Utilization of GIS Technology to Support Development of Flow and Contaminant Fate and Transport Models at US DOE Sites

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BACKGROUND

The Applied Research Center (ARC) at Florida International University (FIU) has supported the remediation efforts of the U.S. Department of Energy's Oak Ridge Reservation (ORR) in Tennessee through hydrological modeling of the fate and transport of inorganic and organic pollutants of concern with a focus on mercury (Hg).

Integrated surface and subsurface flow, fate and transport models were developed for several watersheds including East Fork Poplar Creek (EFPC), Upper EFPC in the Y-12 National Security Complex (Y-12 NSC) and White Oak Creek (WOC), to provide analysis of contaminant patterns within each watershed. More than a hundred simulations were completed to calibrate the models, derive model uncertainties, and to provide analysis of remediation scenarios, resulting in gigabytes of computed spatial and temporal simulation data for each computation node.

An advanced spatial data structure was needed to address the management, processing, and analysis of spatial and temporal numerical modeling data derived from multiple sources. Geographic Information Systems (GIS) technology was employed to support the hydrological modeling work through storage and geoprocessing of spatial and temporal data required by the models and to produce hydrogeological maps for visualization. An ***ArcSDE geodatabase*** was developed which facilitates centralized storage and management of experimental and computed model data, putting it into a structured, coherent, and logical computer-supported system. Its capabilities were extended over the years using tools such as ***ArcGIS ModelBuilder*** combined with ***Python*** scripting to automate repetitive tasks, perform statistical analyses and generate maps and reports. GIS data processing and automation enabled faster and hence more complex analyses of field test data.

Fig. 1. East Fork Poplar Creek

METHOD

1. **Development of an ArcSDE Geodatabase.**
2. **Pre- and post-processing of hydrological model data using ArcMap and ArcToolbox.**
3. **Use of ArcGIS ModelBuilder & Python scripting to:**
   - Automate repetitive geoprocessing tasks.
   - Perform statistical calculations.
   - Generate maps and reports.
4. **Use of ArcGIS Geodatabase Diagrammer to create, edit or analyze geodatabase schema.**

Development of an ArcSDE Geodatabase

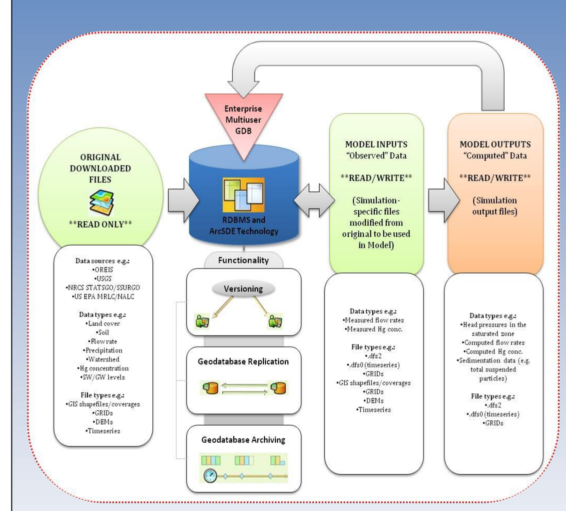


Fig. 2. ORR Geodatabase System Architecture

The ORR Geodatabase (Fig. 2):

