REVIEW OF INTEGRATING PROGRAMS AND CODE STRUCTURES USED FOR DOE ENVIRONMENTAL ASSESSMENTS

Cementitious Barriers Partnership

ACKNOWLEDGEMENTS

Disclaimer

FOREWORD

The Cementitious Barriers Partnership (CBP) Project is a multi-disciplinary, multi-institutional collaboration supported by the United States Department of Energy (US DOE) Office of Waste Processing. The objective of the CBP project is to develop a set of tools to improve understanding and prediction of the long-term structural, hydraulic, and chemical performance of cementitious barriers used in nuclear applications.

A multi-disciplinary partnership of federal, academic, private sector, and international expertise has been formed to accomplish the project objective. In addition to the US DOE, the CBP partners are the United States Nuclear Regulatory Commission (NRC), the National Institute of Standards and Technology (NIST), the Savannah River National Laboratory (SRNL), Vanderbilt University (VU) / Consortium for Risk Evaluation with Stakeholder Participation (CRESP), Energy Research Center of the Netherlands (ECN), and SIMCO Technologies, Inc.

The periods of cementitious performance being evaluated are >100 years for operating facilities and > 1000 years for waste management. The set of simulation tools and data developed under this project will be used to evaluate and predict the behavior of cementitious barriers used in near-surface engineered waste disposal systems, e.g., waste forms, containment structures, entombments, and environmental remediation, including decontamination and decommissioning (D&D) activities. The simulation tools also will support analysis of structural concrete components

of nuclear facilities (spent-fuel pools, dry spent-fuel storage units, and recycling facilities such as fuel fabrication, separations processes). Simulation parameters will be obtained from prior literature and will be experimentally measured under this project, as necessary, to demonstrate application of the simulation tools for three prototype applications (waste form in concrete vault, high-level waste tank grouting, and spent-fuel pool). Test methods and data needs to support use of the simulation tools for future applications will be defined.

The CBP project is a five-year effort focused on reducing the uncertainties of current methodologies for assessing cementitious barrier performance and increasing the consistency and transparency of the assessment process. The results of this project will enable improved risk-informed, performance-based decision-making and support several of the strategic initiatives in the DOE Office of Environmental Management Engineering & Technology Roadmap. Those strategic initiatives include 1) enhanced tank closure processes; 2) enhanced stabilization technologies; 3) advanced predictive capabilities; 4) enhanced remediation methods; 5) adapted technologies for site-specific and complex-wide D&D applications; 6) improved SNF storage, stabilization and disposal preparation; 7) enhanced storage, monitoring and stabilization systems; and 8) enhanced long-term performance evaluation and monitoring.

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1.0   INTRODUCTION

LIST OF ABBREVIATIONS AND ACRONYMS

ASME	American Society of Mechanical Engineers
ASR	Alkali-silica reaction
BC	Boundary condition
BNL	Brookhaven National Laboratory
BLT-MS	Breach, Leach, and Transport-Multiple Species
CAB	Citizen's Advisory Board
CBP	Cementitious Barrier Partnership
DAKOTA	Design Analysis Kit for Optimization and Terascale Applications
DLL	Dynamic-linked Library
DOE	Department of Energy
DOS	Disk Operating System
DUST-MS	Disposal Unit Source Term-Multiple Species
FRAMES	Framework for Risk Analysis in Multimedia Environmental Systems
GS	GoldSim
GMS	Groundwater Modeling System
HLW	High-level waste
LHS	Latin Hypercube Sampling
LLW	Low-level waste
MEPAS	Multimedia Environmental Pollutant Assessment System
MPI	Message Passing Interface
NQA	Nuclear Quality Assurance
NRC	Nuclear Regulatory Commission
PA	Performance assessment
PNNL	Pacific Northwest National Laboratory
PPA	Probabilistic performance assessment
PVM	Parallel Virtual Machine
SAND	Simultaneous analysis and design
SDA	Subsurface Disposal Area
SDF	Saltstone Disposal Facility
SNL	Sandia National Laboratories
SPMD	Single-Program Multiple Data
STOMP	Subsurface Transport Over Multiple Phases
TID	Task IDentifier
TSPA	Total System Performance Assessment
V&V	Verification and validation

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ABSTRACT

A fundamental understanding of the behavior of cementitious barriers will be needed to reduce uncertainty in performance evaluations and to improve designs. These barriers are often one of the primary control mechanisms to prevent or limit radionuclide releases from nuclear facilities. Improved tools are needed to allow performance assessments to fully incorporate and consider the effectiveness of cementitious barriers, which in part limits the types and quantities of contaminants that may be disposed of in shallow land disposal. A set of simulation tools are needed to predict 1) the hydraulic properties, 2) the stability of the relevant cement matrix phases and 3) the release fluxes of contaminants in response to variable boundary conditions and system stresses over relevant time periods. The developed tools should include explicit evaluation of uncertainty in the resulting performance estimates. In this chapter, examples of relevant integration frameworks and couplings are described in the context of the CBP modeling needs. Each of the frameworks described has strengths and weaknesses based on the models that will be selected and the extent and nature of the interactions among the models.

An important objective of the Cementitious Barrier Partnership (CBP) project is to develop a reasonable and credible set of simulation tools to predict the structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over relevant time frames. These barriers are often one of the primary controls to prevent or limit radionuclide release from nuclear facilities. Without adequate tools to estimate future contaminant releases, performance and risk assessments cannot fully incorporate the likely effectiveness of concrete barriers, which may limit the kinds and quantities of radionuclides that may be disposed of in shallow land disposal. Furthermore, understanding the behavior of cementitious barriers at a more fundamental level is needed to evaluate and improve designs for nuclear waste disposal and other critical applications including nuclear power plants and spent nuclear fuel pool storage. A set of simulation tools are needed to predict: 1) the hydraulic properties, 2) the stability of the relevant cement matrix phases and 3) the release fluxes of contaminants in response to variable boundary conditions and system

stresses over relevant time periods. The developed tools should include explicit evaluation of uncertainty in the resulting performance estimates.

A simplified approach to model integration is initially provided that can be used to guide the selection and development of both the models and the needed framework for predicting waste-management related properties of cementitious barriers. Examples of relevant integrations or couplings of models are described in the context of the CBP needs. Each of the integration platforms had strengths and weaknesses depending on the models selected and the nature and extent of interactions among the selected models.

The mechanisms that effect both the structural integrity of cementitious barriers and their capacities to isolate contaminants from the environment can be conceptualized as a series of interacting processes describing physical, hydraulic, and chemical performance. In summary, changes in hydraulic properties, structural performance, and contaminant releases are the net consequences of changes in the physical-chemical structure of the cementitious material in response to ingress and egress of chemical constituents, on-going chemical reactions, and internal and external physical stresses. Contaminants released from the barrier can migrate to human receptors through various exposure media (e.g., vadose zone, groundwater, or surface water) through different potential pathways (e.g., inhalation or ingestion). These potential mechanisms and processes can be abstracted as illustrated in Figure 1[1]. The area of interest for the CBP (i.e., including hydraulic properties and contaminant fluxes from the cementitious barrier) is indicated by a dashed line in Figure 1.

The fluxes of contaminants exiting the cement barrier in question as a function of time are of primary interest to the CBP. However, for contaminants to be released from the cement matrix or barrier at rates above that of simple diffusion, the concrete must undergo some sort of aging or degradation process and a contaminant transport mechanism must be available (e.g., with percolating water or by diffusion). There are a number of processes known to degrade concrete, which will provide for both the release of contaminants from the cement matrix and their subsequent migration from the barrier to the surrounding environment. Some of the known degradation processes include chemical attack (e.g., by chloride, sulfate, oxygen and/or carbonate), frost attack, corrosion of structural members, gas generation, and gel expansion.

Figure 2 provides a simplified conceptual model for many known causes of concrete degradation and how these causes might interact to impact durability, barrier performance, and structural performance (Long, Henderson & Montgomery 2001; Pretorius 2001). The degradation processes that affect durability also tend to impact the performance of the cement as a waste matrix because of changes in pore structure and diffusivity of oxygen and contaminants. Cracking plays a major role in the performance of the concrete barrier by increasing the rate of transport of contaminants to the environment under many scenarios. The development of cracks impacts the transport of oxygen, water, and dissolved species (e.g., sulfate or chloride) into the concrete[2] and contaminants from the cement matrix to the environment (Walton 1992). Degradation also affects the structural properties and performance of the concrete in its ability to withstand

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[1] Figure 1 is based on a presentation entitled "Long-Term Performance of Surface and Sub-Surface Engineered Barriers" by Jacob Philip and Thomas Nicholson of the U.S. Nuclear Regulatory Commission (NRC) to the National Academy of Science on May 26, 2006. The presentation is available at http://dels.nas.edu/besr/docs/PhilipNicholson.pdf (accessed October 1, 2008).

