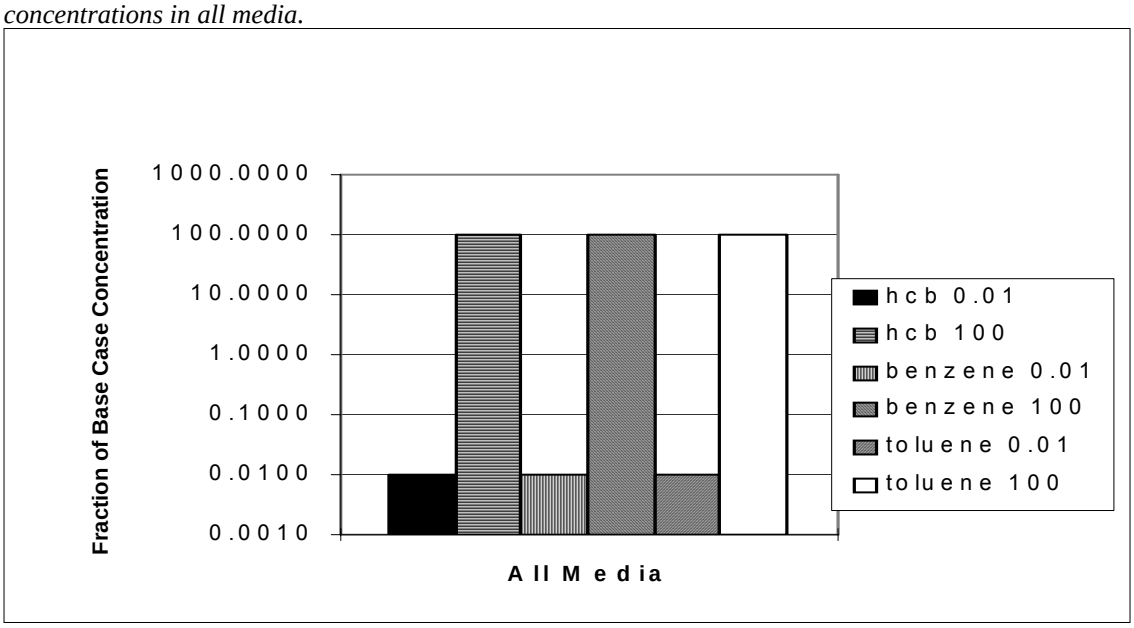



*Figure 3.25: Log (Change in Concentration in All Media) Vs. Fraction of Inflow Water Concentration. The fraction of the chemical concentration of the base case is compared to 0.5 and 2 times the base case inflow water concentration. Increasing the inflow water concentrations results in an increase in chemical concentrations in all media.*



# 4.0 Discussion

## *4.1 Biotic Affects*

An understanding of the ecotoxicological effects of a stormwater system is necessary to determine potential hazards. Stumm (1992) indicates that even in low concentrations, some contaminants can adversely affect aquatic organisms by interfering with inter-organism communication, food-finding or mimicking chemical signals. Some dominant aquatic plants do not assimilate many hydrophobic organic compounds. Consequently, trophic transfer of contaminants is less of a concern. For example, green arrow arum (*Peltandra virginica*), cockspur (*Echinochloa sp*.), and cat-tail (*Typha sp*.) showed minimal bioaccumulation of chlorinated hydrocarbons (e.g. including DDT, DDD, DDE, lindane, chlordane, dieldrin, toxaphene and PCB; Catallo, 1993). For chemicals that are assimilated, plants tend to bind many toxic contaminants (e.g. phenols) in the lignin of their cell wall. In this way, the toxins are removed from interfering with plant metabolism. However, toxins can become bioavailable as they are released from the cell wall while in the digestive system of animals or when the plant matter decays (Deo *et al*., 1994.). Ingestion of plant matter may provide significant exposure to aquatic biota since concentrations in plant matter are predicted to be higher than in air or water.

## *4.2 Reaction Rates*

Poor availability and uncertainty of transformation rate data is a potential source of error with reported transformation rates sometimes spanning two orders of magnitude. There has been little work done describing chemical reaction rates in aquatic plants. A potential source of error is introduced because half-lives in *aquatic* plants are taken from measurements in the soybean. Degradation products from these chemicals, that may even

be more harmful than the original chemical, are not considered. The *Level II* model simply considers that the chemical disappears when it degrades.

### *4.3 Monitoring Programs*

Accurate data for various parameters in stormwater ponds is required and should be measured by field sampling. For example, volumes of plants in stormwater ponds were estimated from biomass in the littoral zone of *lakes* and these values varied by nearly two orders of magnitude. Using these values for much smaller stormwater ponds with different limnological characteristics is a potential source of error. Additionally, loading of benzene and toluene were based on concentrations reported from the NURP study which took place in the late 1970's and early 1980's. Since then, concentrations may have changed significantly due to changes in technology and chemical use, as well as methods of chemical analysis. Data for HCB concentrations in stormwater were collected from various sources with a wide range in reported values. Data are site-specific and variations in contaminant concentration in urban runoff may occur which are significantly different from mean or generalized values.

Measurements taken from different media over a variety of environmental parameters (e.g., different ambient temperatures, sizes of media compartments, chemical sources and transformations, catchment hydrological processes at different scales, inlet and outlet flows, rainfall etc.; Southwood *et al*., 1989; Watt and Maršálek, 1994; van Duin *et al*., 1995) would allow a more accurate description of parameters used in the model under varying conditions. This would also facilitate validation of future, more realistic models by allowing comparisons of predictions with measured data under differing environmental conditions. Also, more realistic modeling runs can be done with

data specific for other common organic contaminants which then can be compared to field measurements. This will help validate future stormwater modeling projects. Finally, if monitoring continued after a stormwater pond is operational, this could continue to test modeling approach and refine its parameters, especially if conditions change.

### *4.4 Modeling*

Field sampling cannot be done to assess chemical accumulation in various media and potential hazards to aquatic biota cannot be considered in stormwater detention ponds that have not been built yet. However modeling can be used to assess the potential concentration and mass distribution and, therefore, the potential bioaccumulation of contaminants in these media in the planning stages, before the pond is actually built and while alternatives can still be considered. The *Level II* model assumes the stormwater system is at equilibrium and at steady state. This is not the case. For example, because of the steady-state assumption, the simplification of the stormwater environment used in this *Level II* model does not allow different inflow and outflow rates, the very reason the ponds are constructed. Additionally, the model's consideration that the stormwater instantaneously reaches equilibrium within the pond is unreasonable, given the rapid flow rates. Stormwater ponds are designed to hold excess stormwater and then release it at a controlled rate over an extended time period to prevent flooding downstream (Taur, 1987).

This model also does not consider the possibility of inter-compartment contaminant transfer. It assumes that an introduced chemical instantaneously partitions into all compartments. This does not actually occur. For example, by predicting different mass distributions of contaminants in warm and cold ambient temperatures, the *Level II*

model does suggest that contaminants should tend to move between compartments (e.g. from air to sediment from warm to cold ambient temperatures).

The use of a more sophisticated model, such a steady-state, non-equilibrium fugacity model, would consider inter-compartment transfer (Mackay, 1991). However, even this model is inappropriate for describing the stormwater pond system. More realistic modeling is required. An unsteady-state or time dependent model would consider non-equilibrium, unsteady-state situations such as changes in environmental parameters over time (e.g. temperature or ice cover), variable flow rates (e.g. from snow melt, rainfall peak vs. base flow, and the difference between input flow rate and output flow rate to and from the pond; Mackay, 1991; Gibbs, 1994).

### *4.5 Consideration of Pollution Control Measures*

Varying the volume of plant matter or sediment gives an indication of the effect of harvesting and sediment collection on contaminant fate. Results from the cold scenarios suggest that, if plant and sediment were collected when the ambient temperature is colder, more of the less-volatile organic contaminants (e.g., HCB) can be retrieved. There was little change in relative mass distribution in these media for more volatile chemicals, like benzene and toluene. For all chemicals changes in the volume of suspended sediment did not significantly change mass distribution or concentrations in other media, suggesting that removal of this media is not an effective contaminant control strategy. However, sorbed chemicals such as HCB enter the system with suspended particles and, so, the medium should not be ignored.

The effect of decreasing the rate of water inflow (e.g., during a rainfall event, as in downspout deconnection, or decreasing percentage urban impervious substrate; or,

base flow between rainfall events) was tested by the sensitivity analysis. Non-structural best management practices dealing with educational and institutional changes (e.g., encouraging landscaped areas, grass buffers, roadside swales to increase imperviousness) can also achieve a reduction of runoff flow rate (Urbonas, 1994). Using stormwater infiltration through porous pavements, infiltration basins, deep boreholes, land-use planning and using natural drainage are some other options to decrease stormwater flow (Maršálek and Sztruhár, 1994; Field, 1985). Results of the sensitivity analysis indicate that decreasing the rate of water inflow into the system results in a decrease in the concentrations of chemicals in all media because chemical loading is a function of flow rate. This does not consider that many contaminant concentrations in water inflow can vary with flow rate (Ellis, 1986; Helsel *et al*., 1979). Additionally, this does not consider what happens to the contaminants in the stormwater which no longer reach the pond. These contaminants would remain "upstream."

Decreasing contaminants in stormwater through source controls was studied by changing the background concentration of water entering the pond. The results indicate that source control results in proportional decreases in concentrations for organic chemicals in all media in a stormwater pond system. As expected, source control is the most effective way to reduce concentrations of chemicals in all media. This can be achieved through a variety of ways. For example the use of construction materials which add to the pollutant problem, can be regulated. Mikkelsen *et al*. (1994) suggest that retention of pollution at its source may be an option (e.g., directing stormwater into contained infiltration systems) where it can be treated for pollutants. Urbonas (1994) also suggests public education on the proper use and disposal of potentially hazardous

materials such as pesticides and crank case oil, creating and enforcing local government regulations, and finding and eliminating illegal sewer connections. Street cleaning is not effective at reducing organic contaminant concentration in stormwater (Field, 1985; Urbonas, 1994).

