U.S. Environmental Protection Agency

U.S. EPA Office of Research and Development
National Exposure Research Laboratory
Ecosystems Research Division

3MRA Quality Assurance

Science Advisory Board
Review of the 3MRA Modeling Program

Presented by:

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Quality Assurance Objectives

- Ensure a product that is at the same time :
  - Based on sound science
  - Transparent
  - Serves the clients needs
- To establish quantitative measures of model quality (i.e., build user confidence and address “model validation”)

3MRA Approach to Quality Assurance

- Planning
- Documentation
- Peer Review
- Standards-based Implementation
- Verification
- Validation

System Level
- Methodology
- Integrated System Software

Component Level
- Modules/DBs Designs
- Module Software
- Databases
- System Components

Planning

ORD/OSW Integrated Research and Development Plan for the Hazardous Waste Identification Rule (HWIR)

Documentation

http://www.epa.gov/ceampubl/mmedia/3mra/index.htm

- 3MRA Modeling System
- 3MRA Source Code
- 3MRA Source Code Test Packages (*)
- 3MRA Documentation
    - SAB Review Materials
    - 5 Volume Set of 3MRA Modeling System Documents
    - Integrated R&D Plan
    - 3MRA Assessment Strategy
    - 16 Volume set of Data Documents
    - 13 Volume set of Science Module Documents
    - 13 Volume set of System Technology Documents
    - Numerous related reports
    - Peer Reviews of 3MRA Science Modules

3MRA Peer Review

- Formal
- Conference Presentations
- Journal Publications

3MRA Peer Reviews
Formal

- Joint OSW/ORD Research and Development Plan, October 1998
- Public Review via FR Notice of Proposed HWIR Methodology and Example Results, July 2000
- Individual Science Modules, 1998 – 2001
- SAB Review, 2003

3MRA Peer Reviews - Conference Presentations

- **Society for Risk Analysis (SRA): Symposium on Multimedia, Multipathway, and Multireceptor Risk Assessment for Identification of Hazardous Wastes,** Atlanta, Ga., December 5- 8, 1999.

- **Society for Environmental Toxicology and Chemistry (SETAC)**:
  - Interactive Poster Session **on Modeling for National Risk Assessment**.
  - Platform Sessions on **Multimedia, Multipathway, and Multireceptor Risk Assessment.** Philadelphia, Pa. 14 -18, November, 1999.

- **International Conference on Brownfield Sites: Assessment, Rehabilitation and Development; Cadiz, Spain** September, 2002

- **American Geophysical Union, Annual Meeting**, Washington, DC**,** May 30, 2002 .

3MRA Peer Reviews – Journal Publications

- The 3MRA Risk Assessment Framework - A flexible approach for performing multimedia, multipathway, and multireceptor risk assessments under uncertainty. C.M. Marin, Ambiotec Group, Inc.; V. Guvanasen, HGL, Inc, Herndon, VA; and Z. Saleem, US EPA. Appearing as the lead paper in: **International Journal of Human and Ecological Risk Assessment**, December, 2003.

- Investigating uncertainty and sensitivity in integrated, multimedia environmental model: Tools for FRAMES-3MRA. J.E. Babendreier, US Environmental protection Agency, Athens, GA and K.J. Castleton, Battelle Pacific Lab, Richland, WA, in publication, **Journal of Environmental Modeling and Software**, 2003.

Standards-based Implementation

Documentation for the 3MRA Technology Software System Volume 9: Software Development and Testing Strategies

Prepared for
U.S. Environmental Protection Agency
Office of Research and Development
National Environmental Research Laboratory
U.S. Environmental Protection Agency

Pacific Northwest National Laboratory
Battelle Boulevard, P.O. Box 999
Richland, Washington 99352

1997

Software Development and Testing Strategies Document (Table of Contents)

