

AN ABSTRACT OF THE THESIS OF

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Ian J. Tinsley

Abstract: In 1993 The Oregon Department of Environmental Quality developed a Cross-media Comparative Risk Assessment model to address certain regulatory concerns. Due to budget constraints the model was never beta tested. Now in 1995, the X-media project has been reopened, and the model revised, and tested. Specific revisions include: 1) Upgrade from a Level II to a Level III Fugacity Model, 2) Incorporation of compound specific Mass Transfer Coefficients and Molecular diffusities into the Level III Fugacity model 3) redefining the exposure factor from total compound amount to media specific concentrations 4) refinement of procedures for using the model and 5) conversion of the model from Oracle 7 to an Excel spreadsheet format. The model generates a Human and Ecological Risk Index for a facility releasing toxins into the environment. The Risk Indices are based on chemical fate and transport predictions, toxicity, population density and ecological sensitive areas. The model can be used to rank facilities for inspection or as a tool to assess the progress of pollution prevention programs. Regulatory permitting departments can use the model to address the cross-media transfer of pollutants from one environmental compartment to another. The versatility of the model allows adaptation to each specific users needs.

Assessing Cross-Media Impacts; A Comparative Risk Approach.

by

David S. Borys

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
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CONTRIBUTION OF AUTHORS

Regina D. Skarzinskas, MPH was involved in the design, analysis, and editing of each manuscript. Lynn Green assisted in model design and data analysis.

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Chapter 1

Assessing Cross-Media Impacts; A Comparative Risk Approach

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INTRODUCTION

Problem Definition

To update the current Oregon Department of Environmental Quality Cross-Media Comparative Risk Assessment model to better address environmental concerns and perform Beta testing to ensure the accuracy and usefulness of the model.

Background

In 1991 the Department Of Environmental Quality (DEQ) was awarded a grant from the US Environmental Protection Agency (EPA) to develop a methodology for incorporating cross-media risk assessment considerations into agency programs. These programs traditionally have been focused on single-media concerns in air pollution, water pollution, or waste management. The three main foci of the project were: to ensure cross media coordination within DEQ, to develop a methodology for performing cross-media risk analysis and to develop a more integrated approach to problem solving that enhances the DEQ's goal of pollution prevention.

After reviewing the models available, project staff determined that there were no suitable models in use and no one was addressing true cross-media impacts. Further

selective reviews of several approaches focused on a suitable prototype to answer the questions posed by the project.

A quantitative comparative risk approach developed by Dr. Gerald Carney at EPA Region VI (Carney, 1992) was selected as the prototype for the cross-media model for three reasons: 1) Carney's model addressed almost all of the needs of the project with the exception of cross-media impacts of pollutants but allowed for the modification of the original format for such a model to be easily included. 2) A Fugacity Model developed by Dr. Donald MacKay was selected to address the cross-media transfer of pollutants. 3) The flexible structure of Carney's approach allowed for the incorporation of fate and transport modeling within the developed structure of comparative risk. The resulting model was a cross-media comparative risk model.

The Oregon Department of Environmental Quality Cross-Media Comparative Risk Assessment Model (X-Media) incorporates the Fugacity Model, as a predictor of the cross media transfer of chemicals in the environment, within the Carney Comparative risk methodology. The model calculates a Human Risk Index (HRI) and an Ecological Risk Index (ERI) (Bridwell, 1993). A HRI is determined by the amount of a toxin present in a specific media, its corresponding toxicity, the degree of vulnerability associated with populations at high risk and the population density living within a four mile radius surrounding a facility. This area is essentially a cylinder defined by a four-mile radius surrounding a facility, and 1000 meters high. An ERI takes into account Sensitive Environments within the defined study area (e.g. wild life refuge, National Forest, etc....),

a chemical's persistence in the environment and its corresponding toxicity. The methodology employed by the X-media model is sound and the process is quick. The X-Media model is not meant to replace the need for detailed Risk Assessments but only to be used as a tool to aid in decision making.

Inclusion of X-media model data can aid in certain regulatory decision making processes. An example of this approach is the Facility Inspection Ranking System (FIRS) developed as a modification of the DEQ X-media model where HRI and ERI values represent potential chemical toxicity. Five facility specific criteria, including the HRI, are used to rank those facilities posing the greatest risk to human health. The flexibility of the X-media methodology allows the model to be adapted to individual needs or concerns such as modifying the study area to account for sensitive populations living close to the source of pollution. Additional criteria can easily be added to the existing ranking system to account for specific enforcement issues which could include the economic factors of replacing machinery to reduce the amount of toxins released into the environment.

Another example of the versatility of the model is its adaptation to DEQ Pollution Prevention Programs (P2). Often lacking in P2 programs is a methodology by which progress can be effectively evaluated. Can it be assumed that if a facility has reduced its releases that its pollution prevention program is working? The X-media model, through the risk indices provides a methodology by which the progress of pollution prevention programs can be quantitatively represented.

In response to the White House's 25 Top Priorities, 'reinventing environmental protection for the 21st century' (Clinton and Gore, 1995), agenda regarding improvements of existing regulatory systems to facilitate a better environmental management system, EPA is currently consulting environmental scientists to find or develop a tool which can characterize the potential risks associated with impacts from industrial chemicals on ecosystems, on air quality, on surface and below surface conditions, and human and animal populations (USEPA Work Statement). Six models have been chosen for further review. Among the top six of those being considered is the Oregon Department of Environmental Quality (DEQ) Comparative Cross-Media Risk Assessment Model (X-Media). With emphasis being placed on the impacts of the cross-media transfer of pollutants and measuring overall reduction in toxic effects, the X-media model has scored high in the initial screening of the models.

The EPA recently selected DEQ's X-media model as one of six to be incorporated on the EPA's mainframe for further testing. One model will eventually be selected as part of the EPA's methodology for enforcement targeting.

The X-Media model was completed in 1993 but due to lack of time and sufficient funds the model was never Beta tested. In 1994, through Ian Tinsley, I (Dave Borys) was introduced to Regina Bridwell and the X-Media model. As a Graduate Thesis Project in Toxicology I proposed to test the model and make any modifications needed to enhance it. The proposal was accepted and I began working on the project in April of 1995. Several changes have been made to the original version of the X-media model including: 1) Upgrade from a Level II to a Level III Fugacity Model, 2) Incorporation of compound

specific mass transfer coefficients and molecular diffusivities into the Level III Fugacity Model 3) redefinition of the exposure factor from total compound amount to media specific concentrations, 4) refinement of procedures for using the model and 5) conversion of the model from Oracle 7 to an Excel spreadsheet format. Throughout the rest of this paper I will be describing the old version of the X-media model and the changes I have made to it along with specific uses for the model.

FUGACITY MODEL

The X-Media model incorporates two important principles currently at the forefront of environmental decision making. A comparative risk approach (USEPA, 1987) for evaluating environmental problems and fate and transport modeling to address the impacts posed by the cross-media transfer of pollutants. The latter being represented by Donald MacKay's fugacity Approach.

Definition

Fugacity is a concept introduced in 1901 by G.N. Lewis and is defined as a chemicals ability to leave a specific media. In 1981 Donald MacKay revisited the concept and made use of the fact that unlike the chemical potential, fugacity is inversely related to concentration. This makes the complex mathematical equations associated with environmental modeling much simpler. By defining a Fugacity Capacity (Z), the ability of

a chemical to stay in a specific media, a simple equation relating fugacity (f) and concentration(C) can be written as:

$$C=Zf.$$

Because MacKay has developed procedures by which Z values can be estimated for any given environmental compartment, equilibrium concentrations can be deduced using f as a common criterion of equilibrium.

Using this concept MacKay developed three separate Fugacity Models each increasing in complexity and predictive estimates of the environmental behavior of chemicals.(MacKay et al., 1986, 1991 and 1992) The level I Fugacity model defines a closed system in which only 5 compartments exist: air, water, soil, biota and sediment. Equilibrium is assumed to be instantaneous within and between compartments. No air or water flow is assumed, the system is closed to all external forces. A level I model allows a quick and easy method to get a rough estimate of the distribution of a chemical into the environment. It should be noted that this approach is overly simplistic and does not represent actual environmental conditions.

The level II Fugacity model goes one step farther in its predictability by defining an open system that allows a chemical to enter or leave the environment (advection and reaction). A continuous source is also assumed. This greatly increases the utility of the model because industry can be considered a continuous source. Equilibrium is still considered to exist within and between compartments but advection and degradation rates can be estimated to mimic actual environmental conditions. This decreases the error

associated with the equilibrium assumption. This model, though more representative than a level I Fugacity Model, still has limitations, especially when a chemical is discharged by a facility into the river. The level II model does not distinguish between the different types of media releases. (e.g. stack, water and soil). As Table 1 shows, if a facility releases 2000 lb/yr of formaldehyde into the river and 2000lb/yr of formaldehyde into the air, the level II model gives the same results. In actual fact one would expect a higher water concentration of formaldehyde if it was being released in the water than when it is being released in the air due to its high water solubility (as much as 50%).

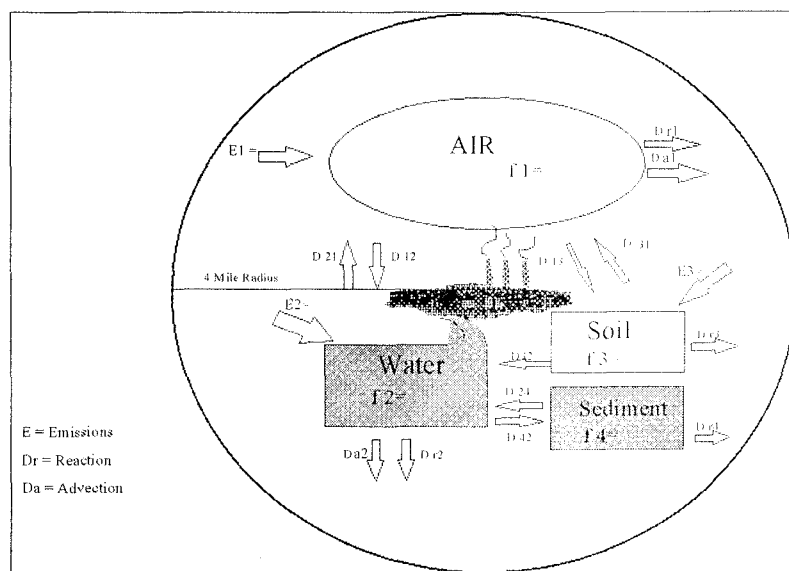
Table 1. Level II Fugacity Model Calculation, Air and Water Releases.

Chemical: Formaldehyde						
Amount Released: 2000lb/yr Air or Water						
Compartment	Volume	Density	Z-Values	Conc.	Amount	% Amount
	(m3)	(kg/m3)	(mol/m3Pa)	(mol/m3)	(moles)	(moles)
Air	1.3E+11	1.185413	0.000403	8.773E-08	11422.11	92.02%
Water	1705774	1000	0.15478	3.366E-05	57.41368	0.46%
Soil	12967349	1500	0.330841	7.194E-05	932.9323	7.52%
Sediment	3411.548	1500	0.661681	0.0001439	0.490886	0.00%

Because equilibrium is assumed to exist between compartments another inherent problem arises. If a facility is releasing a water soluble compound into the air one would expect deposition to be a major factor (e.g. rainfall). The level II model assumes equilibrium between compartments which does not account for processes like deposition. This results

in an under estimation of ground concentrations of water soluble compounds released by a facility into the air. Further refinements were incorporated into a level III model to address these problems.

Figure 1. Processes Involved in a Level III Fugacity Model



A level III Fugacity Model unlike its predecessors does not assume equilibrium between compartments, only within them. This is done by defining a separate fugacity for each of the four defined compartments and allowing all between compartment movement of a chemical to be defined by D-value or more simply, transport equations. **Figure 1** shows the processes involved in a typical Level III Fugacity Model. A lot of information can be incorporated into each D-value equation making it very descriptive of each defined

process. These assumptions make the mathematical calculations more difficult but add an entire layer of evaluative ability to the fate and transport predictions because now individual processes like rainfall or water runoff can be included. Table 2 lists the D-Value parameters that are constant and those that are derived in the Level III Fugacity Model used in the X-media model. Another important added feature is the ability to specify the media of discharge (E). No longer are Z values defined by a single media. In a Level III approach Z-values are defined as bulk Z-values where the air compartment is also composed of particles, the soil compartment is also composed of air and water and the water compartment is also composed of suspended particles (MacKay et al., 1985).

Table 2. D-value Processes and Values

Parameter	Default value or Derivation	Default Parameter	Value
Air-side MTC over water	Calculated separately for each chemical	Dry Deposition (m/h)	10.8 m/h
Water-side MTC	Calculated separately for each chemical	Sediment Deposition Rate	4.6E-07 m ³ /m ² h
Air-side MTC over soil	1 m/hr	Sediment Resuspension rate	4.6E-07 m ³ /m ² h
Water-side MTC over Sediment	.01 m/hr	Sediment Burial Rate	3.4E-09 m ³ /m ² h
Molecular Diffusivity in Air	Calculated separately for each chemical	Water run-off rate from soil	3.9E-05 m ³ /m ² h
Molecular Diffusivity in Water	Calculated separately for each chemical	Solid run-off rate from soil	4.6E-08 m ³ /m ² h
Effective Molecular Diffusivity in Soil	Calculated separately for each chemical	Volume Fraction Aerosols	2E-11
Effective Molecular Diffusivity in Water	Calculated separately for each chemical	Volume Fraction Air in Soil	.2
Effective Molecular Diffusivity in	Calculated separately for each chemical	Volume Fraction Water in Soil	.3
Average Rain Rate (m ³ rain/m ² area.h	8.4E-04 m/h	Volume Fraction Water in	.8
Average Wind Speed (m/s)	3.0 m/s	Advective flow rate Air	1.09E10m ³ /h
Scavenging Ratio	200,000	Advective flow rate Water	1.09E10m ³ /h

Several of the chemical parameters needed for the Level III Fugacity Model, specifically the D-value equations, are unknown. However, Mackay has derived a list of default values to be used (Mackay, 1991). MacKay's rationale for using these default

values is that the fugacity capacity (Z) will be the controlling process in the model estimations of media specific concentrations not fugacity(f) (MacKay and Patterson, 1991). The D -values are used to calculate fugacity only, so close approximations of the default values are sufficient. The most common unknown chemical parameters include: molecular diffusivities and mass transfer coefficients. Both of these chemical parameters significantly alter the outcome of the model when changed. Other uncertain information includes: rainfall rate, dry deposition velocity, water and solids runoff from soil, and sediment deposition, resuspension and burial rate. Table 2 also lists all of MacKay's default parameters.