## 5.0 Conclusion

This modeling exercise has demonstrated that stormwater ponds can fulfill some of their objectives. They collect some chemicals in one place (e.g., HCB in sediment) but this may make these chemicals more available to biota. For more volatile contaminants such as benzene and toluene, stormwater ponds facilitate a redistribution of chemicals into other media, making them more difficult to collect. Thus, there is a need for caution in the use of stormwater detention ponds.

This model has demonstrated the need for continued research on characterizing organic contaminants in urban stormwater by creating more-sophisticated models, and using site-specific monitoring data, which more accurately define the dynamics of the stormwater environment. It has identified data requirements, knowledge gaps and potential sources of error in the modeling process and has suggested a future direction for this work. Monitoring programs and modeling must work together for the best results. Modeling can suggest which parameters need to be monitored closely while monitoring provides data which the modeling requires. An understanding of the dynamics and fate of organic contamination from urban runoff in these stormwater ponds is essential, especially when assessing control measures (Andoh, 1994). By the year 2000, more than 50% of global population will be living in urbanized areas (Massing, 1994). Therefore, not only will the sources of organic pollutants increase, but so will exposure of these

contaminants to human and ecological receptors. It is therefore highly important that these issues be addressed and dealt with effectively.

## 6.0 Recommendations

- Despite possessing a relatively small mass distribution, plant matter is an important medium in stormwater ponds because it possesses high chemical concentrations and can promote chemical degradation. Thus, ingestion of plant matter may be an important vector for contamination to biota. Therefore, parameters which can affect concentration such as reaction rates should be investigated.
- Reaction rates should be studied further because of the scarcity of rate data, the wide range in reported values, and to quantitatively describe the effect of temperature (i.e., reaction rates increase with temperature).
- Extensive monitoring and sampling is required to obtain accurate data required for input parameters (e.g., concentration and rate of inflows) and media characterization (e.g., volume). Some estimates used in the model, such as plant volume or fraction of organic carbon in sediment, were not specific to stormwater ponds. Concentrations in stormwater were based on older data sources (e.g., benzene and toluene from NURP) or showed a wide range in reported values (e.g., HCB). This can affect loading rates into stormwater ponds. Additionally, for a given site, generalized inflow concentrations from different sites found in the literature should not be used because concentration may vary significantly between two sites for different chemicals.
- Sampling of concentrations should be conducted from a variety of media and during different environmental conditions, allowing comparisons of measured and predicted values. This allows validation of more complex models. Monitoring should be done

throughout the year to assess modeling predictions under differing conditions (e.g., flow rate, temperature).

- Baseline measurements (i.e., sampling taken at the beginning of a study to assess the initial state of the environment), such as initial flow rate and concentrations of contaminants in runoff, should also be measured when stormwater ponds are constructed in order to provide a reference for any future changes in these parameters (ESP, 1996).
- A Level IV fugacity model, which considers unsteady-state conditions, is recommended as the next step of this research.
- More contaminants should be modeled and predicted values should be compared to sampled measurements.
- Modeling exercises should be conducted and results should be analyzed with a detailed understanding of natural history of relevant species and biotic effects which occur within the stormwater pond environment.
- Modeling should also consider the availability of contaminants to aquatic organisms (Lee and Jones-Lee, 1995). For example, contaminants that are found in high concentrations in sediment may be incorporated into benthic organisms through ingestion as well as contact (Landrum, 1989).
- The fate of contaminants that remain upstream if the rate of stormwater runoff is decreased should be investigated.

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# Appendix A

Additional Calculations and Tables

*Table A1: Level II Fugacity Model Equations*

| | |
|---|---|
| ***Level II* Model** | • identifies environmental sinks<br>• considers the chemical reaction and advection removal rates |
| **REACTION LOSS**<br>$N_R = k_R CV$<br>$= D_R f$ | $N_R$ = overall reaction rate (mol/h) in the considered compartment<br>$k_R$ = overall reaction rate constant ($h^{-1}$)<br>C = concentration of the chemical in the compartment ($mol/m^3$)<br>V = the compartment volume ($m^3$) |
| $C=Zf$ | Z = the capacity of compartment for the chemical |
| $N_R = k_R ZfV$<br>$D_R = VZk_R$ | f = fugacity of the chemical<br>$D_R$ = transport parameter (mol/Pa.h) |
| **ADVECTION LOSS**<br>$N_A = D_A f$ | $N_A$ = overall advection rate in the considered compartment (mol/h)<br>$D_A$ = transport parameter (mol/Pa.h) |
| for each compartment,<br>$f = I/(D_R + D_A)$ | I = input rate (mol/h)<br>f = fugacity (Pa) |
| $I = E + \sum GC$<br><br><br><br>$O = I = E + \sum GC$ | E = emission rate, a quantity of contaminant directly introduced to the system at a constant rate (mol/h)<br>G = an inflow of water ($m^3/h$), with<br>C = concentration of chemical<br>O = output = input, assuming a steady state condition |
| $O = D_A f + \sum D_R f = \sum (D_A + D_R) f$<br>$f = (E + \sum GC)/ \sum (D_A + D_R)$<br>$f = I/ \sum D$ | |
| $Q = \sum Q_i$<br>$Q_i = C_i V_i = f Z_i V_i$<br>$Q = f \sum Z_i V_i$ | Q = total quantity in the system<br>$Q_i$ = is the quantity of chemical in each compartment |

*Adapted from:* Bacci, E. 1994. *Ecotoxicology of Organic Contaminants.* Lewis Publ., Chelsea, Michigan.

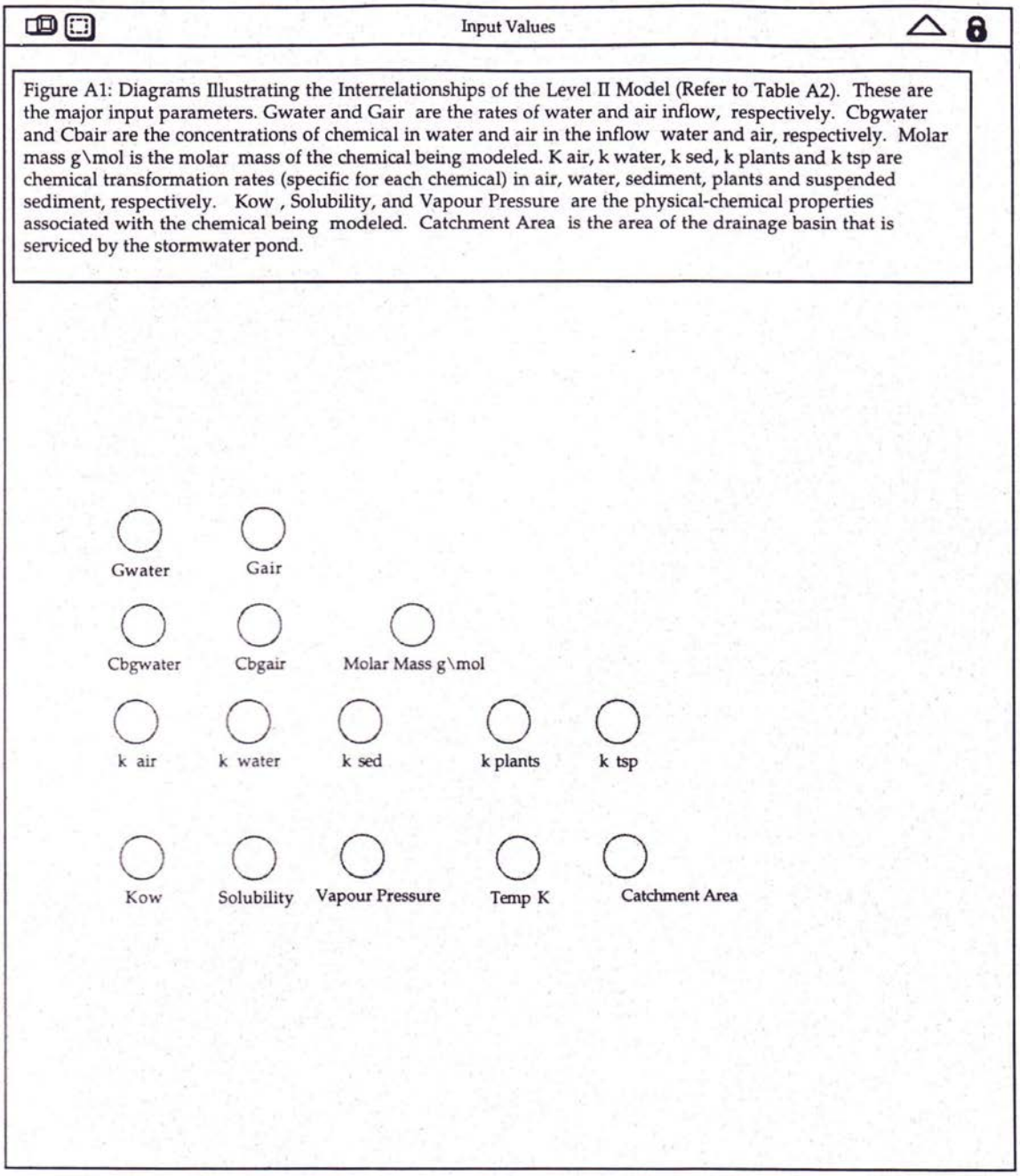



Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (Refer to Table A2). These are the major input parameters. Gwater and Gair are the rates of water and air inflow, respectively. Cbgwater and Cbair are the concentrations of chemical in water and air in the inflow water and air, respectively. Molar mass g\mol is the molar mass of the chemical being modeled. K air, k water, k sed, k plants and k tsp are chemical transformation rates (specific for each chemical) in air, water, sediment, plants and suspended sediment, respectively. Kow , Solubility, and Vapour Pressure are the physical-chemical properties associated with the chemical being modeled. Catchment Area is the area of the drainage basin that is serviced by the stormwater pond.

