
**Pacific Northwest
National Laboratory**

Operated by Battelle for the
U.S. Department of Energy

Examining the Linkage Between FRAMES and GMS

G. Whelan
K.J. Castleton

February 2006

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830



DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor Battelle Memorial Institute, nor any of their employees, makes **any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.** Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or Battelle Memorial Institute. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

PACIFIC NORTHWEST NATIONAL LABORATORY

operated by

BATTELLE

for the

UNITED STATES DEPARTMENT OF ENERGY

under Contract DE-AC05-76RL01830

Printed in the United States of America

Available to DOE and DOE contractors from the
Office of Scientific and Technical Information,
P.O. Box 62, Oak Ridge, TN 37831-0062;
ph: (865) 576-8401
fax: (865) 576-5728
email: reports@adonis.osti.gov

Available to the public from the National Technical Information Service,
U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161
ph: (800) 553-6847
fax: (703) 605-6900
email: orders@ntis.fedworld.gov
online ordering: <http://www.ntis.gov/ordering.htm>



This document was printed on recycled paper.

Examining the Linkage Between FRAMES and GMS

G. Whelan
K.J. Castleton

February 2006

Prepared for the
U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Division of Systems Analysis & Regulatory Effectiveness
Rockville, Maryland 20852
under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99352

Contents

1.0 Introduction.....	-4-
2.0 Groundwater Modeling System	-5-
3.0 Framework for Risk Analysis in Multimedia Environmental Systems	-7-
4.0 Examining the Linkage Between FRAMES and GMS.....	-8-
5.0 Recommendations.....	-15-
6.0 References.....	-17-

Figures

2.1. Three-Dimensional Rendition of a Leachate Plume Migrating Through Heterogeneous Porous Media using MT3DMS, as part of the Groundwater Modeling System (GMS).....	-6-
4.1. Schematic Illustration of the Connection of RT3D to Upstream and Downstream Modules Within in the FRAMES-2.0 Workspace	-10-
4.2.	

Demons

1.0 Introduction

The objective is to provide the U.S. Nuclear Regulatory Commission (NRC), Office of Nuclear Regulatory Research, Division of Systems Analysis & Regulatory Effectiveness with a dose-assessment tool for licensing decisions with sufficient power, flexibility, and utility that it can serve as their primary platform for analyzing the hazards associated with licensing actions at those “complex” sites at which the traditional dose-assessment tools are inappropriate. To meet this objective, this work will further the design and development of the evolving Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) software to enable the integration of or linkage to models of complex domain-specific processes to evaluate the potential for human exposure to radioactive contaminants in complex natural environments.

The U.S. Department of Energy (DOE) Pacific Northwest National Laboratory (PNNL), in conjunction with NRC, has developed a design for linking FRAMES Version 2 (FRAMES-2) and the Groundwater Modeling System (GMS). The objective of the linkage is to facilitate the exchange of model data (inputs/outputs) between the two modeling systems. Although the term GMS is used frequently and rather loosely, in the context of this work, it specifically refers to the computer models housed within GMS.

FRAMES is a software platform that allows users the ability to select and implement environmental software models for risk assessment and management problems. This program is a flexible and holistic approach to understanding how activities affect humans and the environment. It links models that integrate across scientific disciplines, allowing for tailored solutions to specific activities, and it provides meaningful information to business and technical managers. FRAMES is the key to identifying, analyzing, and managing potential environmental, safety, and health risks. The purpose of FRAMES is to assist users in developing environmental scenarios and to provide options for selecting the most appropriate computer codes to conduct human and environmental risk management analyses.

GMS is one of the most sophisticated and comprehensive groundwater modeling packages, containing numerous numerical models and support features for modeling the groundwater environment. GMS provides tools for every phase of a groundwater simulation including site characterization, model development, calibration, post-processing, and visualization.

Because GMS provides so many features, of which some are also addressed by FRAMES, it could represent a platform to link to FRAMES, or FRAMES could represent a platform to link to GMS. The focus of this summary is to examine the strengths and weaknesses of the potential linkage direction and provide recommendations for the linkage between FRAMES and GMS.

2.0 Groundwater Modeling System^a

GMS is one of the most sophisticated and comprehensive groundwater modeling software available. GMS provides tools for every phase of a groundwater simulation including site characterization, model development, calibration, post-processing, and visualization. GMS supports both finite-difference and finite-element models in two and three dimensions, including MODFLOW 2000, MODPATH, MT3DMS/RT3D, SEAM3D, ART3D, UTCHEM, FEMWATER, PEST, UCODE, MODAEM, and SEEP2D. The program's modular design enables the user to select modules in custom combinations, allowing the user to choose only those groundwater modeling capabilities that are required. Additional GMS modules can be purchased and added at any time. The software will dynamically link to these subsequent modules at run time—automatically adding additional modeling capability to the software.