Model Comparisons

In the Original version of the X-media model a Level II Fugacity Model was used because of data availability. However, since a Level III Fugacity Model was more representative of true environmental conditions, an upgrade was made. MacKay has published default values which along with the modifications made to the Level III Fugacity Model, allow for order of magnitude concentration estimates to be generated. **Table 3** clearly shows the differences between the two fugacity level comparisons when dealing with toxic releases by facilities to all environmental media.

Table 3. Level II vs Level III Fugacity Model Calculation, Air Release

Compound:		Acetone			
Media Released:		Air - (2 mol/hr)			
Level II				Relative	
Compartment	Z-Values	Fugacity	Conc.(ug/m3	Conc.	% mol
Air	.000403	4.92E-10	1.98E-13	6.59%	97.3%
Water	.005588		2.75E-12	91.4%	2.69%
Soil	4.05E-5		1.99E-14	.662%	.0008%
Sediment	8.09E-5		3.98E-14	1.324%	.0001%
Level III				Relative	
Compartment	Bulk Z-Values	Fugacity	Conc.(ug/m3	Conc.	% mol
Air	.0004	4.98E-10	1.99E-13	4.25%	98.06
Water	.0055	3.41E-10	1.90E-12	40.6%	1.87
Soil	.0017	6.95E-10	1.23E-12	26.3%	.054
Sediment	.0039	3.41E-10	1.34E-12	28.6%	.006

In the first comparison acetone was emitted to the atmosphere. The level II and level III Fugacity model both predicted the total amount of chemical released that will remain in the air (98%). However, differences in the water, soil and sediment concentration are seen. The Level II model predicts the highest concentration will be in the water (91%) and hardly any of the chemical will reside in the soil or sediment. The Level III model predicts about the same concentration of acetone will reside in the water (40%), soil (26%) and sediment (29%). The Level III predictions make sense because the process that is transporting the chemical to the ground is mainly rainfall. When the chemical was released to the water or the soil the level II model could no longer predict the correct fate of the pollutant in the environment as shown in **Table 4**.

Table 4. Level II vs Level III Fugacity Model Calculation, Water Release

Compound:		Acetone			
Media Released:		Water-(2 mol/hr)			
Level II					Relative
Compartment	Z-Values	Fugacity	Conc.(ug m3)	Conc.	% mol
Air	.000403	4.92E-	1.98E-13	6.59 ^a %	97.3
Water	.005588		2.75E-12	91.4%	2.69
Soil	4.05E-5		1.99E-14	.662 ^a %	.0008
Sediment	8.09E-5		3.98E-14	1.324 ^a %	.0001
Level III					Relative
Compartment	Bulk Z-Values	Fugacity	Conc.(ug/m3)	Conc.	% mol
Air	.0004	3.36E-	1.36E-13	.002 ^a %	2.133
Water	.0055	5.6E-07	3.12E-09	58.66%	97.52
Soil	.0017	4.78E-	8.49E-13	.01 ^a %	.0011
Sediment	.0039	5.6E-07	2.2E-09	41.31 ^a %	.3434

The results of the level III calculations clearly show a significant portion of the acetone will remain in the water. Another good example of the inherent inaccuracy of the level II model, as shown in **Table 5**, when benzene is emitted to the air and water. The level II model predicts all of the benzene will partition to the air. Benzene, however, has a relatively high solubility and therefore an appreciable amount would be expected to be in the water, as the level III fugacity calculation predicts.

Table 5. Level II vs Level III Fugacity Model Calculation, Air and Water Releases

Compound:		Benzene				
Media Released:		Air-(5 mol/hr)				
		Water-(10 mol/hr)				
Level II						
Compartment	Z-Values	Fugacity	Conc.(ug/m3)	Relative Conc.	% mol	
Air	.000403	4.92E-	1.98E-13	6.59%	97.3	
Water	.005588		2.75E-12	91.4%	2.69	
Soil	4.05E-5		1.99E-14	.662%	.0008	
Sediment	8.09E-5		3.98E-14	1.324%	.0001	
Level III						
Compartment	Bulk Z-Values	Fugacity	Conc.(ug/m3)	Relative Conc.	% mol	
Air	.0004	3.36E-	1.36E-13	.002%	2.133	
Water	.0055	5.6E-07	3.12E-09	58.66%	97.52	
Soil	.0017	4.78E-	8.49E-13	.01%	.0011	
Sediment	.0039	5.6E-07	2.2E-09	41.31%	.3434	

Improvements to Model

In an effort to improve the reliability of the level III fugacity model, a sensitivity analysis was performed to ensure the appropriateness of selected default values as well as to identify the variables controlling the output of the model. The sensitivity analysis was performed by increasing individual model parameters 5% for seven chemicals, each varying in physical chemical parameters (e.g. high water solubility, high vapor pressure). A % difference was calculated for each chemical by comparing original media concentrations with the concentrations altered after individual model parameters were changed. The % difference average and standard deviation and the parameters altered for

the sensitivity analysis are presented in **Table 6**. Influential % differences occurred in one of the media when one of the following parameters were altered: emission rate, air and water residence time, rain rate, water runoff, fugacity capacity, and $\log K_{ow}$. With the exception of the residence times, rain rate, molecular diffusivity and volume fraction, the above influential parameters change for every chemical. As long as the physical chemical parameters are accurate, the error in the fugacity model associated with these parameters should be minimal (since the physical chemical parameters are the back bone off the Fugacity Model). If estimation methods are used to obtain physical chemical parameters more error will be introduced. Changing the individual level III fugacity parameters (see Table 2) held constant did not alter model concentrations to any appreciable degree. This is not an invalid assumption they be held constant for all chemicals.

The above sensitivity analysis was performed by only varying one parameter at a time. Though only a small difference was observed when air-water and water-water side mass transfer coefficients (MTC's) and air and water molecular diffusivities were changed individually, a different trend was seen when they were changed simultaneously. It is not an invalid assumption to change all these parameters simultaneously since they are all interrelated. Instead of a concentration varying by less than 1% separately, a % difference of up to 5.77% was seen. Because these parameters can vary widely from chemical to chemical, default values are not appropriate.

Table 6. Level III Fugacity Model Sensitivity Analysis Showing Average % Difference of Seven Chemicals for the Tested Parameters (Including standard deviation).

Parameter	% Difference			
	air	water	soil	sediment
MTC (air/water)	0.0051±.01	-0.0336±.05	0.0051±.01	-0.0336±.05
MTC (air/soil)	0.0265±.07	-0.0155±.04	-0.0448±.08	-0.0155±.04
Half Life(air)	0.4201±.57	0.0592±.10	0.4201±.57	0.0592±.10
Soil Area	0.0000	0.0000	0.0000	0.0000
Dry Deposition	0.0000	0.0000	0.0000	0.0000
Volume Fraction	0.0244±.06	-0.0163±.03	0.0507±1.02	-0.0163±.03
Scavenging Ratio	0.0000	0.0000	0.0003	0.0000
Molecular diff. (air)	0.0010	-0.0033±.01	-0.4189±.91	-0.0033±.01
Residence time (air)	4.042±1.29	0.2638±.48	4.042±1.29	0.2638±.48
Residence time (water)	0.0680±.08	3.608±.52	0.0680±.08	3.608±.52
Emmissions	5.0000	5.0000	5.0000	5.0000
Log k _{ow}	-0.0025	-0.0271±.04	0.7240±2.33	0.8724±1.20
Water Runoff	-0.0376±.10	0.05427±.08	-1.133±1.67	0.05427±.08
Z-value (soil)	-0.0025	-0.0256±.04	0.7241±2.33	0.0256±.04
Rain Rate	-0.4810±1	0.3088±.58	2.779±1.82	0.3087±.58

Note: Bold values represent variables that control model output

Instead, separate molecular diffusivities (air and water) and mass transfer Coefficients (MTC) were calculated based on equations from Verschueren, K (Handbook of Environmental Chemistry, 1983). Mackay and Patterson have stated that as more mass transfer coefficients become available the ability of the model to estimate real environmental situations will improve dramatically (MacKay and Patterson, 1989). Sensitivity analysis shows that when the air and water side MTC are calculated, for example, for benzene, there is a resulting 13.2% and 57% decrease from the default values of 5 m/h and .05m/h. When the same calculations and comparisons were completed for a water soluble compound like methanol there is a resulting decrease in air and water side

MTC of 97% and 45% respectively. For compounds with high vapor pressure and low water solubility the default values are adequate.

However as the water solubility increases, the default MTC's no longer reflect an accurate value (as shown above). The calculated MTC's also produce a significant change in the predicted media concentrations. For benzene the calculated MTC resulted in a .01% increase in air and soil concentrations, and a 46% decrease in water and sediment concentration. The differences in predicted media concentrations become even more pronounced when separate MTC's are calculated for a water soluble compound like methanol. The resulting changes in media concentrations were: .6% increase in air and soil, and a 88% decrease in water and sediment. Use of the default values results in an overestimation of water and sediment concentrations, and an underestimation of air and soil concentrations. With such a large change in predicted concentrations from only a small change in MTC value, it becomes evident that the closer the estimate of the chemical specific parameters, the better the model predictions. Another rationale for calculating separate MTC and molecular diffusivities lies in the transport equations or D-value equations. When default values are used the amount of chemical that is distributed from the atmosphere to the water is not significantly different from that distributed from the water back to the atmosphere. For methanol the difference is 4.5%. When separate MTC's and molecular diffusivities are calculated there is a resulting 51% difference. Now, once the chemical is in water it stays. This is exactly what is expected with a chemical like methanol. For compounds that have a high vapor pressure and a low water

solubility just the opposite is observed. More of the chemical is moving from the water to the air than from the air to the water. Making such distinctions for the transfer of chemicals between specific environmental media help to improve the reliability of the Fugacity Model. A comparative risk approach does not require the data intensity of a traditional risk assessment. Therefore estimates that clearly define the differences between pollutants based on their chemical properties sufficiently satisfy this data requirement.

Data Requirements

The Level III fugacity model used in the current version of the X-media Model requires only 8 specific chemical parameters, release data and compartment areas and volumes. The chemical parameters include: molecular weight, melting point, vapor pressure, solubility, octanol water partitioning coefficient (K_{ow}), temperature and Henry's law constant. Chemical Specific parameters were obtained from current literature or estimated.(Howard et al., 1991, Howard, 1989, and Lyman et al., 1990, MacKay et al., 1992, Verschueren, 1983 and MacKay, 1991) Chemical release data are obtained from the EPA Toxic Release Inventory (TRI) and specific site compartment area data are obtained from a Geographical Information System (GIS). Appendix A lists the chemicals and their physical properties included in the X-media chemical database.

RISK INDICES

Human Risk Index

A Human Risk Index, adapted from an EPA Region VI Comparative Risk Approach (Carney, 1991) is calculated using a number of pre-defined hazard and exposure criteria:

$$\text{HRI} = (\text{Ef} * \text{DI}) * (\text{PR} * \text{DV})$$

Ef - Exposure Factor

DI - Degree of Impact

PR - Population Ratio

DV - Degree of Vulnerability

The Ef (exposure factor) has been defined as the media specific concentration (ug/m³) which is predicted by the Fugacity fate and transport model. The exposure factor is defined by concentration because as a chemical builds up in an environmental media the potential toxicity of the compound increases.

The degree of impact (DI) is an index of the relative toxicity of each compound, and is based on a chemical's cancer and non-cancer effects. The non-cancer DI is based on the chemical Reference Dose (RfD) for water, soil and sediment and its Reference Concentration (RfC) for air. A RfD is defined as the acceptable amount of a chemical which an individual can ingest over a life time and expect no adverse effects. It is used as the basis for the water, soil and sediment compartments because the primary exposure route is assumed to be ingestion. A RfC is defined as the amount of chemical that can be inhaled over a lifetime with no expected

adverse health effects. The primary exposure route in the air compartment is inhalation. The RfD's and RfC's were obtained from IRIS (1995), and Sax and Lewis (1987). Cancer Potency factors for ingestion and inhalation are used to define a DI for chemicals that are carcinogens. These factors are mathematically derived estimates from the concentration of a chemical (mg/kg/day) necessary to produce a given level of excess risk. The cancer slope factors are also obtained from IRIS (1995). Appendix B lists the chemicals and their corresponding compartmental Degree of Impacts included in the X-media chemical database.

To calculate a DI the cancer and non-cancer ranks for a chemical in a specific media are summed. **Table 7** outlines the ranking scale which was adapted from EPA's TRI Hazard Ranking Index (1990).

Table 7. Degree of Impact Ranking Scale

RfD or RfC	Assigned Weight	EPA Cancer	Rank
Rf > .00005	10,000	50	1000000
.00005 < Rf < .0005	1,000	.5 - .49	100000
.0005 < Rf < .005	100	.5 - .4	10000
.005 < Rf < .05	10	.05 - .4	10000
.05 < Rf < .5	1	.005 - .04	100
.5 < Rf	.1	.0005 - .004	10

If a chemical has a reference dose of .5 mg/kg/day then it is given a corresponding DI of .1. If this chemical is also a carcinogen and has a potency factor of .0005 then its total DI is the sum of $.1 + 10 = 10.1$.

The Population Ratio is simply the population density within a 4 mile radius of the facility (Study Area), divided by the population density of the state. The population living within the 4-mile radius of the study area have been selected as the population at risk. The population ratio of the study area is obtained from the Geographical Information System. The population data is based on 1991 Census information.

Defining population in the HRI calculation is very useful because now a distinction can be made between a facility located in the city and one located in a rural area. If a facility is located in a city, the population density will be higher so the probability of an adverse health effect could increase. The facility located in a rural area will have a smaller population located within study the area, so the probability of seeing an adverse health effect may decrease. It should be noted that, if there are no people living within a study area, there is no threat of human exposure and thus no HRI.

The Degree of Vulnerability term can be used as a measure of the vulnerability of the population exposed. For example if an unusually high number of children or other sensitive individuals live within a study area the DV term could be used to account for the sensitive population. The DEQ model currently uses a default value of 1, because of the lack of an sensitive individual identification and ranking system, so no additional weight is given to vulnerable individuals.

