3MRA Modeling System
Technology

Science Advisory Board
Review of the 3MRA Modeling System

Presented by:
Karl Castleton, DoE/PNNL
August 26, 2003
System Technology

• Need for the 3MRA technology

• Overview of the 3MRA technology
  – Science-based requirements
  – Software/Hardware requirements

• Design Features
  – Software system challenges
  – Description of 3MRA software
  – 3MRA modeling system outputs
Science-Based Requirements

- Provide comprehensive human and ecological risk
- Accommodate 2 stage Monte Carlo
- Accommodate site-based modeling
- Provide for multimedia mass balance
- Provide for appropriate aggregation of risk results
- Provide a modeling tool for research in sensitivity analyses and variability and uncertainty assessments
Software Requirements

- Implementation on Windows-based PC environment (Pentium or higher)
- Object Oriented Design (with respect for the “real world”)
- Accommodate legacy codes
- Accommodate multiple programming languages (FORTRAN, C++, Java)
- Automatic QA/QC
- 100% Distributable
Design Features

- Overview of the system design
- 3MRA module data exchange
- Potential dimensionality
- Actual dimensionality
FRAMES 3MRA Modeling System

System User Interface (SUI)
- Waste Management Facility Loop (201 National Sites)
- Waste Management Unit Loop (5 Source Types)
- Sampled Input Data Iteration Loop ($n_r$)
- Chemical Loop (43 Metals & Organics)

$C_w \equiv$ Waste stream concentration  
$C_w$ Loop

Key:
- User Interface
- Data File
- Processor
- Database
- Header Info from SUI
- Warnings/Errors to SUI

List of Sites
- Site-Based Database
- Regional Database
- National Database

List of Chemicals
- Chemical Properties Processors

Chemical Properties Database

Cw Exit Level Processing

Site Input Data
- Site Definition
- Multimedia Multipathway Simulation
- Global Simulation Files
- Exit Level Processor I
- Risk Visualization Processor
- Risk Summary Output File
- Protective Summary Output File

List of Sites
- Site-Based Database
- Regional Database
- National Database

List of Chemicals
- Chemical Properties Processors

Chemical Properties Database

Cw Exit Level Processing
Software System Challenges

• 3MRA Complexities
  – Hardware/Software Requirements
  – Diversity of Software Development Team
  – Software System Solutions
    • Standardizing the way model developers communicate data to each other
    • Standardizing the impacts one media/object on another
Meta Data & Data Transfer Protocols

**Data Dictionaries (DIC files)**
- Sufficient dimensionality
- Designed as “data packets”, i.e., logical grouping of data

**Application Program Interface (API/IOdll)**
- Facilitates data transfer throughout system
- Conducts QA checks on data (e.g., units, range)
- Accesses Model Meta Data to check validity of CSM and inform models regarding locations of incoming data
Relationship Between Dictionary Files and Data Files

**Data Files**: Contain simulation-based values per variable

**Dictionary Files**: Contain information about variables found in Data Files (Meta Data of the data)
Meta Data: Dictionary Files

Ecological Exposure Example

- Chemical Properties SSF Dic.
- Ecological Exposure SSF Dic.

Key Data Inputs
- Food consumption rate
- Body weight
- Dietary preferences

- SR GRF Dic.
  - Surface Impoundment Module
- SW GRF Dic.
  - Surface Water Module
- TF GRF Dic.
  - Terrestrial Food Web Module
- AF GRF Dic.
  - Aquatic Food Web Module

- SI Concentrations
- Water Column and Sediment Concentrations
- Soil, Plant, and Prey Concentrations
- Aquatic Plant and Prey Concentrations