[2] Transport impacts and cracking are coupled in that the movement of sulfate and other species (originally by diffusion) into the concrete can cause cracking of the concrete, which then may result in increased transport. It has been suggested by Walton (1992) that in "the absence of cracks, high quality concrete will almost always do an outstanding job of isolating waste because of its low permeability and high available surface area for sorption. In the presence of cracks, concrete only sometimes works well for waste isolation."
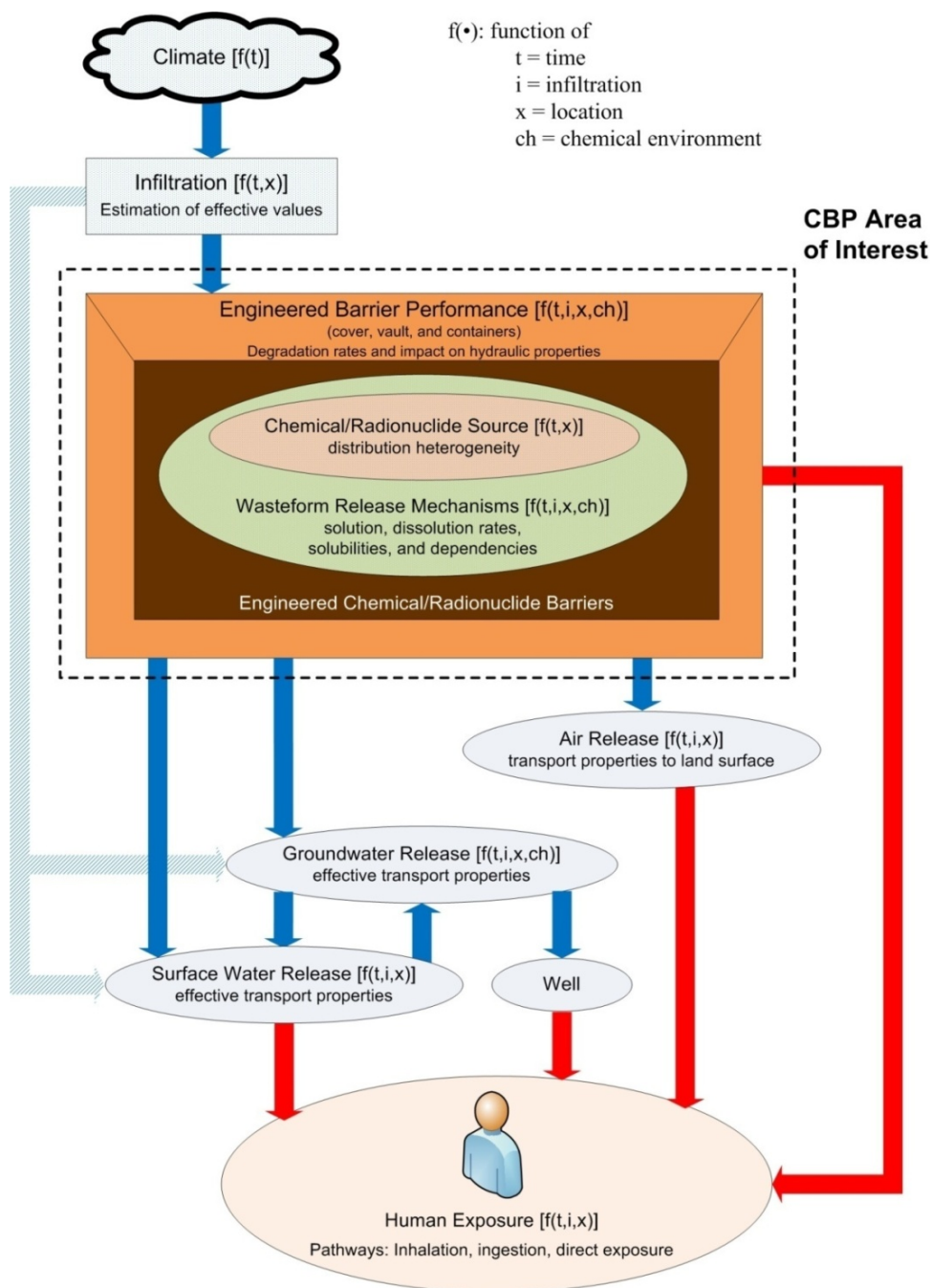
Figure 1. Generalized Performance Assessment Conceptualization (Adapted from A Diagram from Philip and Nicholson (2006)[1])
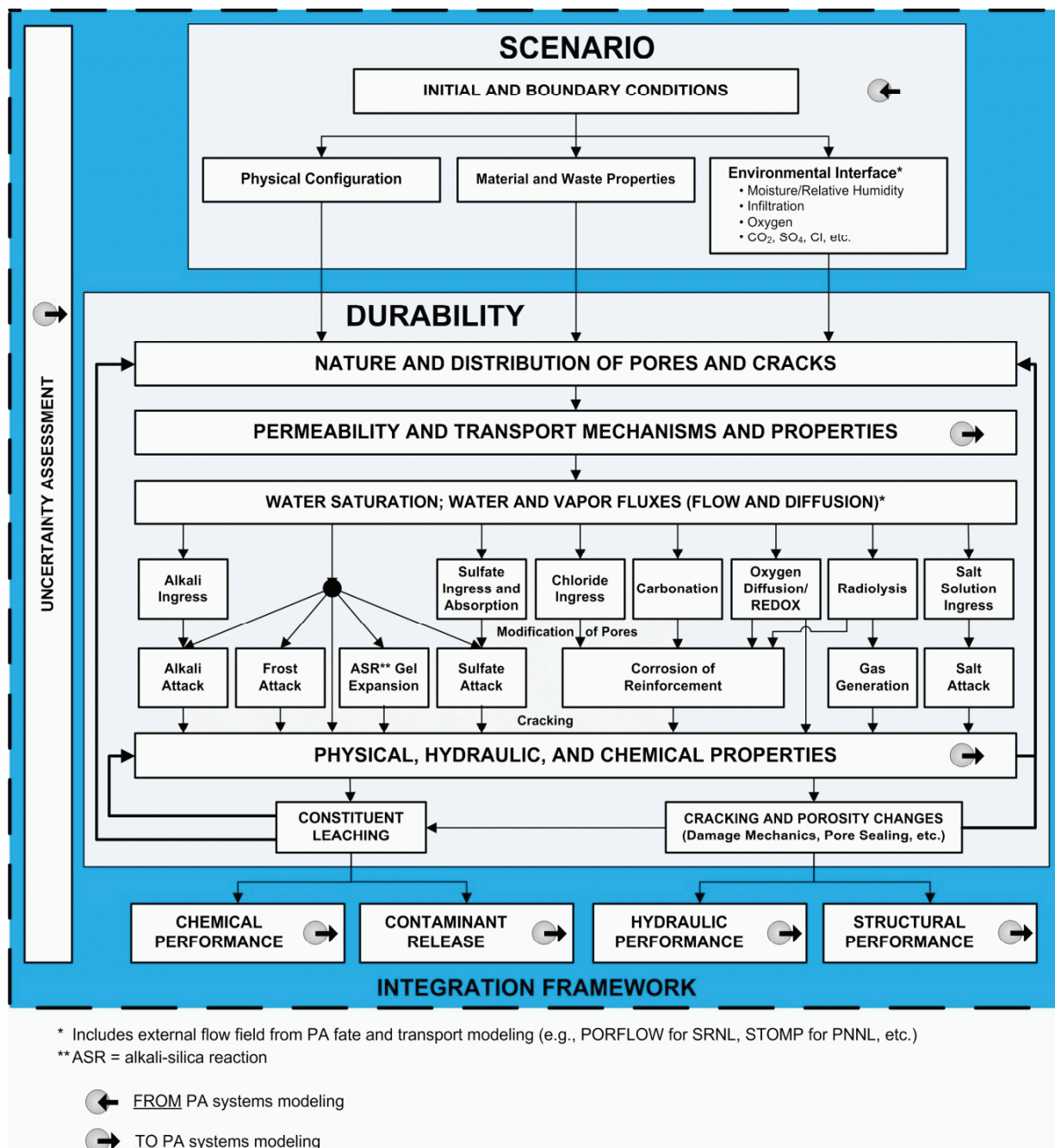
Figure 2. Specifications, Properties, and Phenomena for the Evaluation of Performance of Cementitious Barriers (Adapted from Long et al. (2001) and Pretorius (2001))

loads and limit load-induced cracking.

Another aspect of modeling concrete deterioration and subsequent contaminant transport apparent from the conceptualization in Figure 2 is that it may be possible to represent concrete degradation as a coupled set of modular process that interact with the broader performance assessment computations. Modules can be developed (if not already available) for important degradation processes and then coupled to provide a comprehensive model of concrete deterioration. For example, models are available for many of the important degradation and transport processes represented in Figure 2 (e.g., sulfate and chloride ingress and attack or carbonation). Thus a coupled, modular approach is the expected CBP approach to develop state-of-the-art tools to model concrete behavior for nuclear applications[3]. A modular approach to software design also generally results in easier development and produces better quality results than monolithic design and programming approaches (Lee 1994).

2.0   A SIMPLIFIED APPROACH FOR MODEL INTEGRATION

At a fine enough level of detail, any model integration problem could likely be considered unique; each may use a different framework, require different models, or answer different questions than another integrated solution. However, model integration approaches often have many elements in common, and a process to be followed can be generalized. Figure 3 provides a simplified conceptual framework that was used to develop the screening risk tool for U.S. Department of Energy (DOE) shallow land burial wastes (Brown 2008). Although the framework in Figure 3 was followed for a specific purpose, it can be used to develop a more general integrated model development

framework to inform any such integration process including that for cementitious barriers.

As illustrated in Figure 3, one of the first steps is to conceptualize the problem in terms of the necessary solution and the characteristics that must be captured in order to solve the problem. The approach adopted should be commensurate with the importance, complexity, and maturity or "stage" (e.g., screening, cleanup level definition) of the problem to be solved. These considerations impact not only model selection and integration efforts but also how input data and model parameters should be managed.

Because of the expense involved with quantitative assessment of uncertainties in a simulation (e.g., design and analysis of data, defining relevant probability distributions, structuring uncertainty analyses, or updating), the ability to perform sensitivity analyses is critical to the efficient use of resources. The parameters that most influence model outputs should be identified so that efforts and resources can be focused appropriately. The most typical sensitivity analysis examines the impacts of parameters or input data one-at-a-time and may omit important interaction effects. More sophisticated sensitivity analysis techniques are available depending on the nature and importance of the problem and whether the additional complexity is warranted. These alternative methods may be called externally much in the same manner as the models used to predict needed cementitious barrier behavior. Furthermore, sensitivity and uncertainty analyses are rarely performed in a vacuum; insights from model developers and users are often available and represent an excellent starting place for these analyses.

2.1. Nature of Coupling

How individual models in the CBP framework will be

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[3] A monolithic approach to software development is also possible where all needed functionality is programmed in a single, monolithic code and tight coupling can be instituted. However, the gain in coupling and efficiency from a monolithic code structure may occur at a cost of increased development time (especially if modules or callable programs already exist) as well as the typical issues of low re-usability and interoperability when compared to more modular or component-based schemes. It has been assumed that because programs are available with much of the necessary functionality that a modular scheme will be adopted for the CBP.
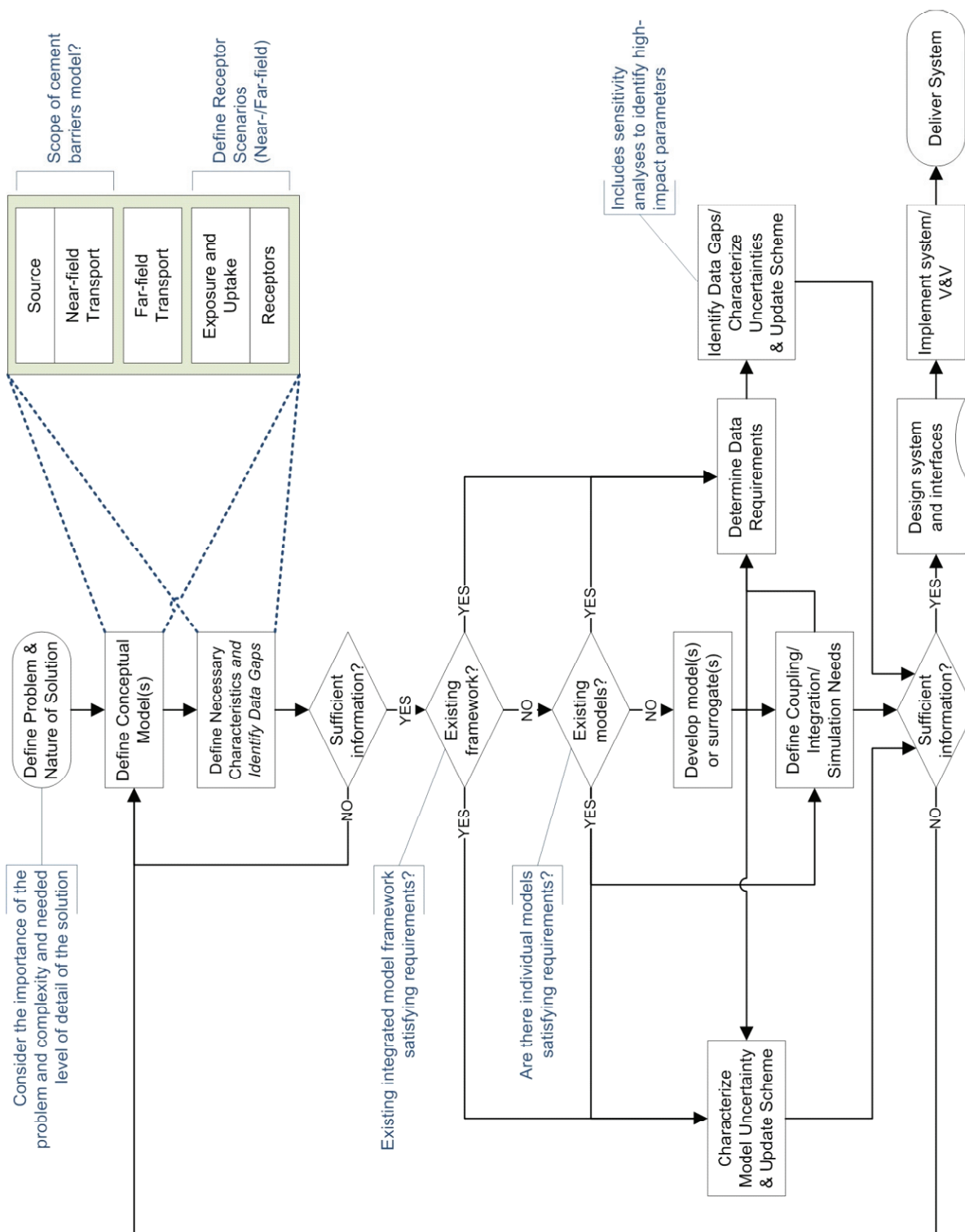
Figure 3.   Simplified Approach to Model Integration for the Risk Screening Tool for Department of Energy (DOE) Buried Wastes (Brown 2008)

implemented and the nature of the dependencies (i.e., coupling) among the model implementations (denoted subordinate codes) requires examination. The degree and directions of the coupling required among the individual subordinate codes will depend on numerical stability considerations for the physical phenomena modeled. Coupling can be classified along the following lines for the integrated simulation framework[4]:

- **None** – The subordinate codes are not related
- **Unidirectional** – The codes are run once in an appropriate sequence with "downhill" information flow and without internal feedback loops between subordinate models.
- **Very weak** – There is coupling between simulations; that is, each subordinate can run independently for an entire transient with iteration needed between transients to synchronize results.
- **Weak** – There is coupling between timesteps; that is, subordinates must be synchronized after each timestep or at defined timestep intervals.
- **Strong** – There is coupling within timesteps; that is, the subordinate programs must proceed together during each timestep.