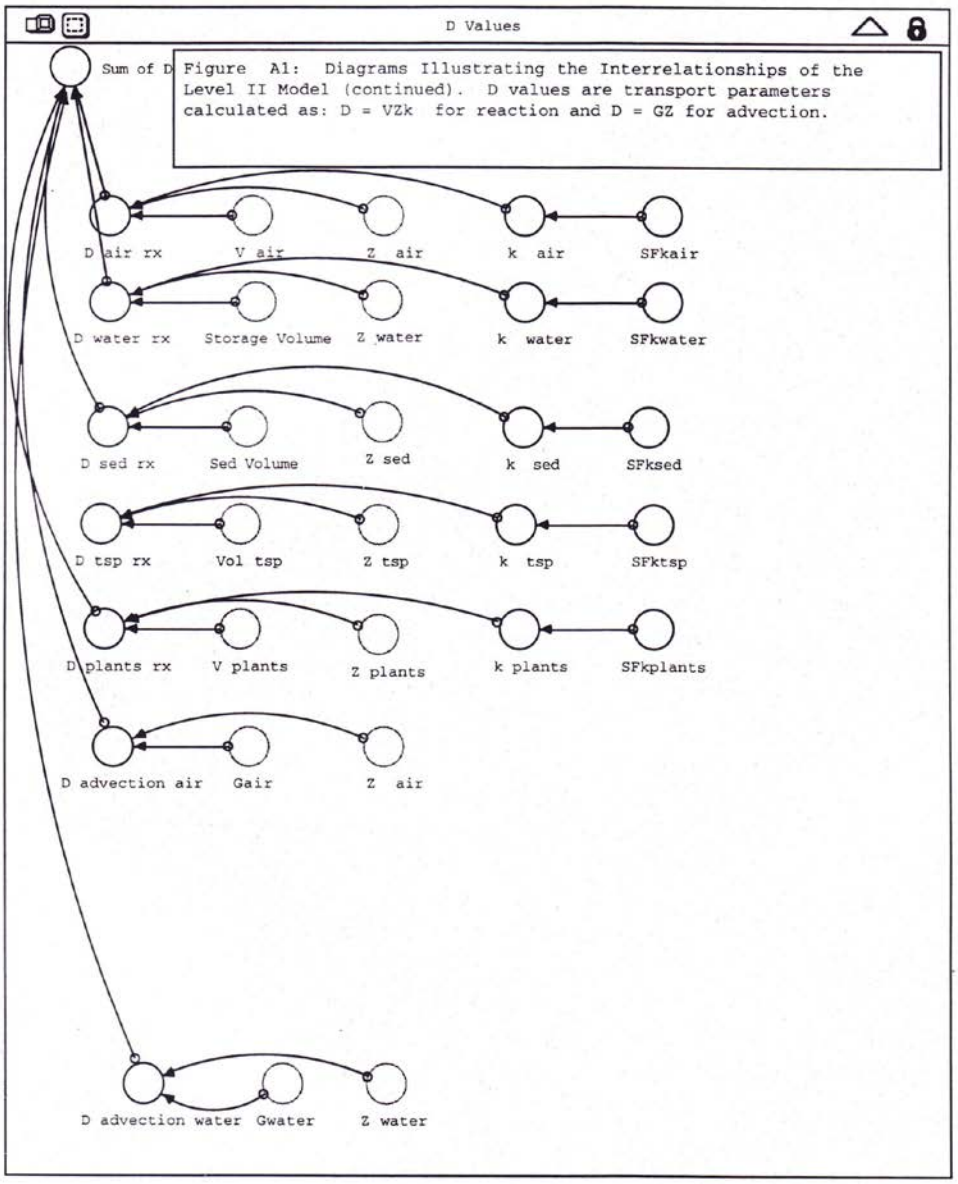
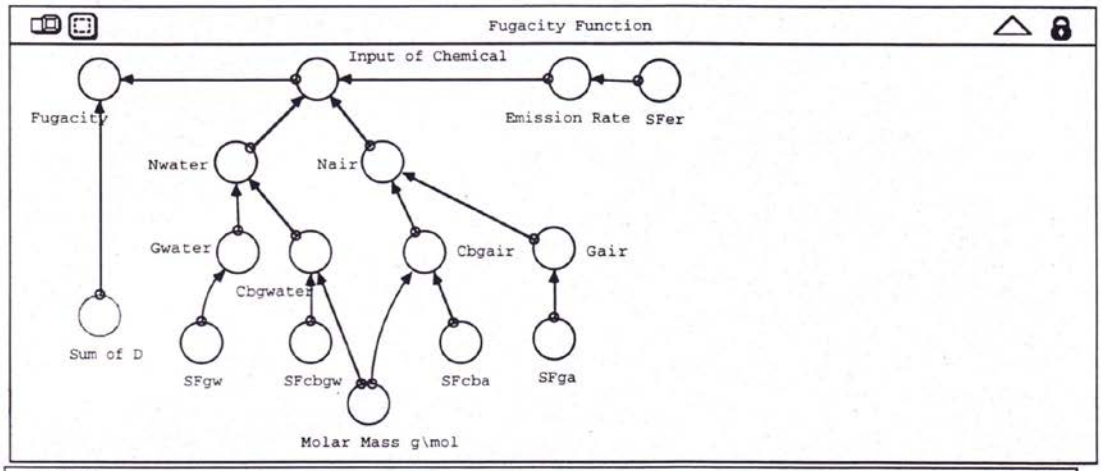

D Values
Sum of D
Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued). D values are transport parameters calculated as: D = VZk for reaction and D = GZ for advection.
D air rx
V air
Z air
k air
SFkair
D water rx
Storage Volume
Z water
k water
SFkwater
D sed rx
Sed Volume
Z sed
k sed
SFksed
D tsp rx
Vol tsp
Z tsp
k tsp
SFktsp
D plants rx
V plants
Z plants
k plants
SFkplants
D advection air
Gair
Z air
D advection water
Gwater
Z water

Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued). Input of Chemical into the stormwater pond system is calculated as the sum of Emission Rate, loading of chemical through water (Nwater) and loading of chemical through air (Nair). Loading through air and water is the product of advection and inflow concentrations for air and water, respectively. Fugacity is calculated as: Input of Chemical/Sum of D.