Ecological Exposure Module

Applied Doses

Ecological Risk Module
### Some Entries From a Dictionary

<table>
<thead>
<tr>
<th>Code</th>
<th>Dim</th>
<th>Type</th>
<th>Min</th>
<th>Max</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AnnInfil</td>
<td>2</td>
<td>float</td>
<td>0</td>
<td>0.03</td>
<td>m/d</td>
<td>leachate infiltration rate (annual avg., WMU subarea(s) only)</td>
</tr>
<tr>
<td>CE</td>
<td>1</td>
<td>float</td>
<td>0</td>
<td>1E+08</td>
<td>g/m2/d</td>
<td>constituent mass emission rate-PM30</td>
</tr>
<tr>
<td>CENY</td>
<td>0</td>
<td>integer</td>
<td>0</td>
<td>10000</td>
<td></td>
<td>number of years in outputs</td>
</tr>
<tr>
<td>CEYR</td>
<td>1</td>
<td>integer</td>
<td>1</td>
<td>10000</td>
<td>year</td>
<td>year associated with output</td>
</tr>
<tr>
<td>CTda</td>
<td>3</td>
<td>float</td>
<td>0</td>
<td>1000000</td>
<td>ug/g</td>
<td>depth averaged soil concentration (from zava to zavb)</td>
</tr>
<tr>
<td>CTdaNY</td>
<td>2</td>
<td>integer</td>
<td>0</td>
<td>10000</td>
<td></td>
<td>number of years in outputs</td>
</tr>
<tr>
<td>CTdaYR</td>
<td>3</td>
<td>integer</td>
<td>1</td>
<td>10000</td>
<td>year</td>
<td>year associated with output</td>
</tr>
<tr>
<td>CTss</td>
<td>3</td>
<td>float</td>
<td>0</td>
<td>1000000</td>
<td>ug/g</td>
<td>soil concentration (annual average, all subareas)</td>
</tr>
<tr>
<td>CTssNY</td>
<td>2</td>
<td>integer</td>
<td>0</td>
<td>10000</td>
<td></td>
<td>number of years in outputs</td>
</tr>
<tr>
<td>CTssYR</td>
<td>3</td>
<td>integer</td>
<td>1</td>
<td>10000</td>
<td>year</td>
<td>year associated with output</td>
</tr>
</tbody>
</table>
IO DLL in SYSTEM CONTEXT

Component 1 → Intermediate Data File → IO dll → Component 2
Description of 3MRA Software

• Multiple Environmental Modules
  – 13 different modules to be invoked per run
• Multi-pathway
  – 4 types of releases (air, surface water, watershed, and vadose zone)
• Multi-receptor
  – 4 receptors, with 5 cohorts (4 used for decision making)
• Software system that allows you to run both production runs as well as answer science questions
Integrating Environmental Models
3MRA Modeling System Outputs

- Requirements of ELP I, ELP II and RVP
- Human Risk Outputs
- Human Risk Roll Ups
- Ecological Risk Outputs
- Ecological Risk Roll Ups
## Potential Dimensionality for 3MRA National Assessment

### Simulations

<table>
<thead>
<tr>
<th>Source Types (5)</th>
<th>Site (201)</th>
<th>Waste Level (5)</th>
<th>Chemical (43)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Realization (10000)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Receptor Type (9)</td>
<td>Risk Bins (7)</td>
<td>Pathways (13)</td>
<td>Cohort (6)</td>
</tr>
<tr>
<td>Risk Bins (7)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Time (10000)</td>
<td>Receptor Locations (677)</td>
<td>Distances (3)</td>
<td>Risk Measure (2)</td>
</tr>
</tbody>
</table>

### Storage

<table>
<thead>
<tr>
<th>Total Simulations (900,850,000)</th>
<th>Total Numbers Potentially Stored (1.8e20)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Total Bytes (1.8 Billion 10 GB hard drives)</td>
</tr>
</tbody>
</table>
## Actual Dimensionality for 3MRA National Assessment

### Simulations
- Realization (1)
- Source Types (5)
- Site (201)
- Waste Level (5)
- Chemical (43)

### Storage
- Receptor Type (5)
- Risk Bins (7)
- Pathways (13)
- Cohort (4)
- Distances (3)
- Risk Measure (2)
- Time (1)
- Receptor Locations (1)

---

<table>
<thead>
<tr>
<th>Simulations</th>
<th>Storage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Realization (1)</td>
<td>Receptor Type (5)</td>
</tr>
<tr>
<td>Source Types (5)</td>
<td>Risk Bins (7)</td>
</tr>
<tr>
<td>Site (201)</td>
<td>Pathways (13)</td>
</tr>
<tr>
<td>Waste Level (5)</td>
<td>Cohort (4)</td>
</tr>
<tr>
<td>Chemical (43)</td>
<td>Distances (3)</td>
</tr>
<tr>
<td></td>
<td>Risk Measure (2)</td>
</tr>
<tr>
<td></td>
<td>Time (1)</td>
</tr>
<tr>
<td></td>
<td>Receptor Locations (1)</td>
</tr>
</tbody>
</table>

---

Total Simulations (90,085)

Total Numbers Stored (.96 Billion)

Total Bytes (Single 10 GB hard drives)
Conclusions 3MRA Software System

• Achieves balance
  – Between modern software (Object Oriented) and legacy
  – Complexity and simplicity
  – Runtime versus storage requirements

• Allows for testing at multiple levels and at different times
  – Modules and system
  – During development and running
Future System Enhancements

• Support more programming languages
• Develop the ability to use different modules, module dictionaries and data-sets more easily
  – A user interface for checking/updating a site-based simulation
• Automated testing for module and system components
  – Cost of manual testing is restrictive