The degree of coupling required by the physical processes modeled will have a critical impact on the software integration, and methods have been developed for handling complexities arising from coupling (Matthies, Niekamp & Steindorf 2006). Because the integrated framework to be developed by the CBP is intended to provide temporally- and spatially-varying constituent fluxes and important hydraulic properties as input to a higher-level performance assessment (PA) code (e.g., PORFLOW or STOMP), the considerations raised in these sections also apply to interactions between the CBP framework and PA code.

It may be preferable to tightly couple models if the models run sufficiently fast and have interfaces that allow them to be tightly coupled with each other. Under these conditions, the integration framework would be primarily a passer of information amongst individual models and a collector of results (i.e., a blackboard) for resulting evaluation. However, the interactions and interdependencies (i.e., coupling) likely to exist among any set of models (especially complex phenomenological models) needed to solve a sophisticated, real-world problem are such that a tight coupling of models is likely to present logistical and computational difficulties[5]. The temporal nature and spatial complexity of the solution likely needed for a state-of-the-art analysis of concrete barriers will likely exacerbate any model coupling and surrogate model development issues. The coupling of individual subordinate models within the integrated framework (as well as the framework and PA model) will be as loose (or weak) as possible based on the numerical stability of the physical phenomena being represented (Cole 2002; Weaver, Tomlinson & Aumiller 2000; Weaver, Tomlinson & Aumiller 2001). This "weak coupling" strategy will allow the CBP tools to leverage off existing programs and maintain as much fidelity as possible to the original codes and solutions.

2.2 Computing Environment

The hardware and software platforms that are used to develop and run an integrated framework are also important considerations. One possible classification for computing environments is:[6]

- **Heterogeneous environment** – Multiple operating systems (e.g., LINUX and Microsoft Windows) and different hardware platforms are needed.

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[4] The classification is taken from a personal communication from G. Flach of SRNL on March 31, 2009. There are additional classification schemes for coupling considerations (King 2005; Page-Jones 1980; Stevens, Myers & Constantine 1974).

[5] Individual models may have performances too slow for use in an integrated framework. Under these circumstances, it may be possible to develop surrogate models or to extract the underlying relationships for direct implementation in the simulation framework, which would make their coupling more straightforward. The technique is also influenced by the quality of the supporting information. Ultimately, the sophistication of the integrating model will be commensurate with the nature of the supporting information.

[6] The classification is taken from a personal communication from G. Flach of SRNL on March 31, 2009.

- **Homogeneous environment** – The same operating system and hardware platform can be used.
- **Single machine** – The coupled software runs on a single machine (although possibly with parallel or multiple processors).

For example, if necessary models must be run on different operating systems, then a framework is necessary that operates in a heterogeneous environment with communication among subordinate codes over a network. On the other hand, a homogeneous environment or single machine could be used if 1) all needed models can run on a single operating system/ hardware configuration or 2) surrogate models can be developed, when needed, to run under the selected configuration. This consideration also applies to the integrated CBP framework and PA model.

The option that requires the least work from model developers would be to call legacy model codes (running in a single operating system) as external, standalone processes from the framework system. However, the needed models may not run on the necessary operating system or executing a model may be computationally too expensive especially if a large number of runs are needed during a simulation (e.g., for an uncertainty analysis). A common alternative to improve computational efficiency is to develop surrogate models that can be integrated directly into the simulation framework and called instead of the more complex models (Field Jr. 2005; Qian et al. 2006). However, using surrogate models not only tends to increase overall model uncertainty (which must be accounted for), it can also change the fundamental nature of the uncertainties in the models because of the tendency of the surrogate model development process to smooth the results. Properly constructed surrogate models must not lose any important model response information.

2.3 Programming Languages Used

Another important aspect that impacts coupling in the system is model implementation (e.g., development environment or native language). Often the native language used to implement a model impacts the manner in which another program can interact with the model code. For example, in the Parallel Virtual Machine (PVM) described in Section 3.5, the C and C++ bindings for the user interface library are implemented as functions; whereas, those for FORTRAN codes are implemented as subroutines (Geist et al. 1994). The CBP framework program, expected to be composed of coupled, subordinate models selected to describe necessary physical phenomena, is intended to supply temporally- and spatially-varying contaminant fluxes and hydraulic properties to a PA model. Thus, linking considerations extend beyond the CBP framework itself.

2.4 Additional Considerations

There are aspects of the conceptual framework in Figure 3 that are non-technical but still very important to the successful development of a credible simulation tool. First, the software tools must follow applicable design guidelines not only because this is a requirement for DOE software[7], but because software design is good programming practice. Because of the desire to maintain fidelity to legacy codes, the nature of the simulation tool should lend itself to modular software design, which will further promote ease of understanding, maintenance, and extensibility. Modularity in a software system will make it easier to stage required development and testing among multiple developers. Finally, the level of required verification and validation (V&V) will also impact the development and, ultimately, acceptance of the cementitious barrier simulation tools.

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[7] Software development for use by the U.S. Department of Energy (DOE) must satisfy the requirements of ASME NQA-1 (ASME 2000).

2.5 Selection Criteria for the CBP Model Framework

A modular approach to software design, development, and maintenance is expected for the tools to be developed for the CBP. This approach has many potential benefits to both developers and end users. Some of the benefits of a modular design include (Lee 1994; Shorter & Adair 2008; Tuchschmid et al. 2006):[8]

- **Development** – Program development can be easily staged or performed in parallel using multiple developers.
- **Prototyping** – This is the stage between design and coding where complex algorithms can be demonstrated or alternative algorithms tested in modules.
- **Testing and Debugging** – Since modules will have well-defined interfaces, modules can often be evaluated independently by testing the interfaces. Some modules may be tested alone; others may need to be coupled with stub procedures to simulate related modules.
- **Understandability** – The modular nature of the system lends itself to being much easier to understand than a monolithic, procedural code.
- **Extensibility** – New results or components can be integrated into the system quickly and easily.
- **Scalability** – Additional computational resources can be utilized (when needed) in a scalable fashion.
- **Real-time capability** – Realistic simulator behavior requires compliance with various real-time constraints including execution in reasonable time on accessible hardware.
- **Maintainability** – The system can be sustained in a research environment often subject to changing information and innovations.
- **Flexibility** – Modules and components should be exchangeable to supporting different application domains and situations.

Various frameworks—modular and otherwise—have been developed to model complex systems. Examples of the various types of approaches available to simulate complex systems, especially those related to the CBP, follow.

3.0 EXAMPLES OF INTEGRATED MODELING APPROACHES AND PLATFORMS

Examples of approaches and platforms that have been used to develop integrated simulation tools for environmental assessments are described to illustrate alternatives to the problem posed by the CBP. These examples of approaches and platforms include

- **Monolithic Approach** – Implement all functionality in a single, monolithic code
  » CEMENT code (Seitz & Walton 1993)
- **Fidelity Approach** – Maintain fidelity to original programs
  » Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) (Whelan et al. 1997)
- **Hybrid Approach** – Adopt principles of both Monolithic and Fidelity Approaches to strike the needed balance between coupling and fidelity
  » Design Analysis Kit for Optimization and Terascale Applications (DAKOTA) (Eldred et al. 2006a; Eldred et al. 2006b; Eldred et al. 2006c)
  » GoldSim Monte Carlo simulation program (GTG 2005b; GTG 2005c)
- **Custom Interface Approach** – Develop custom interface for information passing
  » Parallel Virtual Machine (PVM) (Cole 2002; Geist et al. 1994).

Other tools are briefly described (i.e., BARRIER and 4Sight) to illustrate the breadth of available tools. Finally, the modeling effort to couple flow and transport, infiltration, geochemistry, etc. to support

[8]Although presented as benefits, many elements in the list can also be considered *requirements* for a successful modular system.

the SRS Saltstone performance assessment (PA) is described. The tools that will be developed by the CBP will provide the source term information for a PA like that described for Saltstone.

3.1 Monolithic Approach Example: CEMENT Code

The CEMENT computer code was developed by the Idaho National Engineering Laboratory to implement simplified models describing the processes critical to concrete service life and performance as a barrier to flow and transport for use in performance assessments for concrete vaults and waste forms (Seitz & Walton 1993). Multiple concrete degradation processes are modeled (i.e., reinforcement corrosion, sulfate attack, freeze/thaw, and alkali-aggregate reactions) with an emphasis on rebar corrosion and cracking. The CEMENT code was developed as a monolithic FORTRAN 77 program with subroutines representing the various degradation and transport processes. The subroutines and thus the various processes were not meant to be run in a coupled fashion.

3.2 Fidelity Approach Example: Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES)

The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) was developed by the Pacific Northwest National Laboratory (PNNL) in conjunction with the US NRC[9] (Whelan & Castleton 2006a; Whelan et al. 1997). FRAMES is a platform that allows users to integrate selected legacy environmental software models for risk assessment and management problems (Whelan & Castleton 2006a; Whelan & Castleton 2006b; Whelan et al. 1997). The program is a flexible and holistic approach to understanding how industrial activities may affect

humans and the environment. With specific changes, legacy models can be integrated across scientific disciplines allowing for tailored solutions to specific activities and providing meaningful information to stakeholders and decision makers. FRAMES can be used to develop environmental scenarios and provide options for selecting appropriate models to conduct human and environmental risk management analyses.

The FRAMES program is a visual, object-oriented platform for linking potentially disparate legacy models and databases for conducting assessments. The design facilitates addition of new objects and modules to provide a highly adaptive modeling environment for evaluating a wide variety of exposure and risk scenarios. FRAMES couples user-defined models, databases, and legacy models and systems to transfer data and perform assessments. The FRAMES program (Whelan & Castleton 2006a)

- allows the problem to be conceptualized visually;
- allows the user to choose from different models and databases to address the problem;
- provides sensitivity and uncertainty analysis capabilities; and
- provides tools to visualize, tabulate, and document the results.

The FRAMES program is a Windows-based/Plug&Play system that allows users to import models into the system without the aid of a developer (Whelan & Castleton 2006a). Virtual constructs of real-world objects can be "dragged and dropped" into the system allowing analysts to visually analyze the problem as illustrated in Figure 4. Minimum data are required and models only transfer pertinent information. Monte Carlo sensitivity and uncertainty wrappers provide integrated models with a means to perform probabilistic analyses. The user can also link to external models and/or databases remotely via