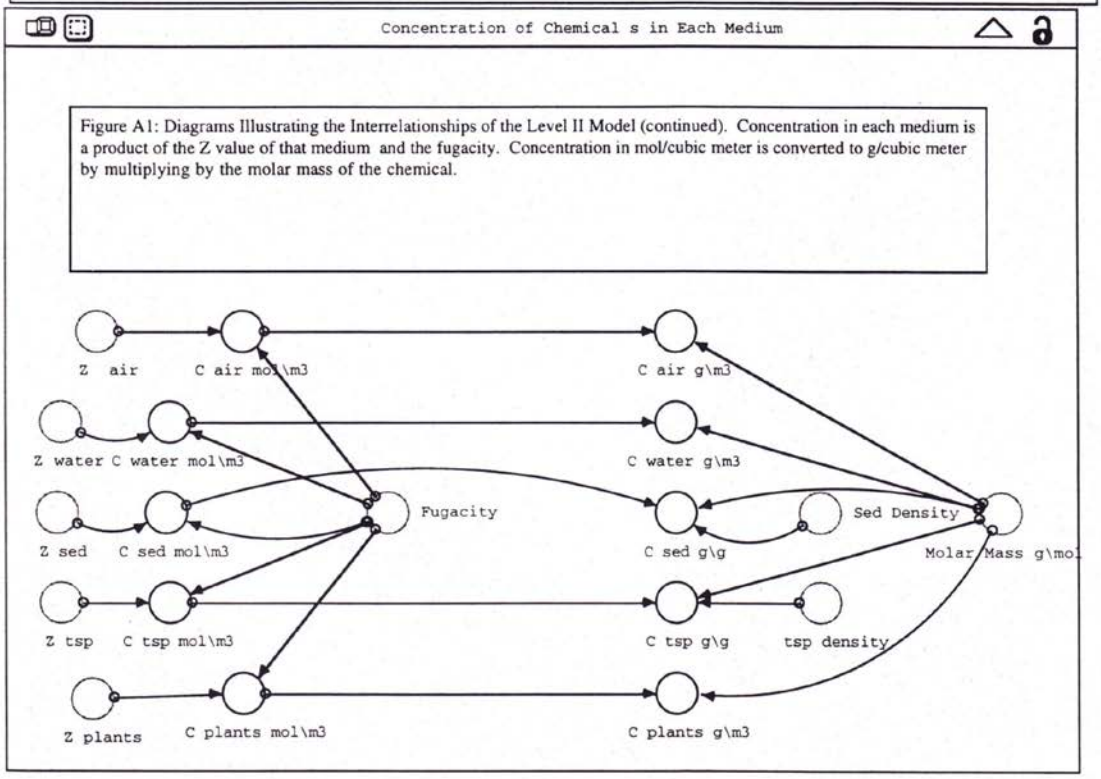
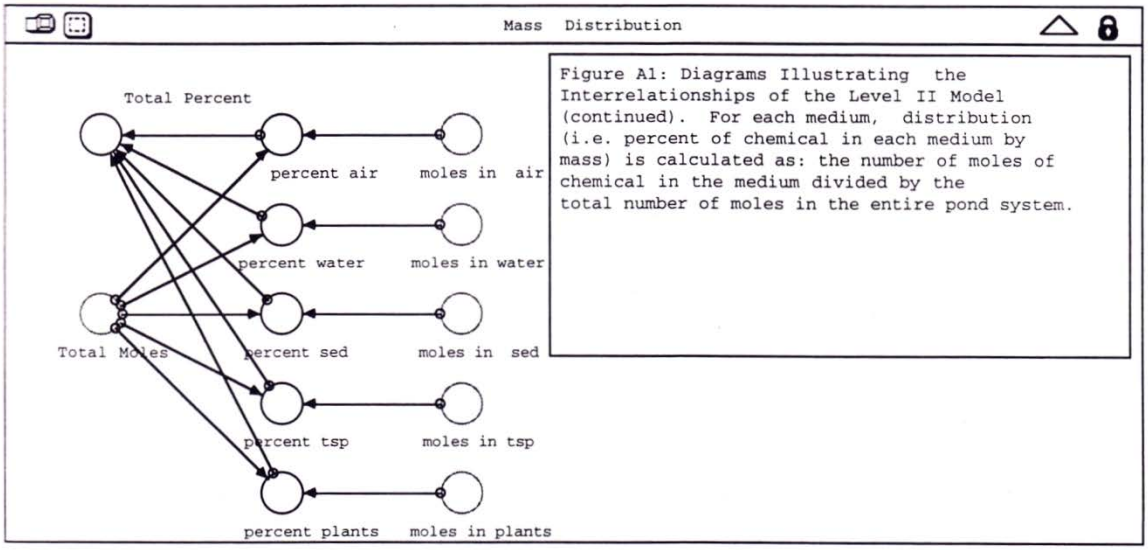
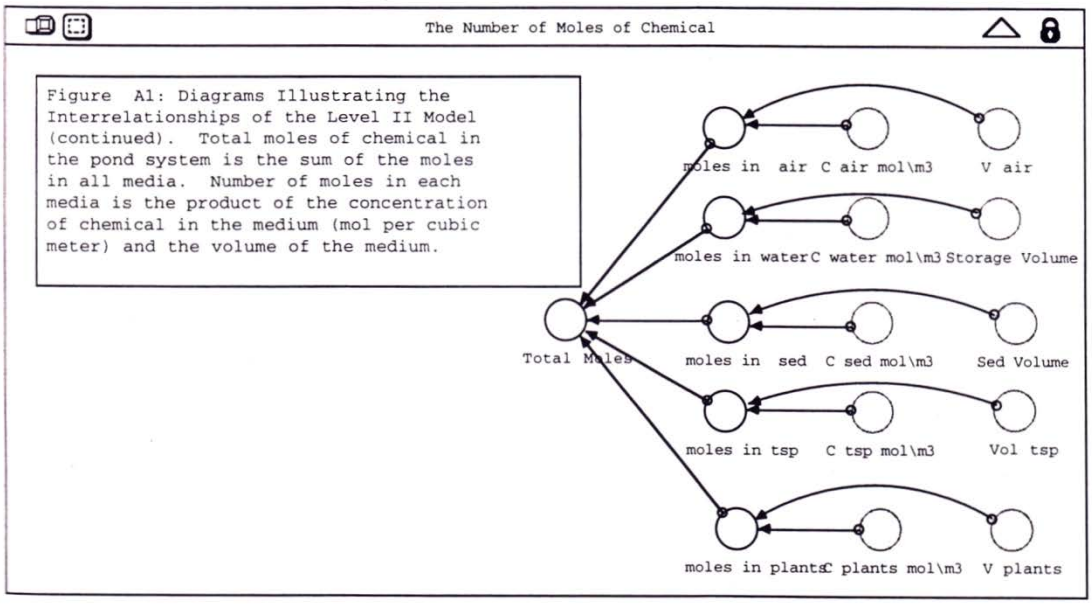




Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued). Concentration in each medium is a product of the Z value of that medium and the fugacity. Concentration in mol/cubic meter is converted to g/cubic meter by multiplying by the molar mass of the chemical.


Mass Distribution
Total Percent
percent air
moles in air
percent water
moles in water
Total Moles
percent sed
moles in sed
percent tsp
moles in tsp
percent plants
moles in plants
Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued). For each medium, distribution (i.e. percent of chemical in each medium by mass) is calculated as: the number of moles of chemical in the medium divided by the total number of moles in the entire pond system.


The Number of Moles of Chemical
Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued). Total moles of chemical in the pond system is the sum of the moles in all media. Number of moles in each media is the product of the concentration of chemical in the medium (mol per cubic meter) and the volume of the medium.
moles in air
C air mol\m3
V air
moles in water
C water mol\m3
Storage Volume
Total Moles
moles in sed
C sed mol\m3
Sed Volume
moles in tsp
C tsp mol\m3
Vol tsp
moles in plants
C plants mol\m3
V plants

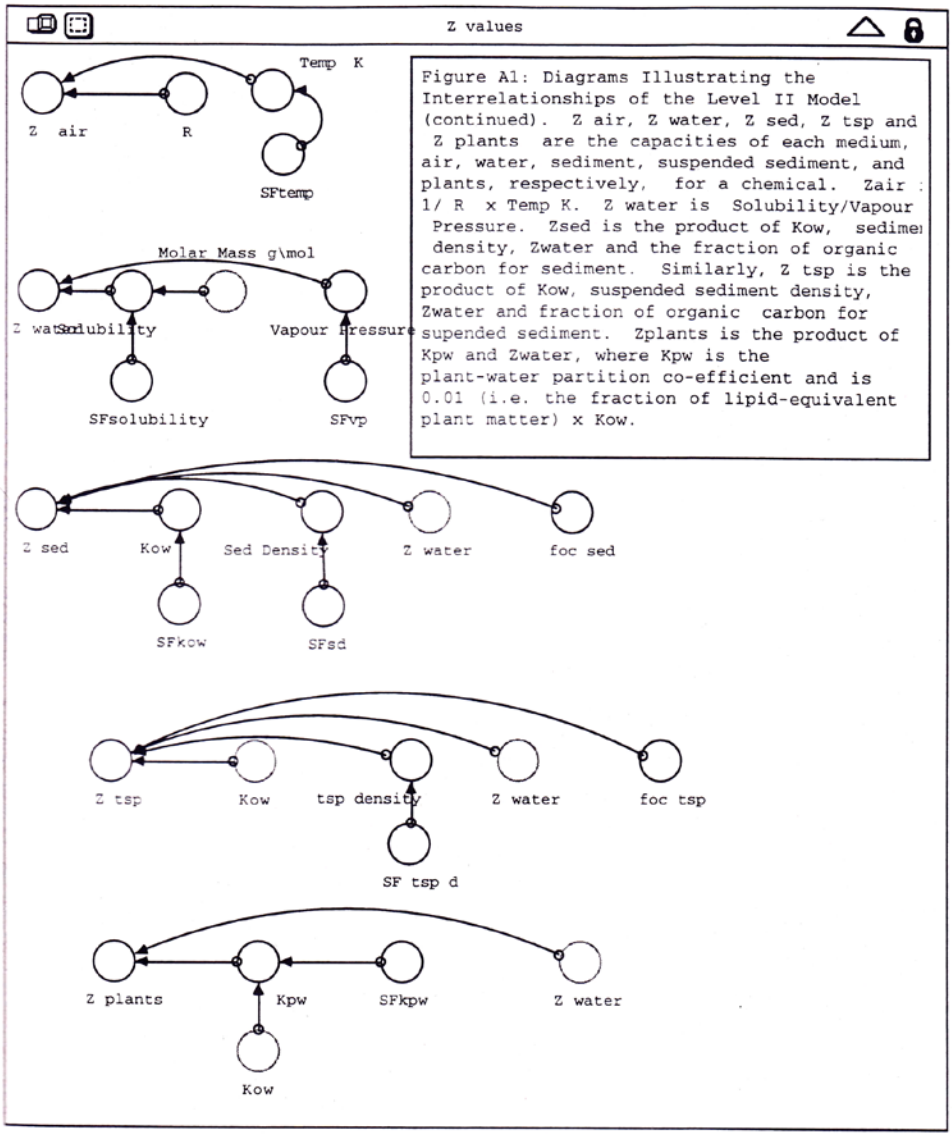
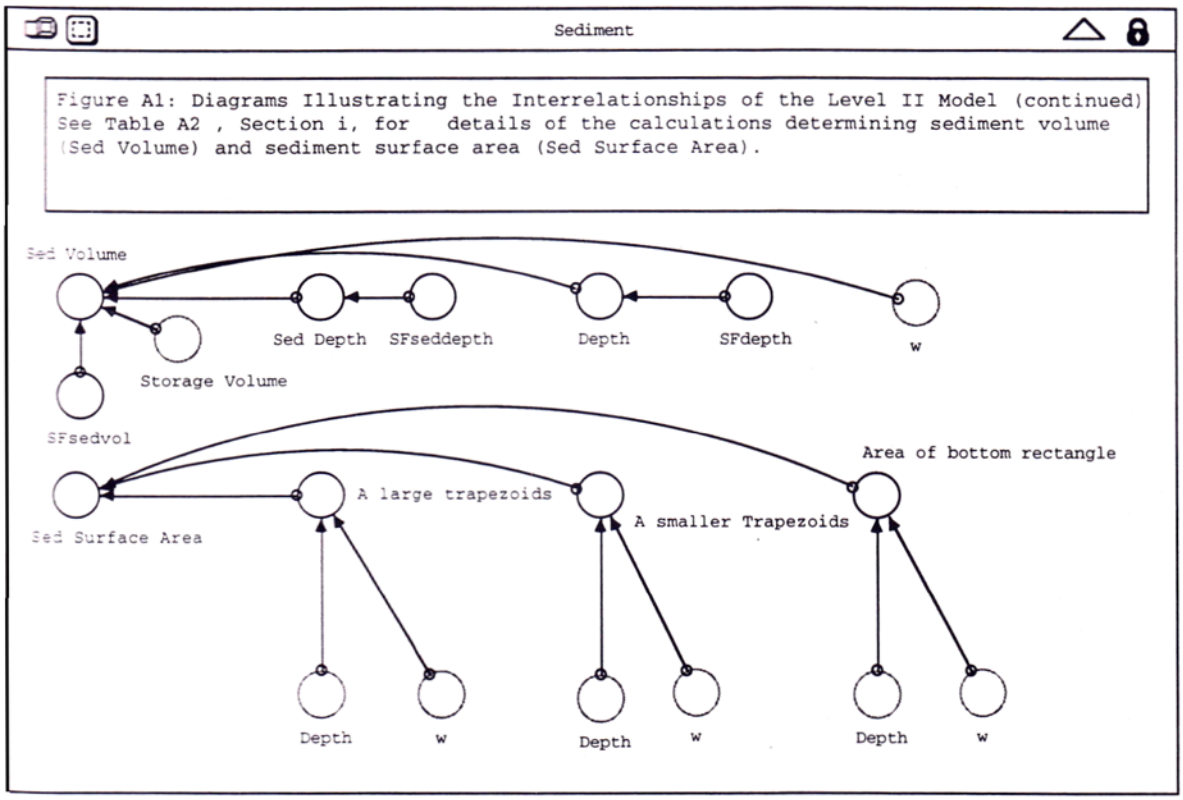



Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued). Z air, Z water, Z sed, Z tsp and Z plants are the capacities of each medium, air, water, sediment, suspended sediment, and plants, respectively, for a chemical. Zair = 1/ R x Temp K. Z water is Solubility/Vapour Pressure. Zsed is the product of Kow, sedimen density, Zwater and the fraction of organic carbon for sediment. Similarly, Z tsp is the product of Kow, suspended sediment density, Zwater and fraction of organic carbon for supended sediment. Zplants is the product of Kpw and Zwater, where Kpw is the plant-water partition co-efficient and is 0.01 (i.e. the fraction of lipid-equivalent plant matter) x Kow.


Sediment
Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued)
See Table A2 , Section i, for details of the calculations determining sediment volume
(Sed Volume) and sediment surface area (Sed Surface Area).
Sed Volume
Sed Depth
SFseddepth
Depth
SFdepth
w
Storage Volume
SFsedvol
Area of bottom rectangle
A large trapezoids
A smaller Trapezoids
Sed Surface Area
Depth
w
Depth
w
Depth
w

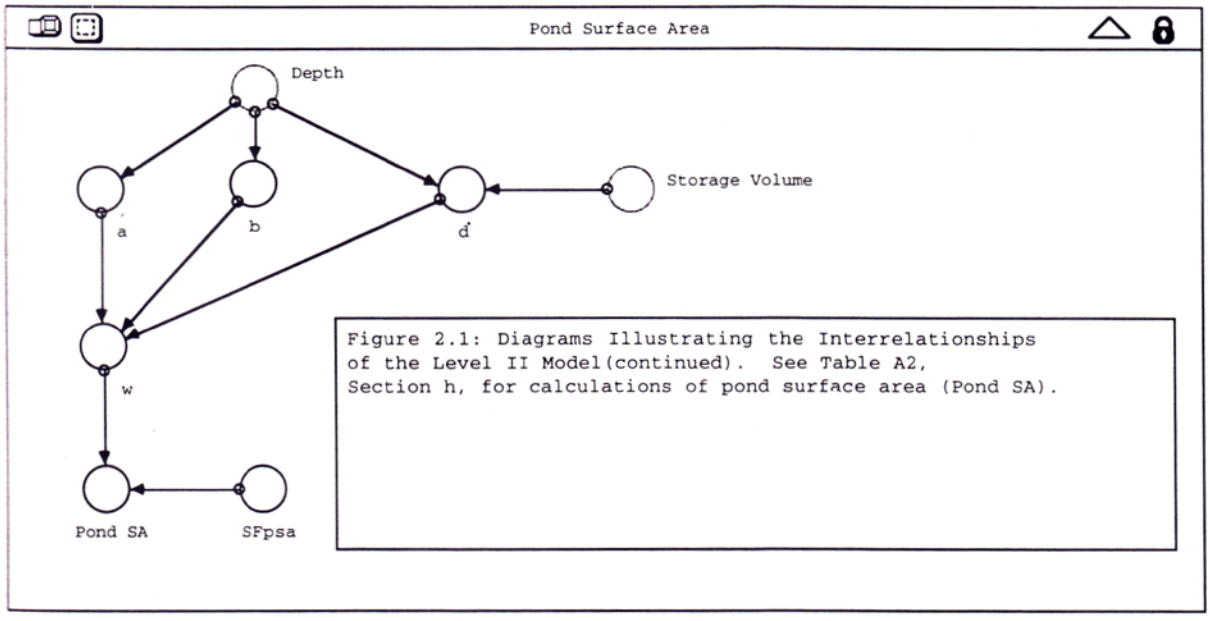

Pond Surface Area
Depth
Storage Volume
a
b
d
w
Pond SA
SFpsa
Figure 2.1: Diagrams Illustrating the Interrelationships
of the Level II Model(continued). See Table A2,
Section h, for calculations of pond surface area (Pond SA).

Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued). Storage volume is the product of catchment area and volume of water required per hectare of catchment (vol per ha). Vol per ha is dependent on the level of environmental protection (Level) and the percent imperviousness of the catchment (Imperviousness). See Table A2, Section 1 for complete calculations.

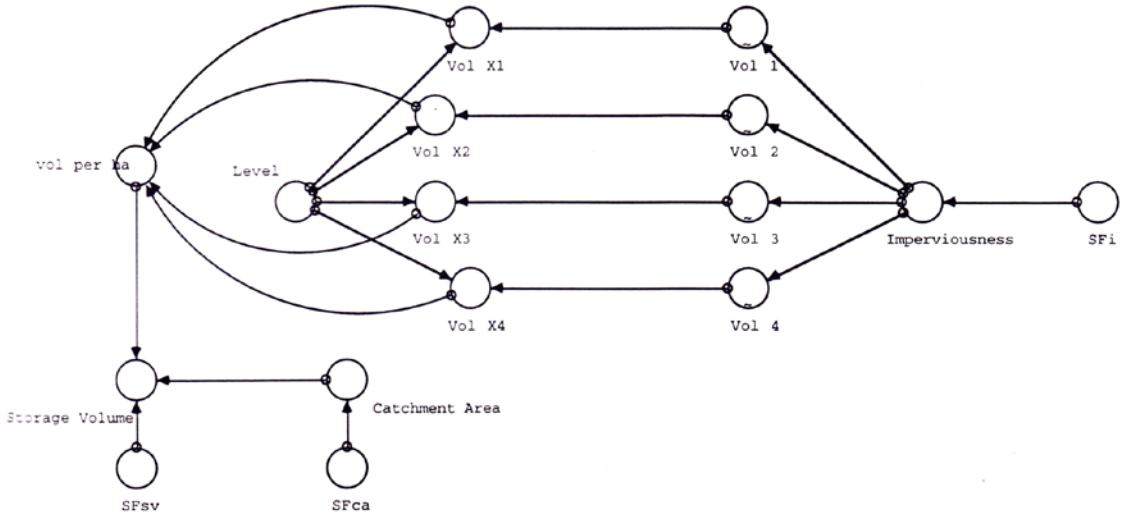


Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued). Volume of air (V air) is the product of pond surface area (Pond SA) and atmospheric height (Atmos Height).

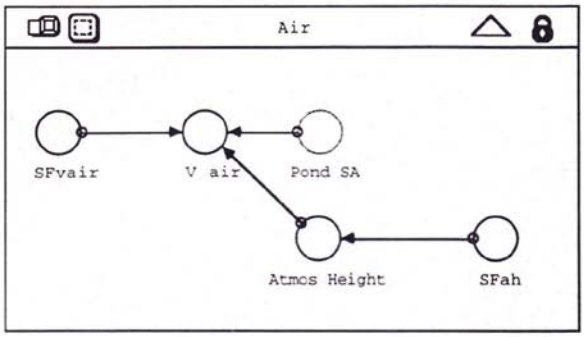



Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued). Plant volume (V plants) is the total plant biomass in the stormwater pond divided by the density of plant matter (Plant Density). Total plant biomass (Total Biomass kg) is the product of the plant biomass per square meter (Biomass kg\ Sq Meter) and the sediment surface area (Sed Surface Area).

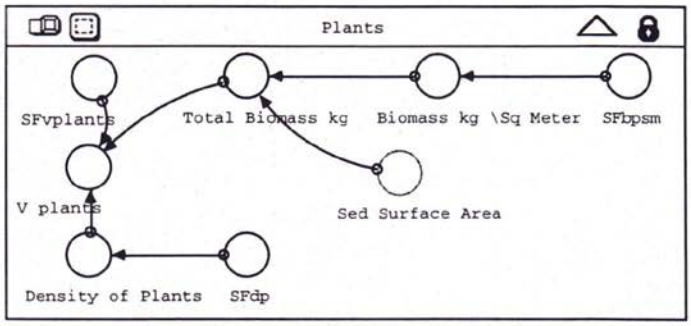



Figure A1: Diagrams Illustrating the Interrelationships of the Level II Model (continued). Volume of suspended sediment (Vol tsp) is suspended sediment concentration in the stormwater pond (tsp concentration) divided by suspended sediment density (tsp density) multiplied by the volume of water in the pond (Storgae Volume).

