



3MRA Uncertainty and Sensitivity Analysis

SAB Review 3MRA Version 1.0 Panel Meeting: August 26, 2003

Justin Babendreier

Office of Research and Development, U.S. EPA

Presentation Outline

- Modeling System Overview; 3MRA Versions
- 3MRA Version 1.0
- National-scale Assessment Dimensionality
- SuperMUSE: Windows-based Supercomputer
- 3MRA Ver1.x UA/SA Software Tools
- Model Evaluation Approaches
- 3MRA Version 1.0 UA/SA Plan
- Example Model Output Using Version 1.x



Modeling System Version Overview:

FRAMES and 3MRA

Definition and Relationship between FRAMES and 3MRA

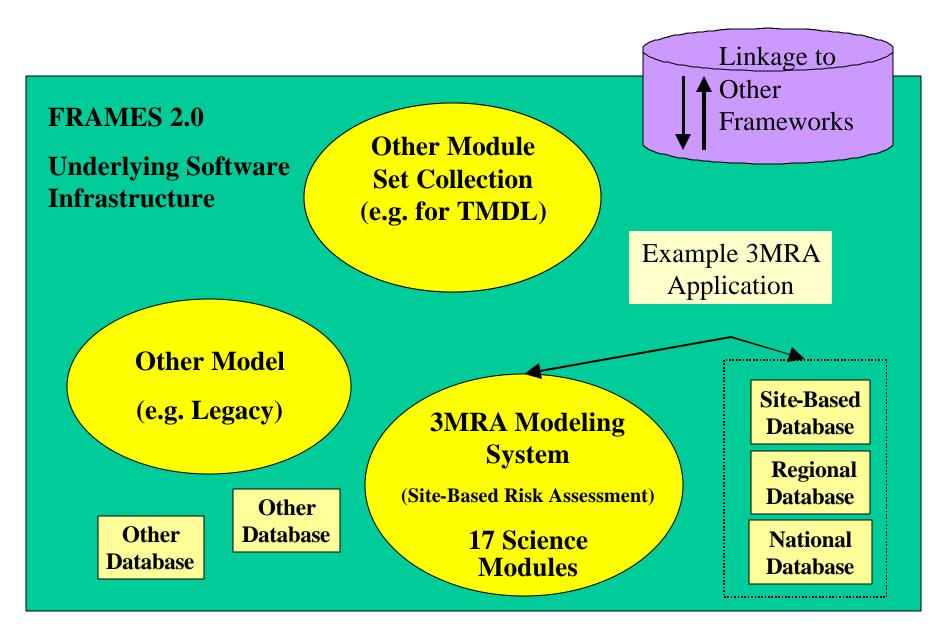
FRAMESFramework for Risk Analysis in MultimediaEnvironmental Systems

Underlying software infrastructure for 3MRA and other models and modeling systems

3MRAMultimedia, Multipathway, Multireceptor, Risk
Assessment

A specific set of models for conducting site-specific or site-based risk assessments, and "rolled-up" studies on regional and national scales.

Conceptual Relationship Between Framework Technology, Models and Modeling System, and Applications



FRAMES 3MRA Versions

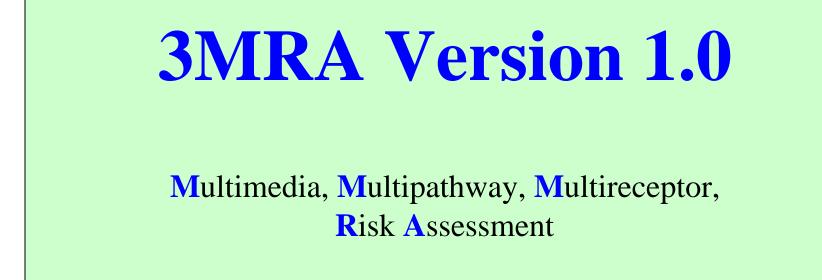
3MRA Version 1.0: National site-based risk assessments

3MRA Version 1.x: A tool set extension to facilitate:
(1) Parallel processing of 3MRA model runs
(2) Uncertainty and sensitivity analyses studies

3MRA Version 2.0 Beta: Same science and data with an extension to facilitate site-specific risk assessments. Significantly advances the design of the underlying FRAMES infrastructure.

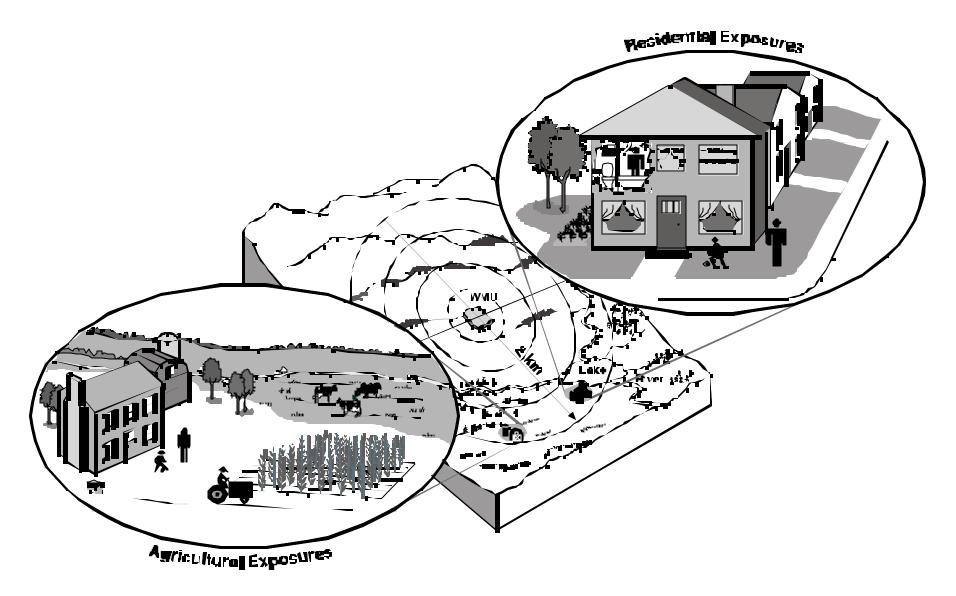
FRAMES 2.0 joint, multi-agency development