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[9] Additional information for the version 2.0 of FRAMES can be found on the PNNL Earth: Environmental Assessment and Risk Tools site at http://mepas.pnl.gov/earth/ and http://mepas.pnl.gov/Frames, V2/index.stm (accessed October 1, 2008).
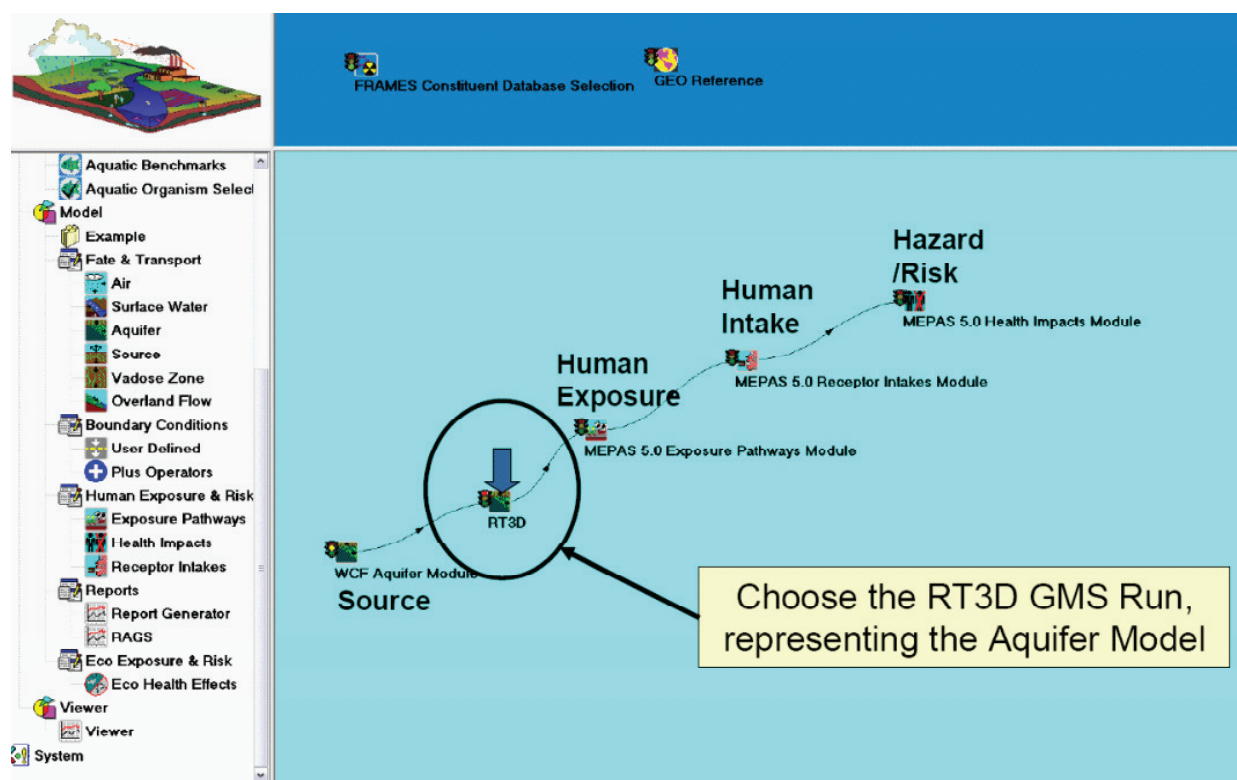
Figure 4. Connecting the RT3D Program to Upstream and Downstream Modules within the FRAMES-2.0 Workspace (Reproduced from Whelan and Castleton (2006a))

web access (although this can significantly compromise computational efficiency). Available databases include those for properties of chemicals 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.

Conceptually, FRAMES acts as middleware[10] to assure the seamless communication among modeling components (Whelan & Castleton 2006b)[11]. No model

or framework actually exists inside FRAMES—the FRAMES program acts as a portal to the model. Figure 5 provides an example of how middleware functions. The user chooses and runs a source-term model to produce the information (e.g., mass flux rates) needed by FRAMES. FRAMES then transfers this information to the user-selected aquifer model (e.g., RT3D in GMS[12]) assuring appropriate conversions are made. The aquifer model is then run and produces data (e.g., concentrations) also for use by FRAMES, which makes the necessary conversions,

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[10]Typically, "middleware" is software connecting components or applications.

[11]The OpenMI interface is another standard for linking environmental models (OpenMI 2007). The standard defines an interface that allows existing time-dependent models to exchange data at run-time.

[12]The Groundwater Modeling System (GMS) is a graphical interface created by the Brigham Young University for various groundwater models—one of these models is the PNNL RT3D. The RT3D code solves coupled partial differential equations to describe reactive-flow and transport of multiple mobile and/or immobile species in a three-dimensional saturated porous media (Clement & Jones 1998).
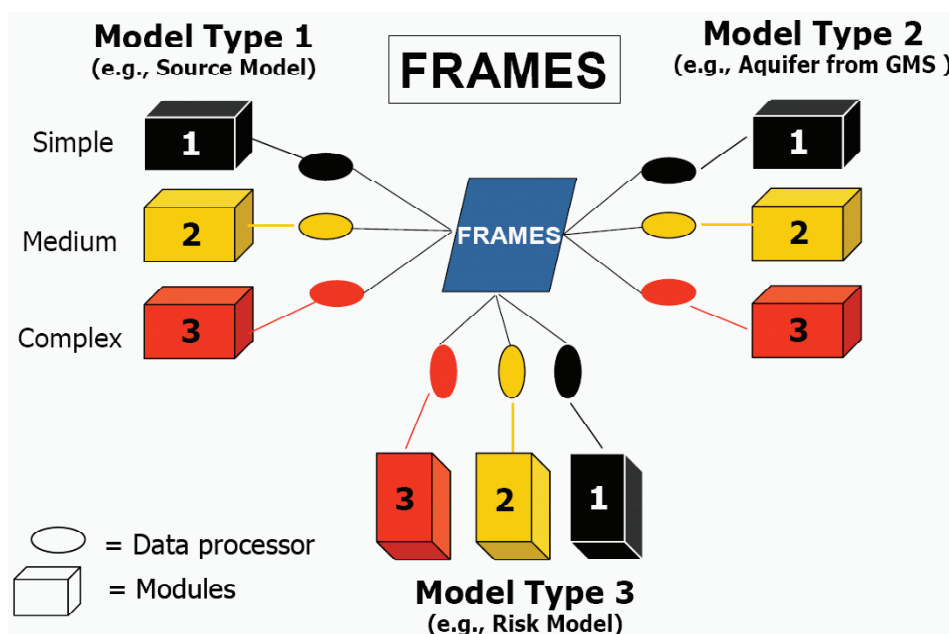
**Figure 5. Illustrating the Linkage of Three Models of Differing Scale and
Resolution Using Frames as Middleware
(Reproduced from Whelan and Castleton (2006b))**

and transfers the data to the selected exposure, intake, and risk models of choice.

3.3 Hybrid Approach Example: Design Analysis Kit for Optimization and Terascale Applications (DAKOTA)

The Design Analysis Kit for Optimization and Terascale Applications (DAKOTA) toolkit provides a flexible and extensible interface among simulation codes and allows new optimization and uncertainty quantification algorithms to be developed (Eldred et al. 2006a; Eldred et al. 2006b; Eldred et al. 2006c). DAKOTA provides algorithms for optimization, uncertainty quantification, parameter estimation, and sensitivity/variance analysis with design of experiments and parameter study methods. These components may be used independently or within advanced

strategies including surrogate-based optimization, mixed integer programming, or optimization under uncertainty (Eldred et al. 2006c). By using object-oriented design principles to implement the key components for iterative systems analyses, DAKOTA provides a flexible and extensible environment for design and analysis of computational models on high performance computers.

One advantage that DAKOTA offers is access to a broad range of iterative capabilities that can be obtained through a relatively simple interface between DAKOTA and the simulator (Eldred et al. 2006c). Figure 6 illustrates the typical loosely-coupled relationship between DAKOTA and a simulation code[13]. Data is exchanged between DAKOTA and the simulation code using data files; DAKOTA does not require access to simulation program source code. During

[13]The solid lines in Figure 6 indicate file input/output operations. Dotted lines indicate passing data that must be handled by the user. DAKOTA writes a parameters file that contains the current variables and then starts the simulation code. When the simulation completes, DAKOTA reads the response data from a results file. This process is repeated until all runs have been completed.
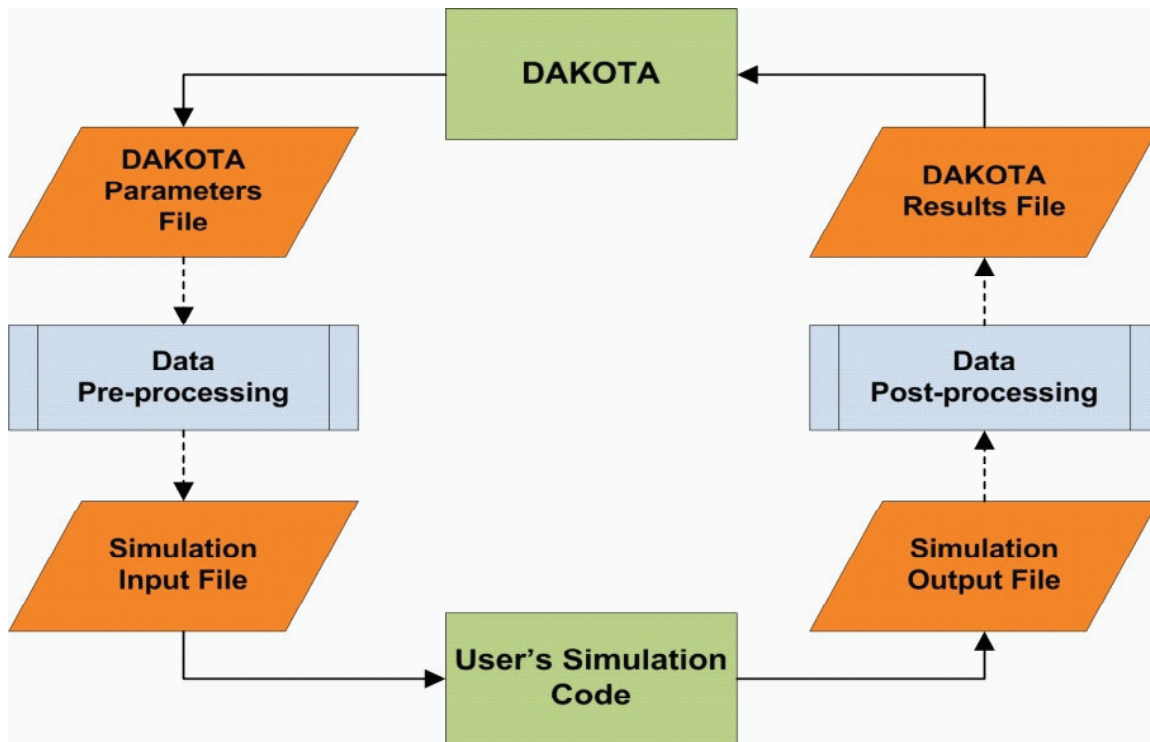
**Figure 6.   The Loosely-coupled or "Black-box" Interface Between DAKOTA and
A User-supplied Simulation Code (Adapted from Eldred et al. (2006c))**

operation, DAKOTA executes the simulation code in a separate external process.

In some cases, it is necessary to have a closer coupling between DAKOTA and a simulation code than that represented in Figure 6. This close coupling is accomplished through either a direct interface or a simultaneous analysis and design (SAND) interface (Eldred et al. 2006c). For the direct interface, the simulation code is modified to act as a subroutine in DAKOTA[14]. The major advantage of a direct interface is the elimination of the overhead resulting from file I/O and process creation. A SAND interface requires extensive modifications to the simulation code so that the optimizer has access to the internal

matrices in the simulation code. Both the optimization routine and simulation code converge simultaneously. While this approach can greatly reduce the computational expense, considerable software development must be expended to achieve this intrusive coupling.

DAKOTA is both a production tool for engineering design and analysis and a research tool for developing new optimization and uncertainty quantification algorithms (Eldred et al. 2006c). Because of the object-oriented design of DAKOTA, new algorithms, strategies, methods, etc. can be added easily. DAKOTA can also serve as a rapid prototyping tool for new algorithm development. By making a broad range of components available, new capabilities can be constructed

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[14] The direct interface can be considered "semi-intrusive" because it requires relatively minor modifications to the simulation code (Eldred et al. 2006c).

rapidly to leverage off previous software investment. DAKOTA has been used to solve engineering design and optimization problems and has provided motivation for research into new areas of optimization.

3.4 Hybrid Approach Example: GoldSim Monte Carlo Simulation Program

GoldSim is commercial Monte Carlo simulation software for dynamically modeling complex systems (GTG 2005a; GTG 2005b; GTG 2005c). The GoldSim simulation software:

- Includes modules for finance, reliability, and contaminant transport,
- Supports risk and decision analysis by simulating future performance,
- Quantitatively represents uncertainties and risks inherent in complex systems,
- Performs deterministic (often point-value) simulations, and
- Simulates simultaneously both continuous and discrete processes (i.e., it is a hybrid simulator[15]).

The GoldSim software has been used in many applications including modeling environmental, business, and engineered systems[16]. A typical use is to support the development of performance assessments for proposed and existing engineered waste management sites. GoldSim can be used to either develop simplified models or couple to existing models; examples for both are provided.