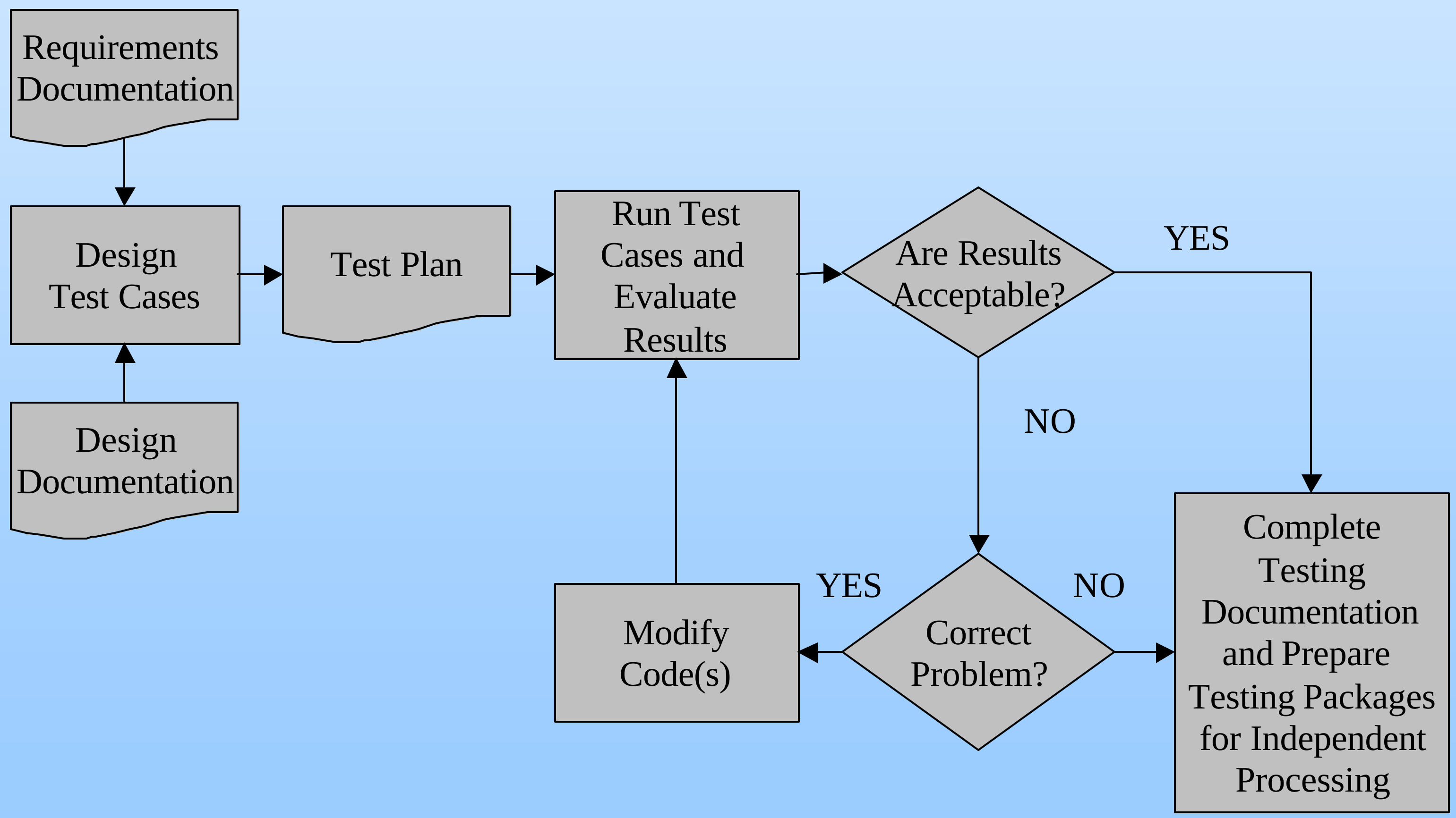
Verification –
Software Development

ELEMENTS OF A TEST PLAN

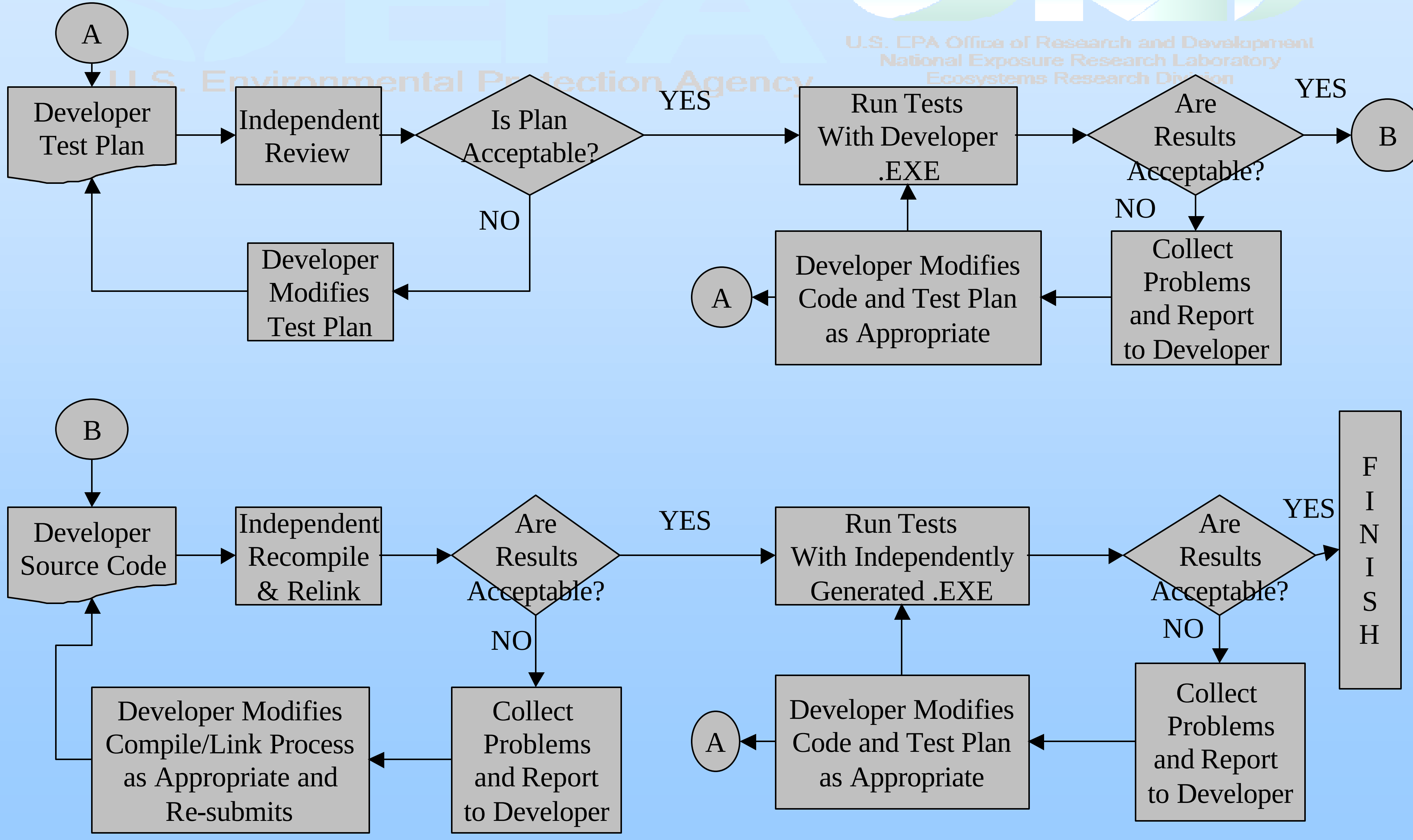
- Background and Scope
- Requirements
- Test Cases
  - Test Case Name
  - Description and Rationale
  - Input Data
  - Expected Results
  - Special Procedures
- References

	Test Cases				
REQUIREMENTS		1	2	3	4
	1	X			X
	2		X	X	
	3			X	
	4				X

3MRA TECHNOLOGY SOFTWARE SYSTEM (DEVELOPER TESTING PROCESS)