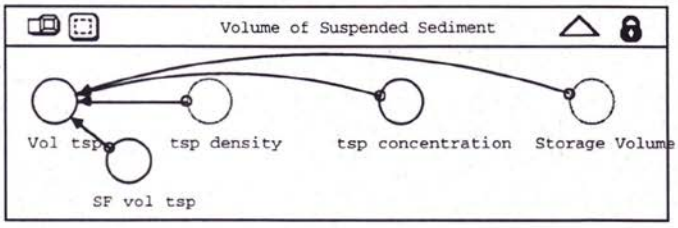


*Table A2: List of Parameters and Input Equations Used in the Level II Fugacity Model*

| | |
|---|---|
| **a. <u>Air Volume</u>**<br>Atmos_Height (m) = 500 m x SFah<br>V_air ($m^3$) = (Pond_SA ($m^2$) x Atmos_Height (m)) x Sfvair<br><br>SFah = 1<br>SFvair = 1 | **<u>Comments</u>** (Refer to Section 2.2: Modeling Parameters)<br><br>Atmos_Height<br>V_air |
| **b. <u>Concentration of Chemical in Each Medium</u>**<br>C_air ($g/m^3$) = C_air ($mol/m^3$) x Molar_Mass (g/mol)<br>C_air ($mol/m^3$) = Z_air ($mol/m^3Pa$) x Fugacity (Pa)<br>C_plants ($g/m^3$) = C_plants ($mol/m^3$) x Molar_Mass (g/mol)<br>C_plants ($mol/m^3$) = Z_plants ($mol/m^3Pa$) x Fugacity (Pa)<br>C_sed (g/g sed) = C_sed ($mol/m^3$) x Molar_Mass (g/mol) x (1/Sed_Density (kg/L)) x (1kg/1000g) x ($1m^3$/1000L)<br>C_sed ($mol/m^3$) = Z_sed ($mol/m^3Pa$) x Fugacity (Pa)<br>C_tsp (g/g tsp) = (C_tsp_$mol/m^3$) x (Molar_Mass_g/mol) x (1/tsp_density ) x (1/1000) x (1/1000)<br>C_tsp_$mol/m^3$ = Z_tsp ($mol/m^3Pa$) x Fugacity (Pa)<br>C_water_($g/m^3$) = C_water_$mol/m^3$ x Molar_Mass (g/mol)<br>C_water_$mol/m^3$ = Z_water ($mol/m^3Pa$) x Fugacity (Pa) | |

*Table A2: List of Parameters and Input Equations Used in the Level II Fugacity Model (continued)*

| | |
|---|---|
| **c. <u>D Values</u>**<br>D_advection_air (mol/Pa.h) = Gair x Z_air (mol/$m^3$Pa)<br>D_advection_water (mol/Pa.h) = Gwater x Z_water (mol/$m^3$Pa)<br>D_air_reaction (mol/Pa.h) = V_air x Z_air (mol/$m^3$Pa) x k_air ($h^{-1}$)<br>D_plants_reaction (mol/Pa.h) = V_plants x Z_plants (mol/$m^3$Pa) x k_plants ($h^{-1}$)<br>D_sed_reaction (mol/Pa.h) = Sed_Volume x Z_sed (mol/$m^3$Pa) x k_sed ($h^{-1}$)<br>D_tsp_reaction (mol/Pa.h) = Vol_tsp x Z_tsp (mol/$m^3$Pa) x k_tsp ($h^{-1}$)<br>D_water_reaction (mol/Pa.h) = Storage_Volume x Z_water (mol/$m^3$Pa) x k_water ($h^{-1}$)<br><br>Sum_of_D (mol/Pa.h) = (D_advection_air) + (D_advection_water) + (D_air_reaction) + (D_plants_reaction) + (D_sed_reaction) + (D_water_reaction) | |
| **d. <u>Calculation of Reaction Rates (k values)</u>**<br>k_air ($h^{-1}$)= (Ln2/$t_{1/2a}$) x SFkair<br>k_plants ($h^{-1}$) = (Ln2/$t_{1/2p}$) x SFkplants<br>k_sed ($h^{-1}$)= (Ln2/$t_{1/2s}$) x SFksed<br>k_tsp ($h^{-1}$) = (Ln2/$t_{1/2t}$) x SFktsp<br>k_water ($h^{-1}$)= (Ln2/$t_{1/2w}$) x Sfkwater<br><br>SFkair = 1<br>SFkplants = 1<br>SFksed = 1<br>SFktsp = 1<br>SFkwater = 1 | k = reaction rate of chemical in respective median (e.g. plants, sediment, etc.)<br>$t_{1/2}$ = half-life of chemical in respective median (e.g. $t_{1/2a}$ = half-life in air) (See *Table 2.2*) |

*Table A2: List of Parameters and Input Equations Used in the Level II Fugacity Model (continued)*

| | |
|---|---|
| **e. <u>Fugacity Function</u>**<br>Cbgair (mol/$m^3$) = (? /Molar_Mass (g/mol)) x SFcba<br>Cbgwater (mol/$m^3$)= (Concentration (g/$m^3$)/Molar_Mass (g/mol)) x SFcbgw<br>Emission_Rate (mol/h)= 0 x SFer<br>Fugacity (Pa)= Input_of_Chemical (mol/h)/Sum_of_D (mol/Pa.h)<br>Gair ($m^3$/hr) = 7920 ($m^3$/hr) x SFga<br>Gwater ($m^3$/hr) = 44136 ($m^3$/hr) x SFgw<br>Nair (mol/h) = Gair ($m^3$/hr) x Cbgair (mol/$m^3$)<br>Nwater (mol/h) = Gwater ($m^3$/hr) x Cbgwater (mol/$m^3$)<br>Input_of_Chemical (mol/h) = Emission_Rate (mol/h)+ Nair (mol/h) + Nwater (mol/h)<br>Molar_Mass (g/mol) = ?<br><br>SFcba = 1<br>SFcbgw = 1<br>SFer = 1<br>SFga = 1<br>SFgw = 1 | Cbgair; ? is background air concentration (g/$m^3$) which differs for each chemical<br>Cbgwater is the background water concentration which differs for each chemical.<br>Emission_Rate=direct input of chemical into the system<br><br>Gair is the rate of air movement through the atmosphere above the stormwater pond. The value of 7920 $m^3$/hr was derived from MOEE (1994)<br><br>Gwater is the rate of water flow through the stormwater pond. 44136 m3/h is the rate of inflow which was taken from Neighbourhood 5-D (CPWL,1995).<br><br>Nair and Nwater is the rate of chemical input in air and water, respectively.<br>Molar Mass is the molar mass of the chemical contaminant in question (See *Table 2.0*).<br>It was assumed that the input of water flow into the pond equals the output of water from the pond. |

*Table A2: List of Parameters and Input Equations Used in the Level II Fugacity Model (continued)*

| | |
|---|---|
| **f. <u>Percentage Distribution of Chemical in Each Medium</u>**<br>percent_air = moles_in_air/Total_Moles x 100<br>percent_plants = moles_in_plants/Total_Moles x 100<br>percent_sed = moles_in_sed/Total_Moles x 100<br>percent_tsp = moles_in_tsp/Total_Moles x 100<br>percent_water = moles_in_water/Total_Moles x 100<br><br>Total_Percent = percent_air + percent_plants + percent_sed + percent_water + percent_tsp | |
| **g. <u>Plants</u>**<br>Biomass ($kg/m^2$) = (3 $kg/m^2$) x SFbpsm<br>Density_of_Plants (kg/m3) = 1000 (kg/m3) x SFdp<br>Total_Biomass (kg) = Biomass_($kg_/m^2$) x Sed_Surface_Area ($m^2$)<br>V_plants ($m^3$)= (Total_Biomass (kg) /Density_of_Plants ($kg/m^3$)) x Sfvplants<br><br>SFbpsm = 1<br>SFdp = 1<br>SFvplants = 1 | V_plants is the volume of plant/detritus matter. |
| **h. <u>Pond Surface Area</u>**<br>a = 5 x Depth (m)<br>b = -24 x (Depth (m))$^2$<br>d = 64/3 x (Depth (m))$^3$-Storage_Volume ($m^3$)<br>w (m) = (-b+(SQRT($b^2$-4x a x d)))/(2 x a)<br>Pond_SA ($m^2$)= (5 x w x w) x Sfpsa<br><br>SFpsa = 1 | a, b, and d are constants from the Quadratic Formula and are used to interrelate Storage Volume, water depth (Depth), Pond Surface Area (Pond_SA), pond length to width ratio (i.e. 5:1; width = w and length =5w), and a slope of the sides of the pond of 1:4. This allows the modeler to change some parameters without needing to recalculate others. |

*Table A2: List of Parameters and Input Equations Used in the Level II Fugacity Model (continued)*

| | |
|---|---|
| **i. <u>Sediment</u>**<br>Area_of_bottom_rectangle ($m^2$) = (5 x w-8 x Depth (m) x w-8 x Depth (m))<br>Area_large_trapezoids = Depth (m)x SQRT(17) x (5 x w - 4 x Depth (m))<br>Area_smaller_Trapezoids = Depth (m) x SQRT(17) x (w - 4 x Depth (m))<br>Depth (m) = 2.0 m x SFdepth<br>Sed_Depth (m) = 0.10 m x SFseddepth<br>Sed_Surface_Area ($m^2$) = Area_of_bottom_rectangle ($m^2$) + Area_large_trapezoids ($m^2$) + Area_smaller_Trapezoids ($m^2$)<br>Sed_Volume ($m^3$) = (4 x (Sed_Depth (m)+Depth (m)) x (1/3 x ((-4 x Depth (m))$^2$)-(6 x w (m) x Depth (m))+1.25 x $w^2$ ($m^2$))-Storage_Volume ($m^3$)) x Sfsedvol<br><br>SFdepth (m) = 1<br>SFseddepth (m) = 1<br>SFsedvol = 1 | Since the pond was assumed to be a hexahedron. To calculate the surface area, the surface area was broken down into two larger trapezoids, two smaller trapezoids and a rectangle at the bottom of the pond.<br><br>Sed_Volume is the volume of sediment. |
| **j. <u>The Number of Moles of Chemical</u>**<br>moles_in_plants = C_plants (mol/$m^3$) x V_plants ($m^3$)<br>moles_in_tsp = C_tsp (mol/$m^3$ )x Vol_tsp ($m^3$)<br>moles_in_water = C_water_(mol/$m^3$) x Storage_Volume ($m^3$)<br>moles_in_air = C_air (mol/$m^3$) x V_air ($m^3$)<br>moles_in_sed = C_sed (mol/$m^3$) x Sed_Volume ($m^3$)<br><br>Total_Moles = moles_in_air + moles_in_plants + moles_in_sed + moles_in_water + moles_in_tsp | |
| **k. <u>Volume of TSP</u>**<br>tsp_concentration = 50 (mg/L) x (1kg/1000000mg)<br>Vol_tsp ($m^3$)= (tsp_concentration (kg/L) /tsp_density(kg/L) x Storage_Volume ($m^3$) x SF_vol_tsp<br><br>SF_vol_tsp = 1 | tsp_concentration = the concentration of suspended sediment. |