3.4.1 Screening Risk Tool for USDOE Buried Wastes

To provide a foundation for risk-informed decision making, a framework and methodology were developed for the consistent and transparent evaluation of the life-cycle risks and risk trade-offs associated with the disposition of wastes in shallow land burial and corresponding site remedial activities (Brown 2008). According to the U.S. Nuclear Regulatory Commission (NRC), risk is one of the inputs needed (along with costs, technical feasibility, cultural and societal impacts, etc.) to make a risk-informed decision.

To demonstrate the usefulness of the risk analysis framework, a general conceptual burial model was developed to describe the wide variety of possible waste, contaminant release, and environmental conditions at DOE shallow land burial sites (Brown 2008). Because no available tool incorporated all necessary features, the necessary elements (e.g., contaminants, transport processes, environmental media, and receptors) of the conceptual model were incorporated into a screening risk tool developed in the GoldSim Monte Carlo simulation software. Because a screening level analysis was the purpose of the tool, it was considered reasonable to use only built-in GoldSim functionality to maximize the efficiency of the simulation (i.e., no external programs or databases were called)[17]. The screening risk tool was used to evaluate exposure and accident risks for buried waste disposition over relevant spatial and temporal scales (Brown 2008).

The GoldSim screening risk tool incorporates simple models, simplifying assumptions, and minimal system site information to estimate life-cycle risks for

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[15] The term "hybrid" to describe the simulator type (i.e., simulates both continuous and discrete processes) is used in a different sense than when this term when applied to the code development approach. For the code development approach, "hybrid" indicates that concepts from the monolithic style and that maintaining the fidelity of the existing codes are adopted. GoldSim can be considered both a hybrid simulator and a hybrid approach to implementation because algorithms can be directly implemented in GoldSim or existing codes can be called externally.

[16] Examples of the types of problems to which GoldSim has been applied are listed at http://www.goldsim.com/ (accessed October 1, 2008).

[17] A similar approach was taken by Esh et al. to develop an independent performance assessment model to facilitate review of DOE' s non-HLW determination for the Saltstone Disposal Facility (SDF) at the Savannah River Site (Esh, Ridge & Thaggard 2006).

shallow land burial site disposition (Brown 2008). The manners in which contaminant transport and environmental media are implemented in the screening risk tool are illustrated in Figure 7. As indicated in this figure, a more detailed and accurate risk tool can also be developed by using GoldSim as an integrating platform from which more detailed codes that can be called as external programs. The screening risk tool provides an integrated platform for quantitatively evaluating the life-cycle risks and risk trade-offs needed as input to decision-making for shallow land burial site disposition (Brown 2008). The framework and methodology as implemented in the screening risk tool has promoted transparency and consistency in DOE risk analysis[18].

3.4.2   SNL Coupled GoldSim-BLT-MS Software Package

GoldSim can be used as an integrating framework from which extant, external programs can be called and their results dynamically coupled into the simulation. One example is the software package developed by the Sandia National Laboratories (SNL) in which GoldSim was coupled with the deterministic Breach, Leach, and Transport-Multiple Species (BLT-MS) external code to provide probabilistic analysis capability. The resulting software package has been used for the preliminary assessment of candidate low-level waste repository sites (Mattie, Knowlton & Arnold 2007).

SNL developed a paradigm for the probabilistic performance assessment (PPA) of candidate low-level radioactive waste (LLW) disposal sites using legacy U.S. Nuclear Regulatory Commission (NRC) sponsored software within a Monte Carlo framework. The Breach, Leach, and Transport-Multiple Species (BLT-MS) code (Sullivan et al. 1996) has been used to evaluate potential releases from a candidate disposal facility[19]. The BLT-MS code (which provides point-value estimates) was coupled with GoldSim to create a framework for evaluating uncertainties in a potential LLW repository system.

The BLT-MS code includes the following functionality (Mattie, Knowlton & Arnold 2007):

*   The code is able to simulate the degradation of waste containers (i.e., source term) for both localized and generalized corrosion;
*   The code includes four types of waste-form release or leaching mechanisms including rinse release, diffusion release, dissolution, and solubility-limited release; and,
*   The code incorporates a finite element-based transport solver for the far-field transport of radionuclides including advection, sorption, ingrowth and decay, sources and sinks for Neumann, Cauchy, and Dirichlet-type boundary conditions.

The BLT-MS code was originally developed in FORTRAN and compiled to run under DOS. The functionality of the code was not altered; however, modifications to the input/output constructs of the model were made to couple the code with GoldSim (Mattie, Knowlton & Arnold 2007).

Figure 8 illustrates a highly simplified conceptual

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[18] The information described was developed for the Idaho Site high-level waste (HLW) calcined bin sets and Subsurface Disposal Area (SDA) (Brown et al. 2005; Switzer et al. 2005) and was presented to the Idaho Site Citizen's Advisory Board (CAB) in July 2005. The Idaho Site CAB endorsed the reports and strongly recommended to the DOE that the provisions of the reports be followed. The CAB recommendations (i.e., #123 and #124) are available at http://www.cresp.org/ (accessed October 1, 2008).

[19] The BLT-MS code was developed by Brookhaven National Laboratory (BNL) for the NRC for LLW compliance analyses (Mattie, Knowlton & Arnold 2007). Two codes have the needed capability to simulate source-term releases and transport of radionuclides. These are the two-dimensional BLT-MS and the one-dimensional Disposal Unit Source Term-Multiple Species (DUST-MS) code (Sullivan 2001). BLT-MS was selected for the performance assessment model because of its multidimensional capabilities (Mattie, Knowlton & Arnold 2007).
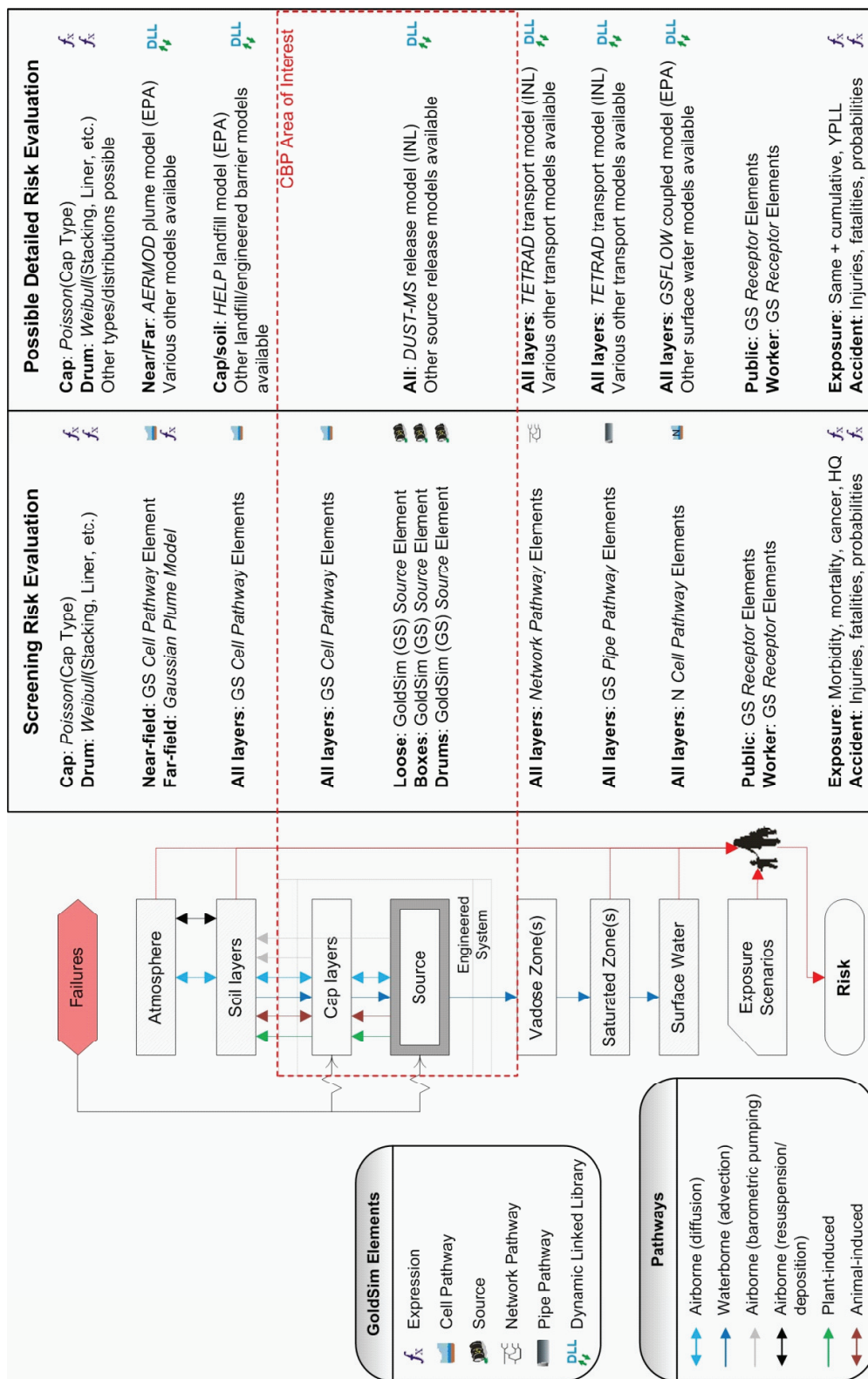
Figure 7.   Implementation of the Screening Risk Tool and Proposed Detailed Risk Tool Using the GoldSim Monte Carlo Simulation Software

model describing how a point-value relationship (or, in this case, the BLT-MS model) can used to estimate uncertainties in predicted risks. A set of input values are generated representing the random variables and provided to the model from which a corresponding risk is predicted—this describes a single realization. A sufficient number of realizations provide the uncertainty distribution for risk.[20]

The conceptual model illustrated in Figure 8 typically oversimplifies the analysis of uncertainties in predicted human health risks because (Brown 2008):

- Probabilistic exposure analysis is performed (i.e., toxicity is fixed and often overly conservative[21]) not probabilistic risk analysis.
- To be more accurate, uncertain parameters should be separated into those that are stochastic and those that are variable and a two-dimensional Monte Carlo simulation performed (Burmaster 1997; Cullen & Frey 1999; Frey 1998; Frey & Bharvirkar 2002; Frey & Rhodes 1998; Hattis & Burmaster 1994; Hoffman & Hammonds 1994).
- Uncertain parameters are often assumed to be independent or uncorrelated, which may or may not be the case and will change the resulting uncertainty distribution estimates.

The parameters that are considered fixed versus those that are considered uncertain in the GoldSim-BLT software package are listed in Table 1.

A conceptual model of how to apply Monte Carlo to risk analysis was illustrated in Figure 8. The manner in which the BLT-MS program is coupled with GoldSim to provide risk analysis for candidate low-level waste (LLW) disposal sites is summarized in Figure 9 (Mattie, Knowlton & Arnold 2007). The user initially (1) constructs a BLT-MS Model using the BLT-MS preprocessor to generate a master input file (where numbers correspond to those in Figure 9). Then in GoldSim, the user (2) specifies the uncertain parameters and distributions and (3) the duration of the simulation and number of realizations desired. The user (4) saves the GoldSim/BLT-MS Integration Model and (5) runs the integrated model.

Upon execution, GoldSim (6) samples uncertain distributions using Latin Hypercube Sampling (LHS). The first realization is (7) started and GoldSim passes the uncertain values to the input dynamic linked library (DLL) using predefined arrays. Another DLL (8) reads the BLT-MS input file and writes a new input file containing point-values for uncertain parameters replaced with sampled values. Upon completion of the read DLL, GoldSim then (9) runs the launch DLL, which executes the BLT-MS model for the input file (constructed in Step 8). Upon completion of the BLT-MS run, the launch DLL (10) extracts selected data from the BLT-MS output files and passes the output to the integrated GoldSim model for storage and use. To save copies of the BLT-MS output files during local or networked runs using GoldSim's Distributed Processing Module (GTG 2007), the file capture DLL is used to (11) copy selected output files to a central location. Steps 7-11 are (12) repeated until all realizations have been executed. Upon completion of the simulation, the integrated model (13) is saved and the user can review the results in GoldSim.