The GMS approach for establishing the conceptual model makes it possible to build a conceptual model in the GMS Map Module using Geographical Information System (GIS) feature objects (points, arcs, and polygons). The conceptual model defines the boundary conditions, sources/sinks, and material property zones for a model. The model data can then be automatically discretized to the model grid or mesh. The conceptual model approach makes it possible to deal with large complex models in a simple and efficient manner. GMS provides tools for creating complex stratigraphy and translating 3-D objects directly to a finite-difference grid or finite-element mesh.

GMS has a powerful graphical tool for creating models and visualizing results. Models can be built using digital maps and elevation models for reference and source data. During the model building process, the graphical representation of the model allows quick review and presentation of your work. Fully 3-D views, with contouring and shading, of your model allow anyone to see and understand the domain and parameters of your analysis. Figure 2.1 illustrates the 3-D rendition of a leachate plume migrating through heterogeneous porous media using MT3DMS.

GMS features a suite of tools for performing stochastic simulations with MODFLOW and accompanying transport models. The Risk Analysis Wizard is a new tool associated with the stochastic modeling tools in GMS. Two types of analyses are currently supported: probabilistic threshold analysis and probabilistic capture zone delineation. This wizard allows you to quantify the risk of a contaminant exceeding critical levels in groundwater or the risk of a capture zone including key areas at a site. Such analysis helps determine appropriate action to be taken in design or remediation.

GMS includes a suite of tools to assist in the process of calibrating a groundwater model to point and/or flux observations. Calibration is the process of modifying the input parameters to a groundwater model until the output from the model matches an observed set of data. When a computed solution is imported to GMS, the point and flux residual errors are plotted on a set of calibration targets and a variety of plots can be generated showing overall calibration statistics. Most of the calibration tools can be used with any of the models in GMS. Automated parameter estimation is supported in GMS, using well known parameter estimation tools such as PEST and UCODE (i.e., sometimes called “inverse models”).

I() To confirm accuracy, the text for this section is based on http://www.ems-i.com/GMS/GMS_Overview/gms_overview.html.

GMS Using MT3DMS

Three-dimensional aquifer modeling of contaminant transport through heterogeneous porous media

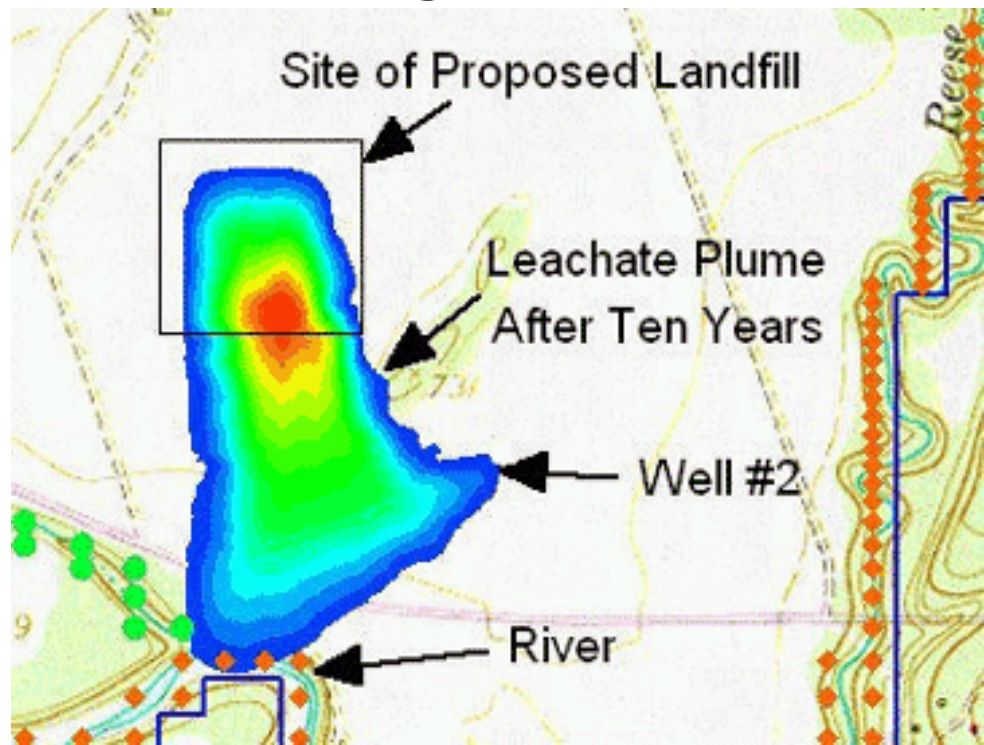


Figure 2.1. Three-Dimensional Rendition of a Leachate Plume Migrating Through Heterogeneous Porous Media using MT3DMS, as part of the Groundwater Modeling System (GMS)