The sensitivity of the HRI is determined by each of the four defining terms. At this time the DV term is one so it does not affect the result of the HRI. The Ef, DI and PR are all first order terms, equally contributing to the calculated HRI (in theory). Because of

the order of magnitude of each parameter, one term could significantly influence the overall HRI. After completion of a Pilot Study it was found the exposure factor, followed by the population ratio influenced the HRI more than does the Degree of Impact.

HRI Model Comparison (old vs new)

In the original version of the model the Ef was defined as the amount (moles) of chemical present in each of the environmental media (air, water, soil and sediment) defined by the Fugacity Model. To calculate the Ef, the percentage of chemical present in each media (predicted by the Fugacity Model) was multiplied by the total amount of chemical reported released. If one required chemical parameter was missing for a toxin being released by a facility, a % amount could not be calculated and the total amount of chemical released was used as a default value for the Ef.

The idea behind the calculation of the exposure factor by using total moles released is sound because if a chemical cannot be modeled due to missing data, a HRI can still be calculated due to the known amount of chemical released. A flaw in the logic arises though, when dealing with potential exposure. By using total moles the air will almost always have the greatest amount of moles present, due to its greater volume and thus contribute the most to the total facility HRI. It is true that the air compartment will have the greatest number of moles, but it is not true that the air will necessarily contribute the greatest amount to the total facility HRI.

When dealing with exposure, media concentration is of greater concern than the total amount of chemical present. Even though the air has the greatest mass of toxin present, that does not mean it has the highest concentration. In fact the air compartment because of its vast volume will usually have the smallest concentration. So calculating the Ef in this manner severely overestimates the relative risk posed by the air compartment and under estimates the relative risk posed by the other compartments. For example if a chemical is water soluble one would expect a significant portion to migrate to the ground by a deposition process and potentially build up. If the Ef was defined by media concentration instead of total amount of chemical present, the X-model would more accurately predict the HRI posed by a facility releasing toxins into the air.

As shown in **Table 8** an Ef for acetone in air, water, soil, and sediment is 14308, 449, 4577 and 1 calculated using a level II Fugacity Model. Using a level III fugacity approach an Ef for acetone in air, water, soil and sediment is .0091, 4, 292 and 3 (amount released are also given to help clarify between the differences between the Ef's). As shown here with acetone and in Table 8 for the other chemicals the old method severely overestimates the Ef factor for air which tends to skew the HRI to reflect this compartment only. Because the new method uses concentration instead of total amount, the Ef for the air compartment is not over estimated and actually better reflects the exposure overall. This can be seen by comparing the Ef for phenol. For both the original and modified model the soil has the greatest Ef, but the former still overestimates the air and water Ef. This overestimation stems from the fact that deposition is the main process by which phenol is transported to the ground compartments.

TABLE 8. Exposure Factor Comparison

COMPOUND	AMOUNT RELEASED (lbs/yr)		
	AIR	WATER	SOIL
PHENOL	1938	250	5
ACETONE	19150	180	5
MEK	3101	180	5
FORMALDEHYDE	105600	5	5
METHANOL	390640	11000	250
CHLORINE	250		
AMMONIA	250	1200	
HYDROCHLORIC ACID	200000		
SULFURIC ACID	33800		

COMPOUND	NEW COMPARTMENT Ef				OLD COMPARTMENT Ef			
	AIR	WATER	SOIL	SEDIMENT	AIR	WATER	SOIL	SEDIMENT
PHENOL	0.004	4	398	3	193	145	1855	0
ACETONE	0.091	4	292	3	14308	449	4577	1
MEK	0.014	3	37	2	2325	371	590	1
FORMALDEHYDE	0.164	1	174	1	95211	359	10039	1
METHANOL	2	185	810	148	358732	27303	15812	44
CHLORINE					250	0	0	0
AMMONIA					250	1200	0	0
HYDROCHLORIC ACID					2000000	0	0	0
SULFURIC ACID					33000	0	0	0

The area of water within the study area is about 100 times less than the that of the soil area so one would expect less phenol to be deposited in the river than in the soil and thus less risk if exposed. The original calculation does not amplify the difference between the Ef of the water and the Ef of the soil as accurately as the modified Ef. Thus the modified version better reflects the potential exposure because it is the actual concentration not the total amount of the chemical.

In Table 9 and 10 both an original and modified HRI were calculated for three facilities: Facility 1 (Furniture Company), Facility 2 (Wood Treater) and Facility 3 (Paper

Mill). Year to Year comparisons were also calculated for Facility 3. Facility 1 and Facility 2 both reported releasing chemicals only to the air where as Facility 1 reported air, land and water releases.

For all three Facilities there is a considerable difference in the magnitude of the old method and new method HRI's. This difference is due to the change from level II to Level III Fugacity model and the change from using total amounts of a chemical released for calculating the Ef to using actual compartment concentrations instead.

As **Table 9** shows for both Facility 1 and Facility 2, calculating the HRI using the original model results in the air compartment contributing the greatest to the total Facility HRI whereas using the modified version, the soil compartment contributes the most to the total Facility HRI. Because of the vast volume of the air compartment and thus the minimal concentration, it should not contribute the most in terms of exposure and risk to the total HRI. The modified model, by using concentrations for the Ef does not give the same predictions. Here the soil contributes the most to the HRI because of deposition processes carrying the water soluble chemicals to the ground compartments.

Another interesting comparison can be shown between these facilities. Facility 1's HRI using the old method is greater than Facility 2 whereas just the opposite is true for the new HRI's. Why is this? The answer is simple. Facility 1 releases a greater amount of each chemical than Facility 2. Because of the way the old HRI was defined Facility 1's HRI is greater. Looking closer at both facilities, Facility 2 releases three more chemicals (of which two can have HRI's calculated for) than Facility 1.

TABLE 10. Original and Modified Yearly HRI Comparisons

Facility Name: FACILITY 3 1992										
AMOUNT RELEASED (lbs/yr)										
COMPOUND	AIR	WATER	SOIL	SEDIMENT						
PHENOL	2400									
ACETONE	18830	180								
MEK	4037	170								
FORMALDEHYDE	1E+05	5								
METHANOL	4E+05	13000								
CHLORINE	250									
AMMONIA	250	2000								
HYDROCHLORIC	1E+05									
SULFURIC ACID	41000									
OLD COMPARTMENT HRI						NEW COMPARTMENT HRI				
COMPOUND	AIR	WATER	SOIL	SEDIMENT	TOTALS	AIR	WATER	SOIL	SEDIMENT	TOTALS
PHENOL	8E+07	226522.8	127505.05	226522.08	78891651	33	10	3137	8	3188
ACETONE	3E+06	1076544	12204.57	1076544	5608925.1	1	242	17659	195	18097
MEK	8E+05	1891428	66536.4	1891428	4616056.2	0	1878	22527	1520	25925
FORMALDEHYDE	4E+10	1.4E+08	6130320	140118930	4.416E+10	1000	50	10158	40	20253
METHANOL	8E+08	642936	2134.398	1076544	757418122	159	1403	3833	1124	6479
					4.501E+10					73942
Facility Name: FACILITY 3 1993										
AMOUNT RELEASED (lbs/yr)										
COMPOUND	AIR	WATER	SOIL	SEDIMENT						
PHENOL	1938	250	5							
ACETONE	19150	180	5							
MEK	3101	180	5							
FORMALDEHYDE	1E+05	5	5							
METHANOL	4E+05	11000	250							
CHLORINE	250									
AMMONIA	250	1200								
HYDROCHLORIC	2E+06									
SULFURIC ACID	33000									
OLD COMPARTMENT HRI						NEW COMPARTMENT HRI				
COMPOUND	AIR	WATER	SOIL	SEDIMENT	TOTALS	AIR	WATER	SOIL	SEDIMENT	TOTALS
PHENOL	7E+07	207085.2	116438.7	207085.2	72105833	27	27	2562	20	2636
ACETONE	4E+06	1096374	12428.85	1096374.0	5707683	1	244	18797	196	19238
MEK	6E+05	1476136	51958.2	1476136.2	3602871.3	0	1976	23716	1599	27291
FORMALDEHYDE	5E+10	1.48E+08	6474141.2	147972468	4.664E+10	1056	53	11185	43	21846
METHANOL	7E+08	633591	2104.494	633591	746050834	158	1194	5217	957	7486
					4.746E+10					78497

This is why the new HRI for Facility 2 is greater than the new HRI for Facility 1. Just releasing more of a chemical does not necessarily imply that Facility 1 should pose a greater relative risk than Facility 2. The new method for calculating the HRI makes this distinction by predicting exposure based on concentration instead of the total amount of a chemical released.

Another problem encountered with the old method of calculating the HRI arose during Yearly Facility Comparisons as seen in **Table 10**. In the X-media models' original form the actual emissions were used in the calculation of the HRI. This resulted in very large numbers wherein order of magnitude differences were the only logical parameter upon which ranking could be based. The resulting loss in sensitivity of the HRI to potential impacts diminished the usefulness of the comparison when no order of magnitude difference were generated. This can be seen by looking at the 1992 and 1993 Facility 3 old HRI's. Sensitivity is lost for yearly comparisons using the original model whereas using the modified version the total HRI values are considerably significantly lower so sensitivity is retained and difference can be seen on a relative ranking scale.

Ecological Risk Index

The Ecological Risk Index (ERI), adapted from Region VI, is a compilation of hazard and exposure criteria defined by:

$$ERI = \left[\sum_{i=1}^n [(SAR * DV)]_i \right] * (Ef * DI)$$

SAR - Sensitive Area Ratio

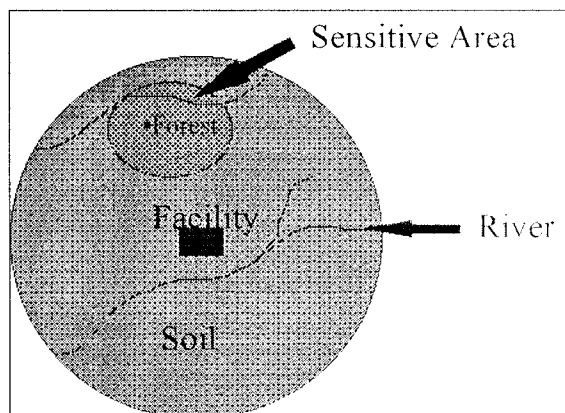
DV- Degree of Vulnerability

Ef- Exposure Factor

DI - Degree of Impact

SAR is the area of each exposed sensitive ecosystem within the study area divided by the study area (4-mile radius). **Figure 2** illustrates a Forest (Sensitive Area) within a study area.

Figure 2. Illustration of a Sensitive Environment within the Study Area.



The Degree of Vulnerability term is measured in terms of the sensitivity of the ecosystems within the study area. A number of sensitive environments have been classified by the EPA (

DEQ, 1993). This classification is also used in the X-media model. **Table 11** outlines the sensitive areas and their corresponding ranks.

Table 11. Sensitive Areas and their Ranking included in the X-Media Model.

SENSITIVE AREAS	RANK
Biotic Areas of Critical Concern	25
Coordination Areas	25
Range experiment stations	50
Research Forest	25
National Wildlife Refuge	75
Misc. Sensitive Areas	100
National Monument	100
Oregon Cascades Recreation Area	75
Oregon Designated Conservation Area	25
Federal Research Natural Area	75
Oregon Scenic Waterway	25
Oregon Wildlife Refuge	75
Federal Wilderness Area	100
Federal Designated Scenic River	50

The E_f is the media specific concentration in $\mu\text{g}/\text{m}^3$ predicted by the Fugacity model. Because of the lack of data correlating ecological impacts with air pollution, only water and soil concentrations are used to calculate the ERI. It should be noted that wet and dry deposition from the air compartment are accounted for in the Fugacity model. In other words if the rain transports a portion of the chemical to the soil and it does not evaporate, it is accounted for in the E_f for the ERI.

The DI for the ERI is based on a chemicals K_{ow} and No Observable Adverse Effect Level (NOAEL). This DI is calculated by weighting a chemicals Log K_{ow} or solubility (if the K_{ow} is unavailable) against its NOAEL. **Table 12** outlines the ERI DI ranking scale. The

toxicity values for each chemical are ranked using an EPA based scale developed for the TRI (USEPA, 1990). The X-Media model ERI results have not been evaluated at this time so results will not be included in this article.

Table 12. Ecological Degree of Impact Ranking Scale

Bioaccumulation Water Solubility	Log K _{ow}	BCF (l/kg)	>100	Chronic 10-100	NOAEL 1-10	(mg/kg/day) 0.1-1	<0.1
>1500	<.08	<1	0.5	5	50	500	5000
500-1500	.08-2	1-10	5	50	500	5000	50000
25-500	2-3.2	10-100	50	500	5000	50000	500000
-	3.2-4.5	100-1000	500	5000	50000	500000	5000000
-	4.5-5.5	1000-10000	5000	50000	500000	5000000	50000000
<25	5.5-6	>10000	50000	500000	5000000	50000000	500000000

The sensitivity of the ERI is primarily controlled by the DI, then the Ef and the DV playing a lesser role. The SAR does not control the sensitivity of the equation because it is always one.

ERI Model Comparison (old vs new)

The Ef for the ERI has also been redefined as concentration instead of total amount. The reasoning behind this is identical to that of the HRI. By defining the Ef as concentration instead of total amount, exposure in each medium is better addressed. One additional problem encountered with the ERI is when no sensitive environments were present in a study area. In the original X-media model a ERI could not be calculated if this were to occur. Surprisingly a

study area not containing a sensitive area is quite common. The null ERI arises from the fact that if no sensitive environments were located within a study area the SAR and DV both equal zero so a Zero ERI would result. To remedy the problem a default value of one was added if no sensitive area is present within the study area since there is usually an ecological risk posed by facilities releasing toxics. Now an ERI can be calculated for every facility. A distinction can still be made between ERI's for those facilities that pose a greater relative Eco risk by the sensitive area and degree of impact terms in the equation. If a sensitive area is present within the environment the calculation is carried out by dividing the sensitive area by the total land and water area of the study zone, multiplying it by its corresponding Degree of Vulnerability, next subtract the total sensitive area by the total land and water area of the study zone and divide it by the total land and water area of the study zone, add these two values together and multiply them by the Ef and the DI. Now the sensitive areas and the non-sensitive areas are taken into account in the ERI calculation. Because an ERI could not be calculated using the old method no comparisons were made between it and the new method.

Note: For both the HRI and the ERI, problems will arise using the concentration approach with metals since these components are not amendable to a fugacity approach. A possible solution would be to estimate missing chemical parameters, such as using a low vapor pressure and solubility for metals, so a fugacity could be calculated. Z - Values could no longer be estimated but instead actual partition coefficients would be used. When more partition coefficients become available, this solution could be developed.