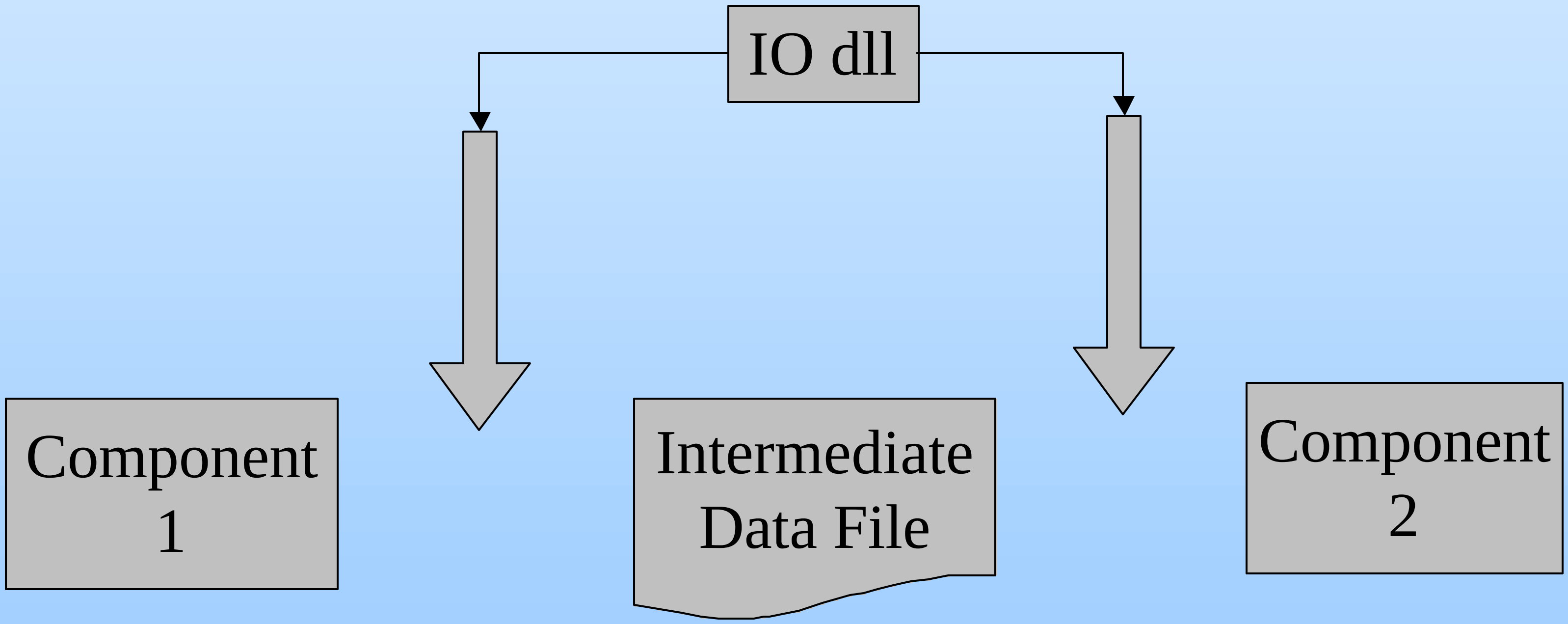


3MRA TECHNOLOGY SOFTWARE SYSTEM (INDEPENDENT TESTING PROCESS)



Example Requirements-based Testing Protocol : IO dll

IO DLL in SYSTEM CONTEXT



IO dll Requirements

Requirement Number	Requirement
1	Correctly read data (all strings, logicals, integers, and floats having from 0 to 6 dimensions) from the format required for the Site Definition Files (SDF)/SSF and the GRF
2	Correctly write data (all strings, logicals, integers, and floats having from 0 to 6 dimensions) to the format required for the SDF/SSF and the GRF
3	3 Recognize only the variables listed in a data group dictionary (*.dic)
4	Correctly access arguments passed from the calling program
5	Create an error file (ASCII)
6	Create a warning file (ASCII)
7	Write an error message to the error file and halt program execution when a designated error condition occurs (for instance, the program attempts to access a data group or variable that is undefined in a data dictionary, data accessed is outside the range allowed for that variable as defined in the data dictionary, and so forth)
8	Write a warning message to the warning file when a designated warning condition occurs (example, calling subroutine OpenGroups twice before calling CloseGroups)
9	Destroy the error file
10	Destroy the warning file
11	Support the Borland C++ Version 4.0 compiler
12	Support the Microsoft® Visual C++ Version 5.0 compiler
13	Support the Lahey FORTRAN-90 Version 4.0 compiler
14	Support the Digital Visual FORTRAN-90 Version 5.0 compiler
15	Be a 32-bit DLL
16	Run under Windows® 95