3.0 Framework for Risk Analysis in Multimedia Environmental Systems

FRAMES (<http://mepas.pnl.gov/FRAMESV1/index.html>; <http://mepas.pnl.gov/earth/>), developed by PNNL and in conjunction with NRC, is a visual, object-oriented platform for linking disparate models and databases for conducting exposure and effects assessments. This object-oriented system design facilitates adding new objects and modules and provides a highly adaptive modeling environment for evaluating a wide array of exposure/risk scenarios. FRAMES follows the Environmental Software Systems Compatibility and Linkage guidelines, as outlined under the Interagency Steering Committee on Multimedia Environmental Models (ISCMEM; <http://iscmem.org/Proceedings.htm>). FRAMES seamlessly links user-defined disparate models, databases, and modeling systems to transfer data. FRAMES

- represents a deployable system
- provides a means to visually conceptualize the problem
- allows the user to choose the most appropriate models and databases to address the problem
- provides sensitivity/uncertainty analyses
- provides tools to visualize and tabularize the results
- provides a mechanism to document the results
- increases credibility as it automatically provides a mechanism to reproduce the results.

FRAMES provides the following major attributes: (1) PC Windows-based, (2) Plug&Play to allow users to import their own models into the system without the aid of a system developer, (3) Drag&Drop real-world icon objects to allow analysts to visually display the problem to be solved, (4) minimum data transfer requirements, so models only receive pertinent information, (5) system viewers (graphical & tabular) to provide managers with a means to view input/output, (6) Monte Carlo sensitivity/uncertainty wrapper to provide all models with a means to perform probabilistic analyses, (7) capability to begin the assessment at any point in the problem to eliminate unnecessary modeling, (8) new classes of models to enter into the system to seamlessly communicate with other models, (9) web accessibility to allow the user to link any model to any database at a remote location, (10) an aliasing capability to allow the user to define surrogates for chemicals and organisms for those databases that lack specific chemical and organism data of interest, (11) import spreadsheet data and user-supplied data to confirm that site-specific information is used, and (12) databases, including properties for chemical constituents and radionuclides, human exposure parameters and risk factors, aquatic and terrestrial toxicity reference values, biological species life-history profiles, food bioaccumulation factors, and biota sediment accumulation factors.

4.0 Examining the Linkage Between FRAMES and GMS

As noted in Section 3, the NRC hosted and documented Environmental Software Systems Compatibility and Linkage guidelines, as outlined under the Interagency Steering Committee on Multimedia Environmental Models (ISCMEM; <http://iscmem.org/Proceedings.htm>). This workshop and subsequent documentation provided a foundation of software attributes for those frameworks that would represent some aspect of middleware. Middleware represents that software that provides linkage capabilities between models, databases, and/or frameworks. Frameworks are defined herein as software representing a confederation of models and databases.

Communication through integration between FRAMES and GMS essentially represents the first attempt to link two stand-alone frameworks with inherently different designs and purposes. FRAMES was specifically designed as middleware, where as GMS was specifically designed to provide one of the most sophisticated and comprehensive groundwater modeling software systems for every phase of a groundwater simulation. The attributes and features exhibited by GMS are formidable and impressive. Gaining access to and using the GMS features would provide modelers with enhanced capabilities to address, not only the needs of NRC but also, the needs of multiple government agencies. Because GMS provides so many features, of which some are also addressed by FRAMES, it could represent a platform to link to FRAMES, or FRAMES could represent a platform to link to GMS.

By reviewing the Environmental Software Systems Compatibility and Linkage guidelines, it becomes apparent that using GMS as *de facto* middleware to link to FRAMES does not meet many of the 19 attributes recommended by the Interagency Steering Committee on Multimedia Environmental Models. GMS was never designed to represent middleware to link to other models or frameworks. As such, its site characterization, model development, calibration, post-processing, and visualization tools have been designed to address the needs of the models that are immediately contained within the system, although other models could (and do) use the peripherals contained within GMS, like the grid or mesh generators. Access to these components for use by FRAMES or other models linked to FRAMES would not confirm that FRAMES or these other models would enjoy the same immediate benefits as those models fully coupled in GMS.

There are many features and attributes that need to be considered when deciding on the best way to link to and use framework functionality. Some considerations are as follows.

- Parallel Development Efforts – GMS is a very sophisticated modeling system. There is no intent to, nor should we, recreate GMS in FRAMES. There are too many models in GMS, whose linkages are model-specific and whose complexities are not intended for the casual user. The most efficient way to take advantage of new software developments in GMS is to allow the developers of GMS to continue their parallel efforts without being encumbered by FRAMES-specific specifications. In this manner, GMS developers can continue on a parallel track where new features are accessed by FRAMES through a universal linkage mechanism, similar to the one exercised with RT3D (Whelan and Castleton 2006).^a

I() Castleton KJ. 2006. *FRAMES-2.0 Software System: Groundwater Modeling System (GMS) Importer*. Pacific Northwest National Laboratory, Richland, WA. (Draft).