Summary of Model Assumptions

It is assumed that the Fugacity Model will provide an estimate of environmental concentrations based on the underlying assumption that the TRI emission estimates reported by each facility are correct. The Fugacity Model assumes steady state and only gives corresponding order of magnitude estimates of compartment concentrations. These values should not be viewed as definitive. The average wind speed and rainfall data used are generally descriptive of Oregon. (NOAA, 1993). It should be noted that the Fugacity Model has the capability to handle incoming, or background concentrations of a chemical entering the study area. No factor is included to account for overlapping study areas. All sources within the study are considered to be continuous. The DI's for air are based on the RfC. The DI for soil, water, and sediment are based on the RfD. The assumption is made that potential risks to the population within a 4 mile radius of the facility (study area) are representative of the potential risks posed by the site.

HRI AND ERI RANKING CATEGORIES

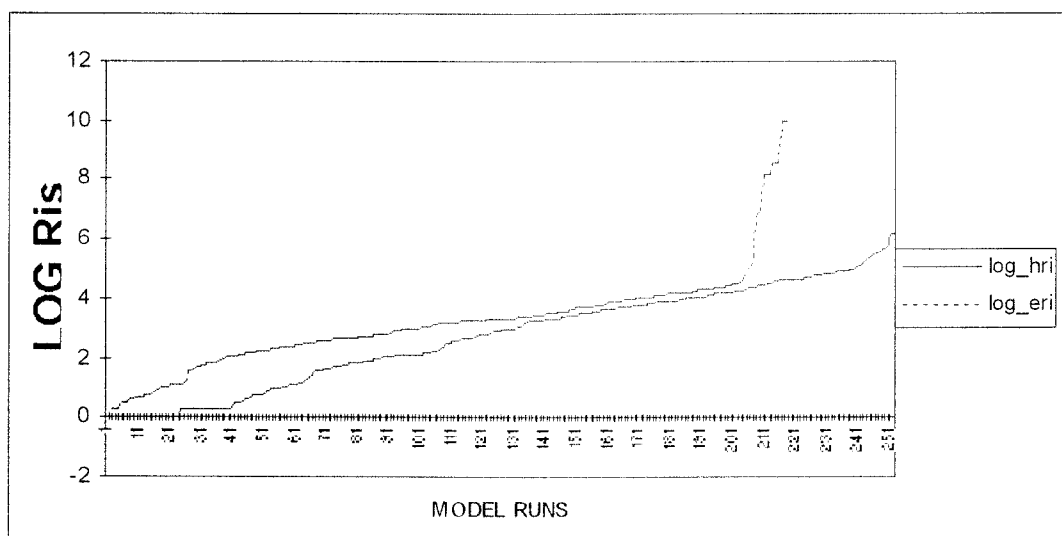
Before reviewing the results, it is important to fully understand the parameters upon which the HRI and ERI are calculated. The Risk Indices employed in the X-Media model take into account five separate, but equally important factors: Population in the study area, chemical toxicity and amount released, sensitive populations and compartment specific concentrations. It is important to note that a high HRI and ERI could be associated with

several different factors. For example: if facility A received an HRI of 75000, this could mean there is a high population density within the study area, the concentration in one media could be significant, or a chemical released from the facility may have a high toxicity ranking. If a facility received an ERI of 40000 this could mean that there are several sensitive eco-systems with large Degrees of Vulnerability within the study area, a ground compartment has a significant concentration, or a chemical released from the facility has a large DI corresponding to high toxicity and persistence in the environment. The results of the model provide an analysis of potential cross-media impacts but do not define 'increased risk' due to those impacts. The model merely provides a basis for comparison based on a relative ranking scale. This is why it is so important to look at the original calculations to determine which factor is the main contributor.

To determine the relative significance of the HRI and ERI numbers a 138 facility pilot study was undertaken. Because the original intent of the model was to maintain data sensitivity throughout the calculation process, Carney's method of ranking all equation parameters from 1 to 4 was not adopted. The more advantageous approach was taken to retain actual values and then convert them to a relative ranking scale. The facilities chosen for the pilot study all released organic chemicals either in the air, water or land. The facility release information was obtained from the EPA's TRI database for Oregon. At the completion of the study, summary statistics were run on the HRI and the ERI to try and obtain one relative ranking scale for both indices. Ascending plots of both the HRI and ERI showed non-linearity, a severe statistical

limitation. Several transformations to force a normal distribution were unsuccessful. **Figure 3** contains ascending Log plots of both the HRI and the ERI.

Figure 3. Ascending Log HRI and Ascending Log ERI Plot



HRI CATEGORIES

Due to the large spread of the data a simple relative ranking scale would result in a loss of model sensitivity at both ends of the scale. With a single ranking scale, about 60 of the Pilot Facilities received a rank of one or zero. In order to preserve the sensitivity of the X-media model each data set was broken into three categories, High, Medium and Low. The categories were delineated by inflections in the curves (See **Appendix C**). Within each marked category a relative ranking scale from 1 to 100 is established. First each category value is standardized and

then normalized from 1 to 100. **Table 13** lists the standardization and ranking formulas for each category.

Table 13. HRI Relative Ranking Scale

HRI			
Category	HRI Ranges	Standardization (S)	Ranking
Low	1 - 250	$(\text{HRI}-41.25)/52.75$	$S*22.8+18$
Medium	251 - 34600	$(\text{HRI}-7051.57)/7689.37$	$S*22.3+20$
High	34601 - 1640000	$(\text{HRI}-197332)/326364$	$S*20.25+11$

Low

Facilities that received a low ranking category had total releases in lb/yr ranging from 10 to 131300 of mainly volatile chemicals with over 90% being emitted into the air either by a stack or non-point source. The higher volatility of the chemicals explains the low category ranking. The toxins being released by these facilities have a very high vapor pressure and a low water solubility resulting in a loss of a majority of the chemical by advection in the air. With almost all of the toxin leaving the study area, the air concentration remains low and because of the low water solubility the ground compartment concentrations also remain low. Low compartment concentrations mean low HRI's. A few facilities released small quantities of chemicals which were less volatile and more water soluble. These chemicals are expected to build up in all the compartments due to their slow advective properties. These facilities received a low category rank for two reasons: only minute quantities were released and the

surrounding population density was almost non-existent due to a rural location. Facilities that fell into a low ranking category generally released between one and three volatile chemicals into the air and were located in a rural area.

Medium

The next category of facilities released between 250 and 1.1E6 lb/yr of less volatile and more water soluble chemicals, which have a moderate degree of impact associated with their presence in the ground compartments. More facilities also released toxins into the water and land compartments. The major contribution from this group was from the build-up of chemicals in the soil compartment due to deposition processes. Common chemicals released among the facilities which fell in the medium category were acetone, methanol, methyl ethyl ketone and methyl isobutyl ketone (MIK). These facilities released between one and five chemicals of which 1 to 3 tended to be water soluble and the remaining were volatile chemicals which do not contribute much to the HRI. The population density of the facilities tended to be larger than the low category facilities suggesting a more urban setting.

High

Those Facilities falling into the high category released from 1000 to 529000 lb/yr of highly soluble chemicals which had a moderate to high degree of impact in the air and ground compartments. All of the chemicals released by those facilities falling within the medium

category were also released by the high category facilities, but in much greater quantities. High Category facilities release between 1 and 8 chemicals to the air, water or land. Also included in this group were significant releases of more toxic chemicals such as epichlorohydrin, phenol, 2,4-D, dicofol and carbaryl. A high Population Density was associated with these facilities implying most were located within metropolitan areas. Facilities fell within the high category because of the combination of the large quantity of chemicals they released, the degree of impact associated with these chemicals and the large surrounding populations.

A common trend, of water soluble chemicals, was found among facilities scoring high in all the categories. The water soluble chemicals most commonly released by these facilities were: acetone, ethylene glycol, methanol, methyl ethyl ketone, methyl isobutyl ketone and n-butanol. Two other trends were also seen, the higher the category the greater the amount of one or more of the previous list of chemicals are being released, and the higher the category the more the soil compartment contributes to the total facility HRI. The problem associated with these chemicals were their water solubility. In a state like Oregon, where it rains constantly, a water soluble chemical will tend to be carried to the surface by such a deposition process. When on the ground these water soluble chemicals will become associated with the moisture in the soil and then become trapped as they move further into the ground. Unlike the water and air compartment which have significant advection processes by which a chemical could leave the study area, reaction and volatilization is the only process by which these chemicals could leave the soil. Fate and transport modeling predicts high concentrations

remain in the soil. This and the fact that the soil compartment is 100 times greater than the water compartment is why it contributes the greatest amount to the total facility HRI.

ERI Categories

The ERI was also split into 3 separate categories for identical reasons to the HRI, loss of sensitivity. Three inflection points were chosen just (as with the HRI) to define the low, medium and high categories. **Table 14** lists the ERI standardization and ranking formulas for each category. Unlike the large HRI the larger ERI's were not reflective of water soluble chemicals. ERI values tended to be larger when a facility released more volatile than water soluble chemicals. The reason being the ERI DI, which is defined by a chemicals NOAEL and K_{ow} . The more volatile chemicals in general have a greater K_{ow} than the water soluble chemicals and thus a greater ERI.

Table 14. ERI Relative Ranking Scale

Category	Ranges	Standardization (S)	Ranking
Low	1 - 1150	$(ERI-297)/322.80$	$S*28.2+27$
Medium	1151 - 50000	$(ERI-9653)/9619.66$	$S*19.65+18$
High	50001 - 10000000	$(ERI-2099397)/3578161$	$S*35.7+26.02$

Low

Unlike the HRI those facilities falling within the low ERI Category Ranking release a considerable amount of water soluble chemicals and only small amounts of highly volatile, low water soluble compounds. Because population is not defined in the ERI equation urban or rural setting of facilities are not directly taken into account. Because of the large HRI's associated with these facilities falling within the low ERI ranking Category indicates they are located in urban areas. Sensitive Eco-systems are not usually present in the study areas of facilities falling in this category. This makes sense because if a facility is located in a city one would expect fewer ecosystems and thus less exposure to eco-systems because much of the ground compartment is covered by buildings or asphalt.

Medium

Those Facilities falling within the Medium Category tended to release more volatile chemicals or chemicals with high K_{ow} 's than water soluble chemicals. Study Areas with one Sensitive Area are quite common within this category. The HRI values are grouped more closely to the medium ERI category than the low ERI Category.

High

All the Facilities falling in the High ERI Category have one or more sensitive environments located in their study areas. These facilities tend to be rurally located and release chemicals that are either volatile or have a considerably high K_{ow} . The chemicals that tend to be associated with facilities receiving high ERI's are those releasing: xylene, toluene, styrene, ethylene glycol, n-butyl alcohol, phenol, and pesticides.

INTERPRETATION OF RESULTS

What do these Risk Indices mean? The X-media model was developed as a tool to aid in the decision making process, it is not intended to provide a sole basis for action. HRI and ERI values only have meaning in a comparative framework when ranking similarly evaluated facilities. Specifically, comparisons can only be made with the same facility under different operating conditions or for different facilities in which HRI or ERI values have been generated using the same criteria. The Risk Indices provide an estimate of the relative likelihood of each facility to cause harm when compared to other facility ranks. The Ef or fugacity results however can be viewed as separate entities. The predicted concentrations provide a rough screening for partitioning of chemicals released to the environment. When comparing two facilities HRI or ERI values, the Risk Indices become relevant. Specifically when the Facilities Risk Indices are compared from year to year. When comparing two HRI or ERI

values, the larger the number, the greater the relative risk. **Table 15** shows the results from two facilities run through the X-media model.

Facility A is a furniture company located in a populated section of a rural area. It reported to EPA TRI releases of xylene, toluene, methyl isobutyl ketone and methyl ethyl ketone (MEK). The individual HRI's are 12, 9, 514 and 45843. Looking at each chemicals compartment HRI, it is obvious that MEK is the major contributor to the total HRI, specifically in the soil compartment. Is this conclusion valid? Looking at the large solubility (270,000 mg/l) compared to the vapor pressure (13,300 Pa) one would expect a significant portion of the MEK released into the air from a stack to be carried down to the soil and water and thus into the sediment by rainfall and wet deposition processes. This is exactly what the Fugacity model predicts. Xylene and toluene are highly volatile chemicals which are carried out of the study area quickly by advection. This is why both have a corresponding low HRI. Methyl isobutyl ketone is not as soluble as MEK so less will be deposited to the surface compartments.

Table 16 lists facility A's ERI values. No sensitive areas were present within the study area. Xylene and methyl ethyl ketone both contributed the same weight to the total Facility ERI. Normally the more volatile chemicals contribute a significant portion to the total ERI but in this case the Ef for MEK is large which increases the Risk Index even though the DI is low.