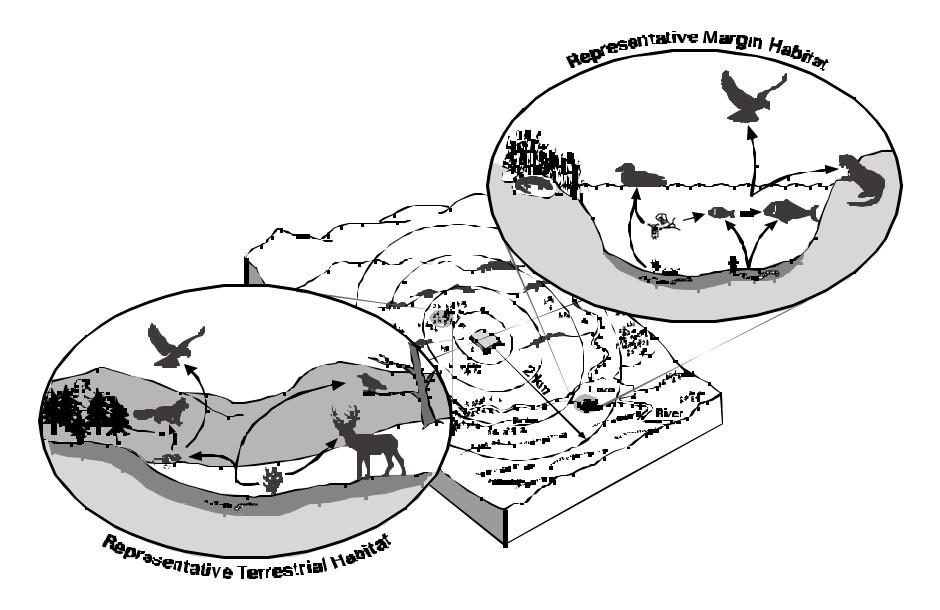


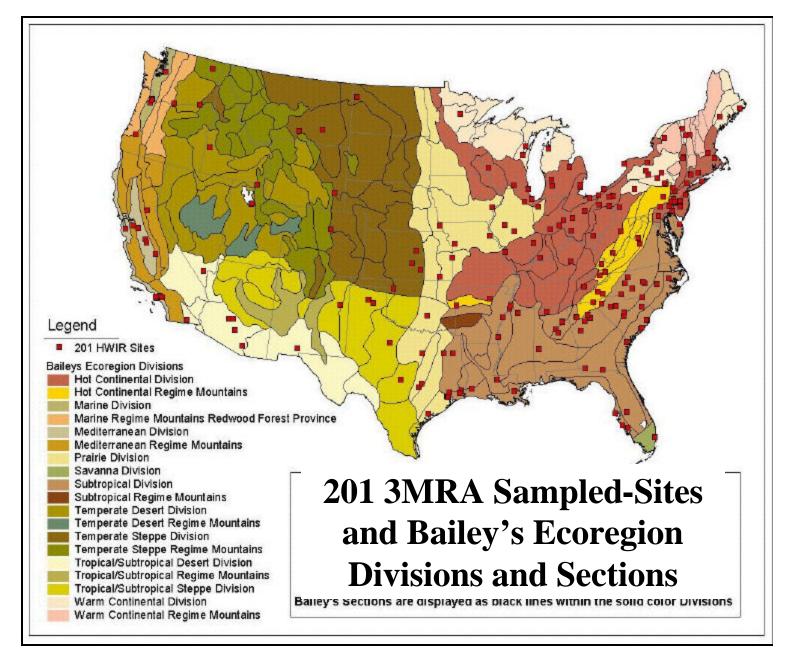
...A screening-level, site-based modeling approach for nationalscale assessment of land-based hazardous waste disposal.

Conceptual Framework For Human Receptors



Conceptual Framework For Ecological Receptors





...419 Site-WMU Combinations in 3MRA databases

Overview of 3MRA National Study

Source Types (WMUs)

Surface ImpoundmentAerated Tank

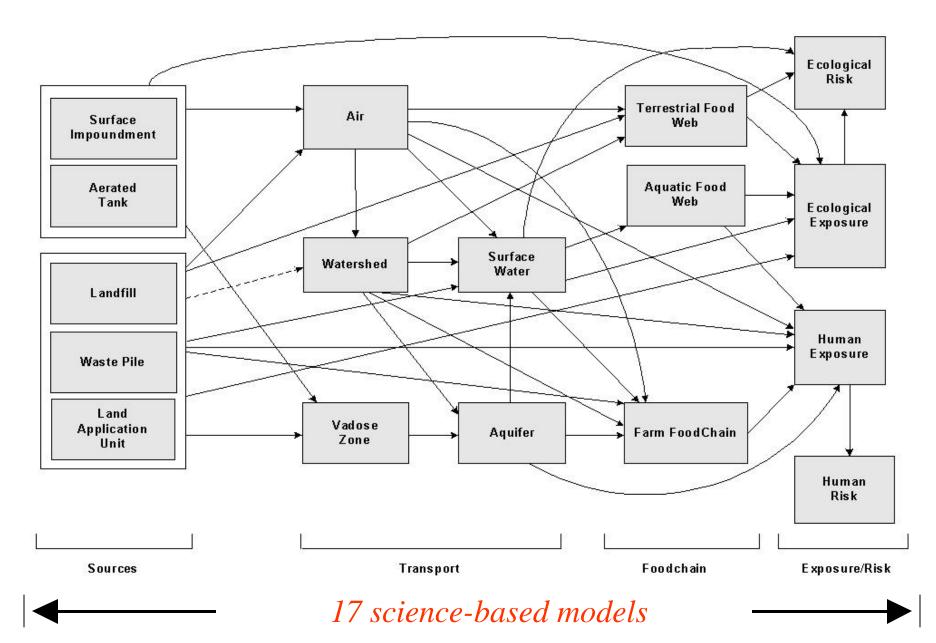
- •Landfill
- •Waste Pile
- •Land Application Unit

Problem Statement Conceptual Model Modeling System Input Data Sampling-Based Simulation Output Data

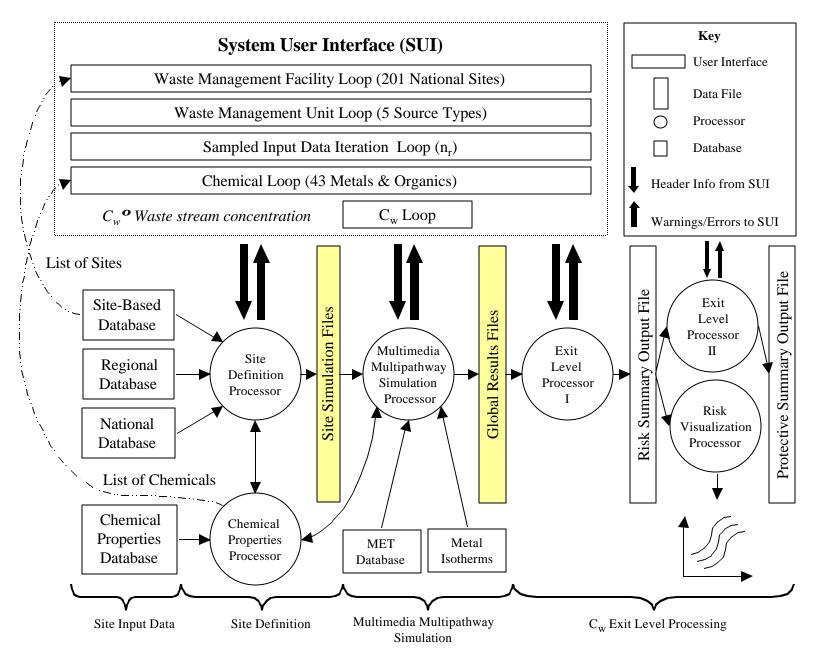
"Exit Level" Post-Processing

Variability, Uncertainty and Sensitivity
Cancer (risk probability)
Noncancer (hazard quotient)
Population weighted risk distribution
Multiple protection measures