*Table A2: List of Parameters and Input Equations Used in the Level II Fugacity Model (continued)*

| | |
|---|---|
| **I. <u>Volume of Water (Storage Volume)</u>**<br>Catchment_Area (ha) = 62 (ha) x SFca<br>Imperviousness = 0.35 x Sfi<br>Level = 2<br>Storage_Volume ($m^3$) = (vol_per_ha ($m^3$/ha) x Catchment_Area (ha)) x Sfsv<br><br>vol_per_ha ($m^3$/ha) = Vol_ x1 + Vol_ x2 + Vol_ x3 + Vol_ x4<br><br>Vol_ x1 = IF(Level=1) THEN(Vol_1) ELSE(0)<br>Vol_ x2 = IF(Level=2) THEN(Vol_2) ELSE(0)<br>Vol_ x3 = IF(Level=3) THEN(Vol_3) ELSE(0)<br>Vol_ x4 = IF(Level=4) THEN(Vol_4) ELSE(0)<br><br>Vol_1 = GRAPH(Imperviousness)<br>(0.00, 1.25), (0.05, 21.2), (0.1, 41.2), (0.15, 60.0), (0.2, 80.0), (0.25, 100), (0.3, 119), (0.35, 140), (0.4, 151), (0.45, 164), (0.5, 176), (0.55, 190), (0.6, 201), (0.65, 212), (0.7, 224), (0.75, 232), (0.8, 242), (0.85, 250), (0.9, 260), (0.95, 273), (1.00, 280)<br>Vol_2 = GRAPH(Imperviousness)<br>(0.00, 1.25), (0.05, 13.8), (0.1, 25.0), (0.15, 36.2), (0.2, 50.0), (0.25, 61.2), (0.3, 75.0), (0.35, 90.0), (0.4, 95.0), (0.45, 100), (0.5, 105), (0.55, 110), (0.6, 118), (0.65, 122), (0.7, 130), (0.75, 135), (0.8, 141), (0.85, 150), (0.9, 158), (0.95, 164), (1.00, 171)<br>Vol_3 = GRAPH(Imperviousness)<br>(0.00, 0.00), (0.05, 9.00), (0.1, 18.0), (0.15, 25.5), (0.2, 31.5), (0.25, 42.0), (0.3, 51.0), (0.35, 60.0), (0.4, 66.0), (0.45, 69.0), (0.5, 73.5), (0.55, 75.0), (0.6, 79.5), (0.65, 82.5), (0.7, 85.0), (0.75, 88.5), (0.8, 91.5), (0.85, 95.0), (0.9, 100), (0.95, 105), (1.00, 108)<br>Vol_4 = GRAPH(Imperviousness)<br>(0.00, 0.00), (0.05, 10.0), (0.1, 18.8), (0.15, 30.0), (0.2, 38.8), (0.25, 46.2), (0.3, 52.5), (0.35, 60.0), (0.4, 60.0), (0.45, 60.0), (0.5, 60.0), (0.55, 60.0), (0.6, 60.0), (0.65, 60.0), (0.7, 60.0), (0.75, 60.0), (0.8, 60.0), (0.85, 65.0), (0.9, 65.0), (0.95, 65.0), (1.00, 65.0)<br><br>SFca = 1<br>SFi = 1<br>SFsv = 1 | vol_per_ha ($m^3$/ha) calculates the required storage volume for each hectare of catchment area and for desired protection level (See *Table 2.1*)<br><br>Vol_ x = GRAPH(Imperviousness) creates a function where (x, y) are points along a curve which related "a required volume per ha of catchment to percent imperviousness" (see *Table 2.3; MOEE, 1994*).<br><br>MOEE (1994) guidelines for stormwater ponds are for catchment sizes between 5 and 100 hectares. |

*Table A2: List of Parameters and Input Equations Used in the Level II Fugacity Model (continued)*

| | |
|---|---|
| **m. <u>Z values</u>**<br>foc_sed = 0.05<br>foc_tsp = 0.17<br>Kow = (Kow?) x Sfkow<br>$K_{PW}$ = (0.01x $K_{OW}$) x SFkpw<br>R = 8.314 Pa.$m^3$/mol.K<br>Sed_Density = (1.5 kg/L) x Sfsd<br>Solubility = (?)/ Molar_Mass x SFsolubility<br>Temp (K) = 298 (K) x SFtemp<br>tsp_density = (1.5 kg/L) x SF_tsp_d<br>Vapour_Pressure = (?) x SFvp<br><br>Z_air = 1/(R (Pa.$m^3$/mol.K) x Temp(K))<br>Z_plants = Kpwx Z_water (mol/$m^3$Pa)<br>Z_sed = Sed_Density (kg/L) x 0.41 (L/kg) x Kow x Z_water (mol/$m^3$Pa) x foc_sed<br>Z_tsp = tsp_density (kg/L) x 0.41 (L/kg) x Kow x Z_water (mol/$m^3$Pa) x foc_tsp<br>Z_water (mol/$m^3$Pa) = Solubility (mol/m3)/Vapour_Pressure (Pa) x SFkow = 1<br><br>SFkpw = 1<br>SFsd = 1<br>SFsolubility = 1<br>SFtemp = 1<br>SFvp = 1<br>SFtsp_d = 1 | Temp_K was either 274K (1$^{o}$C) or 298K (25 $^{o}$C)<br><br>Fraction of organic carbon (foc) in sediment and suspended sediment were 0.05 and 0.17 based on Mackay (1991). Octanol equivalent matter in plants was set at 0.01 based on Mackay (1991) and Paterson *et al.* (1991).<br><br>Kow? represents the Kow of a specific chemical.<br><br>Z values describe the capacity a medium has for a specific chemical<br><br>Temp (K) = the temperature in Kelvin<br><br>"?" indicates chemical specific data |

*Table A3: Sizes of The Five Media. Air is the largest medium, followed by water, sediment and plants. Suspended sediment is the smallest medium. See* Table A2 *and for a detailed description of how these volumes were calculated, including the assumptions that were made.*

| **<u>Media</u>** | **<u>Volume ($m^3$)</u>** |
|---|---|
| Air | 2.0 x $10^6$ |
| Water | 5580 |
| Sediment | 279 |
| Plants | 8.6 |
| Suspended Sediment | 0.19 |

*Table A4: Temperature Correction for Vapour Pressure and Solubility for Benzene and Toluene*

| Chem-ical | m.p. | b.p. | P | Solubility | Temp. | Phase | A | B | C |
|---|---|---|---|---|---|---|---|---|---|
| | ($^o$C) | ($^o$C) | (Pa 25 $^o$C) | (g/m3 25 $^o$C) | ($^o$C) | **(at Temp)** | | | |
| **benzene** | 5.53 | 80 | 12700 | 1780 | 1 | solid | 6.09[a] | 1204.65[a] | 220.079[a] |
| **toluene** | -95 | 111 | 3800 | 515 | 1 | liquid | 6.38[a] | 1575.01[a] | 249.37[a] |

| Chem-ical | P | P | Fugacity | P at temp | P used | Solubility | Solubility** | Sol. used |
|---|---|---|---|---|---|---|---|---|
| | (mmHg) at Temp. | (Pa) at Temp | **Ratio** (F) | (Pa) | (Pa) | (g/m3) at Temp | (g/m3) at Temp | (g/m3) |
| **benzene** | 4.38 | 583.79 | 0.89 | 521.80 | 521.80 | 1249.92 | | 1117.19 |
| **toluene** | 1.23 | 163.73 | N/A* | N/A | 163.73 | 361.63 | N/A | 361.63 |

*Sources for Antoine's Constants: Boublík, 1984*
**N/A because toluene is a liquid at this temperature so one does not need to convert solid liquid vp to solid vp*
***Solubility, Phase Corrected*

*Table A5: Temperature Corrections for Vapour Pressure and Solubility for HCB*

| Chemical: | m.p. | b.p. | P | Solubility | Temp K | Phase | |
|---|---|---|---|---|---|---|---|
| **HCB** | $^o$C | $^o$C | (Pa) 25 $^o$C | g/m3 25 $^o$C | | (at Temp.) | |
| | 230 | 322 | 0.0023 | 0.005 | 274 | solid | |
| **Log P** | **P** | **Fugacity** | **P used** | **Log S** | **Solubility** | **Solubility** | **Sol. used** |
| | (Pa) | **Ratio** | (Pa) | | (mol/m$^3$) | (mol/m$^3$) | (g/m3) |
| -3.91 | $1.23 \times 10^{-4}$ | 0.00343 | $4.23 \times 10^{-7}$ | -4.54 | $2.87 \times 10^{-5}$ | $9.86 \times 10^{-8}$ | $2.81 \times 10^{-5}$ |