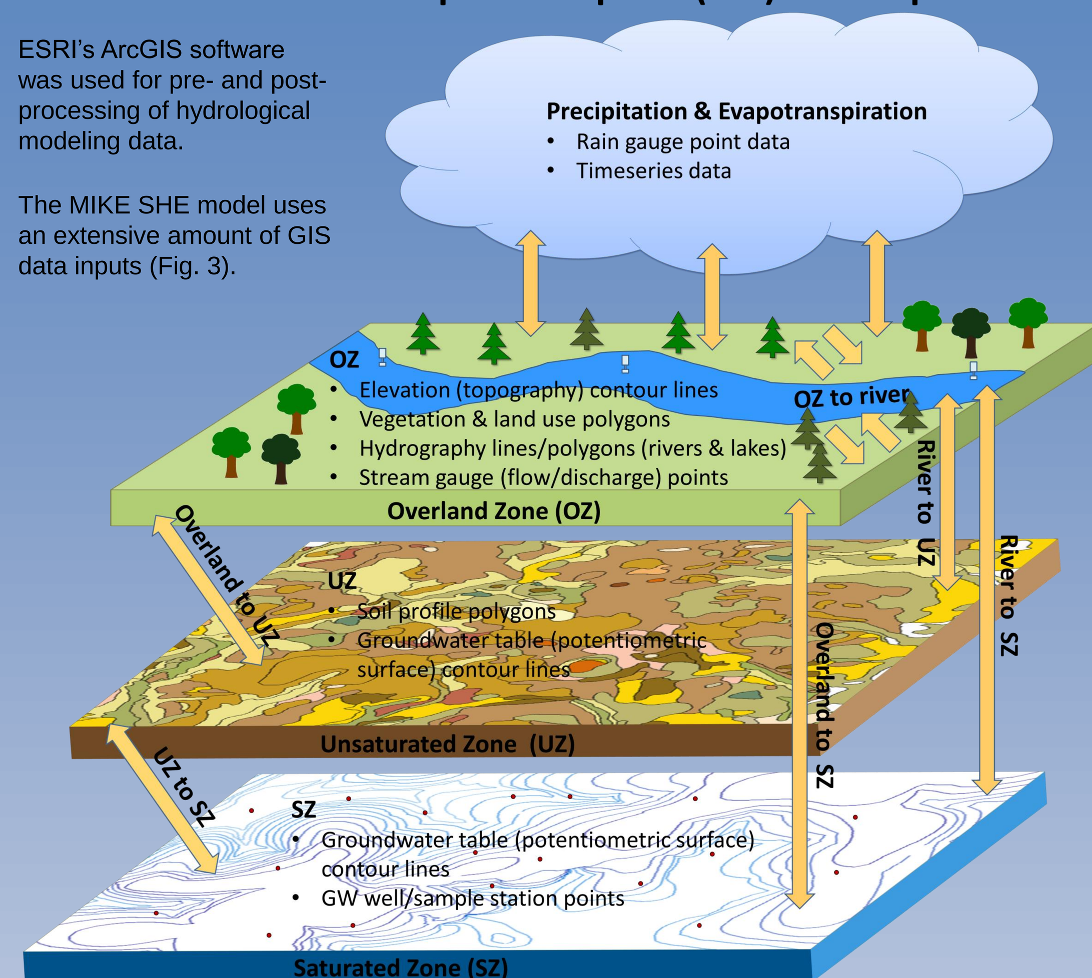
- A multiuser relational database management system (RDBMS) deployed on advanced Windows server using ArcGIS for Server.
- Based on ArcHydro and ArcGIS Base Map data models which had several input data types in common with ORR Geodatabase.
- ArcHydro has tools to support water resources applications within the ArcGIS environment.
- Modifications were then made for project specific input parameters.

- Serves as a centralized data management system.
- Provides access to data generated from simulations of contaminant fate and transport to all users.
- Facilitates storage, concurrent editing and import/export of model configuration and output data specific to the hydrologic and transport models being used.
- Structured to be replicable for application at other DOE sites.

Pre- and Post-Processing of Model Data using ArcGIS

- ESRI's ArcGIS software was used for pre- and post-processing of hydrological modeling data.
- The MIKE SHE model uses an extensive amount of GIS data inputs (Fig. 3).

Fig. 3. MIKE SHE Model Spatiotemporal (GIS) Data Inputs



- Development of hydrological models requires data that may include thousands of groundwater monitoring wells, boreholes, stream reaches with gauges, weather stations, land cover, vegetation, soil type, topography, geology, water quality and satellite imagery (Fig. 4).
- GIS enables hydrologists to pre-process and integrate data derived from multiple sources that are usually in different coordinate systems, have different spatial references, are at different scales, and are from different time periods, into a single manageable system.
- GIS-based approaches in hydrological modeling can provide the benefit of combining different layers of geographic data to create new integrated information which can be quite useful for creating dependent or independent hydrological variables.
- GIS can also serve as a useful tool in visually displaying research results via maps, graphs and reports which help to enhance the understanding and interpretation of model-derived data and to obtain a perception closer to reality.