Table 15. Facility A & B X-Media Model HRI Results

Facility A			Total HRI = 46371 Category = HIGH Rank = 1		
Population Density		613	Compartment Concentrations (ug/m3)		
			Degree of Impacts		
			Human Risk Indexes		
Compound Name	Amount Released (lb/yr)	Air	Water	Soil	Sediment
Methyl Ethyl Ketone	21807	0.101	0.845	215.351	0.68
DI		0.1	10	10	10
HRI		0	179	45521	144
Methyl Isobutyl Ketone	18402	0.065	0.18	23.32	0.157
DI		10	1	1	1
HRI		14	4	493	3
Toluene	33108	0.138	0.09	2.38	0.286
DI		1	0.1	0.1	0.1
HRI		3	0	5	1
Xylene	38128	0.133	0.1	4.46	0.526
DI		1	0.1	0.1	0.1
HRI		3	0	9	1

Facility B			Total HRI = 9314 Category = Medium Rank = 27		
Population Density		302	Compartment Concentrations (ug/m3)		
			Degree of Impacts		
			Human Risk Indexes		
Compound Name	Amount Released (lb/yr)	Air	Water	Soil	Sediment
Ethyl Benzene	3300	0.013	0.005	0.176	0.015
DI		0.1	1	1	1
HRI		0	0	2	0
Ethylene Glycol	4800	0.017	0.001	0.006	0.001
DI		1	1	1	1
HRI		0	0	0	0
Glycol Ethers	21000	N/A	N/A	N/A	N/A
DI		N/A	N/A	N/A	N/A
HRI		N/A	N/A	N/A	N/A
Methyl Ethyl Ketone	5400	0.025	0.463	53.3	0.373
DI		0.1	10	10	10
HRI		0	48	5555	39
N-Butyl Alcohol	12600	0.039	28.9	3461	24.2
DI		10	0.1	0.1	0.1
HRI		4	30	3605	25
Xylene	27000	0.094	0.071	3.16	0.374
DI		1	0.1	0.1	0.1
HRI		1	0	3	0

Table 16. Facility A & B X-Media Model ERI Results

Facility A		Total ERI = 583				
		Category = LOW				
Population Density 613		Rank = 52				
Compartment Concentrations						
Compound Name	Amount Released (lb/yr)	Water	Soil	Sediment	DI	ERI
Methyl Ethyl Ketone	21807	0.645	215.351	0.68	0.5	228
Methyl Isobutyl Ketone	18402	0.18	23.32	0.157	5	115
Toluene	33108	0.09	2.38	0.286	5	12
Xylene	38128	0.1	4.46	0.526	50	228

Facility B		Total ERI = 2025				
		Category = MEDIUM				
Population Density 302		Rank = 2				
Compartment Concentrations						
Compound Name	Amount Released (lb/yr)	Water	Soil	Sediment	DI	ERI
Ethyl Benzene	3300	0.005	0.176	0.015	500	91
Ethylene Glycol	4800	0.001	0.006	0.001	0.5	0
Methyl Ethyl Ketone	5400	0.463	53.3	0.373	0.5	27
N-Butyl Alcohol	12600	28.9	3461	24.2	0.5	1745
Xylene	27000	0.071	3.16	0.374	50	162
Glycol Ethers	21000	N/A	N/A	N/A		

Facility B is a Bottling company in the industrial section of a big city. These sections of a city tend to be scarcely populated. It reported to EPA TRI releases of xylene, ethylbenzene, butanol, MEK, ethylene glycol (monoethyl ether) and glycol ethers. The corresponding HRI's are 4, 2, 3664, 5642, 0 and N/A. MEK accounts for the greatest contribution to the total HRI with 1-Butanol next. One would expect butanol to accumulate more in the surface compartments than MEK because of its low vapor pressure (931 Pa) and high solubility (74,000 mg/l). Looking at the environmental fate predictions proves this theory correct. So why does MEK have a greater HRI than butanol. The answer is simple, MEK has a higher

Degree of impact in the soil, water and sediment then butanol. Ethyl benzene, ethylene glycol (monoethyl ether) and xylene are highly volatile chemicals so both are advected from the study area quickly. Glycol ethers can not be run by the Fugacity model at present due to incomplete chemical data.

ERI values for Facility B are also listed in **Table 16**. No Sensitive areas were present in Facility B's study area. N-butyl alcohol contributed the most to the ERI because of its high ground compartment Ef. Both xylene and ethyl benzene have significant DI,s but in the case both small ground compartment Ef's keep the corresponding chemical specific ERI's low.

When evaluating the results it is only necessary to first look at the category rank. For example, Facility A's HRI falls into the high category where as Facility B's HRI falls into the medium category. Because Facility A received a high category rank it poses a greater relative risk than Facility B which received a medium category rank. To account for facilities that receive similar category ratings each category has been divided into a scale from 1 to 100. The higher the score the greater the relative risk within each category. Splitting each Risk Index into three categories allows a higher degree of sensitivity to be retained. By doing this small changes in the human risk indices can be noticed within each ranking category. Using the comparative risk approach a user can compare a facilities Risk Index with the highest value in its category. This will give the user an idea of the degree of relative risk associated with the facility. ERI values are evaluated similarly to the HRI with the only difference being the ranking scale.

It should be noted that facility A has a larger population density living within the study area than facility B. In terms of the comparative risk assessment employed in the model, the higher the population the greater the potential for human exposure. Since facility A has more people living around it the threat of exposure is greater and the human risk is greater. If there is no population living within the study area there is no risk of human exposure so there will be no HRI associated with the corresponding facility. Neither facility has a sensitive eco-system within their study area so no additional weight is given to either facility ERI.

The HRI and ERI values at this point in time must be viewed as separate entities. No correlation has been established between the two indices. This means that if a facility receives a higher ERI than HRI, it can not be concluded that this facility poses a greater risk to eco-systems than to humans. These risk indices are used to indicate to environmental professionals, the users, of potential risks. Once flagged, the user should go back to the data and pinpoint the high contributors to risk for both the HRI and the ERI. The information by which the risk indices are defined will aid in the decision making process concerning which direction should be taken if further action is needed.

USES OF MODEL

Because of the X-media model's ability to address cross-media impacts of pollutants and convert these impacts into HRI and ERI values for purposes of comparative risk, it occupies an important niche in a number of environmental programs such as: Pollution

Prevention (P2), Toxics Use Reduction (TUR), Enforcement Targeting, and permitting processes.

Facility Inspection Ranking System (FIRS)

As our industrial base grows, the potential for pollution from industry increases. Environmental agencies are issuing more and more permits restricting releases. The sheer increase in the number of permitted facilities raises concerns for the future regarding adequate monitoring. A Facility Inspection Ranking System (FIRS) was derived using the X-media model and other facility specific information to prioritize facilities for inspection. This will ensure regular inspection of facilities which pose the greatest risk to human health.

For each facility the X-media model is run to generate an HRI. In addition to the organic chemicals accounted for in the HRI the amount of SO₂, NO_x, CO₂ and particulate matter (<10 microns) are considered. Also facilities within Ozone non-attainment areas and those with compliance histories receive an additional rank. Some discretion is left up to the inspector to include a judgment factor. Each one of these five categories are weighted differently to derive an inspection ranking for each facility. The individual category ranks are given in **Table 17**.

Table 17. FIRS Ranking Categories and Scales

Ran	HRI	Ran	No _x , So _x , CO	Rank	Non-attainment Area	Ran	Compliance History
1	<59	1	<10 tpy	1	Particulate NAA	1	Complaints Reported
2	59-116	2	11-50 tpy	3	Ozone NAA	3	Non-Compliance in past 2 years
3	117-233	3	51-100 tpy			4	Formal Enforcement action in past 2 years
4	234-468	4	>100 tpy				
5	469-937						
6	938-1874						
7	1875-3749						
8	3750-7499						
9	7500-14999						
10	>15000						

The HRI is given the highest weight because it is a summary of the quantity and type of chemical released, fate and transport predictions, compartment specific toxicity and study area population data. The other categories in the FIRS were adapted from the ODEQ Northwest Region Air Quality Department. The amount of SO₂, NO_x, CO₂ and particulate matter (<10 microns) is an important consideration because such compounds lead to acid rain and contribute to photo-chemical smog. (Walcerk and Chang, 1987) If a facility is releasing Hazardous Air Pollutants (HAP's) in an ozone non-attainment area the health effects associated with the compounds become worse. For example, exposure to sulfuric acid produces a more severe health effect on the lungs in the presence of ozone. (Schlesinger, 1989) Because of the health implications, facilities within Ozone-non-attainment areas are given a higher rank than facilities located outside non-attainment areas.

Compliance History proves to be a good indication of a facilities willingness to obey permit limits. Facilities with poor compliance history tend to have recurring problems with the

environmental permitting agency (ODEQ). For this reason facilities with prior enforcement actions are ranked higher than those with a clean record. Inspector Judgment is irreplaceable when it comes to ranking facilities for inspection. Each inspector has written and issued the permit for their facilities. So when it comes to knowing which facilities are going to be non-compliant no one has a better idea than the individual inspectors. The inspector judgment category can also be used in the presence of an inspection rank tie between two facilities.

A facility is ranked in each of the five categories and the sum is the corresponding inspection rank. The higher the number the higher the priority for inspection. An example of 10 facilities differing in release severity, including individual category ranks, is given in **Table 18**. Even though a facility has a significant HRI rank it does not necessarily mean the inspection rank will be high. This reflects the influence of criteria in the remaining categories. It is a combination of all 5 categories that ultimately defines the inspection ranking order. Using this type of methodology provides environmental professionals with a consistent way to rank facilities for inspection.

Table 18. FIRS Facility Comparison

Facility Name	HRI	Rank	Quantity of Particulate		Non-Attainment Area	Inspector's Judgment	Compliance History	Sum
			SO _x , NO _x , CO(TPY)	Rank				
D	14179	7	<50		2	3		12
E	9283	6	<10		1	3	3	13
F	12	1	<50		2	3	3	9
G	370185	9	>100		4	3	1	17
H	3181	5	<50		2	0		7
I	14819	7	<10		1	3		11
J	13167	7	<10		1	3	1	14
K	689	4	<50		2	3	1	10
L	13	1	<50		2	3	1	8
M	28766	7	<10		1	3		11
N	1964	5	<50		2	3		10
O	27	1	<50		2	3		6
FIRS								
Inspection order								
1 G		7 N						
2 J		8 K						
3 E		9 F						
4 D		10 H						
5 I		11 L						
6 M		12 O						

Pollution Prevention

As illustrated above the results of the X-media model become more useful when coupled with other facility specific information. Other uses for the model include quantifying the progress of Pollution Prevention or Toxic Use Reduction Programs. An example is given in **Table 19**. Facility C, a Paper Company, in 1993 stopped using methyl ethyl ketone and also had a resulting 93% decrease in the use of methanol and a 66% decrease in the use of acetone. This process change resulted in an 33% decrease in air, 100% increase in water and a 97.6% decrease in land releases for methanol and a 48% increase in air, 106% increase in water and a 92.8% decrease in land releases for acetone. This information is ironic because if there is

a decrease in chemical use one would expect a resulting decrease in chemical release. Just the opposite was observed. Similar comparisons should be followed by facility interviews to see if the information reported is false and where the reporting system is flawed. In terms of pollution prevention the question here is whether the increased amount of acetone released to the air and water and the increased amount of methanol discharged to the water is less harmful to human health than the release of methyl ethyl ketone (MEK) to the air. Model results for both years shows that complete substitution of MEK resulted in a 11% increase in facility C's HRI from 1992 to 1993. Because the HRI is used for comparative purposes the resulting number can not be converted to a 'percent increase in risk' methodology. All that can be said is the HRI for facility C, when completely substituting MEK, is higher than when using MEK.

Because of the higher HRI it is assumed the potential for human health risk is higher. This makes sense because acetone and methanol are both water soluble compounds so considerable amounts will be carried to the surface compartments by rain. Even though MEK has a higher degree of impact and is more persistence in the surface compartments than acetone or methanol the increased release and thus increased concentration of both in the study area outweigh the effects of releasing MEK. Using the HRI in this manner gives Pollution Prevention Programs a new piece of information. Progress!! Without a similar process to rank progress these programs are lacking a vital piece of data.

Table 19. Facility Pollution Prevention Yearly Comparisons

Facility 1992					Total HRI = 3251			
No Sensitive Areas					Category = Medium			
					Rank = 9			
					Compartment Concentrations (ug/m3)			
					Degree of Impacts			
					Human Risk Indexes			
Compound Name	Amount Used (lb/yr)	Amount Released lb/yr)			Air	Water	Soil	Sediment
		Air	Water	Soil				
Acetone	64000	21807	3300	18	0.06	1716	236	1378
DI					0.1	1	1	1
HRI					0	908	125	729
Methanol	2111000	176300	30100	18	0.826	15465	278	12388
DI					1	0.1	0.1	0.1
HRI					0	818	15	655

Facility 1993					Total HRI = 2897			
No Sensitive Areas					Category = Medium			
					Rank = 8			
					Compartment Concentrations (ug/m3)			
					Degree of Impacts			
					Human Risk Indexes			
Compound Name	Amount Released (lb/yr)	Air	Water	Soil	Air	Water	Soil	Sediment
Acetone	190000	14750	1600	250	0.07	867	745	696
DI					0.1	1	1	1
HRI					0	459	394	368
Methanol	3.00E+06	274000	0	750	1.28	55	955	44
DI					1	0.1	0.1	0.1
HRI					1	3	51	2
Methyl Ethyl Ketone	20000	5805	250	5	0.027	132	66.6	106
DI					1	10	10	10
HRI					0	702	352	565

Other Uses

The X-media model can aid environmental agency permitting departments in detouring the cross-media transfer of chemicals. Permittees can run the model for their facility and determine if any of the chemical they release to one media is likely to be transported to another

(eg water to air). If a chemical is being transferred from one media to another other permitting departments can be notified.

Alternative Technologies is another useful application of the model. If a facility is thinking of changing processes, the X-media model can determine the relative risk for both human health and the environment before performing any changes. Some examples are switching chemicals or installing solvent recovery systems.

The best location for new facility sites can also be determined by the model before any ground is broken. Running each potential location for the facility through the model will allow the best site to be chosen which poses the least relative risk to both human health and the environment.

LIMITATIONS OF MODEL

One of the major limitations of the model is its fate and transport modeling. The predicted concentrations are not definitive but only order of magnitude estimates. These concentrations should not be viewed as true values because of the many limiting assumptions in default values used in the model. For example, the model assumes steady state, but often the chemicals within the study area will not have time to reach steady state conditions. Often chemical specific parameters have to be estimated because values are not available in the literature. Such estimations can lead to relatively large errors in the predicted concentrations. The Fugacity Model can not handle metals or compounds with negligible vapor pressures.

Without fate and transport predictions, a HRI for a facility can not be calculated. So a facility that releases several metals but only one organic compound, will have a resulting HRI based only on the one organic compound. Either a sensitivity analysis is needed to give error bounds to account for release data unable to be handled by the Fugacity model, or an alternative partitioning model is needed to account for metals. One alternative would be to use a plume model to predict maximum ground level concentrations of metals downwind of the site as the corresponding E_f . It could be assumed that this would be the maximum exposure anyone within the study area would be exposed to. This is a very conservative estimate.

Facility Release Data are obtained from EPA's Toxic Release Inventory (TRI) data. TRI was used because it was the only source for chemical specific release data, which the model requires. This data is a compromise because reported values are in lb/yr even though actual release amounts may be different from day to day depending on specific running conditions. The lb/yr is not based on sampling data but on use and process data. Some compounds are reported as mixtures, e.g. glycol ethers, making it impossible to distinguish specifically which types of a pollutant are being released, and the TRI database is lagging by about two years. (Ross and Associates, 1994) All these oversimplifying assumptions leads to model prediction uncertainties. Since the TRI is the only chemical specific release information available it has been adopted for model release data. It should be noted that the model is not limited to TRI data only. More accurate data can be used when it is available. The study area is defined by a four mile radius surrounding a facility in which there is no incoming pollution.