*Table A6: D values and Fugacity of Chemicals, Warm and Cold Runs*

| | D values (mol/Pa.h) | | | | | | | Fugacity (Pa) |
|---|---|---|---|---|---|---|---|---|
| **Chemical** | **Air advection** | **Water advection** | **Air reaction** | **Plants reaction** | **Sed. reaction** | **TSP. reaction** | **Water reaction** | **f** |
| **Benzene warm** | 3.20 | $7.92 \times 10^{1}$ | $1.12 \times 10^{2}$ | $5.15 \times 10^{-6}$ | $3.00 \times 10^{-2}$ | $6.78 \times 10^{-4}$ | 1.44 | $2.38 \times 10^{-2}$ |
| **Benzene cold** | 3.48 | $1.21 \times 10^{3}$ | 1.24 | $1.37 \times 10^{-5}$ | $2.51 \times 10^{-3}$ | $1.30 \times 10^{-4}$ | $2.76 \times 10^{-1}$ | $3.84 \times 10^{-3}$ |
| **Toluene warm** | 3.20 | $6.49 \times 10^{1}$ | $2.38 \times 10^{2}$ | 0 | $8.93 \times 10^{-2}$ | $1.94 \times 10^{-3}$ | 1.14 | $1.64 \times 10^{-2}$ |
| **Toluene cold** | 3.48 | $1.06 \times 10^{3}$ | 5.96 | 0 | $1.32 \times 10^{-1}$ | $3.00 \times 10^{-4}$ | $1.76 \times 10^{-1}$ | $4.72 \times 10^{-3}$ |
| **HCB warm** | 3.20 | $1.78 \times 10^{3}$ | $1.59 \times 10^{-1}$ | 3.81 | 3.26 | $7.40 \times 10^{-3}$ | $6.71 \times 10^{-3}$ | $5.32 \times 10^{-8}$ |

Table A7 (a to j): Sensitivity Analysis Results

**a. Concentration**

| SF kplants | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 1000 | 0.32 | 0.32 | 0.32 | 0.32 | 0.32 |
| benzene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

**Percent Distribution**

| SF k plants | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

**b. Concentration**

| SF k sed | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 1000 | 0.36 | 0.36 | 0.36 | 0.36 | 0.36 |
| benzene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 1000 | 0.87 | 0.87 | 0.87 | 0.87 | 0.87 |
| toluene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 1000 | 0.77 | 0.77 | 0.77 | 0.77 | 0.77 |

**Percent Distribution**

| SF k sed | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

**c. Concentration**

| SF k air | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 1000 | 0.69 | 0.69 | 0.69 | 0.69 | 0.69 |
| benzene 0.001 | 2.33 | 2.33 | 2.33 | 2.33 | 2.33 |
| benzene 1000 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| toluene 0.001 | 4.41 | 4.41 | 4.41 | 4.41 | 4.41 |
| toluene 1000 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

**Percent Distribution**

| SF k air | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

**d. Concentration**

| SF k tsp | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

**Percent Distribution**

| SF k tsp | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

**e. Concentration**

| SF k water | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.001 | 1.01 | 1.01 | 1.01 | 1.01 | 1.01 |
| benzene 1000 | 0.12 | 0.12 | 0.12 | 0.12 | 0.12 |
| toluene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 1000 | 0.21 | 0.21 | 0.21 | 0.21 | 0.21 |

**Percent Distribution**

| SF k water | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.001 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 1000 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

f. Concentration

| SF sed vol | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

Percent Distribution

| SF sed vol | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.5 | 1.90 | 1.90 | 0.95 | 1.90 | 1.90 |
| HCB 2 | 0.51 | 0.51 | 1.03 | 0.51 | 0.51 |
| benzene 0.5 | 1.00 | 1.00 | 0.50 | 1.00 | 1.00 |
| benzene 2 | 1.00 | 1.00 | 2.00 | 1.00 | 1.00 |
| toluene 0.5 | 1.00 | 1.00 | 0.50 | 1.00 | 1.00 |
| toluene 2 | 0.99 | 0.99 | 1.99 | 0.99 | 0.99 |

g. Concentration

| SF v plants | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

Percent Distribution

| SF v plants | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.5 | 1.00 | 0.50 | 1.00 | 1.00 | 1.00 |
| HCB 2 | 0.99 | 1.98 | 0.99 | 0.99 | 0.99 |
| benzene 0.5 | 1.00 | 0.50 | 1.00 | 1.00 | 1.00 |
| benzene 2 | 1.00 | 2.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.5 | 1.00 | 0.50 | 1.00 | 1.00 | 1.00 |
| toluene 2 | 1.00 | 2.00 | 1.00 | 1.00 | 1.00 |

h. Concentration

| SF gw | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.5 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 |
| HCB 2 | 1.01 | 1.01 | 1.01 | 1.01 | 1.01 |
| benzene 0.5 | 0.63 | 0.63 | 0.63 | 0.63 | 0.63 |
| benzene 2 | 1.42 | 1.42 | 1.42 | 1.42 | 1.42 |
| toluene 0.5 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 |
| toluene 2 | 1.65 | 1.65 | 1.65 | 1.65 | 1.65 |

Percent Distribution

| SF gw | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

i. Concentration

| SF cbgw | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 |
| HCB 100 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| benzene 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 |
| benzene 100 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| toluene 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 |
| toluene 100 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |

Percent Distribution

| SF cbgw | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.01 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 100 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.01 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 100 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.01 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 100 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

j. Concentration

| SF vol tsp | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| HCB 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| benzene 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 0.5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| toluene 2 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

Percent Distribution

| SF vol tsp | Air | Plants | Sed. | TSP | Water |
|---|---|---|---|---|---|
| HCB 0.5 | 1.00 | 1.00 | 1.00 | 0.50 | 1.00 |
| HCB 2 | 1.00 | 1.00 | 1.00 | 2.00 | 1.00 |
| benzene 0.5 | 1.00 | 1.00 | 1.00 | 0.50 | 1.00 |
| benzene 2 | 1.00 | 1.00 | 1.00 | 2.00 | 1.00 |
| toluene 0.5 | 1.00 | 1.00 | 1.00 | 0.50 | 1.00 |
| toluene 2 | 1.00 | 1.00 | 1.00 | 2.00 | 1.00 |

*Table A8: Sensitivity Analysis Results. Decreases or increases are reported as percentage changes over the range of SF values. Sensitivity Runs were made with background air concentration equal to zero.*

**Reaction Rates**

**Concentration**

**k plants**

Benzene: decrease in all media, by <1%
Toluene: no change
HCB: Decreasing trend in all media: from SF = 0 to 1, by <1%; from SF = 1 to 1000, by approx. 68%

**k sed**

Decreasing in all media (all chemicals)
Benzene: from SF = 0 to 1, by <1%; from SF = 1 to 1000, by 13% for all media
Toluene: from SF = 0 to 1, by <1%; from SF = 1 to 1000, by 23% for all media
HCB: from SF = 0 to 1, by <1%; from SF = 1 to 1000, by 64% for all media

**k air**

Decreasing in all media (all chemicals)
Benzene: from SF = 0 to 1, by 133%; from SF = 1 to 1000, by 99.8% for all media.
Toluene: from SF = 0 to 1, by 342%; from SF = 1 to 1000, by 99.8% for all media.
HCB: from SF = 0 to 1, by <1%; from SF = 1 to 1000, by 31% for all media.

**k tsp**

No changes were observed for all chemicals in all media.

**k water**

Decreasing in all media (all chemicals)
Benzene: Decreases for all media. from SF = 0 to 1, by <1%; from SF = 1 to 1000, by 88%
Toluene: Decreases for all media. from SF = 0 to 1, by <1%; from SF = 1 to 1000, by 79%
HCB: from SF = 0 to 1, by <1%; from SF = 1 to 1000, by 0.04%

**Percent Distribution**

No changes were observed with changes in reaction rate (k) over a range of six orders of magnitude for all chemicals in all media.

*Table A8: Sensitivity Analysis Results (continued).*

**Media Volumes**

**Sediment Volume**

**Concentration**

Decreasing in all media (all chemicals)
Benzene: Decreases for all media. from SF = 0 to 2, by <1%
Toluene: Decreases for all media. from SF = 0 to 2, by <1%
HCB: Decreases for all media. from SF = 0 to 2, by <1%

**Percent Distribution**

Benzene and toluene showed increases in sediment which were proportional to increases in SF. They showed decreases in all other media which were <1%. HCB showed smaller increases in sediment: from SF = 0.25 to 2, 15%. For all other media: from SF = 0 to 1, decrease of 19.5 times; from SF = 1 to 2, a decrease of 49%.

**Plant Volume**

**Concentration**

Benzene and toluene showed no observed changes in concentration. HCB showed a decrease in all media <1%.

**Percent Distribution**

All chemicals showed a decrease in all media, except for plants, by <1%. For plants, all chemicals showed increases which were proportional to increases in SF.

**Volume of Suspended Sediment**

**Concentration**

Concentration did not vary with changing SF values for all chemicals and media.

**Percent Distribution**

For all chemicals, percent of chemical decreased in all media except for suspended sediment by <1%. Suspended sediment exhibited a proportional increase in chemical.

*Table A.8: Sensitivity Analysis Results (continued).*

| |
|---|
| **Rate of Water Inflow**<br>**Concentration**<br>Increasing the rate of water inflow increased the concentrations of chemicals in all media and for all chemicals.<br>Benzene: from SF = 0.25 to 1, by 64%; from SF = 1 to 2, by 42%.<br>Toluene: from SF = 0.25 to 1, by 70%, from SF = 1 to 2, by 65%<br>HCB: from SF = 0.25 to 1, by 4%; from SF = 1 to 2, by <1%.<br><br>**Percent Distribution**<br>No changes in percent distribution of chemical are associated with changing rates of water inflow for all chemicals and all media. |
| **Concentration in Water Inflow**<br>**Concentration**<br>Changes in background water concentration resulted in proportional changes in concentrations of chemical in every media for every chemical.<br><br>**Percent Distribution**<br>There were no observed changes in percent distribution resulting from changes in background concentration of water over a range of four orders of magnitude. |