- Framework-to-Framework Access – Using GMS as a starting point, there is no simple mechanism to access FRAMES or any other software system that exists outside of the GMS structure. Access to a GMS simulation from an outside software system can be relatively easily implemented, especially through FRAMES-2.0. A GMS simulation can be accessed through the FRAMES-2.0 Conceptual Site Model (CSM) workspace, using a FRAMES-2.0 icon and GMS Project File (Whelan and Castleton 2006). For example, access to a GMS saturated zone model (e.g., RT3D) would be through a FRAMES saturated zone icon (a.k.a. GMS icon). Because the CSM allows for information to be transferred to and from the icon, containing the GMS Project File (i.e., GMS icon), information can be consumed by the GMS model from another upstream module in the FRAMES-2.0 workspace, and information can be produced by the GMS model for consumption by other downstream modules in the FRAMES-2.0 workspace. Figure 4.1 illustrates the connection of RT3D to upstream and downstream modules within in the FRAMES-2.0 workspace. Figure 4.2 demonstrates how a user chooses a GMS Project File, representing RT3D. In this figure, the RT3D module is associated with the baseline calibrated run, titled GWTest1. Choosing this “Applicable Model” allows the user simple and easy access to GMS’ RT3D.
- Sensitivity/Uncertainty – Both FRAMES-2.0 and GMS have their own internal mechanisms for executing Sensitivity/Uncertainty (S/U) analyses. GMS internally contains Monte Carlo capabilities, and FRAMES-2.0 contains a different sampling mechanism (e.g., Latin Hypercube in FRAMES-2.0), reconciliation between the two potentially different sampling schemes maybe desired before full consistency between the frameworks can be attained. Because upstream icons can be linked to the GMS icon in the FRAMES-2 workspace (see Figure 4.1) to produce input for its consumption, the FRAMES-2.0 Sensitivity/Uncertainty (S/U) icon can also be linked to the GMS icon, allowing for random sampling of any input, which is passed to GMS through the GMS icon User Interface in the FRAMES-2.0 workspace. A simple solution is to eliminate one of the sampling schemes. Because both FRAMES and GMS run as a stand-alone systems, this solution would not be acceptable. Barring this solution, several options, associated with the S/U linkage between FRAMES and GMS, are available.
 - Hold GMS Static and Only Use FRAMES – Random sampling of GMS input parameters occurs within the FRAMES-GMS icon, using the FRAMES-2.0 S/U module(s), before passing the information on to GMS (i.e., RT3D). Under this situation, for each set of the random samples passed from FRAMES-2.0 to GMS, a single deterministic execution of the GMS model would occur, producing one set of output results per realization. The input at the FRAMES-2.0 level (e.g., source-term concentrations) is subsequently randomly sampled and supplied to GMS, resulting in a series of GMS output results based on deterministic GMS runs. In other words, FRAMES-2.0 controls and implements the S/U analysis by controlling which input parameters are varied, while GMS just performs deterministic runs. The statistics would be captured and collated at the downstream end by FRAMES-2.0. This option has many positive attributes. For example, the S/U module could be easily separated into an iterator, sampler, and summarizer, so the user has choices to use different statistical packages, when warranted. Additional S/U capabilities can be added, as needed (e.g., partial r^2 s).
 - Hold FRAMES Static and Only Use GMS – At the other extreme, input at the FRAMES-2.0 level is held static and is supplied to GMS, where the GMS Monte Carlo capabilities are exercised. In other words, FRAMES-2.0 provides static data, and GMS controls and implements the S/U analysis by controlling which parameters are varied.

- Use FRAMES and GMS Simultaneously – Because FRAMES-2.0 and GMS both contain Monte Carlo capabilities, both could be exercised simultaneously. This inherently creates problems as different approaches are being used to sample and implement the analysis. In addition, inconsistencies could arise if both systems were sampling the same parameter.