IO dll Requirements-based Test Cases

REQUIREMENTS	TEST CASES																									
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
1		x			x		x																			x
2			x	x																						
3																									x	
4	x																									
5		x															x	x	x							
6		x																								
7						x		x	x	x	x	x	x	x	x		x		x	x	x	x	x	x	x	
8																x										
9			x																							
10			x																							
11	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
12	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
13	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
14	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
15	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
16	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x

IO dll Test Cases

IODL_1 This case verifies that the NumArgs, GetArgInt, and GetArgString functions of the DLL are operating correctly.

IODL_2 This simple case verifies that the DLL read operations can be performed successfully for all four data types (string, logical, integer, and float) from 0 to 6 dimensions.

IODL_3 This case verifies that the DLL can correctly write to the format required for the SDF/SSF and GRF. Write operations for all four data types (string, logical, integer, and float) from 0 to 6 dimensions are performed.

IODL_4 This test case verifies that the DLL correctly reads from a SSF/GRF file previously created by the DLL.

IODL_5 This case verifies that the DLL can accurately locate and read parameters from a very large (6.9 MB) data group file. It is assumed that if one or two parameters can be read from this file without error, the DLL should be able to read all the parameters in this file.

IODL_6 This case verifies that the DLL does not allow the user to write to a data group file that it is reading from if the file is not the last file listed in the ARGUMENTS environment variable. Of the files listed in ARGUMENTS, all files can be read from, but only the last file can be written to.

IODL_7 This case verifies that the DLL allows a program to read simultaneously from several different data group files. The files HD.SSF, AR.SSF, and EE.SSF are all read from.

IODL_8 This test attempts to read a variable of a particular data type as if it were some other data type (that is, attempt to read an integer variable as if it were a float).

IODL_9 This case verifies that DLL writes an error message when an element is requested from an array that is outside the range of the elements defined in the data group file.

Test Case IODL_5

Description and Rationale

This case verifies that the DLL can accurately locate and read parameters from a very large (6.9 MB) data group file. The DLL reads from the SSF file "SW.SSF." This file is too large to be included in this test plan, but it is available electronically. Only a sampling of reads is performed. It is assumed that if one or two parameters can be read from this file without error, the DLL should be able to read all the parameters in this file.

Test Case IODL_5 (cont'd)

Conducting the Test

To run this case, double click on "runc.bat." At the prompt, type "iodl_5" and press return. The program runs and creates an output file called "iodl_5c.out," located in the SSF directory, and an output file called "hdjunk.grf," located in the GRF directory. The "iodl_5c.out" file lists the functions called and the results returned. The "hdjunk.grf" file is empty because no write calls are made. The "iodl_5c.out" file is shown as follows. The results returned can be compared to the expected results comment in the "iodl_5.tst" file. To run the Microsoft® Visual C++ test program, repeat the previous steps using "runmscp.bat." The output file is called iodl_5m.out.

Call OpenGroups

Call ReadReal1 sw.ssf sw_var100 m 10

Returned 6.000000001

Call ReadReal4 sw.ssf sw_var53 g/day 1 1 1 4

Returned 12.4

Call CloseGroups

Test Case IODL_5 (cont’d)

Input Data

The input file to the testing program is as follows:

"OpenGroups"
"ReadReal1",
"sw.ssf","sw_var100","m",10, ; should return 6.00000001
"ReadReal4",
"sw.ssf","sw_var53","g/day",1,1,1,4, ; should return 12.4
"CloseGroups"
"Stop"

Expected Results

The data listed in the test output file (IODL_5.OUT) are expected to exactly match the corresponding data in SW.SSF.