3MRA Science Modules and Connectivity



3MRA Stand-Alone Design: Input-Output



3MRA Model Input Variables (966)

SystemGroup	3MRA10	Ŧ	
DictCode	ssf	+	
Number of Inputs		-	
ModGroup	 Dictionary Description 	•	Total
af	aquatic foodweb		21
aq	saturated zone		14
ar	air		23
at	AT		24
ср	chemical properties		142
ee	ecoexposure		14
er	ecorisk		4
ff	farm foodchain	1	45
hđ	header		63
he	human exposure		105
hr	human risk		7
lau	LAU		51
lf	LF		44
si	SI		25
sl	site layout		208
sw	surface water		24
tf	terrestrial foodweb		31
vz	vadose zone		3
wp	WP	50	
ws	watershed	23	
Grand Total			921

Broken down by 20 iconic input dictionaries

Each input - up to 3 dimensions...

3MRA Model Output Variables (372)

SystemGroup	3MRA10	÷
DictCode	grf	•
Number of Inputs		
ModGroup	- Dictionary Description	- Total
af	aquatic foodweb	18
aq	saturated zone	11
ar	air	17
ee	ecoexposure	3
er	ecorisk	27
ff	farm foodchain	39
he	human exposure	78
hr	human risk	39
sl	site layout	4
sr	source	38
sw	surface water	19
tf	terrestrial foodweb	60
VZ	vadose zone	5
ws	watershed	14
Grand Total		372

Each output up to 5 dimensions...

These are further postprocessed into more useful risk endpoints....



3MRA National Assessment Strategy

... screening-level, site-based modeling approach for national-scale assessment of land-based hazardous waste disposal.

National-Scale Problem Statement

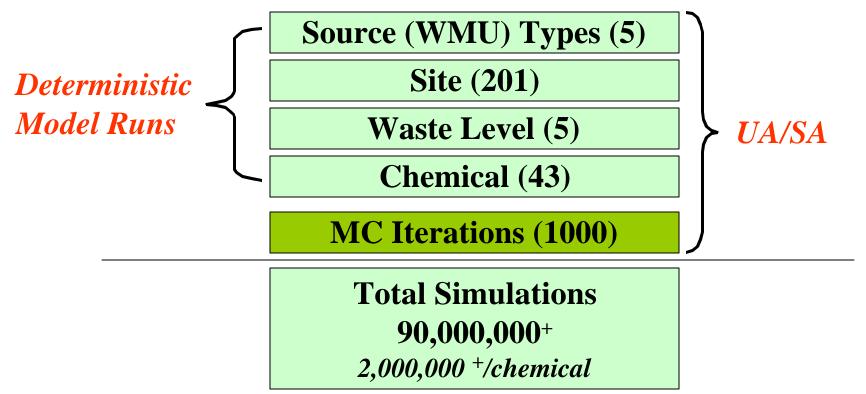
At what waste stream concentration (C_w) will wastes, when placed in a non-hazardous waste management unit over the unit's life, result in:

- 1. (Human) Greater than A% of the people living within B distance of the facility with a risk/hazard of C or less, and
- 2. (Ecological) Greater than D% of the habitats within E distance of the facility with an ecological hazard less than F,
- 3. (National) At G% of facilities nationwide,
- 4. (Uncertainty) With confidence H% accounting for subjective input uncertainty, and confidence I% accounting for output sampling error.



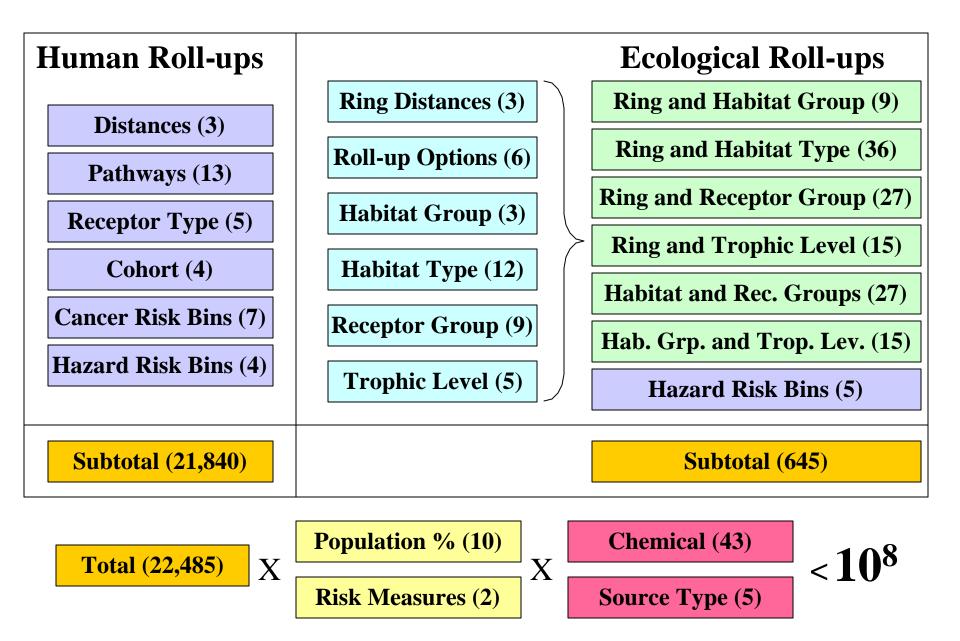
Monte Carlo Simulations Needed for 3MRA National Assessment