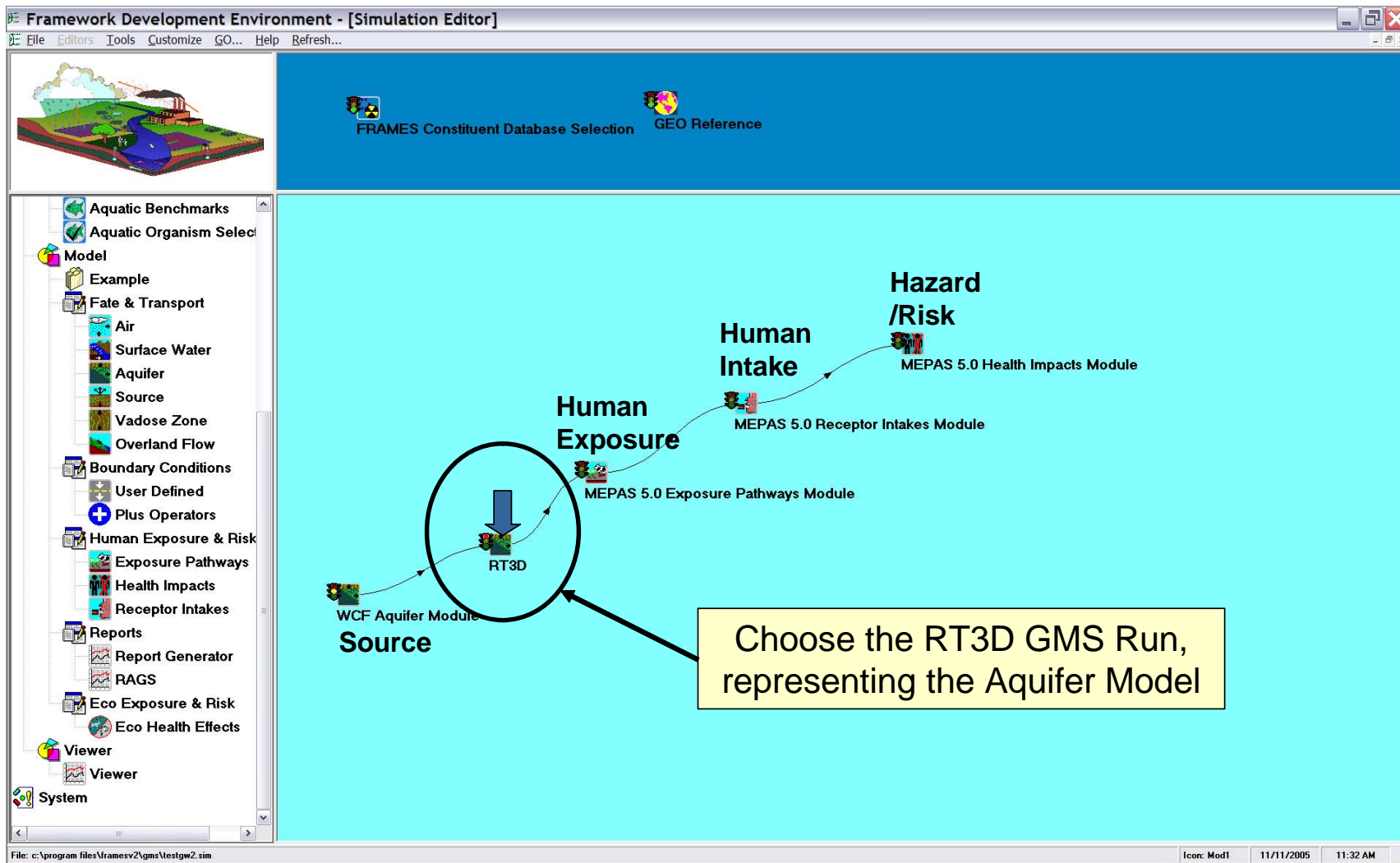


Figure 4.1. Schematic Illustration of the Connection of RT3D to Upstream and Downstream Modules Within in the FRAMES-2.0 Workspace