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Verification

Data Collection and Database Organization

Data Verification

- Data collection plan specifying data sources and how data would be collected from those sources
- QA/QC protocols that were specified as part of the data collection plan, including
  - data entry checks,
  - independent calculations to verify correct processing,
  - automated checks of critical parameters, formats, and processes
- Independent testing of the major site-based elements
  - review and compare data collection and model documentation for consistency
  - review QA/QC history for completeness
  - review selected data methodologies, programs, and results

3MRA “Validation”

- Modules
  - Legacy
  - Newly developed
- System
  - Site Assessment
  - Model Comparison
  - UA/SA

Module Validation : Legacy Codes

- ISC
  - Point Sources : extensive validation studies of dispersion algorithms varying terrains,
  - Area sources; Dry/Wet Deposition : scarce field studies, extensive development during 1990’s to improve these algorithms (significant testing and comparison to existing models was performed)
  - Plume Depletion : existing scheme replaced for 3MRA with extensive testing including comparisons with numerical solutions to eddy diffusivity equation
- EXAMS
  - Several calibration/validation studies across a number of surface water types (streams, rivers, ponds, etc.) for a variety of chemicals
- Vadose/Aquifer Modules :
  - Based on EPACMTP which itself has undergone validation at four unique sites
  - Vadose zone module (modified) predictions compared with soil column study

Module Validation : Non-Legacy Codes

- **Wastewater Source Modules** : based on and compared to CHEMDAT8, which itself has undergone significant field-based testing
- **Land-based Source Modules** : compared with HELP and soil column experimental data
- **Farm Food Chain/Terrestrial Food Web** : based on existing MPE methodology, which itself is based on the IEM
- **Aquatic Food Web** : based on existing science in peer reviewed literature, methods are used on various EPA guidance documents and rule makings
- **Human Exposure** : no validation conducted, based on widely accepted state of the science formulations
- **Human Risk** : no validation is possible, based on generally accepted and well used methods
- **Ecological Exposure** : no validation conducted, based on generally accepted science-based formulations
- **Ecological Risk** : no validation

Site Assessment / Model Comparison Study

Objective : To initiate work leading to an increased knowledge of how 3MRA compares with observed data and other MM modeling approaches

Approach : Design and execute collaborative study with OAQPS TRIM.Fate modeling team

- Select Industrial D type site, multimedia contaminant, multimedia monitoring data
- formulate modeling inputs for each model
- select specific exposure endpoints for model comparison (eco endpoints)
- compare and explain modeling results relative to observations
- report results