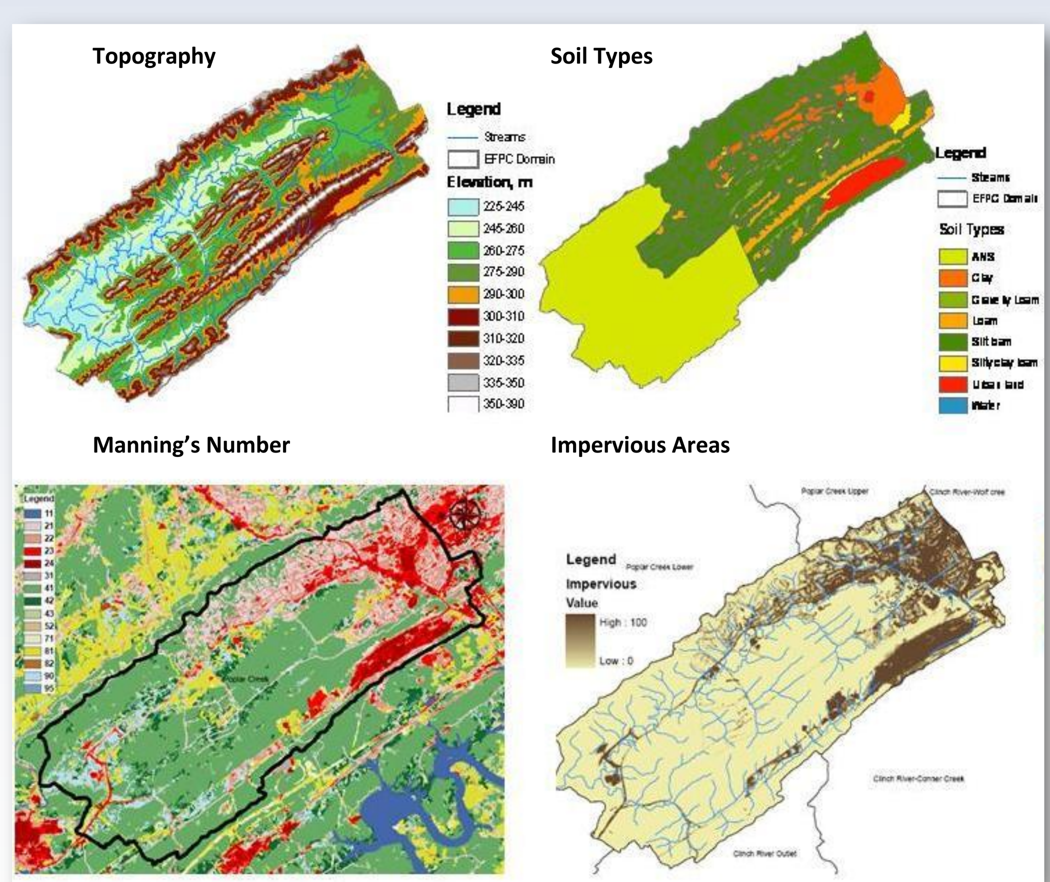


Fig. 4. Gridded input data files used for model development

ArcGIS ModelBuilder & Python

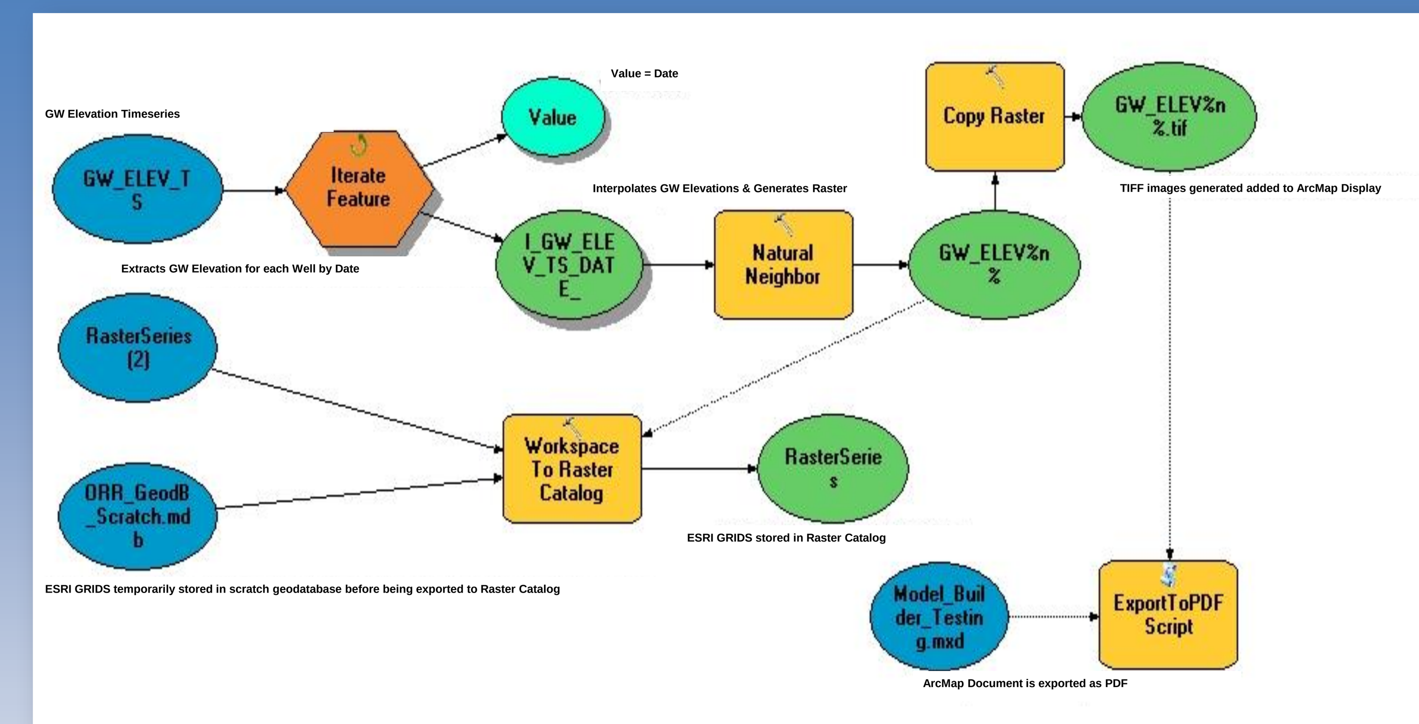


Fig. 5. ArcGIS ModelBuilder Workflow Diagram

Geoprocessing Automation

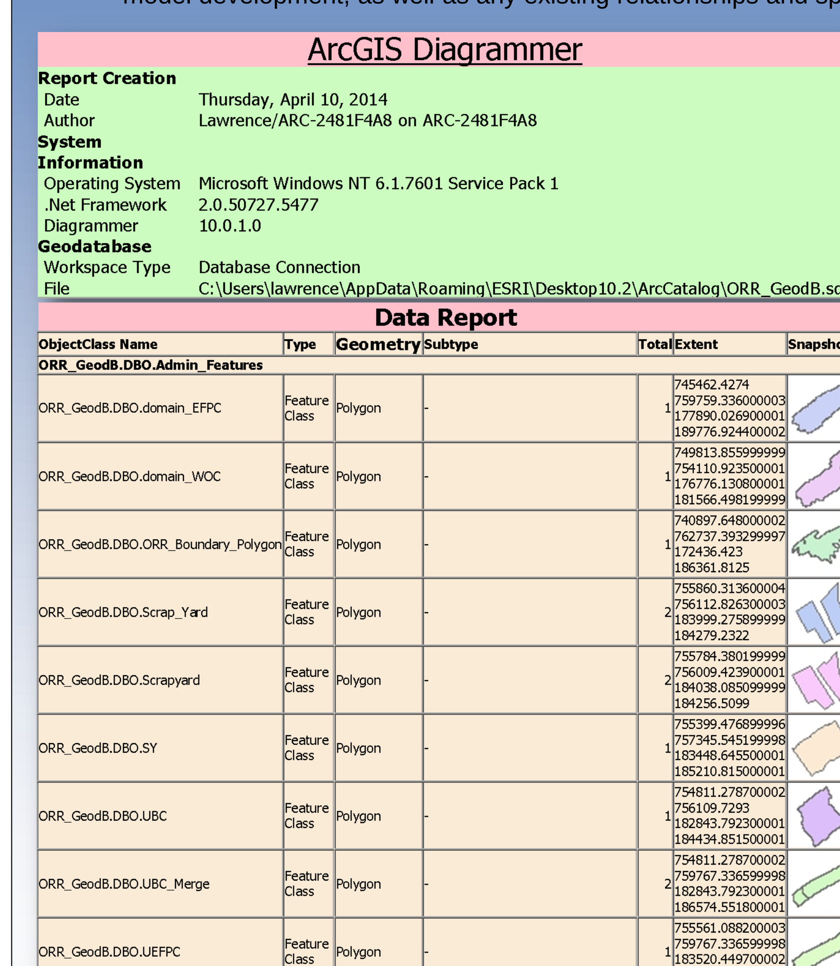
- Python scripts were used to customize built-in ArcGIS tools to automate repetitive model-specific geoprocessing tasks using ArcGIS ModelBuilder.
- A toolbox was developed for use with the EFPC model, but is scalable and reusable with geodatabases containing data relevant to other DOE sites.
- Customized tools and scripts automate the query and retrieval of timeseries data and contaminant flow and transport parameters from the ORR geodatabase.
- The ArcGIS data model iterates through selected features and exports the results in tabular format.
- The toolbox has capabilities to:
  - Add GIS files to ArcMap and create layer files.
  - Select features within a specified area (e.g. the study domain) and zoom to selected features.
  - Clip/extract selected features and create a new layer file of selected subset.
  - Export clipped feature in format to be used by MIKE SHE/11 model.
  - Export attributes of clipped feature in MS Excel or text format for statistical analysis and generation of graphs and reports.
  - Export map extent in various formats (e.g. JPEG, TIFF or PDF) for development of reports.
  - Interpolate timeseries data collected at various monitoring points, generate gridded surfaces, and create and export mapped results.
- ArcGIS ModelBuilder generates model workflow diagrams (Fig. 5) to document and visually represent tools and scripts incorporated in the data model.