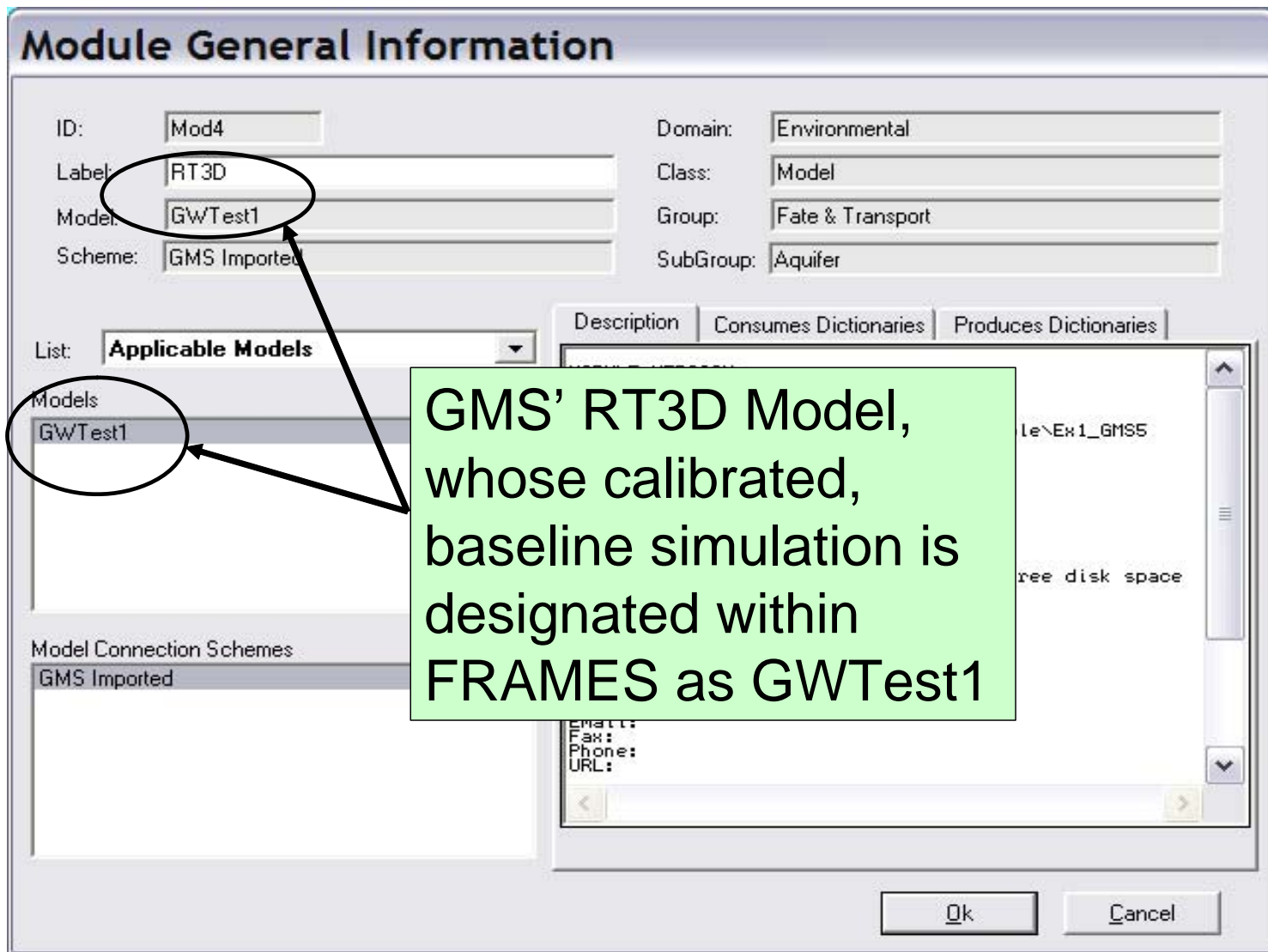


Figure 4.2. Demonstration of How a User Chooses a GMS Project File, Representing RT3D

- Use GMS in Serial or Parallel Execution – The linkage and subsequent execution could occur either in serial or parallel. A serial execution occurs when GMS produces output representing one realization set at a time. A parallel execution has GMS producing all output realizations, and FRAMES then accesses and imports the set of choice.
- Proprietary – Initiating the linkage from FRAMES addresses the difficult issue associated with proprietary software. By separating GMS from FRAMES, the user can maintain an appropriate distance from the legal entanglements that surround GMS. FRAMES represents open software that allows anyone to link his/her model to the system. If this coupled software (i.e., FRAMES and proprietary models in FRAMES) becomes proprietary, it is because the models linked to the system are proprietary; as the FRAMES system is free. Conversely, when a user pays a licensing fee for GMS, he/she licenses the peripherals that provide the added value to the models inside GMS. The model executables are not under the GMS license. If allowed by the model developer, the model executables are free to use. In other words, GMS can be used to set up a problem, using a particular model within GMS, but a FRAMES user is free to package a simulation, including the GMS portion of the simulation, and send it to anyone without violating the license. This is done by only packaging the groundwater model’s executable, as only the executable is required by FRAMES.
- ISCMEM Requirements – The FRAMES-2 design tried to follow the recommended 19 attributes documented by ISCMEM. This allows FRAMES the capability to provide more universal linkages to other software packages.
- Universal Linkage – The most important by-product of linking FRAMES and GMS is the linkage process/procedure that is developed. This process/procedure can be extended and used as a universal approach/template to link to FRAMES to other frameworks and more sophisticated, science-support models, in addition to GMS.
- Viewers – Viewers vary in complexity, purpose, and requirements. Viewers are typically designed for a specific purpose (i.e., communicate datasets or process flow). Viewers are used to describe the CSM, input and output results, spatial attributes, and summaries, just to name a few. The GMS CSM focuses on automatically discretizing model grids or meshes and defining the immediate boundary conditions, sources/sinks, and material property zones for a specific model. GMS also has powerful graphical tools for digitizing maps and visualizing results, but these are specific to the models in the GMS system. The peripherals in GMS, although impressive, are focused on only one medium, groundwater (i.e., vadose and saturated zones). GMS was not designed to present a multimedia (i.e., intermedia) CSM of the assessment, involving multiple models. FRAMES is a more likely mechanism to initiate the construction of a multimedia CSM, of which the groundwater pathway is one component. It also allows the user to plug and play viewers. This does not preclude a GMS expert from using the GMS viewers, but they would be used as part of the stand-alone GMS system.
- Contaminant Tracking – Not all models track contaminants in the same way. The range of choices is from internal tracking, to dependence on the integrating system to track, to no tracking at all. Not all models in GMS track contaminants of concern, as some may only accept one contaminant at a time. An iterator could be set up in FRAMES to feed these GMS models each contaminant in sequence. If appropriate, a module could be developed to roll up the output results, so the output is statistically captured. FRAMES tries to address the issue that not all models track contaminants in the same way. FRAMES assumes that all contaminants are, in effect, “parents” when being passed between models.