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[20] Haldar and Mahadevan (2000) discuss how to determine sufficiency in sampling as well as techniques for more efficient sampling than Monte Carlo. GoldSim includes Latin Hypercube and Importance Sampling methods to supplement Monte Carlo (GTG 2005b; GTG 2005c).

[21] Attempts have been made to quantify exposure likelihoods for ecological risk assessments (Hope 2000; Hope 2001; USEPA 2001); however, few attempts appear to have been made for human receptors. It has also been indicated that the ecological dose-response relationship may be treated probabilistically for regulatory purposes (USEPA 2001). Thus it appears that ecological probabilistic risk assessments may often be more faithful to traditional probabilistic risk assessment methods than their human health counterparts.
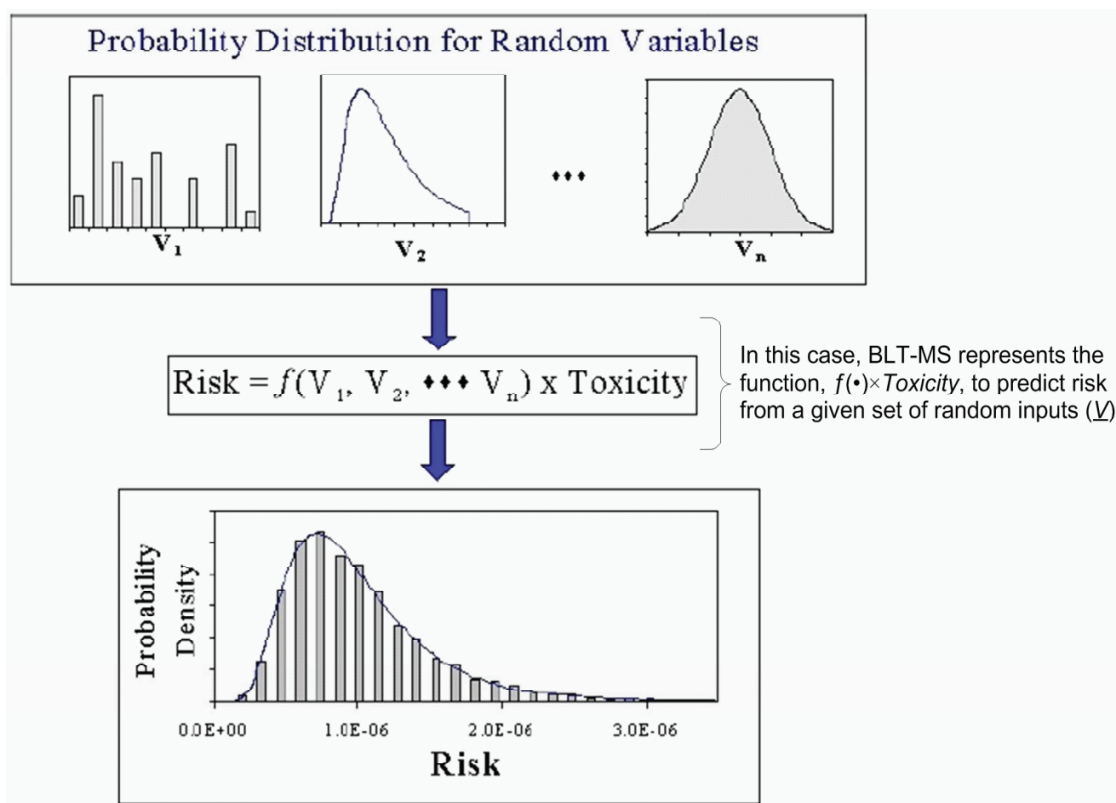
Figure 8. Conceptual Model of A Monte Carlo Risk Analysis (Reproduced from USEPA (2001))
Random Variables (V_1, V_2, ..., V_n) Refer to Variables That can be Characterized by Probability Distributions. A Point-value Risk is Predicted for Each Set of Random Values—in this Case, the BLT-MS Code would Be Used. Repeated Sampling Results in A Frequency Distribution of Risk.

Table 1. Examples of Fixed and Uncertain Parameters in the GoldSim BLT-MS Integrated Software Package (Mattie, Knowlton & Arnold 2007)

Fixed Parameter or Parameter Set	Uncertain Parameter or Parameter Set
Finite-element mesh design parameters/specifications	Initial concentrations within the source term
Material properties within the finite element mesh	Boundary flux/concentration quantities
Finite element nodes for boundary conditions (BC's), including fixing the BC type for a given node	Breaching characteristics for a given container type
Number of isotopic species	Leaching characteristics for a given waste type
Number of decay chains and branching fractions	Transport characteristics of host rock/soil
Number of container types	Darcy flux and moisture content within host rock/soil
Number of waste types	
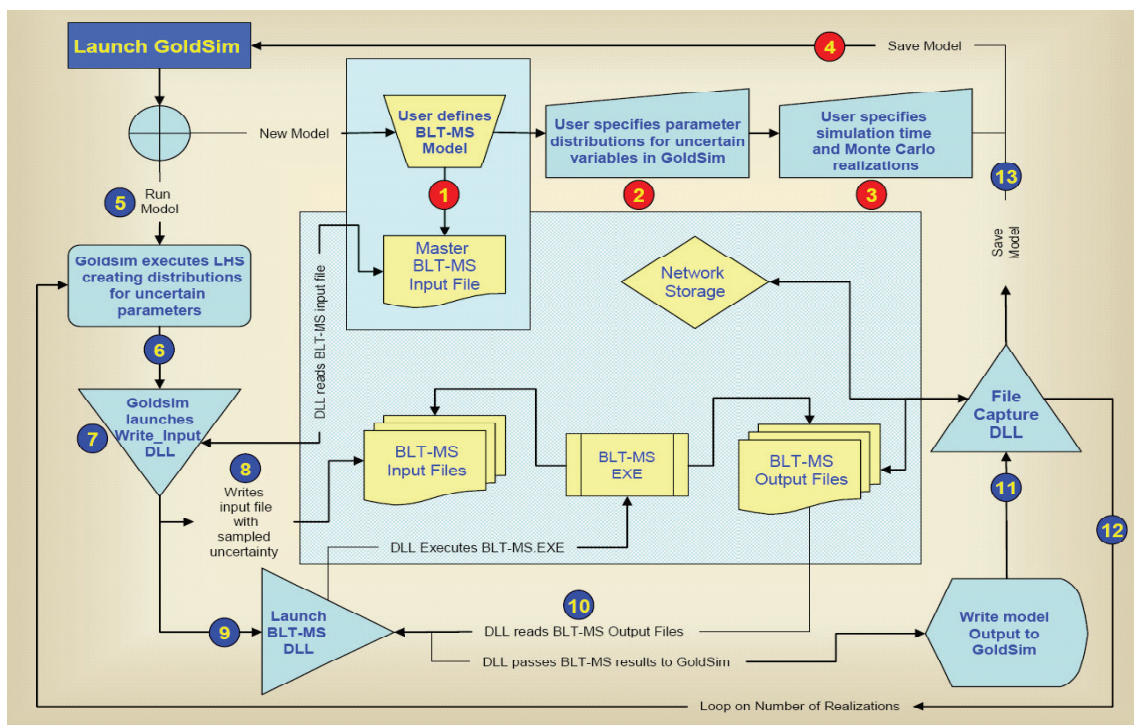
**Figure 9.   Flow Chart for GoldSim/BLT-MS Integration Model
(Reproduced from Mattie et al. (2007))**

3.4.3   Coupled GoldSim-PHREEQC Geochemical Code

Another example involves coupling a complex geochemical code to GoldSim using the external linkage capability in GoldSim via a dynamic linked library (DLL)[22]. Situations where linking GoldSim to a geochemical model may be useful include (Eary 2007):

- **Mixing problems** – In systems where the effects of variable inputs to a mixture must be modeled, linkage to a geochemical model may be needed.
- **Chemical equilibration** – Hydrochemical systems where equilibria from changes in conditions or reactants must be modeled may benefit from linking to a geochemical model.

- **Aqueous speciation** – Systems where the speciation of dissolved species must be considered will likely require a geochemical model.

Figure 10 provides a schematic of how the PHREEQC (Parkhurst & Appelo 1999) geochemical code can be coupled with GoldSim to perform geochemical calculations.

There are several considerations when determining whether or not a DLL should be used to couple a geochemical model to GoldSim for a particular modeling problem (Eary 2007). Advantages of this approach include:

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[22] Other examples are provided at www.goldsim.com coupling the PHREEQC geochemical code to GoldSim using either a Lookup table or spreadsheet.
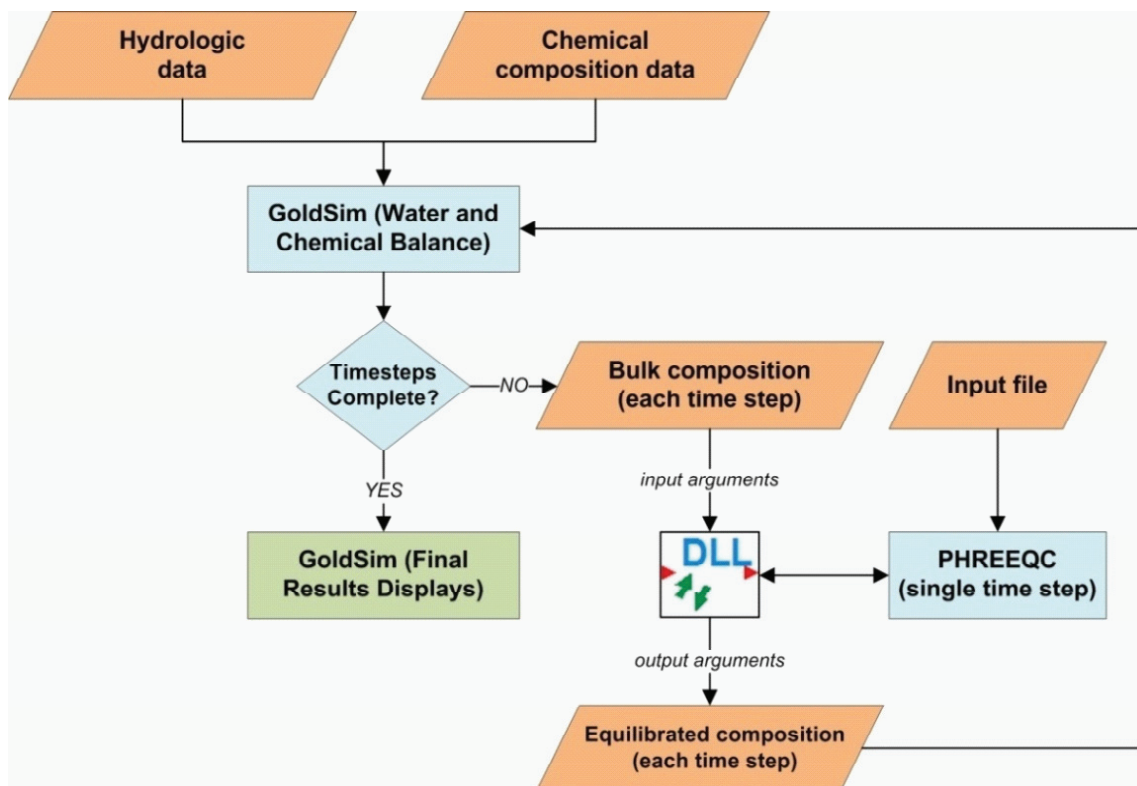
Figure 10. Schematic of Data Flow for the Method of Direct Linkage Between GoldSim and PHREEQC Using a Dynamic-linked Library (Adapted from Eary (2007))

- Applicability to multiple chemical systems with careful development of the conceptual model,
- Ability to integrate the effects of a large number of different chemical processes on solution compositions for each time step, and
- Relatively fast execution when compared to a spreadsheet linkage approach because the need for a spreadsheet as an intermediary is eliminated.

Disadvantages of using a DLL to couple a geochemical code to GoldSim include:

- Requires a large amount of time to define charge-balanced solution compositions if there are more than a few inflows,

- Questions concerning the robustness of the approach to real-world problems, and
- Requires a working knowledge of C++ to modify and rebuild the DLL code for different modeling scenarios and species lists.