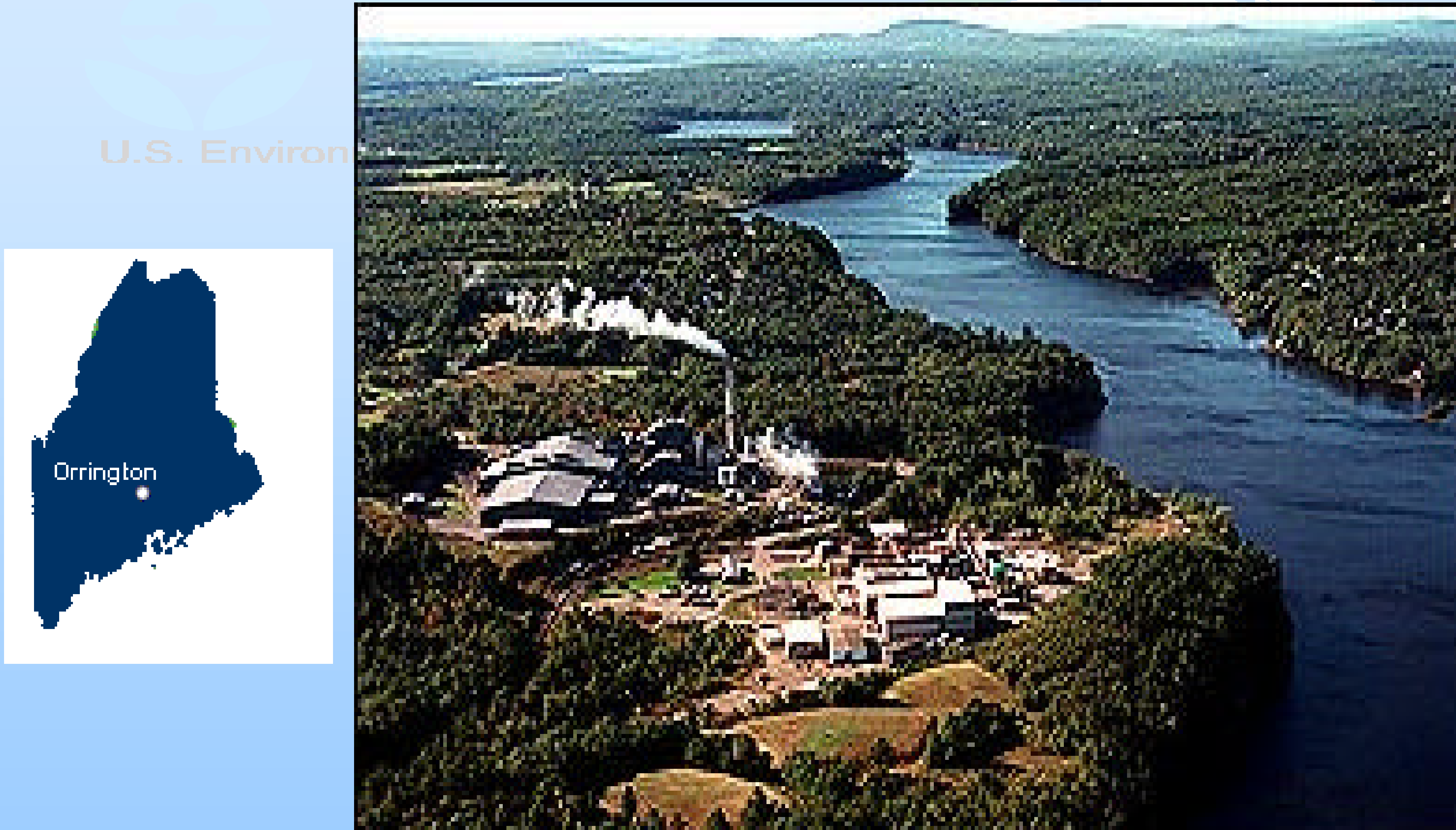

Figure 1 : HoltraChem Manufacturing Site

Limitations to Study

Data

- Source term based on characteristics of chlor-alkali facility
- Monitoring data provides snapshot of Hg and not continuous time series
- Contributions from other Hg sources (on/off site) not considered

Modeling

- TRIM simulates multimedia F&T and foodweb only
- 3MRA does not simulate subsurface F&T for deposited contaminants, thus no vadose zone or aquifer simulation
- TRIM does not simulate land-based disposal

Available Data

On-site

- Surface soil
- Subsurface soil
- Deer Mouse
- Earthworm

Off-site

- Ambient air
- Surface Water
  - River
  - Ponds
  - Lakes
- Sediment
  - Ponds
  - Lakes
- Loon
- Deer Mouse
- Earthworm

3MRA(HWIR) Model Quality Assurance

3MRA/TRIM Model Comparison [Comparative Endpoints]

Medium	Endpoints	Hg Species	Locations	Times
Atmosphere	Ambient conc, depostion rates	Divalent	Monitoring Stations, lakes/ponds for deposition	Annual avg (30 yrs)
Soil	Avg surface soil conc	Divalent	On site, S of site, selected watersheds	Annual avg (30 yrs)
Surface Water (water column)	Avg water column conc	Divalent, methyl	River (N/S of facility), Swetts Pond, Brewers Lake, Fields Pond, Thurston Lake	Annual avg (30 yrs)
Surface Water (sediment)	TBD	Divalent, methyl	Same as above	Annual avg (30 yrs)
Biota (terrestrial)	Vegetation, White-tailed deer, deer mouse, short-tailed shrew, earthworm	Divalent, whole body	TBD (Based on Habitat Locations)	Year 30
Biota (aquatic)	Largemouth bass, white perch	Methyl, whole body	Ponds and Lakes	Year 30
Biota (terrestrial/aquatic)	Common Loon, Mink, Raccoon	Divalent, whole body	TBD (Based on Habitat Locations)	Year 30

And while system-based sensitivity and uncertainty analysis are certainly part of the overall Quality Assurance effort, they will be presented in their own right