Statistical Analysis

- Customized Python scripts were also developed to perform statistical analyses on model output data.
- A library of scripts was implemented and coupled with other existing libraries used for mathematics, science, and engineering such as NumPy and SciPy.
- The goal was to create scripts to calculate model performance statistics for a subset of existing flow and contaminant monitoring stations.
- Data for the selected stations are available, in most cases, on an hourly basis and for some stations on a daily basis only.
- The following lists some of the parameters for which scripts were developed.
  - **ME:** Mean error .
  - **MAE:** Mean absolute error .
  - **RMSE:** Root mean square error.
  - **STD:** Standard deviation.
  - **CoVar:** Covariance.
  - **Cor:** Correlation.
  - **PEV:** Percent explained variance.
  - **NS:** The Nash-Sutcliffe model efficiency coefficient.

ArcGIS Geodatabase Diagrammer

- Details of the ORR geodatabase data and schema were generated using the ArcGIS Geodatabase Diagrammer utility for ArcGIS 10.2.
- ArcGIS Diagrammer is essentially a productivity tool used to create, edit or analyze geodatabase schema.
- It generates reports (Fig. 6) and diagrams (Fig. 7) in the form of editable graphics and serves as a visual editor which accepts XML workspace documents that are created from ESRI's ArcMap or ArcCatalog.
- Reports generated depict the ORR geodatabase data structure and details of the features, rasters and tables used during hydrological model development, as well as any existing relationships and spatial references.



ArcGIS Diagrammer

Report Creation
Date: Thursday, April 10, 2014
Author: Lawrence/ARC-2481F4A8 on ARC-2481F4A8
System Information
Operating System: Microsoft Windows NT 6.1.7601 Service Pack 1
.Net Framework: 2.0.50727.5477
Diagrammer: 10.0.1.0
Geodatabase
Workspace Type: Database Connection
File: C:\Users\lawrence\AppData\Roaming\ESRI\Desktop10.2\ArcCatalog\ORR_GeodB.sde

Data Report

ObjectClass Name	Type	Geometry	Subtype	Total	Extent	Snapshot
ORR_GeodB.DBO.Admin_Features						
ORR_GeodB.DBO.domain_EFPC	Feature Class	Polygon	-	1	745462.4274 759759.336000003 177890.026900001 189776.924400002	
ORR_GeodB.DBO.domain_WOC	Feature Class	Polygon	-	1	749813.855999999 754110.923500001 176776.130800001 181566.498199999	
ORR_GeodB.DBO.ORR_Boundary_Polygon	Feature Class	Polygon	-	1	740897.648000002 762737.393299997 172436.423 186361.8125	
ORR_GeodB.DBO.Scrap_Yard	Feature Class	Polygon	-	2	755860.313600004 756112.826300003 183999.275899999 184279.2322	
ORR_GeodB.DBO.Scrapyard	Feature Class	Polygon	-	2	755784.380199999 756009.423900001 184038.085099999 184256.5099	
ORR_GeodB.DBO.SY	Feature Class	Polygon	-	1	755399.476899996 757345.545199998 183448.645500001 185210.815000001	
ORR_GeodB.DBO.UBC	Feature Class	Polygon	-	1	754811.278700002 756109.7293 182843.792300001 184434.851500001	
ORR_GeodB.DBO.UBC_Merge	Feature Class	Polygon	-	2	754811.278700002 759767.336599998 182843.792300001 186574.551800001	
ORR_GeodB.DBO.UEFPC	Feature Class	Polygon	-	1	755561.088200003 759767.336599998 183520.449700002 186574.551800001	