3.5 Custom Interface Approach Example: Parallel Virtual Machine

The Parallel Virtual Machine (PVM) is a set of integrated software tools and libraries that emulates a general-purpose computing framework on inter-connected computers of varied architectures (Geist et al. 1994). The overall objective of the PVM is to enable a collection of heterogeneous computing

environments to be used cooperatively for concurrent or parallel computation. The principles on which PVM is based include (Geist et al. 1994):[23]

- **User-configured host pool**. Computational tasks execute on a set of machines (either single- or multiprocessor) selected by the user for the run. The host pool may be changed at run-time, which is an important feature for fault tolerance.
- **Transparent hardware access.** Applications may view hardware as an "attributeless" collection of virtual processing elements or may exploit the capabilities of specific machines by positioning selected tasks on appropriate computers.
- **Process-based computation**. The basic unit of parallelism is a task, which is an independent sequential thread of control alternating between communication and computation.
- **Explicit message-passing model**. Computational tasks cooperate by explicitly sending messages to and receiving messages from each other.
- **Heterogeneity support**. PVM permits messages containing multiple datatypes to be exchanged between machines having different data representations.
- **Multiprocessor support**. PVM uses native message-passing facilities on multiprocessors to take advantage of the underlying hardware.

The PVM system is comprised of two parts: the daemon[24] and a library of interface routines. The daemon resides on all the computers comprising the virtual machine and performs the basic computational tasks[25]. The library of interface routines contains a functionally complete set of primitives[26] needed for

cooperation among application tasks including those for message passing, creating processes, coordinating tasks, and modifying the virtual machine.

The PVM computing model is based on conceptualizing an application as a series of cooperating tasks (Geist et al. 1994). Each task is responsible for one piece of the application. An application may be parallelized along its functions (i.e., "functional parallelism") where each task performs a different function. More commonly, an application is divided into a set of identical tasks (i.e., "data parallelism" or single-program multiple data (SPMD) model) in which each only solves a small part of the data as illustrated in Figure 11. PVM supports any mixture of functional or data parallelism methods. The potential heterogeneity of the computing systems supported by PVM is illustrated in Figure 12.

PVM currently supports the C, C++, and FORTRAN programming languages to include interfaces for many target applications in the 1990s. The C and C++ bindings for the PVM user interface library are implemented as functions and those for FORTRAN are implemented as subroutines. All tasks are identified by a unique integer task identifier (TID) from which messages are sent and received. The user writes programs containing embedded calls to the PVM library where each program corresponds to a task making up the application (Geist et al. 1994). To execute an application, the user typically starts one copy of a task from a machine within the host pool, which subsequently initiates other PVM tasks that compute locally and exchange messages with each other using TIDs. Because of the ubiquitous nature of the virtual

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[23]According to http://www.mcs.anl.gov/research/projects/mpi/ (accessed May 15, 2009), PVM has been displaced by the Message Passing Interface (MPI) for technical computing; however, both are specifications for libraries that can be used for parallel computing. PVM will be used as an example of the approach.

[24] A computer daemon is a program that continuously runs (typically in the background) that triggers actions when it receives specific input.

[25]An example of a daemon is a mail program that runs in the background and handles all the incoming and outgoing electronic mail on a computer (Geist et al. 1994).

[26]Primitives are the most elementary form available in a programming language (e.g., machine instructions, microcode instructions, interpreted statements, etc.).
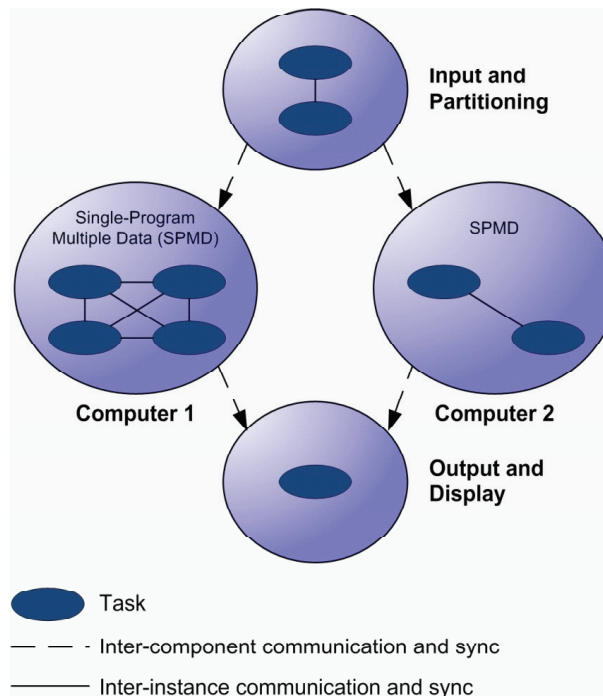
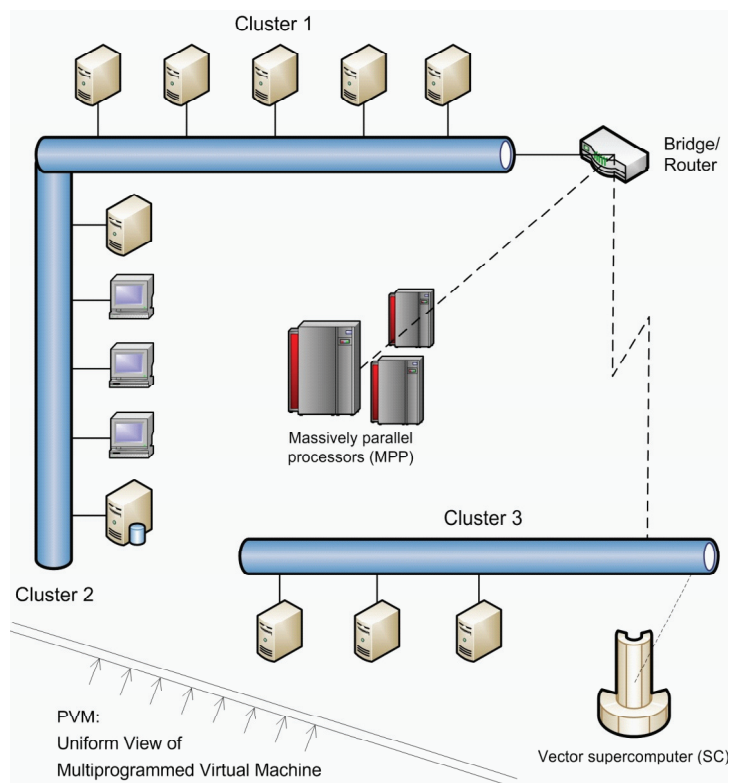**Figure 11. Parallel Virtual Machine Computational Model (Adapted from Geist et al. (1994))**

Figure 12. Parallel Virtual Machine Architectural Overview (Adapted from Geist et al. (1994))

machine concept and its simple but complete inter-face, PVM has gained widespread acceptance in high-performance scientific computing (Geist et al. 1994).

3.6 Other Codes Used for Cementitious Barriers

Additional examples of modeling cementitous barri-ers are provided to give a better indication of extent to which these barriers have been historically modeled. These modeling efforts are:

- **BARRIER code (Rogers and Associates Engineering)** – This code represents one of the first attempts at modeling the long-term perfor-mance of barriers used in low-level waste (LLW) disposal (Icenhour 1995; Shuman et al. 1988). The code provides radionuclide source term, environ-mental transport, and dose calculation capabilities. Release mechanisms include constant leach rate, nuclide-specific leaching, advection with partition-ing between liquid and solid phases, and diffusion. The concrete degradation mechanisms include sulfate attack, calcium hydroxide leaching, freeze-thaw cycling, and corrosion of reinforcing metal.

- **4Sight computer code (NIST)** – This computer program (developed by the National Institute of Standards and Technology for the NRC) (http://concrete.nist.gov/4sight/) was designed as a resource for estimating the service life of new underground concrete structures (Snyder & Clifton 1995). The program uses combined numerical models for ion transport, chemical reaction, and subsequent changes to transport coefficients to model the response of a concrete structure to its environment. 4Sight uses a continuum scale trans-port/reaction model to predict the dissolution and/or precipitation of minerals and salts.

- **Saltstone Disposal Facility Performance Assessment Model (Nuclear Regulatory Commission)** – This model was developed in the GoldSim Monte Carlo software to support NRC review of the Saltstone Disposal Facility (SDF) at the Savannah River Site (Esh, Ridge & Thaggard 2006). The model is comprised of abstracted models representing those processes likely to drive system performance including degradation of the engineered barrier and oxidation and physical degradation (e.g., sulfate attack or cracking) of the saltstone waste form. The model includes source term and near-field release, saturated zone and surface water transport, and dose assessment.

3.7 Radiological Performance Assessment for the Z-Area Disposal Facility Using PORFLOW-3D

The final modeling effort described here is the 1992 performance assessment (PA) model developed for the Z-Area Saltstone Disposal Facility (SDF) at the Savannah River Site (SRS) (Cook & Fowler 1992). The SDF is a near-surface disposal facility that receives DOE low-activity wastes immobilized in a cementitious waste form denoted saltstone that are contained in a reinforced concrete vault (Cook & Fowler 1992). The SDF PA requires understanding of the wastes that will be disposed and the environment into which they will be placed over long periods of time. Thus multiple models have been used to predict the performance of the disposal system.

The manner in which models are integrated for the SDF radiological performance assessment is illustrat-ed in Figure 13 and Figure 14 for intact and degraded vaults, respectively. As can be seen in these figures, the PORFLOW-3D code is used as the primary
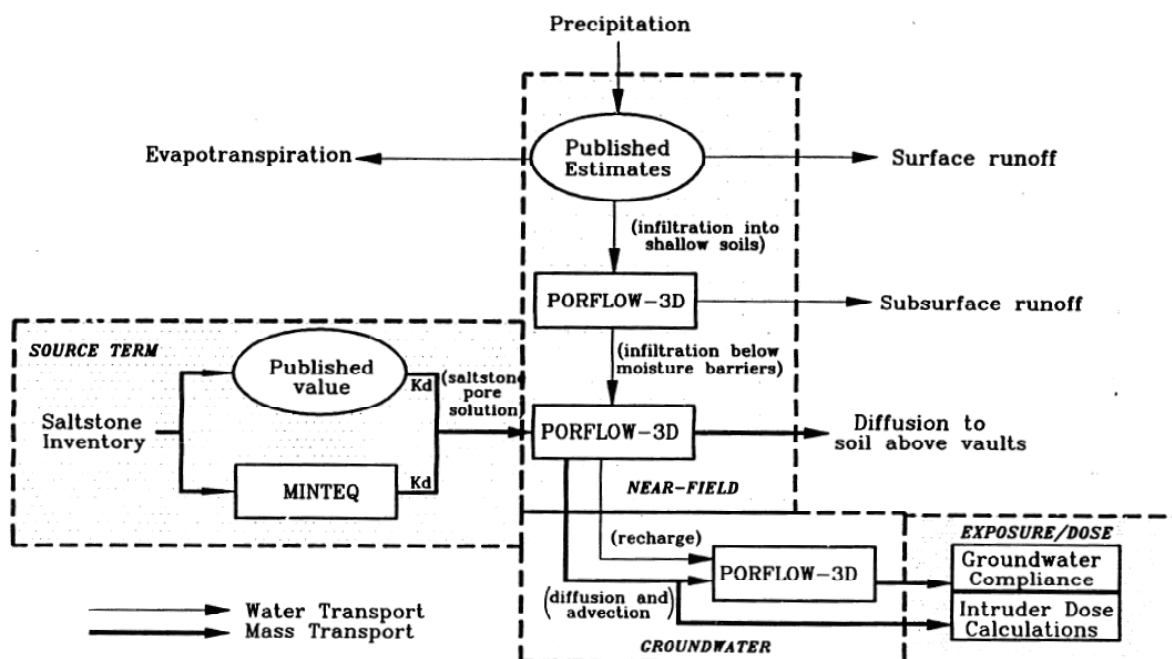
Figure 13. Integration of Computational Methods for the Radiological Performance Assessment of Intact SDF Vaults (Reproduced from Cook and Fowler (1992))
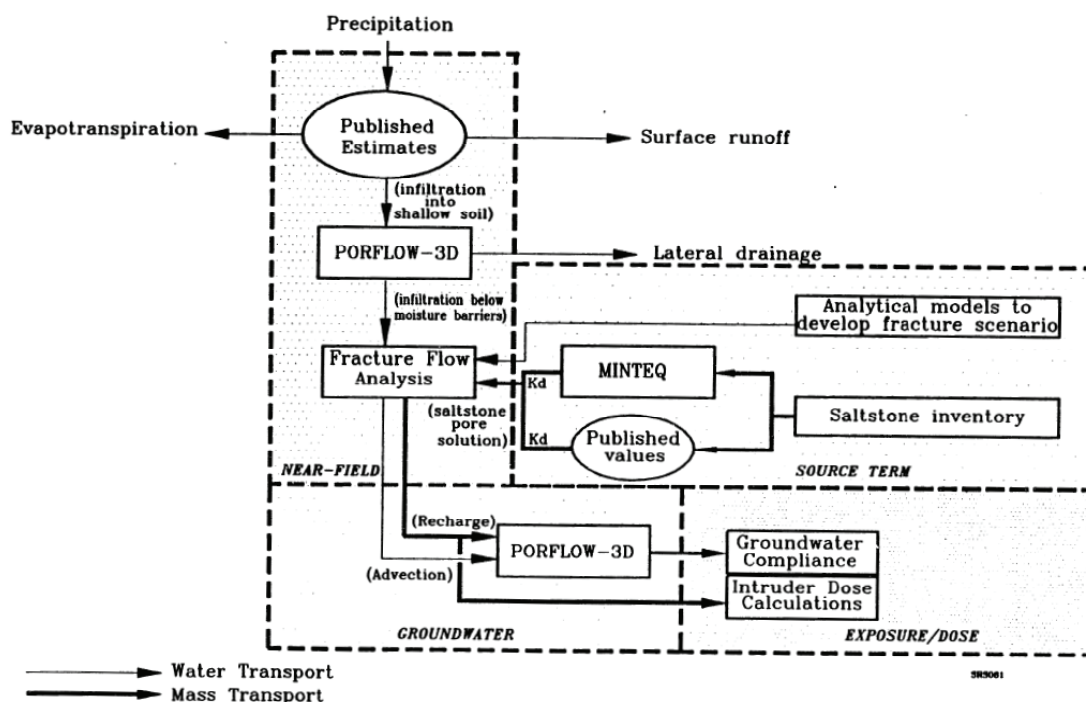