Uncertainties also exist within the HRI algorithm. If the RfC's or RfD's are not known either the values must be omitted, as in the case of the RfD, or estimations made. The RfC is estimated for a compound by dividing its threshold limit value, if available, by 4200. This approximation method under-estimates the RfC, so the resulting DI and HRI will be conservative. The population ratio and hydrology data are only updated every 10 years, so population explosions in certain areas of the state can not be accounted for from year to year. This proves to be a limitation because it should be expected an urban population density increase would occur within a study area each year. Facilities which release chemicals classified as carcinogens, have extremely large HRI values. This may be an overestimate of the comparative risk because many chemicals that are suspect carcinogens do not have a cancer potency factor, but are potentially, just as harmful, but their HRI is considerably lower. Care should be taken when evaluating an HRI from a facility releasing carcinogens.

CONCLUSION

Though the X-media model has limitations, they are out weighed by the benefits. The fate and transport portion of the model addresses the cross-media concerns associated with facilities releasing toxins into the environment, a pioneering effort in itself. The HRI algorithm provides sound logic to address health concerns. The comparative risk approach allows the HRI to be used for assessing the progress of pollution prevention programs or to rank facilities for annual inspections. If used in the facility permitting process, permit writers can be made

aware of the transfer of pollutants from one media to another. With a consistent methodology in place to address cross-media issues associated with industrial releases, environmental agencies are better able to address human health issues when making permitting decisions. The EPA has recognized this and is interested in adapting the X-Media methodology as the basis for a National level Screening Tool for Enforcement Targeting of industries releasing toxins into the environment.

Future Directions

The first direction of future research will be in establishing a relationship between the HRI and the ERI. This will allow weighting of the two different relative risks for each facility. In other words, a distinction will be able to be made between which risk is of greater concern for a facility, human or ecological? The current version of the X-media model, as with the previous version, cannot calculate a relative risk for facilities only releasing metals. To solve this problem the incorporation of a deposition model to the X-media model was thought to be the best and easiest strategy. This method was taken through the conceptual stage and brought into the initial testing stages. Due to lack of time though, is to be postponed until a latter date.

Excel Program

The X-media model has been implemented in an excel spreadsheet adding even more versatility to its usefulness. The model is organized such that each facility is in one workbook.

The first worksheet contains information about the facility and the study area as well as reported TRI chemicals and their corresponding compartment specific HRI. The total HRI is given at the top of the page. The following worksheets give specific data about the release chemicals as well as fate and transport modeling calculations such as rates and concentrations.

Appendix D contains a copy of the program and the operating instructions.

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APPENDICES

Appendix A

CAS CODE	CHEM NAME	MOL MASS	VAPOR PRES. (Pa)	SOLUBILITY (mg/l)	TEMP. (C)	KOW	HALF LIFE AIR (hr)	HALF LIFE WATER (hr)	HALF LIFE SOIL (hr)	HENRY'S LAW Pa/m3/mol
94-75-7	2,4-D	221	1.4	682	25	646	10	72	720	1.38815E-05
106-89-8	2-(CHLOROMETHYL)OXIRANE	92.53	1733.19	60000	20	2.8	1458	672	672	2.43179328
110-80-5	2-ETHOXYETHANOL	90.12	533.29	10000	25	29	30	420	420	
101-14-4	4,4'-METHYLENEBIS(2-CHLOROANIL									
83-32-9	ACENAPTHENE	154.2	0.206	3.47	25	8317.6	5	152	1372	8.024917824
75-07-0	ACETALDEHYDE	44.06	98658.28	10000	20	2.69				9.866
67-64-1	ACETONE	58.1	30797	10000	25	0.58	1535	96	96	3.7186172
79-10-7	ACRYLIC ACID	72.07	426.63	10000	20	1.45	13	96	96	0.0324
7429-90-5	ALUMINUM (FUME OR DUST)	26.98	133.32		1284					
1344-28-1	ALUMINUM OXIDE (FIBROUS FORM)	101.96								
7664-41-7	AMMONIA	17	882000	531000	20	1	100	100	100	30.397416
6484-52-2	AMMONIUM NITRATE	80.06		1.92						
7783-20-2	AMMONIUM SULFATE	132.16								
120-12-7	ANTHRACENE	178.24	0.03	1.29	25	28184	1	1	6120	6.5861068
7440-36-0	ANTIMONY	121.75	133.32		886					
COMPOUND	ANTIMONY COMPOUNDS									
7440-38-2	ARSENIC	75								1
COMPOUND	ARSENIC COMPOUNDS									
1332-21-4	ASBESTOS (FRIABLE)									
7440-39-3	BARIUM	137.36	1333.22		1049					
COMPOUND	BARIUM COMPOUNDS									
71-43-2	BENZENE	78.1	12690.9	1791	25	134.91	276	252	252	547.153488
50-32-8	BENZO(A)PYRENE	252	0.00000074	0.0038	25	6E+06	1	1	7044	0.243179328
92-52-4	BIPHENYL	154	1.33	7.5	25	5754.4	59	102	102	19.55567096
106-99-0	BUTADIENE	54.09	281000	735	25	97.7	5	420	420	382.313
141-32-2	BUTYL ACRYLATE	128.2	533.29	1600	20	1.12	13	96	96	0.333
85-68-7	BUTYL BENZYL PHTHALATE	312.4	0.00114657	2.9	20	60255	33	96	96	0.1317
63-25-2	CARBARYL	201.22	1.81E-04	32	25	229.08	12.6	672	672	1.30E-03
120-80-9	CATECHOL	110.12	133.32	451000	20	0.88	14	10	10	0.1002
7782-50-5	CHLORINE	70.9	6384000	3261	20	0.5511				1957.682
10049-04-4	CHLORINE DIOXIDE									
67-66-3	CHLOROFORM	119.4	26334	9300	25	89	2496	2496	3427	385.033936
108-43-0	CHLOROPHENOL	128.56	15.86	26000	25	316	47.04	1356	1356	0.0571898
1897-45-6	CHLOROTHALONIL	265.91	0.1	0.6	25					0.167

APPENDIX A (Continued)

CAS CODE	CHEM NAME	MOL MASS	VAPOR PRES. (Pa)	SOLUBILITY (mg/l)	TEMP. (C)	KOW	HALF LIFE AIR (hr)	HALF LIFE WATER (hr)	HALF LIFE SOIL (hr)	HENRY'S LAW Pa/m3/mol
7440-47-3	CHROMIUM	52		0	25					
COMPOUND	CHROMIUM COMPOUNDS	100								
7440-48-4	COBALT	58.93								
COMPOUND	COBALT COMPOUNDS									
7440-50-8	COPPER	64	1330	0.001	18700					6302
COMPOUND	COPPER COMPOUNDS									
8001-58-9	CREOSOTE	204	379	5850	25	128825	25	624	2730	0.065
98-82-8*	CUMENE	120.21	611	50	25	4570	53	120	120	1480
110-82-7	CYCLOHEXANE	84.18	10265.79	55	20	2754	13	2496	2496	186.651
5989-27-5	D-LIMONENE	140	0.01	0	25	1	6	300	600	
117-81-7	DI-(2-ETHYLHEXYL)PHTHALATE	390.54	0	0.3	25	5.11	10000	600		
132-64-9	DIBENZOFURAN	168		10	25	15849	10	420	420	
75-71-8	DICHLORODIFLUOROMETHANE	120.91	566618.5	280	20	100	11649	2496	2496	2023.638
75-71-8	DICHLORODIFLUOROMETHANE (CFC-1	120.91	566618.5	280	20	100	11649	2496	2496	2023.638
75-09-2	DICHLOROMETHANE	84.94	58662	13000	25	17.8	2521	420	420	273.576744
115-32-2*	DICOFOL	370.47	1.33E-04	1.2	24	3467.4	70.08	172.8	172.8	5.66E-05
111-46-6	DIETHYLENE GLYCOL	106.14	133	0.01	59	0.01				13300
1746-01-6	DIOXIN	321.98	0.0000002	0.0000002	25	1E+07	123	12046	12046	0.212781912
298-04-4*	DISULFOTON	272.42	0.02	16.3	20	10471	3	252	288	101.32472
	EPICHLORHYDRIN	92.53	1733.19	60000	25	2.799	1458	672	672	2.672868
140-88-5	ETHYL ACRYLATE	100.13	3910.33	20000	20	0.09	13	96	96	0.196
100-41-4	ETHYLBENZENE	106	1330	168	25	1258.9	47	156	156	879.4985696
107-21-1	ETHYLENE GLYCOL	62.07	11.7	10000	25	0.04	46	168	168	0.006079483
110-80-5	ETHYLENE GLYCOL MONOETHYL ETHER	90.12	706	10000	25	0.794	30	420	420	5197
206-44-0	FLUORANTHENE	202	0.254	0.265	25	79433	11	42	6960	0.958
86-73-7	FLUORENE	166.22	1.33	1.98	25	15849	37	1140	1140	21.2781912
50-00-0	FORMALDEHYDE	30.03	516439	10000	25	2.24	4	96	96	6.4608
354-5-8-5	FREON	187.37								
76-13-1	FREON 113	187.37	48329.23	170	25	1445	175200	100000	100000	284.29
COMPOUND	GLYCOL ETHERS									
1024-57-3	HEPTACHLOR EPOXIDE	106.35	29.92	1	25	5	34	24	9000	29.92
67-72-1	HEXACHLOROETHANE	236.74	50	50	25	8511	278400	2496	2496	1

APPENDIX A (Continued)

CAS CODE	CHEM NAME	MOL	VAPOR	SOLUBILITY	TEMP.	KOW	HALF LIFE	HALF LIFE	HALF LIFE	HENRY'S LAW
		MASS	PRES. (Pa)	(mg/l)	(C)		AIR (hr)	WATER (hr)	SOIL (hr)	Pa/m3/mol
7647-01-0	HYDROCHLORIC ACID	36.46	405300	10000	17.8	0				40.53
7664-39-3	HYDROGEN FLUORIDE	20.01	121056.38	10000	25	2				12.106
67-63-0	ISOH (ISOPROPANOL)	60.1	5719	10000	25	1.12	39	96	96	0.820730232
7439-92-1	LEAD	207.19		0						
COMPOUND	LEAD COMPOUNDS									
108-38-3	M-XYLENE	106.18	799.93		20	1585	14	420	420	
108-31-6	MALEIC ANHYDRIDE	98.06	0.01		20					
7439-96-5	MANGANESE	54.94	133.32		1292					
COMPOUND	MANGANESE COMPOUNDS									
78-93-3	MEK (METHYL ETHYL KETONE)	72.1	13300	270000	25	1.8	353	96	96	4.721731952
999999-99-9	METAL									
67-56-1	METHANOL	32.04	12236	10000	25	0.17	392	96	96	13.678837
96-33-3	METHYL ACRYLATE	86.1	9332.54	52000	20	0.034	15	96	96	0.179
108-10-1	METHYL ISOBUTYL KETONE	100.16	1929	20400	20	15.5	25	96	96	9.6258484
101-68-8	METHYLENE BISPHENYL ISOCYANATE	250.27	0.13		40		3	15	15	
80-62-6	METHYL METHACRYLATE	100.13	5119.56	156000	25	23.99	5	420	420	32.82920928
71-36-3	N-BUTYL ALCOHOL (1-BUTANOL)	74.1	931	74000	25	7.6	48	96	96	0.0710036
91-20-3	NAPHTHALENE	128	10.9	31.7	25	1995.3	16	246	775	48.93983976
1313-27-5	MOLYBDENUM TRIOXIDE	143.94		1						
7440-02-0	NICKEL	58.71								
COMPOUND	NICKEL COMPOUNDS									
7697-37-2	NITRIC ACID	63.02	6372.79	10000	20					0.637
11097-69-1	PCB 1254	327	0.01	0.012	25	407380				273.576744
87-86-5	PENTACHLOROPHENOL	266	0.00017	20	20	2089.3	766	56	2412	0.344504048
85-01-8	PHENANTHRENE	178.24	0.91	1.16	25	31623	11	24	2592	2.593912832
108-95-2	PHENOL	94.11	69.7	87000	25	28.8	13	31	132	0.040225914
7664-38-2	PHOSPHORIC ACID	98	3.8	10000	20	0				0
85-49-9	PHTHALIC ANHYDRIDE	148.11	0.03	6200	25	0	2666	1	1	0.000628214
000075569	PROPYLENE OXIDE	58.08	70940.849	476000	25	1.07	463.2	218.4	218.4	8.65
129-00-0	PYRENE	202	0.000882	0.14	25	75858	1	1	25300	607.94832
78-92-2	SEC - BUTANOL	74.12	2439.7999	181000	25	6.456	39.6	96	96	0.92205
COMPOUND	SILVER COMPOUNDS									
1310-73-2	SODIUM HYDROXIDE	40	133.32		739					

APPENDIX A (Continued)

CAS CODE	CHEM NAME	MOL	VAPOR	SOLUBILITY	TEMP.	KOW	HALF LIFE	HALF LIFE	HALF LIFE	HENRY'S LAW
		MASS	PRES. (Pa)	(mg/l)	(C)		AIR (hr)	WATER (hr)	SOIL (hr)	Pa/m3/mol
100-42-5	STYRENE	104.2	877.8	310	25	891.3	4	504	504	284.7224632
7446-09-5	SULFUR DIOXIDE	64.07	3242391.04	0.08	22					40529888
7664-93-9	SULFURIC ACID	98.08	133.32	10000	25					0.013
62-56-6**	THIOUREA	76.12		91.8	25	0.0216	8.8	96	96	
1314-20-1	THORIUM DIOXIDE	264								
7550-45-0	TITANIUM TETRACHLORIDE	189.7								
108-88-3	TOLUENE	92.1	3777.2	534.8	25	537	57	312	312	601.8688368
584-84-9	TOLUENE-2,4-DIISOCYANATE	174.17	13.33		20					
26471-62-5	TOLUENEDIISOCYANATE (MIXED ISO	174.17								
71-55-6	TRICHLOROETHANE,1,1,1-	133.42	16491.93	347	25	309	29661	4956	4956	6383.45736
79-01-6	TRICHLOROETHYLENE	131.4	9177	1100	25	263	150	6480	6480	1043.644616
75-69-4	TRICHLORODIFLUOROMETHANE									
75-69-4	TRICHLOROMONOFUOROMETHANE	137.36	107031.22	1080	25	338.84	715000	6480	6480	9828
95-63-6	TRIMETHYLBENZENE,1,2,4-	120.19	270	51.9	25	4466	8	370	370	577.550904
108-05-4	VINYL ACETATE	86.09	11332.404	25000	20	5.37	12	175.2	696	48.73
1330-20-7	XYLENE	106.16	877.8	175	25	1318.3	23	420	420	516.756072
7440-66-6	ZINC	5		0	25	18.62				
COMPOUND	ZINC COMPOUNDS									