Individual 3MRA Modeling System Simulations Needed

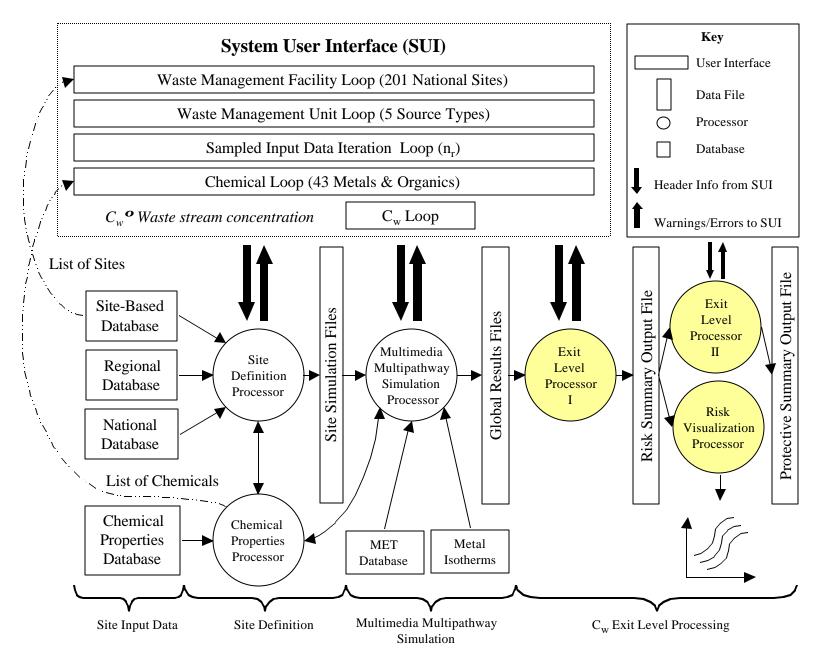


One national iteration for 1 chemical, 1 WMU = 2095 model runs (i.e., for exit levels: $5 C_w * 419$ site-WMUs = one output sample)

Wastestream (C_w) Exit Levels Possible in 3MRA



Importance of the "Exit Level" Processors.....



Problem Statement Revisited

In determining a single exit level waste stream concentration (C_{wexit}):

Output Profile Scenario Description

a. Chemical

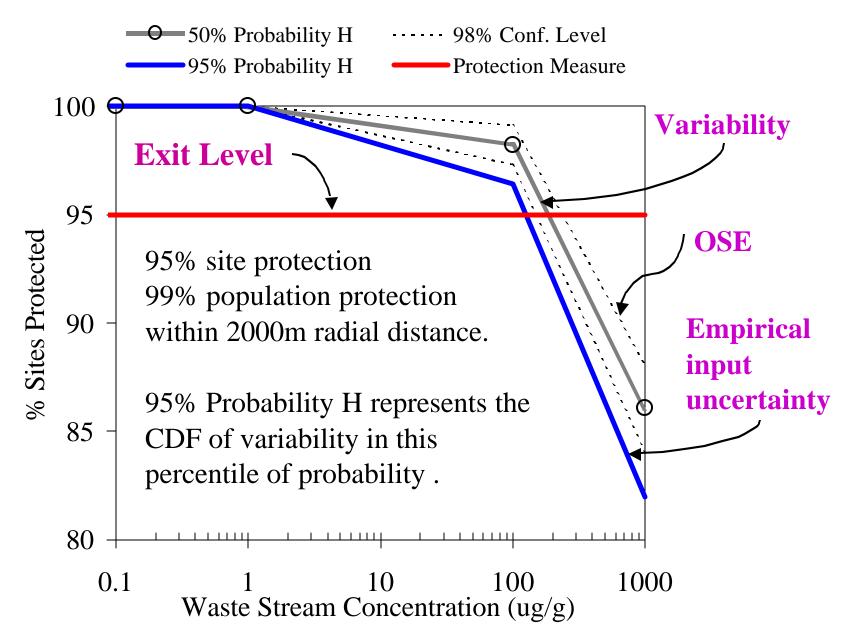
b. Source Type (i.e., WMU)

c. 9-tuple Risk Profile:A% human pop. D% ecol. pop.B distance E ring distance

C risk level F risk level

G% sitesH% uncertaintyI% precision

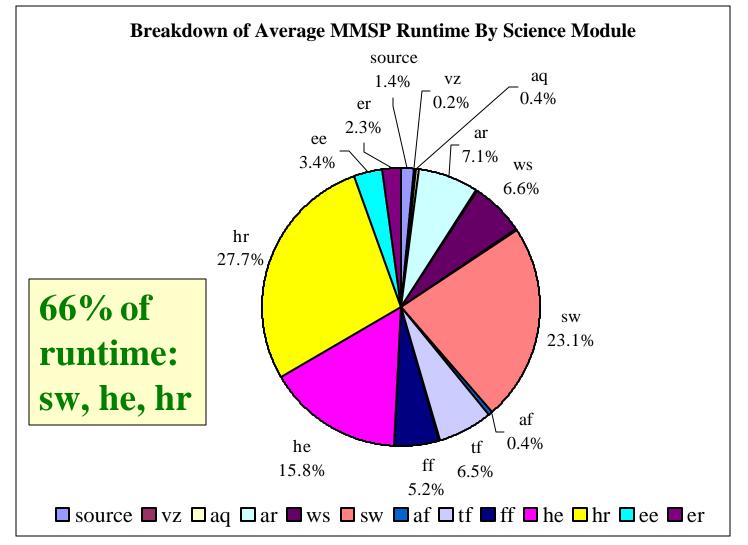
Example 3MRA Exit Level Calculation for Benzene



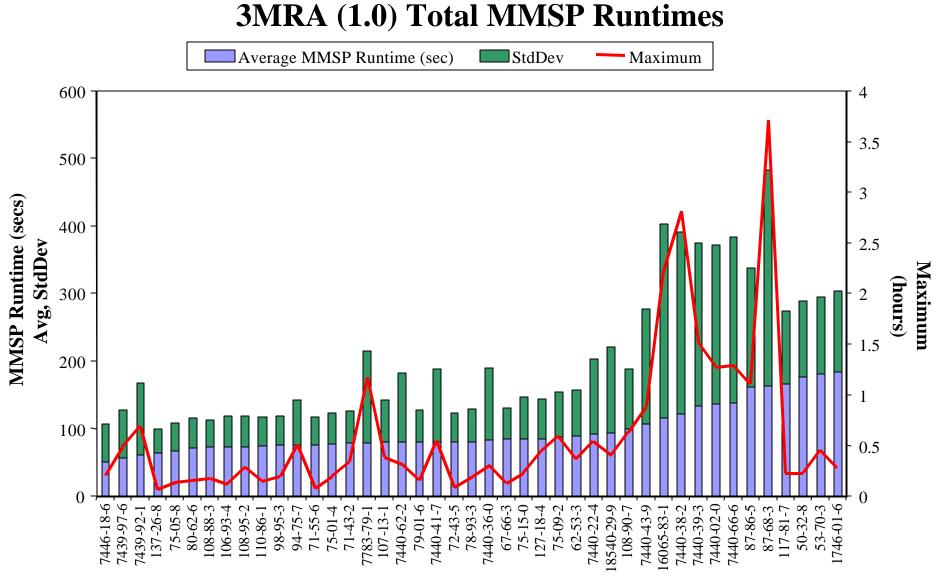
Summary of Dimensionality for National-Scale Problem Statement