Each model is free to address progeny generation and account for the fact that any constituent can produce progeny, even progeny of progeny. As output the model would rename progeny as parents, who then again may produce progeny by the next model. Accounting for progeny in this manner allows the system to not only track progeny generation, but also allows models that do not generate progeny data to consume the information as parents and produce subsequent information in a manner that all models can consume.

- Universal GIS Linkages – Spatial information can be dealt with in number of different ways. Some models track location by noting the distance and offset from an arbitrary source (e.g., 100 m downgradient from the source). Some include a geospacial reference point that is universally based (e.g., latitude and longitude). Others use Geographical Information Systems to help track and display spatial data. GMS has a powerful graphical tool for creating models, building using digital maps and elevation models for reference and source data, and visualizing results. The GMS Map Module uses GIS feature objects (points, arcs, and polygons) to build a visual groundwater model. During the model building process, the graphical representation of the model allows quick review and presentation of the work. The conceptual model defines the boundary conditions, sources/sinks, and material property zones for a specific model. Fully three-dimensional views, with contouring and shading, of a specific model allow anyone to see and understand the domain and parameters of the analysis. The model data can then be automatically discretized to the model grid or mesh. FRAMES has been designed to handle the eventual linkage to the Geospacial Object Library For Environmental Modeling (GEOLEM; http://iscmem.org/WG01_Geolem.htm), which will represent middleware to open GIS systems, so visualization, analysis, and spatial needs would be provided in each model on an as-need-basis. The FRAMES GIS icon represents a place holder for the central distributing spatial data to all models in the system.
- Simulation Input/Output – Unlike GMS, FRAMES was specifically designed as a middleware conduit, shuttling information from one model to another. By using FRAMES as the linkage middleware, the GMS modeler would be required to identify not only which input parameters could be changed but also the location associated with the output results. The FRAMES user would only be allowed to change those input parameters deemed appropriate by the GMS model developer, and the FRAMES user would need the GMS expert to provide the geospacial location of the output results (e.g., node; cell; row, column, layer, etc.).
- Database Linkages and Data Transfer – GMS has fully coupled protocols and databases that support only those models in the system. FRAMES has software linkage tools that allow for communication between host (i.e., local) and remote systems (i.e., running models remotely or accessing data from remote databases). FRAMES has standardized the approach for data transfer, using Application Programming Interface (API) Dynamic Link Libraries (DLLs) and Function Calls, and metadata DICtionaries. These facilitate a more universal capability to communicate with different models and databases. FRAMES has develop several universal data transfer tools, three of which are of particular importance (<http://mepas.pnl.gov/ACC>).
 - a. Data Owner Tool (DOT) – The DOT is support software that allows the Data Owner to map the database structure to a file on the Module Server, which holds the developed extraction plans (mappings), database schema, and the schema of the Database DIC. In effect, the DOT documents the meta-information associated with the database and data to be extracted, when the extraction is invoked.
 - b. Data Extraction Tool (DET) – Data Extraction Tool (DET) extracts the data from the designated database and returns it to the DCE through the Hypertext Transfer Protocol (http).

- When invoked by the DCE, the DET goes out to the DOT database, retrieves the desired extraction plan from the DOT database, extracts the appropriate data through a Structured Query Language (SQL) server, and returns it to the DCE. The DCE then stores these data on the local drive in a designated file for eventual consumption by module icons (and their underlying models) connected to the data-set icon.
- c. Data Client Editor (DCE) – The Data Client Editor (DCE) invokes the Data Extraction Tool (DET), which extracts the data from the designated database and returns it to the DCE through the Hypertext Transfer Protocol (http), meeting the metadata requirements outlined by the Database DIC, containing the appropriate Variable Referencing Keys. Only those data associated with the Variable Referencing Keys are extracted from the database.

PNNL completed two out of the three major phases, each providing successively more complete linkages between the FRAMES and GMS:

1. FRAMES provides input to GMS for GMS to consume. GMS runs remotely, although the remote linkage and execution are not part of this phase. GMS then provides output for FRAMES to consume.
2. FRAMES imports output results from a stand-alone GMS application.

As part of the first two phases, a GMS expert will need to set-up, execute, and calibrate a base case, so it is stable and convergent. The inputs and outputs have been identified for RT3D (Castleton 2006; Whelan and Castleton 2006).