Fig. 6. ArcGIS Geodatabase Diagrammer Data Report

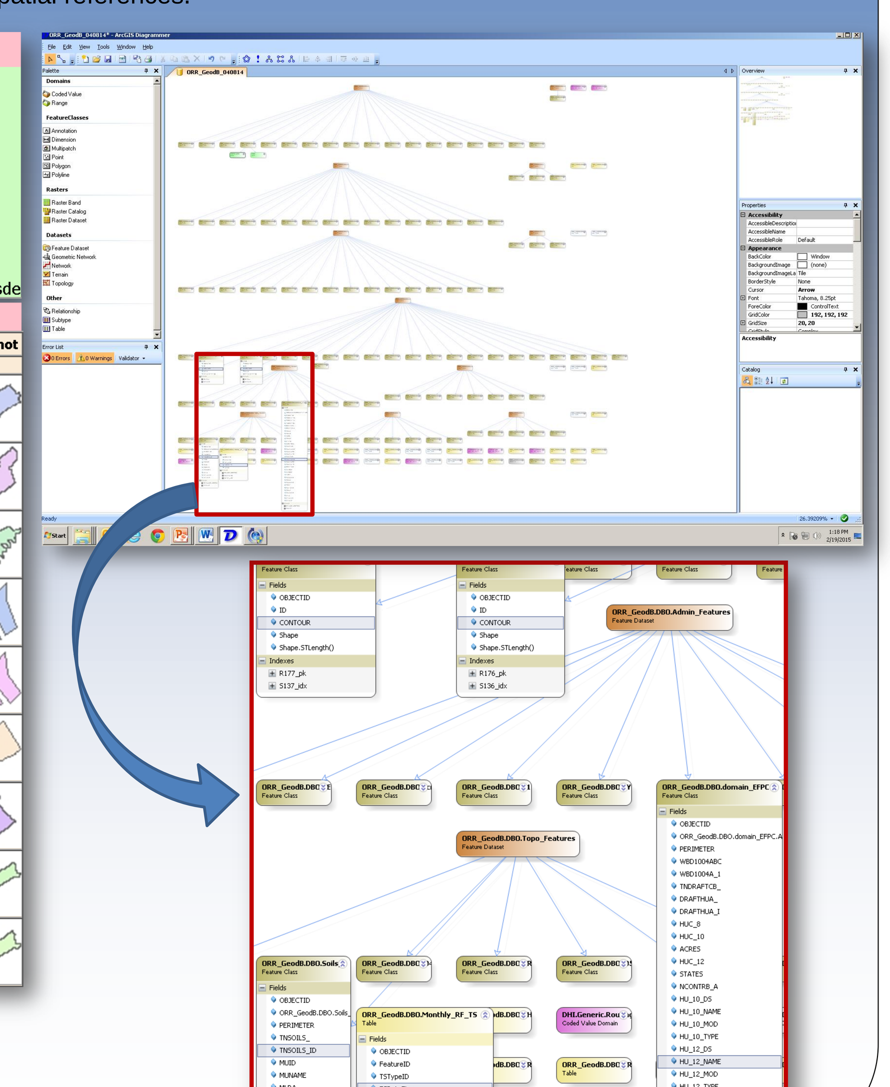


Fig. 7. ORR Geodatabase Schema Diagram

BENEFITS & CONTRIBUTIONS

- GIS-based hydrologic models can provide a spatial element that other hydrologic models lack.
- GIS enables hydrologists to pre-process and integrate data derived from multiple sources into a single manageable system.
- GIS-based approaches in hydrological modeling can be used to combine different layers of geographic data to create new integrated variables.
- GIS can be used for visualization of model-derived research results via maps, graphs and reports.
- GIS technology has proven useful in supporting the hydrological modeling work performed by FIU-ARC at the Oak Ridge Reservation (ORR) through development of a geodatabase which has provided an advanced spatial data structure for management, processing, and analysis of spatial and temporal numerical modeling data derived from multiple sources.
- ArcGIS ModelBuilder coupled with Python scripting enabled the automation of many of the repetitive geoprocessing tasks required for pre- and post-processing of hydrological modeling data. GIS data processing and automation facilitated faster and hence more complex analyses of field test data. The toolbox created is a scalable and reusable application that can be implemented at other DOE sites.
- Finally, a web-based GIS application can facilitate sharing of project derived data with stakeholders including DOE personnel and ORR site contractors.

ACKNOWLEDGEMENTS

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