- # Module/Processor Inputs = 966 per model run (\leq 3D)
- # Module/Processor Outputs = 372 per model run ($\leq 5D$)
- Model runs needed for probabilistic national risk assessment per chemical (i.e., UA_p): ~ 2,000,000 ⁽⁺⁾
- Post-processed exit levels (C_w) possible for a 3MRA national assessment: ~ 10⁸ accounting for:
 - Multiple decision variables in risk context
 - **Population and subpopulation analysis**
 - 43⁺ chemicals, 5 waste management unit types

3MRA Modeling System Runtimes



Average individual site scenario run ~ 2 min.



CASID

3MRA Run Time for National-Scale Problem Statement

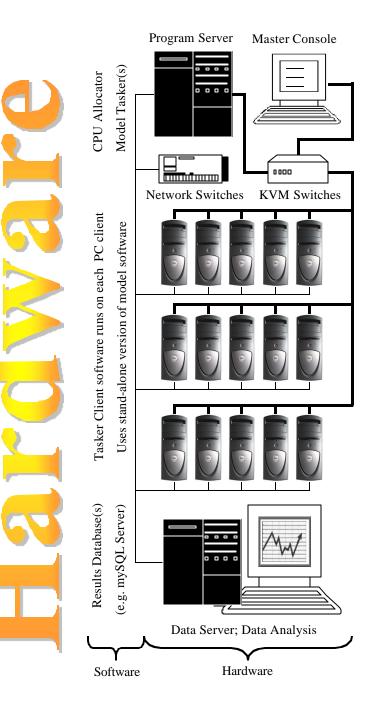
- 1. All chemicals: average model run time ~2 minutes
- 2. On SuperMUSE: ~ 2 days per 100 national realizations of model runs needed for probabilistic national risk assessment <u>per chemical</u> (i.e., UA_p)
- **3.** Single PC: ~ 10 months per chemical per 100 realizations
- 4. Single PC: ~ 8 years per chemical per 1000 realizations
- 5. Single PC: ~ 344 years, 43 chemicals, 1000 realizations



SuperMUSE: Supercomputer for Model Uncertainty and Sensitivity Evaluation

... 180-client nodes,

215 GHz, PC-Based - Windows and Linux both supported



SuperMUSE Supercomputer for Model Uncertainty

& Sensitivity Evaluation

Major Components:

- Front-end program server,
- Back-end data server,
- Currently 180 client PCs
- 16-port Raritan KVM switches,
- 24-port Linksys (10/100) switches
- Master CISCO 3550-24/2 switch.
- Network protocol TCP/IP.
- GigE channel (1000 megabits/sec) data flow to and from servers.

Windows & Linux OS supported

SuperMUSE Parallel Computing Cluster at ORD/NERL/ERD, Athens, Georgia



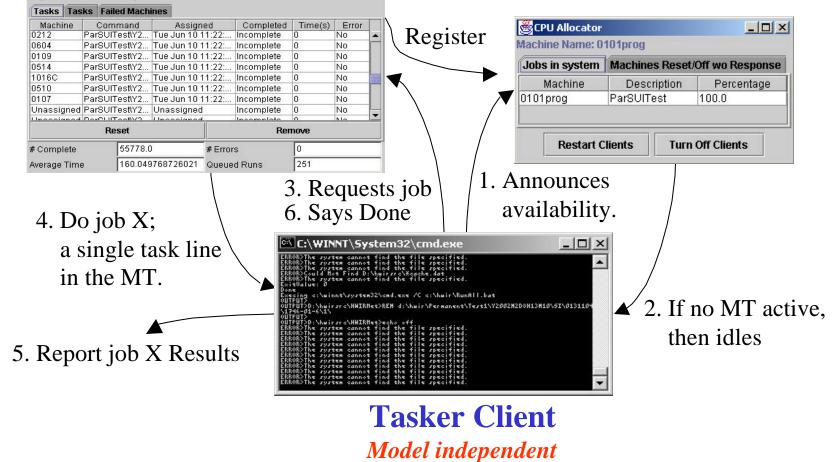


💐 SUI Tasker

Registered with: 0101Prog

Model Tasker (MT) Model dependent

CPU Allocator *Model independent*



- 0 ×

Executes OS-based commands delivered by MT

MiniMUSE Parallel Computing Cluster



Beneficial Impacts of PC-Based SuperMUSE*ing*

- ✓ SuperMUSE is scalable from 2 to 1000^+ PCs.
- ✓ Supports Windows or Linux based modeling systems.
- ✓ Solves "**embarrassingly parallel**" computing problems.
- \checkmark A local solution \rightarrow empowers model developers and users.
- ✓ Simple, inexpensive, can be built/operated by PC novices.
- \checkmark Ideal for debugging models and performing UA/SA.
- ✓ For an average model runtime of 2 minutes, ERD's SuperMUSE can run over 3 million simulations/month.



3MRA Version 1.x Tools to Support UA/SA

...includes both model dependent and model independent tools

Supercomputing Software System Needs

 Facilitating

 Distribution of

 Workloads Among PCs

 •CPU Allocator ✓

 •Model Tasker ✓

 •Tasker Client ✓

•Client Monitor 🖌

Managing files and Data Across PCs

- Update Client 🖌
- Command Tasker 🗸
- Process Messages 🖌
- ELP1 Client Collectors
 Aggregated ✓
 Disaggregated