APPENDIX B

Chemical Name	Degree of Impact (Human)			Cancer Potency Factor		Degree of Impact (Ecological)
	Air	Soil	Water	Ingestion	Inhalation	
Acenaphthene		1	1			50000
Acetaldehyde	10					
Acetone	0.1	1	1			5
Acrylic Acid	100	1				5
Aluminum(fume or dust)	100					
Ammonia	1	0.1	0.1			50
Anthracene	100	0.1	0.1			500000
Antimony	1000	1000	1000			
Arochlor 1254	1000					500000
Arsenic		1000	1000			
Barium	1000	1	1			
Benzene	1000	100	100	100	10	50
Benzo{a}pyrene				100000	100000	
Biphenyl		1				500000
Butadiene	0.1				10	
1-Butanol	10	0.1	0.1			0.5
Butyl Benzyl Phthlate		10	10			50000
Catechol	10					
Chlorine	1000	10	10			
Chloroform	10	10	10			5
2-(Chloromethyl) Oxirane	0.1	100	100			50
Chlorothalonil		10	10			0.5
Chromium	1000	0.1	0.1			
	0					
Cobalt	1000					
	0					
Copper	1000	1	1			
Creosote		1	1			0.5
Cumene	0.1	10	10			
Cyclohexane	1					
2,4-D	100	10	10			5000
D-Limonene		0.1	0.1			
Di-(2-ethylhexyl)- Phthalate	10	10	10			

APPENDIX B (Continued)

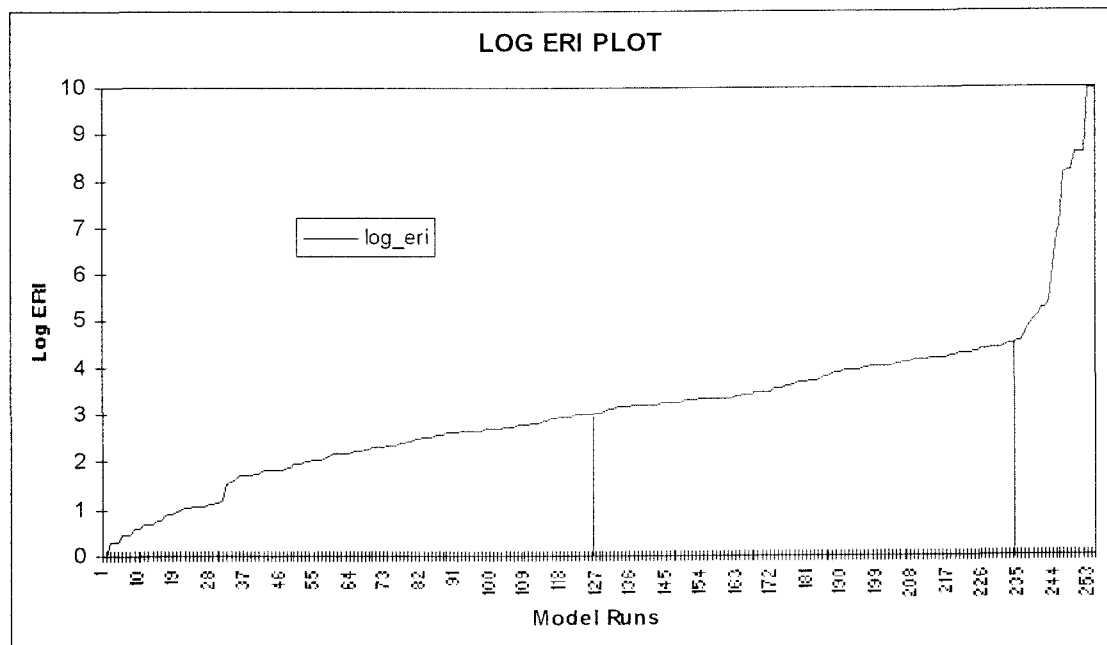
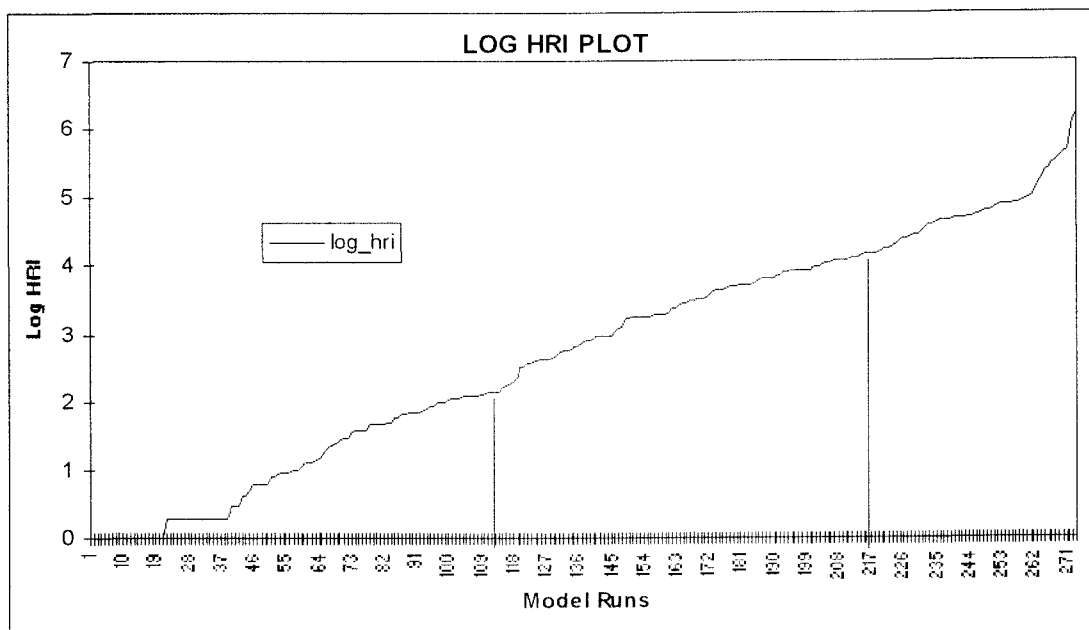
Chemical Name	Degree of Impact (Human)			Cancer Potency Factor		Degree of Impact (Ecological)
	Air	Soil	Water	Ingestion	Inhalation	
Dichlorodifluoro methane	0.1	1	1			
Dichloromethane	10	1	1	100	10	50
Dioxin				1000000	1000000	
Disulfoton	10000	10000	10000			
2-Ethoxy Ethanol	1	1	1			5
Ethyl Acrylate	10					
Ethyl Benzene	0.1	1	1			500
Ethylene Glycol	10	0.1	0.1			0.5
Ethylene Glycol monoethyl ether	1	1	1			0.5
Fluoranthene		10	10			5000
Fluorene		10	10			50000
Formaldehyde	1000	1	1			5
Heptachlor	0.1	10000	10000		10	50000
Epoxide						
Hexachloroethan e		100	100			500000
Hydrochloric Acid	10	10	10			
Hydrogen Fluoride	100					
isopropanol	0.1					
Lead	10000	1000	1000		1000000	
Maleic Anhydride	1000	1	1			
Manganese	1000	10	10			
Methyl Ethyl Ketone	0.1	10	10			0.5
Methanol	1	0.1	0.1			0.5
Methyl Acrylate	10					
Methyl Isobutyl Ketone	10	1	1			5
Methyl methacrylate	1	1	1			50
Methyl Bisphenyl Isocyanate	10000					

APPENDIX B (Continued)

Chemical Name	Degree of Impact (Human)			Cancer Potency Factor		Degree of Impact (Ecological)
	Air	Soil	Water	Ingestion	Inhalation	
Molybdenum Trioxide	100					
Napthalene	10	100	100			
Nickel	1000	10	10			
Nitric Acid	0					
	100					
Pentachlorophen ol	1000	10	10	1000		
Phenol	100	0.1	0.1			5
Phosphoric Acid	1000					
Phthalic Anhydride	100	0.1	0.1			
Propylene Oxide	10			10	100	
Pyrene		10	10			500000
Sodium Hydroxide	100					
Styrene	1	1	1			5000
Sulfur Dioxide	100					
Sulfuric Acid	1					
Tetrachloroethyl ene	1			1000	10	5
Toluene	1	0.1	0.1			5
Toluene-2,4- Disocyanate	1000					
	0					
Trichloroethane	1	1	1			
Trichloroethylen e	1	10	10	100		
Trichlorofluorom ethane	0.1	1	1			
1,2,4- Trimethylbenzen e	10					
Vinyl Acetate	1					5
o-Xylene	1	0.1	0.1			50
Zinc		1	1			5000

* Missing values are due to lack of chemical toxicity and physical data.

APPENDIX C



APPENDIX D

Cross-Media Comparative Risk Assessment Model Operating Instructions

Forward: The Oregon Department of Environmental Quality has developed a Cross-Media Comparative Risk Assessment model (X - Media) to address certain regulatory concerns. The model generates a Human and Ecological Risk Index for a facility releasing toxins into the environment. The Risk indices are based on chemical fate and transport predictions, toxicity, population density and ecological sensitive areas. The model can be used to rank facilities for inspection or as a tool to assess the progress of pollution prevention programs. Regulatory permitting departments can use the model to address the cross-media transfer of pollutants from one environmental compartment to another. The versatility of the model allows adaptation to each specific users needs.

The X-media model accounts for a four mile radius surrounding a facility and defines it as the study area. Study Area information such as water area, population density and ecological sensitive areas are obtained from GIS. Fate and Transport modeling is performed to consider cross-media impacts of toxins released by a facility. The Fate and Transport model divides the study area into four compartments: Air, Water, soil and Sediment. Facility Release information used by the model is obtained from EPA's TRI database.

The X- media model contains two basic Algorithms:

1. Human Risk Index (HRI)

$$HRI = (Ef * DI) * (PR * DV)$$

Ef - Exposure Factor

DI - Degree of Impact

PR - Population Ratio

DV - Degree of Vulnerability

The Ef (exposure factor) is the media specific concentration (ug/m3) predicted by the fugacity fate and transport model.* The exposure factor is defined by concentration because as a chemical builds up in an environmental media the potential toxicity of the compound, or its resulting response, increases upon exposure.

APPENDIX D (Continued)

A degree of impact (DI) is defined for a chemical in each compartment, and is based on a chemicals' cancer and non-cancer effects. The non-cancer DI is based on the chemical Reference dose (RfD) for water, soil and sediment and its Reference concentration (RfC) for air. Cancer Potency factors for ingestion and inhalation are used to define a DI for chemicals that are carcinogens. Appendix A contains the DI ranking scale.

The Population Ratio is simply the population density of the exposed individuals within a 4 mile radius of a facility (Study Area), divided by the population density of the state of Oregon. The population living within the 4-mile radius of the facility has been selected as the population at risk.

An HRI is calculated in each media (air, water, and soil) for every organic chemical released by the facility. The individual media HRI are summed to give a total chemical HRI. A total Facility HRI is calculated by summing the individual chemical total HRI's.

* Fugacity is a procedure used for calculating the behavior of chemicals in an environment.

2. Ecological Risk Index (ERI)

$$ERI = \sum_{n=1}^{n=i} [(SAR * DV)]_i * (Ef * DI)$$

SAR - Sensitive Area Ratio

DV- Degree of Vulnerability

Ef- Exposure Factor

DI - Degree of Impact

SAR is the area of each exposed sensitive environment within the study area divided by the study area (4-mile radius). EPA Classified Sensitive Environments are used.* The Degree of Vulnerability term is measured in terms of the sensitivity of the ecosystem within the study area. Appendix B lists the Sensitive Environments and their corresponding Degree of Vulnerability. The sum and limit signs indicate that each Sensitive Area and corresponding Degree of Vulnerability term is treated separately and then added together before carrying out the rest of the calculation.

The Ef is the media specific concentration in ug/m3 predicted by the fugacity model. Because of the lack of data regarding Ecological Impacts from air pollution, only impacts from water and soil are used to calculate the ERI.

APPENDIX D (Continued)

The DI for the ERI is based on a chemicals K_{ow} * and No Observable Adverse Effect Level (NOAEL). This DI is calculated by weighing a chemicals Log K_{ow} or solubility (if the K_{ow} is unavailable) against its NOAEL. Appendix C outlines the ERI DI ranking scale.

One ERI is calculated for each organic chemical released by the facility. A total facility ERI is calculated by summing all the individual chemical ERI's.

Inorganic compounds such as metals or chemical mixtures such as glycol ethers cannot be run through the model.

The HRI and ERI are not to be summed together, they are to be treated separately.

HRI - ERI Interpretation

Before interpreting the results each total HRI and ERI must be split into three categories low, medium and high. This was done because of the large range of HRI and ERI values resulting in a non-normal distribution. A distribution of the HRI and ERI are included in Appendix D. Once categorized the results are standardized and then ranked from 1 to 100. The following table outlines the category ranges, standardization factors, and ranking equations. It should be noted that these calculations are not performed automatically in the X-Media spreadsheet. These calculations must be performed by the user.

HRI Ranking

Category	Ranges	Standardization (S)	Ranking
Low	1 - 250	$(HRI-41.25)/52.75$	$S*22.8+18$
Medium	251 - 34600	$(HRI-7051.57)/7689.37$	$S*22.3+20$
High	34601 - 1640000	$(HRI-197332)/326364$	$S*20.25+11$

*EPA Classified Sensitive Environments were obtained from the December 14, 1990 Federal Register.

*Octanol/Water Partition Coefficient, used as an indicator of chemical persistence.