Figure 14. Integration of Computational Methods for the Radiological Performance Assessment of Degraded SDF Vaults (Reproduced from Cook and Fowler (1992))

model to estimate the performance of the SDF vault[27]. PORFLOW-3D is a three-dimensional code capable of simulating multi-phase fluid flow in variably saturated porous or fractured media[28].

The PORFLOW-3D code is used in the near-field region, which is also of primary interest to the CBP. Figure 15 illustrates the interrelationships among the various computations needed to predict the performance of SDF vaults. One use of CBP product tools is to generate the source term results for input to the existing radiological PA model.

4.0   DISCUSSION

4.1   General Integration

A set of simulation tools to predict the performance of cement barriers can be developed using various approaches and software tools. Four approaches (i.e., monolithic, fidelity, hybrid, and custom interface) with relevant examples were described that potentially could be used to develop the integrated framework for the CBP model although other tools are available. The tools described all have strengths and weaknesses.

DAKOTA is a powerful, object-oriented tool for solving complex iterative problems (e.g., optimization and uncertainty quantification) on high-performance computing platforms. However, when compared to a tool such as FRAMES or the GoldSim Monte Carlo simulator, the DAKOTA software will likely require additional work to develop the solution needed for the CBP problem. For example, the CBP framework

solution will require a user-friendly interface because of its intended user base; the needed interface would either have to be developed or an existing one integrated into the framework. There are additional essential components (e.g., source release or environmental media and transport) that are already parts of or available in other models considered (i.e., GoldSim and FRAMES) that would need to be developed or selected and integrated into the framework.

FRAMES is another powerful, object-oriented platform for linking potentially disparate legacy models and databases for conducting assessments to understand how industrial activities might affect humans and the environment. Unlike the DAKOTA program, however, FRAMES does have source release and environmental transport and media component models readily accessible. The source term module included in FRAMES, Multimedia Environmental Pollutant Assessment System (MEPAS), describes contaminated aquifers, ponds, or vadose zones (Streile et al. 1996; Strenge 2001). However, it is conceivable that the models created by the CBP could be integrated into a framework like FRAMES to estimate far-field effects.

Because of the ubiquitous nature of the virtual machine concept and its simple but complete interface, the Parallel Virtual Machine (PVM) has gained widespread acceptance in high-performance scientific computing applications. Currently, only models developed in C, C++, and FORTRAN can be coupled using the PVM interfaces. It is unlikely that all models selected for use in the CBP framework will be available in these three languages[29].

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[27] It may be inferred from the representations in Figure 13 and Figure 14 that these systems are coupled; however, any information exchange or coupling is performed by the users and is not programmed into the systems.

[28] Another example of such a code is the Subsurface Transport Over Multiple Phases (STOMP) code developed by PNNL that calculates the time-dependent thermal flow, moisture flow, and contaminant transport (including aqueous and vapor phases) in variably saturated media (White & Oostrom 1996; White, Oostrom & Lenhard 1995). The code can be run in one, two, or three dimensional modes and has been used by the Hanford Groundwater Remediation Project and by the team preparing the Hanford Tank Closure and Waste Management Environmental Impact Statement.

[29] The investigation of models for potential CBP use resulted in the selection of various models including Leach[XS] (C#) and ORCHESTRA (Java) that will not be available in C, C++, or FORTRAN.
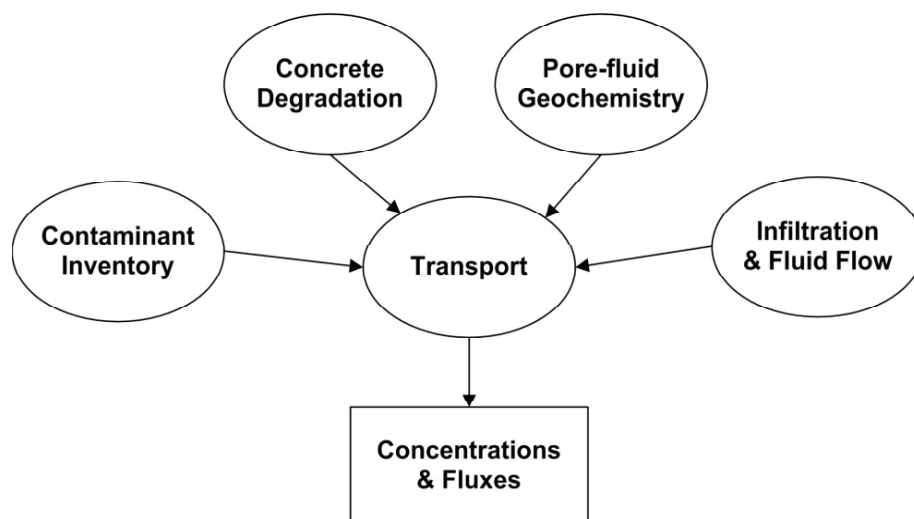
Figure 15. Interrelationships Among Near-field Performance Assessment Computations (Reproduced from Cook and Fowler (1992))

GoldSim possesses a graphical interface as well as built-in source release, environmental transport and media, and sensitivity/uncertainty capabilities. The built-in GoldSim functionality will likely not be sufficient to implement all needed features for the CBP models; however, the external linking capabilities could allow the use of GoldSim as a framework platform.

4.2 General Uncertainty Discussion

The results obtained from the CBP integrated model will be used to develop performance assessments for cementitious barriers in nuclear and other pertinent application. These results will include both the fluxes of contaminants from and the critical hydraulic properties of the concrete barrier. However, in performance assessment space, it is not sufficient to only provide predictions of required properties; the uncertainties or sensitivities in the required results are needed to support the performance assessment (PA) process.

There are times when a "deterministic" or point-value analysis may be sufficient to answer questions posed by decision-makers during a PA. The point-value analysis is typically supplemented by a series of bounding or sensitivity analyses to demonstrate that the actions to be taken will be protective of human health and the environment. However, it is often preferable for complex sites to base decisions on probabilistic performance analyses, and uncertainty quantification analysis becomes critical for these sites[30]. It appears that the DOE is beginning the process of using probabilistic or hybrid deterministic/probabilistic approaches more in the performance assessment process.

Of the example integration frameworks described in this chapter, the GoldSim and FRAMES applications provide built-in capabilities for sensitivity and uncertainty analyses. For example, GoldSim provides basic uncertainty analysis capabilities including Monte Carlo, Latin Hypercube, and Importance Sampling methods (GTG 2005c). Correlations between parameters can be introduced into the GoldSim simulation.

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[30]Uncertainty quantification should be important for either analysis; however, the uncertainties tend to be much more evident in the probabilistic analysis.

If Bayesian methods are required for updating parameter or data uncertainties or if more sophisticated techniques are needed to analyze modeling or other types of uncertainties, then these would be implemented and called as external routines just as with the other integration frameworks examined in this chapter. In contrast, the Parallel Virtual Machine (PVM) provides a basic platform which can support user-defined uncertainty and sensitivity functionality in the same manner as other routines. Extension of the concepts underlying the optimization features in DAKOTA to uncertainty quantification is currently being investigated.

Sensitivity analyses are also needed in the PA process especially during the initial stages of the assessment when the purpose is to identify influential model parameters (that may require detailed or site-specific characterization) and hazardous and radioactive contaminants of potential concern. For example, GoldSim provides two basic sensitivity analysis platforms: tornado charts and X-Y function charts (GTG 2005b)[31]. Both platforms provide graphical representations of the degree to which the selected (dependent) result is sensitive to independent variables. However, both of these methods provide only simple one-parameter-at-a-time-type sensitivity analysis capabilities. DAKOTA also provides sensitivity algorithms. It is likely that more sophisticated and efficient sensitivity methods will be needed for the CBP framework and would be required for any of the frameworks presented in this chapter.

5.0 CONCLUSIONS

Understanding the behavior of cementitious barriers is necessary to evaluate and improve designs. These barriers are often the primary control mechanism to prevent or limit radionuclide releases from nuclear facilities. Without an adequate set of tools to estimate future contaminant releases, assessments cannot fully incorporate and consider the effectiveness of cementitious barriers, which, in turn, limits the nature of those radionuclides that may be disposed of in shallow land disposal. Simulation tools will be needed to predict 1) the hydraulic properties, 2) the stabilities of the relevant cement matrix phases, and 3) the release fluxes of contaminants in response to variable boundary conditions and system stresses over relevant time periods.

The framework conceptualized to provide the set of simulation tools to estimate future performance of cement barriers can be provided by a number of different software tools. Different approaches were described with examples to illustrate the various types of systems that could potentially be used for the CBP application. These approaches ranged from a monolithic structure to hybrid systems to a custom message passing interface. The integration approaches had strengths and weaknesses depending on the models selected and the nature and extent of interactions among the selected models. To leverage off legacy systems to the extent possible, the expected approach for the CBP will be a hybrid, modular approach with weak coupling among the subsystem based on the stability of the overall integrated system.

The outputs from the CBP tools will be used to develop performance assessments for cementitious barriers in nuclear and other pertinent applications. These results will most likely include both the fluxes of contaminants from and the important hydraulic properties of the concrete barrier. However, for performance assessments, it is not sufficient to only provide predictions of these properties; the uncertainties or sensitivities in these parameters will be needed to support the performance assessment process. It is

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[31] To develop the tornado chart, independent variables other than that selected are held at their "deterministic" values and three simulations are executed at the central value and lower and upper bounds (GTG 2005b). To define the X-Y chart, GoldSim performs a series of simulations varying one independent variable at a time through its range of values; it is often thus more computationally intensive than the tornado chart.

likely that more sophisticated and efficient sensitivity and uncertainty methods than available in the platforms examined in this chapter will be needed for the CBP simulation tools.

6.0   REFERENCES

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