Facilitating 3MRA-Specific Data Analysis

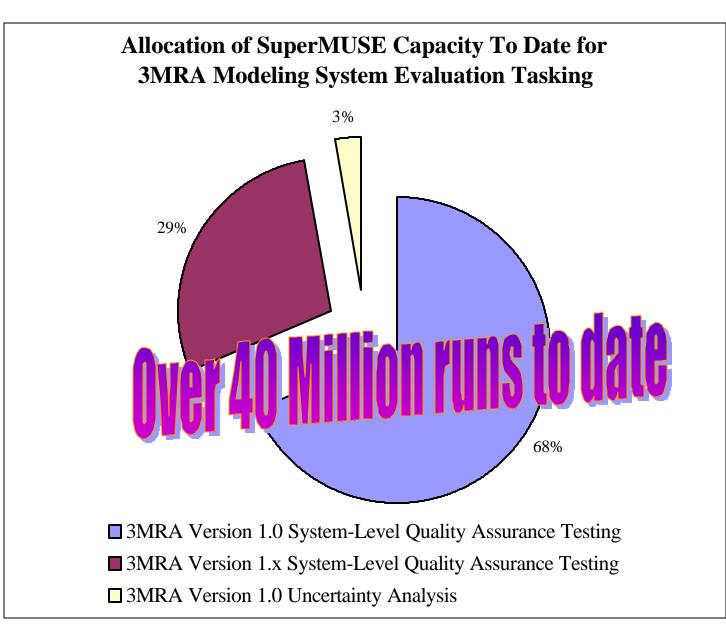
- Site Visualization ✔
- Site Summary ✔
- Aggr. MySQL ELP1 🗸
- Aggr. MySQL ELP1 🖌

- Aggr. ELP2Vis 🗸
- Automated UA/SA Tools
- Disaggregated ELP1
- Disaggregated ELP2
- Enhanced SUI

Example: Server–Side Update Client Tool User Interface

🛃 Editing E:\utils\HwirRunBat.bat			_ 🗆 🗙
File Help			
Execute		Invert Selection	
	0102, [Win98], Win 0103, [Win98], Win 0104, [Win98], Win 0105, [Win98], Win 0106, [Win98], Win 0107, [Win98], Win 0108, [Win98], Win 0110, [Win98], Win 0111, [Win98], Win	WinNT, Power Edge 6400, (e,\hwir1), 2 Disks, 4 CPUs 98, Optiplex GX150, (c,\hwir), 1 Disks, 1 CPUs	
		so, opupiex oxroo, (c,aiwii), r bisks, r or os	

Use of SuperMUSE and 3MRA Version 1.x





Model Evaluation Approaches

...leading to an overall statement of quality assurance in design for a specific intended purpose

(*Beck et al, 1997*)

Classes and Types of Uncertainty

General Classes of Uncertainty

Variability (V)

Empirical Uncertainty (U)

Model Error (ME)

Types of Empirical Uncertainty

Random Error (RE)

Systematic Error (SE)

Sample Measurement Error (SME; see RE, SE)

Input Sampling Error (ISE; see RE)

Output Sampling Error (OSE; see RE)

Inherent randomness

Correlation

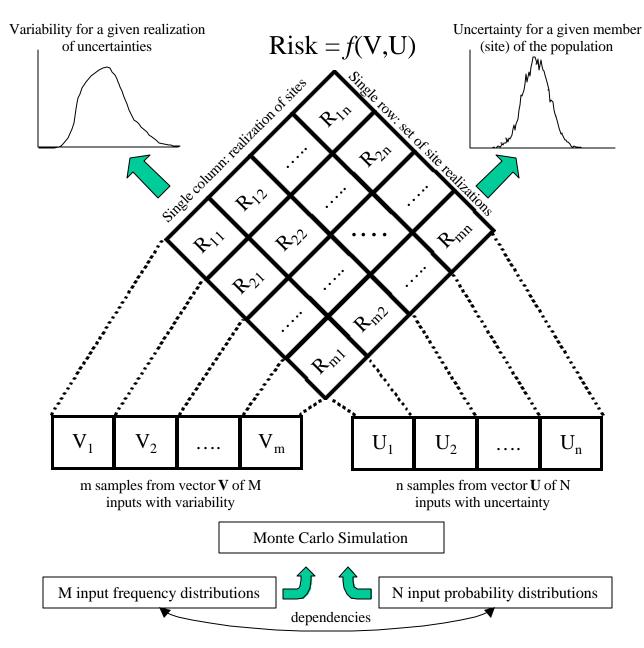
Disagreement

Performance Uncertainty Analysis (UA_p)

...describing potential differences between model predictions and nature.

Uncertainty due to lack of knowledge and data.....

Analysis Approach \rightarrow given uncertainty in both models and their inputs, quantify/qualify uncertainty in model output(s).

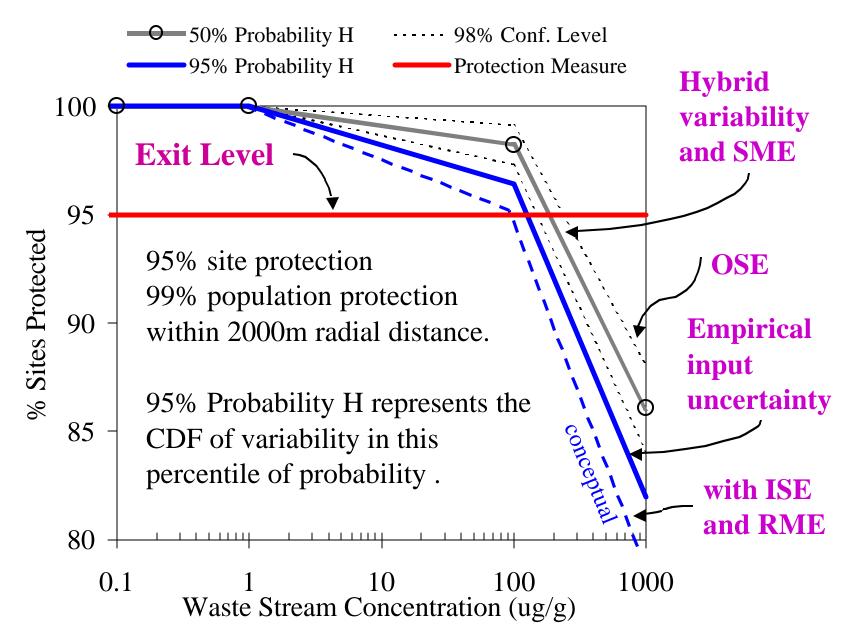


2-Stage Monte Carlo....

Separating <u>uncertainty</u> and <u>variability</u> in output predictions.