ERI Ranking

Category	Ranges	Standardization (S)	Ranking
Low	1 - 1150	$(ERI-297)/322.80$	$S*28.2+27$
Medium	1151 - 50000	$(ERI-9653)/9619.66$	$S*19.65+18$
High	50001 - 10000000	$(ERI-2099397)/3578161$	$S*35.7+26.02$

APPENDIX D (Continued)

Each preceding worksheet contains:

1. Chemical specific parameters of one chemical released by a facility
2. Amount of chemical released
3. Degree of Impact of chemical released
4. Fate and transport predictions of chemical in study zone (media specific concentrations).
 - Concentration ($\mu\text{g}/\text{m}^3$)
 - Amount (moles)
 - Amount of chemical removed from study area by advection or reaction.
 - Overall Residence Times (overall time a chemical spends in the environment)
 - Compartment transport values (amount of a chemical entering or leaving a specific compartment)

Worksheets 2 - 16

	A	B	C	D	E	F	G
1	Worksheet: Toluene						
2			(g/mol)	(Pa)	(mg/l)	(C)	
3	108-88-3	TOLUENE	92.1	3.7772	0.048	25	637
4							
5							
6							
7	Property	Air	Water	Soil	Sediment	Total	
8	Area (m2)		426443.539	129673485	426443.539		
9	Volume (m3)	1.302E+11	1705774.155	12967348.5	3411.54831		
10	Release (lb/yr)	309000	0	0	0		
11	Release (mol/hr)	174.0892933	0	0	0		
12	Background Conc. (mol/hr)	0	0	0	0		
13	Z-Value (mol/m3Pa)	0.000407246	0.001981467	0.00335935	0.00535276		
14	Fugacity (Pa)	3.43801E-05	0.32025E-06	2.5828E-05	3.5819E-06		
15	Conc. (ug/m3)	1.289506144	0.997248483	22.263311	3.0478385	27.598	
16	Amount (mol)	1822.950054	0.017914305	3.13458405	0.0931129	1826.1	
17	Dt	1	0.1	0.1	0.1		
18	D-Reaction (mol/hr)	22.16323487	3.97862E-05	0.01309523	17.5069621		
19	D-advection (mol/hr)	151.9125045	0.00044781				
20	Reaction residence time	82.25108225	450.2640288	239.912808	6.449E-09		
21	Advection residence time	12	40.00422728				
22	Overall residence time	48.72386472					
23							
24	Partition	D-value	D-Value				
25	Data	Mol/Pa hr	mol/hr				
26	Air-Water	14.68555921	0.000504891				
27	Water-Air	14.08940554	8.90486E-05				
28	Air-Soil	988.5882962	0.033987774				
29	Soil-Air	807.2652165	0.020849739				
30	Soil-Water	2.819007563	7.28083E-05				
31	Water-Sediment	0.447042769	2.82542E-06				
32	Sediment-Water	0.447042769	1.77113E-06				

APPENDIX D (Continued)

What is needed to perform a Study?

1. To perform a study you will need the following facility information:
 - a. latitude and longitude
 - b. Toxic release data
 - c. Water area and population density, and sensitive areas within the study zone
 - d. Physical chemical parameters of toxins released

The latitude and longitude and toxic release data are obtained from EPA's TRI database. A copy of the TRI database will be included on disk. The water area and population density of the study zone are obtained from the Geographical information system located on the 5th floor of DEQ head quarters building. Amy Clark (ext. 5370) or Doug Terra (ext. 5044) run the GIS. All that is needed is the facility name and latitude and longitude coordinates. The physical-chemical parameters of several toxins are located in the X-media chemical database. A copy of the data base will be included with the X-media model.

Performing a Study

Before starting a study, the X-Media model and X-media chemical files must be open in excel.

1. The Summary sheet and each preceding sheet contains cells highlighted in yellow. These cells represent spaces where values must be inputted. There is only one exception, the Ecological Sensitive area highlighted cells in the Summary sheet do not require any input values if no sensitive areas are present in the study zone.
2. In the Summary sheet the Water Area and Population density cells must have values inputted.

Summary Worksheet

	A	B	C	D	E	F	G	H
1	Facility Name:	Facility A						
2		123 No Pollution Way						
3		Portland	OR		97503			
4								
5								
6	Water Area	126444	m(2)	TYPE	ORDCA	RHA		
7	Soil Area	100000000	m(2)	AREA	476934	1E+05		
8	Population density	8.83		DV	25	75		
9	YEAR	1993						

APPENDIX D (Continued)

3. Each preceding sheet contains one chemical that the facility is releasing. To input the chemical specific parameter information on each sheet the X-Media chemical database must be open. Within the X-media chemical database find the first chemical that the facility is releasing. (The chemicals within the X-media database are in alphabetical order). Once the chemical is found highlight the entire row containing the chemical of interest and copy it. Next, select sheet 2, row 3, column A, of the X-Media model and paste the chemical specific parameters. Now the specific chemical release information must be inputted for each media the toxin is released (Air, Water, Soil). This information is obtained from the TRI database. For air stack and fugitive releases are added together. Water and land releases are inputted as is. These cells are highlighted in yellow (Row 10 Column C, D, E). If the background concentration is known this information can also be inputted but is not necessary to run the model. (Row 12, Column C, D and E).

Worksheets 2 - 16

	A	B	C	D	E	F	G
1							
2			(g/mol)	(Pa)	(mg/l)	(C)	
3	108-88-3	TOLUENE	92.1	3117.2	133.8	25	154
4							
5							
6							
7	Property	Air	Water	Soil	Sediment	Total	
8	Area (m2)		426443.536	129673485	426443.536		
9	Volume (m3)	1.302E+11	1705774.156	12967348.5	3411.54831		
10	Release (lb/yr)	309000	0	0			
11	Release (mol/hr)	174.0892933	0	0			
12	Background Conc. (mol/hr)	0	0	0			

4. If a chemical is not present in the X-Media chemical database the user can input the physical-chemical parameters by hand in row 3 column A - X or contact D. Borys at 229-6858 or Regina Bridwell 229-6913.

5. Step 3 must be completed for each chemical a facility is releasing. Inorganic chemicals can be inputted but no results will be calculated on the summary sheet. Note, each worksheet only contains one chemical.

APPENDIX D (Continued)

Example: Facility A is releasing the following chemicals:

Chemical	Media Chemical Released (lb/yr)		
	Air	Water	Soil
Acetone	200	123	0
Methanol	2000	0	0
Butanol	0	65	200
Ethylene Glycol	0	6000	0

** The Table is interpreted as follows: Facility A is releasing 200 lb/yr of Acetone to the air, 123 lb/yr to the water and 0 lb/yr to land, 2000lb/yr of methanol to the air and 0lb/yr to the water and soil, etc.

The Study Zone has a water area of 1E06 m2 and a population density of 560.

In the Summary sheet the water area of 1E06 and population density of 560 would be inputted (Row 6 and 8 column C). In sheet 2 the chemical specific parameters for acetone would be pasted on row 3 column A and the 200 lb/yr in air and 123 lb/yr in water release information would be inputted on row 10 column C and D. In sheet 3 the chemical specific parameter information for methanol would be pasted on row 3 column A and the 2000 lb/yr in air release information would be inputted in row 10 column C. The same information would be inputted for butanol on sheet 4 and ethylene glycol on sheet 5.

6. Once all the chemical release information is inputted return to the Summary sheet to view the results. Lines 13 - 16 columns A - H will contain the summary HRI and ERI information. Lines 17 - 27 columns A- H will contain code that links them to worksheets 6 - 16. Lines 17-27 can be deleted if undesirable. If any inorganic chemicals were inputted in sheets 2 - 16, an error message will be seen in the summary sheet. No HRI or ERI values are able to be calculated for inorganic chemicals at this time. If inorganic chemicals are present in the summary sheet type N/A in the cells where that chemicals HRI and ERI values usually appear. For example, if sheet 7 contains an inorganic chemical then N/A should be typed in row 18 columns C-H in the summary sheet.

APPENDIX D (Continued)

Summary Worksheet

	A	B	C	D	E	F	G	H
11	Chemical		Compartment Human Risk Index				Total	
12	Sheet #	Name	Air	Water	Soil	Sediment	HRI	ERI
13	2	ACETONE	0	0	1	0	1	207
14	3	METHANOL	0	324	3183	250	3767	102512
15	4	BUTANOL	0	0	2	0	3	68
16	5	ETHYLENE GLYCOL	0	929	9239	748	10917	2972
17	6							
18	7							
19	8							
20	9							
21	10							
22	11							
23	12							
24	13							
25	14							
26	15							
29	RESULTS							
30							HRI=	14688
31							ERI=	105867

7. The HRI and ERI results (Column G and H) are summed in the Results Section on row 30 and 31. To perform the summing operation click on row 30 column H and type '=sum(G13:G16)'. Repeat for the ERI except sum column H. Always sum the HRI and ERI for all the chemicals present on the summary sheet.

8. If all the inputted information is correct and the results are satisfactory the workbook can be saved. To save the file choose the 'save as' command in the file menu. Give the file an eight character code descriptive of the facility name. This will ensure the same facility is not run twice.

9. To print the summary sheet, click the print icon on the tool bar or choose the print command in the file menu. To Print the sheet 2 - 16, choose the desired sheet, highlight Rows 1 - 32 columns A - G and select the print command from the file menu. When the print window appears choose **selection** and then OK. Repeat for each desired sheet.

Updating Yearly Facility Information

Once a facility has been run for one year it can easily be updated for another year.

1. The water area and population density will not be changed (The GIS data is only updated every ten years).

APPENDIX D (Continued)

- The only changes necessary are in worksheets 2 - 16, the type and quantity of toxin released.

Worksheets 2 - 16

	A	B	C	D	E	F	G
1	108-88-3	TOLUENE	92.1	3771.7	534.6	26.1	537.7
2		(g/mol)	(Pa)	(mg/l)	(C)		
3	108-88-3	TOLUENE	92.1	3771.7	534.6	26.1	537.7
4							
5							
6							
7	Property	Air	Water	Soil	Sediment	Total	
8	Area (m2)		426443.536	126673485	426443.536		
9	Volume (m3)	1.302E+11	1705774.156	12667348.5	3411.54631		
10	Release (lb/yr)	308000	0	0			
11	Release (mol/hr)	174.0892933	0	0			
12	Background Conc. (mol/hr)	0	0	0			

- If the chemicals released for the latest year are the same as the previous year then the only changes to be made are in the amount of each chemical released.
- If the latest year TRI data is different than the previous year, but the total number of chemicals released is unchanged, then changes only have to be made in the type and amount of chemical released. If the type of chemical released is being changed refer to Performing a Study Step 3.
- If the total amount of toxins being released by a facility is greater than the previous year the summary sheet as well as sheet 2 - 16 has to be changed.

- To update the Summary sheet to include the additional chemicals inputted in worksheets 2-16 perform the following instructions:

For the HRI -

- Copy the cells in the last row that contain the compound name and the Air HRI Value.
- Paste the same number of cells as the additional number of chemicals released that were inputted for the new year directly below the copied cells.
- Each pasted cell must be edited starting with the cell closest to the copied cell.

APPENDIX D (Continued)

- The only change that has to be made is the worksheet # present in the Formula. If the new chemical was placed in worksheet 7 then all the 'worksheets' seen in the formula must say 'worksheet7'. To change the worksheet # in the formula just delete the old number and put in the new number. Each row in the summary sheet corresponds to one worksheet number.

Summary Worksheet

	A	B	C	D	E	F	G	H
1	Facility Name:		Facility A					
2			123 No Pollution Way					
3			Portland	OR	97503			
4								
5			SENSITIVE ENVIRONMENT					
6	Water Area		426444 m(2)	TYPE	ORDCA	RNA		
7	Soil Area		100000000 m(2)	AREA	476934	1E+05		
8	Population density		8.83	DV	25	75		
9	YEAR		1993					
10								
11		Chemical	Compartment Human Risk Index				Total	
12	Sheet #	Name	Air	Water	Soil	Sediment	HRI	ERI
13	2	TOLUENE	0	0	1	0	1	207
14	3	ACETONE	0	324	3183	260	3767	102512
15	4	METHANOL	0	0	2	0	3	68
16	5	MEK (METHYL ETHYL KETONE)	0	929	9239	746	10917	2972
17	6	XYLENE	0	0	0	0	0	108
18	7							
19	8							
20	9							
21	10							
22	11							
23	12							
24	13							
25	14							
26	15							
27	16							
28								
29	RESULTS							
30							HRI=	14688
31							ERI=	105867

- After the pasted cells formula worksheet #'s have been updated copy column C of the updated cells and paste them in the first row of the updated cells column D - F.
- Column G contains the formula to sum the preceding HRI's. Copy a cell in Column G that has a value present and paste it in the cells with no values (The cells updated).

APPENDIX D (Continued)

For the ERI -

1. Column G contains all the formulas to calculate the ERI. Essentially the ERI is updated the same way as the HRI.
2. Copy the last cell in column G that contains an ERI and paste the contents in the empty cells below. For example, if two new chemicals were added then two cells directly below the copied cell will have values pasted in them.
3. The Worksheet #'s within the formulas of the pasted cells must be changed to correspond to the worksheet #'s where the new chemicals were inputted. Just like before, if one of the new chemical was inputted in worksheet 7 then all the 'worksheet #'s' within the formula must be changed to 'worksheet7'.

Saving the Updated File

1. Each Reporting year should have a separate directory so facility file names are consistent from year to year.
2. If a directory is not created for the year corresponding to the updated facility one must be created before the updates can be saved.
3. Directories are created in file manager and are named by reporting year. For example, if the reporting year is 1993 the directory is named 1993.
4. Save each updated facility in the directory corresponding to the reporting year data inputted.

- It is important to note that if you do not change the directories before saving the changes the old data will be lost and the new data will be in its place.

APPENDIX D (Continued)

STUDY EXERCISE:

Facility B located at 300 E 50th St. in Portland, Oregon reported releasing the following chemicals in 1993:

Chemical	Media Chemical Released (lb/yr)		
	Air	Water	Soil
Toluene	309,000	0	0
Acetone	717600	0	0
Methanol	46000	0	0
Methyl Ethyl Ketone (MEK)	307000	0	0
Xylene	10050	0	0

The Study Area contains:

Water Area	426444 m2	
Population Density	8.8341	
Type of Sensitive Environment	Area of Sensitive Environment	Degree of Vulnerability
ORDCA	476934.1 m2	25
RNA	1218291 m2	75

** Appendix B contains Sensitive Area abbreviation descriptions.

If all the input parameters were entered correctly the HRI and ERI should have values of:

Chemical Name	Compartment Human Risk Index				Total HRI	ERI
	Air	Water	Soil	Sediment		
TOLUENE	0	0	1	0	1	207
ACETONE	0	324	3183	260	3767	102512
METHANOL	0	0	2	0	3	68
MEK (METHYL ETHYL KETONE)	0	929	9239	748	10917	2972
XYLENE	0	0	0	0	0	108
RESULTS						
					HRI=	14688
					ERI=	105867