PNNL recommends maintaining FRAMES as the middleware to link to independent frameworks, like GMS, which can provide the much needed modeling sophistication that is required by managers for current assessments. Whelan and Castleton (2006) describe the step-by-step procedure for gaining access to and using GMS, and in particular RT3D, for more science-support analyses. Castleton (2006) presents the technical details of the linkage between FRAMES and GMS, again using RT3D as an illustrative example. Both of these documents provide recommendations on how to implement the collaboration between FRAMES-2.0 and GMS.

5.0 Recommendations

The next phase of GMS integration will allow the FRAMES user to 1) export information to GMS models, by modifying model inputs, 2) run the GMS model's calibrated executable, and 3) read outputs from an existing GMS project. PNNL creates the capability to import a GMS Project File (*.gpr) and then generate the information needed to run the imported Project File associated with the RT3D model. This will serve as a prototype approach to access all models contained within GMS.

Based on a review of the attributes associated with linkage options between FRAMES-2 and GMS, the following recommendations are made:

- The Sensitivity/Uncertainty (S/U) algorithms that currently exist in FRAMES-2 and GMS will remain separate and independent. Monte Carlo analysis using the FRAMES-2 S/U tools will only be associated with the input boundary conditions being provided to GMS and not associated with other information already in GMS.
- The initial S/U approach will be to execute GMS in serial mode, where output represents one realization at a time. At a later date, it is recommended to extend the S/U functionality to parallel mode, so GMS produces all output realizations, and FRAMES-2 then accesses and imports the GMS-output set of choice. FRAMES-2 is currently designed to consume an analysis using serial mode, so any modifications to implement this approach would not be extensive.
- It is recommended that FRAMES-2 be used as middleware to access GMS and provide functionality to supply GMS boundary conditions that vary and to integrate GMS output results as input to downstream models. Using FRAMES-2 as middleware allows users to package simulation results, only requiring the GMS model's executable and not GMS. Users receiving a simulation package containing linkages to GMS only need the executable associated with the model used in GMS.
- It is recommended that the FRAMES-2 and GMS software systems remain as separate, independent modeling software systems, linked through boundary-condition Input/Output (I/O) "portals."
- It is recommended that the linkage protocol implemented between FRAMES-2 and GMS represents a template for linking FRAMES-2 to other models in GMS and other software systems.
- The viewers contained in GMS should remain as peripheral support products in the stand-alone GMS system, and linkages to GMS viewers from FRAMES-2 should not be developed at this time, as special training is required to operate GMS.
- FRAMES-2 should eventually be used to link directly to GIS middleware, such as GEOLEM, for universal access to GIS software products, including those that are free. GMS is linked to ArcGIS, which is proprietary software and, therefore, does not lend itself for use without a fee.

Important work to be concluded, which goes beyond the first two phases of development, includes the following:

1. Develop a GMS-friendly structure (similar to a file management structure in GMS) that would capture all of the available GMS-calibrated runs under the Tools section of the FRAMES tool bar.

The user would then be able to choose the pre-runs of interest and place them under the appropriate icons in the Simulation Editor (i.e., work space where the icons are located).

2. Demonstrate the full linkage from source to risk for the following example: source, vadose zone, RT3D in GMS, to a well location, exposure, intake, and risk/hazard. The well location represents the point where contaminated water is removed, and sensitive receptors are exposed to this water. It should be recognized that PNNL developed this linkage in a universal, generic manner, so we should be able to easily map all of the inputs and outputs of GMS, not to mention any other modeling system or set of models. Currently, the spatial grids must match exactly, and locations (i.e., spatial attributes) are not system tracked, as the GIS (i.e., GEOLEM) is not complete.
3. Develop the GMSImport tool, so it is constructed in a way that will allow for easy inclusion for importing additional models within GMS, such as MT3DMS.

6.0 References

American Chemistry Council. *Comprehensive Chemical Exposure Framework*. Available at: <http://mepas.pnl.gov/ACC>

Environmental Modeling Systems, Inc. *GMS 6.0 Overview*. Available at: http://www.ems-i.com/GMS/GMS_Overview/gms_overview.html

Framework for Risk Analysis in Multimedia Environmental Systems. Available at: <http://mepas.pnl.gov/FRAMESVI/index.html>

Framework for Risk Analysis in Multimedia Environmental Systems. Available at: <http://mepas.pnl.gov/earth/>

Interagency Steering Committee on Multimedia Environmental Models. Available at: <http://iscmem.org/Proceedings.htm>

Interagency Steering Committee on Multimedia Environmental Models. Available at: http://iscmem.org/WG01_Geolem.htm

Whelan G, and KJ Castleton. 2006. *Groundwater Modeling System Linkage with the Framework for Risk Analysis in Multimedia Environmental Systems*. PNNL-15654. Pacific Northwest National Laboratory, Richland, WA..