(adapted from Rhodes and Frey, 1996)

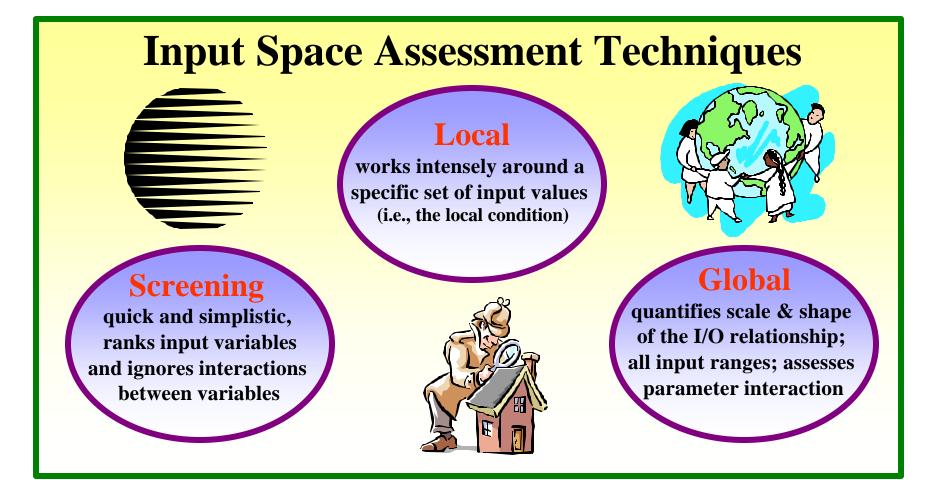
3MRA Exit Level Uncertainty



Sensitivity Analysis (SA):

....a study of how the uncertainty in output of an analytical or numerical model can be apportioned to different sources of uncertainty in the model input.

A. Saltelli



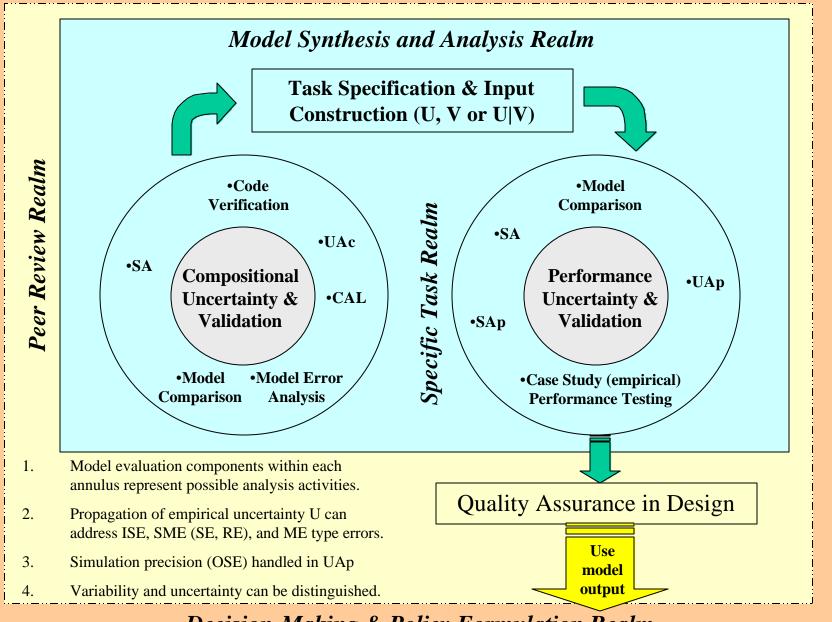
Components of Model Evaluation.

(a.k.a., Verification, Validation, and Predictive Uncertainty Analysis)

Components of Model Evaluation								
Uncertainty (U)								
Variability (V)								
Total Uncertainty (TU)								
Compositional Uncertainty Analysis (UA _c)								
Performance Uncertainty Analysis ($UA_p = UA$)								
Sensitivity Analysis (SA)								
Calibration (CAL)								
Code Verification (CodVer)								
Model Comparison (ModComp)								
Compositional Validity (CompVal)								
Performance Validity (PerfVal)								

Model Validation (ModVal)

Peer review



Decision-Making & Policy Formulation Realm

Sensitivity-Analysis-Based Performance Validation (SA_p)

...assessing and describing the behavioral and non-behavioral characteristics of the modeling system.

A specific construction of performance validation as a reflection, by way of sensitivity analysis, of the evaluation of the external definition of the current task back onto the internal composition of the model.

Model Evaluation: Summary Perspective

Model evaluation is seen as a statement of quality assurance in design (i.e., tool or technology):

.....a result of the model synthesis and analysis effort,

.....viewed as the outcome of the overall model validation effort for the specific task defined.



3MRA Version 1.0 UA/SA Plan

.....for the national-scale assessment problem statement

3MRA UA/SA Plan

- **Performance uncertainty analysis (UA_p)**
- Sensitivity analysis (SA)
- Sensitivity-based Performance Validation (SA_p)
- 7 Chemicals:
 - Benzene,
 - PCE,
 - 2,3,7,8-TCDD,
 - Benzo(a)pyrene,
 - Arsenic,
 - Nickel, and
 - Divalent Mercury.

3MRA UA/SA Plan (UA_p)

Performance Uncertainty Analysis:

• Entails propagation of input uncertainty through the modeling system, while also addressing output sampling error (OSE) associated with computational limitations of the sampling-based MCS strategy.

• Uses a pseudo 2nd-order analysis to separate variability and empirical input uncertainty, while quantifying OSE.

3MRA UA/SA Plan (SA)

Sensitivity Analysis:

• A balanced, tiered formulation of SA is planned for identifying key, important, and redundant model inputs. The basic approach to be undertaken is global input space assessment via sampling-based methods.

• SA to be conducted for this purpose will enhance both compositional and performance validation aspects for the modeling system.

• Will include global based SA techniques:

Correlation /Regression Regional Sensitivity Analysis (RSA) Tree Structured Density Estimation (TSDE)

3MRA UA/SA Plan (SA_p)

SA-based Performance Validation:

o Basically an assessment of a "prior" validity through the execution of a regional sensitivity analysis (RSA) procedure, realized as an assessment of the model's maximum relevancy in predicting model behavior for various population percentiles.

o Will investigate higher order interactions via TSDE.



Example 3MRA Version 1.x Output: 79 National Realizations

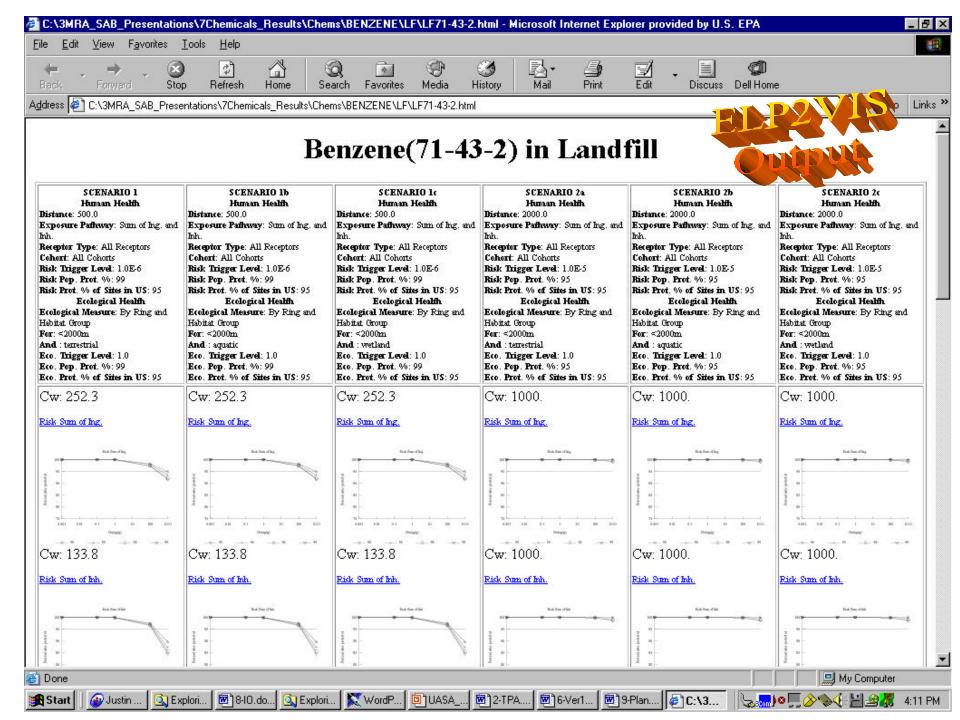
Risk Endpoint Description	Scenario					
Scenario ID	1	2				
% Population Protected	99%	95%				
% Sites Protected	95%	95%				
Protective?	More Less					
Human						
Distance (m)	500	2000				
Cancer Risk	10^{-6}	10^{-5}				
Hazard Risk	0.1	1				
Pathway	Sum Ing. & Inh.					
Receptor Group	All					
Cohort Group	А	.11				
Ecological						
Ring Distance (m)	2000	2000				
Hazard Risk	1	1				
By Ring and Habitat Group	Terr., Aq.	, Wetland				
Simulation						
Sources/Chemicals/Cws	5/7	7/5				
Sites/sources	419					
# National Realizations	79					
# Modeling System Runs	1,158	3,535				

Example Simulation Experiment

Simulated 7 Chemicals & Metals

CASID							
	Chemical Name	Carc	inog	enic	Non- Car	Ecological	
		Inhalatio	n I	ngestion	Inhalation	Ingestion	Leonogreun
127-18-4	РСЕ		\bigcirc	\checkmark		\checkmark	√
71-43-2	Benzene	\checkmark	\bigcirc	\checkmark			✓
1746-01-6	2,3,7,8-TCDD	\checkmark	\bigcirc	\checkmark		\checkmark	✓
50-32-8	Benzo(a)pyrene			\checkmark			✓
7440-38-2	Arsenic	\checkmark		\checkmark		\checkmark	✓
7440-02-0	Nickel	\checkmark				\checkmark	✓
7439-97-6	Dival. Mecury				\checkmark	\checkmark	✓

Additive Risk



Example Exit Level Results 2 Scenarios - 7 Chemicals

(Example, Preliminary Summary)

Source Type	Surface Impoundment 137		Aerated Tank		Land Application Unit 28		Waste Pile		Landfill 56	
#Sites Evaluated										
Total Simulations	378,	378,805 378		,805	77,420		168,665		154,840	
	50 th Percentile (Average) Exit Level (ppm)							2		
Chemical/Scenario	1	2	1	2		2	1.	2	1	2
PCE	0.36	100*	6.5	100*	3.2	5000*	453	5000*	778	5000*
Benzene	0.13	100*	1.5	100*	2.1	1000*	8.1	1000*	109	1000*
Benzo(a)pyrene	0.001*	0.001*	0.001*	0.001*	1.0*	1.0*	1.0*	1.0*	1.0*	1.0*
2,3,7,8-TCDD	2.2E-7	1E-4*	1E-4*	1E-4*	1.4E-6	1.6E-5	2.5E-4	0.001	0.001	0.004
Arsenic	0.095	2.1	50*	50*	0.004	0.59	3.0	18	1.8	298
Nickel	11	1000*	1000*	1000*	6.7	127	352	10000*	446	10000*
Divalent Mercury	0.1*	0.1*	0.1*	0.1*	0.49	2.2	10	10*	10*	10*

* Shows max Cw analyzed in experiment

- **Scenario 1 = more protective**
- **Scenario 2 = less protective**

Dominant Human Pathways, Human Receptors, and Ecological Habitats

(Example, Preliminary Summary)

Chemical	Dominant Risk/Route	200000 SOLC 1	face ndment	Aerated Tank		Land Application Unit		Waste Pile		Landfill	
Scenario		1	2	1	2	1	2	1	2	1	2
PCE	HCancer	Cr,Wa	Сгор	Стор	Стор	Water	Стор	Стор	Стор	Стор	Стор
	Ing.	Fa,G,Fi	Fa,G,Fi	G,Fi	G,Fa,Fi	G,R,Fi	G,Fi	G,Fi,R	G,Fi,Fa	Fa,G,Fi	Fa,G,Fi
Benzene	HCancer	Air,Cr	Air,Cr	Air,Cr	Air,Cr	Air, Sh.	Air	Show.	Air	Show.	Air
	Inh., Ing	G,Fi,R	G,Fi,R	G,Fi,R	G,Fi,R	G,Fi,R	G,Fi,R	Fi,R,G	Fi,R,G	G,Fi,R	All
Benzo(a)pyrene	Low Risk	Cr, Beef		0.75		Сгор		Стор		Bf,Cr	100 00
6 - 6655C - 6		6778		0.00			- *		3778	6 8)	855
2,3,7,8-TCDD	HCamer, Eco	Air	Air	Air		Air	Eco	Fi,Cr,Air	Eco	Eco	Eco
	Inh.	Bf, Oth.		Bf,Oth.		All	Ter,Aq	Fi,G,R	Wet.	Ter,Aq	Ter,Aq
987 - 581 - S						Successory 1	- 201 - 10	and the second	-	Received .	5 82.25
Arsenic	HCamer, Eco	Water	Eco		1994 - 1997 - 19	Wa,Cr	Eco	Wa, Cr	Eco	Water	Eco
	Ing.	Fi	Ter.	<u></u>	0	G,Fi,R	Aq.,Ter	G,Fi,R	Wet.	All	Aq.
Nickel	HBazard, Eco	Water		20		Water	Eco	Water	Eco	Water	Eco
	Ing.	Fisher				R,G,Fi	Ter,Aq	R,G,Fi	Wet.	Fa,Fi	Aq,Ter
Hg~2	HBazard	226	<u>.</u>	0.022	223	Fish	Fish	Fish	Fish	Eco	Eco
	Ing.					Fisher	Fisher	Fisher	Fisher	Ter,Aq	Ter,Aq