

# **DESCRIPTION OF THE SOFTWARE AND INTEGRATING PLATFORM**

## **Cementitious Barriers Partnership**

**December 2009**

**CBP-TR-2009-003, Rev. 0**



**DESCRIPTION OF THE SOFTWARE AND INTEGRATING  
PLATFORM SELECTED FOR THE CEMENTITIOUS BARRIER  
PARTNERSHIP (CBP) PROJECT**

**Cementitious Barriers Partnership**

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and

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An electronic copy of this document is also available through links on the following websites:  
<http://srnl.doe.gov/> and <http://cementbarriers.org/>**



## **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 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 Nuclear Regulatory Commission (NRC) is providing support under a Memorandum of Understanding. The National Institute of Standards and Technology (NIST) is providing research under an Interagency Agreement. Neither the NRC nor NIST are signatories to the CRADA.

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 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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# **CBP SOFTWARE SUMMARIES FOR LEACHXS™/ORCHESTRA, STADIUM®, THAMES, AND GOLDSIM**

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## **LIST OF ACRONYMS AND ABBREVIATIONS**

|           |  |
|-----------|--|
| ASCII     | American Standard Code for Information Interchange     |
| ASME      | American Society of Mechanical Engineers               |
| CBP       | Cementitious Barriers Partnership                      |
| CSF       | Chemical Speciation Fingerprint                        |
| DHA       | Dissolved Humic Acid                                   |
| DOC       | Dissolved Organic Carbon                               |
| DLL       | Dynamic Link Library                                   |
| D&D       | Decontamination and Decommissioning                    |
| ECN       | Energy Research Centre of the Netherlands              |
| EPA       | U.S. Environmental Protection Agency                   |
| FE        | Finite Element   |
| GTG       | GoldSim Technology Group                               |
| GUI       | Graphical User Interface                               |
| HA        | Humic Acid   |
| LAW       | Low Activity Waste                                     |
| LCCA      | Life Cycle Cost Analysis                               |
| LeachXS   | Leaching eXpert System                                 |
| L/S       | Liquid to Solid ratio                                  |
| NPV       | Net Present Value                                      |
| ODBC      | Open Database Connectivity                             |
| ORCHESTRA | Objects Representing CHEmical Speciation and TRANsport |
| PA        | Performance Assessment                                 |
| POM       | Particulate Organic Matter                             |

## **LIST OF ACRONYMS AND ABBREVIATIONS (contd)**

|          |   |
|----------|---|
| QA       | Quality Assurance   |
| REDOX    | REDuction/OXidation   |
| RVE      | Representative Volume Element                                   |
| SCM      | Supplementary Cementitious Material                             |
| SH       | Spherical Harmonic  |
| STADIUM® | Software for Transport and Degradation in Unsaturated Materials |
| THAMES   | Thermodynamic Hydration And Microstructure Evolution Simulator  |
| VBA      | Visual Basic for Applications                                   |

# **CBP Software Summaries for LeachXS™/ORCHESTRA, STADIUM®, THAMES, and GoldSim**

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The goal of the Cementitious Barriers Partnership (CBP) is to develop a reasonable and credible set of tools to predict the structural, hydraulic and chemical performance of cement barriers used in nuclear applications over extended time frames (e.g., >100 years for operating facilities and >1000 years for waste management). The simulation tools and data produced will be used to evaluate and predict the behavior of cementitious barriers used in near surface engineered waste disposal systems including waste forms, containment structures, entombments and environmental remediation. The tools will also support analysis of structural concrete components of nuclear facilities (i.e., spent fuel pools, dry spent fuel storage units, and recycling facilities). Model parameters will be obtained from literature sources and experimentally measured under this project, when needed, to demonstrate application of the simulation tools to three prototype applications (i.e., waste form in concrete vault, high level waste tank grouting, and spent fuel pool).

These cementitious materials are exposed to dynamic environmental conditions that cause changes in material properties via (i) aging, (ii) chloride attack, (iii) sulfate attack, (iv) carbonation, (v) oxidation, and (vi) primary constituent leaching. A set of state-of-the-art software tools has been selected as a starting point to capture these critical aging and degradation phenomena. STADIUM® has been used to predict the behavior of concrete structures exposed to chemically aggressive environments including chloride and sulfate. LeachXS™ is a database and expert decision tool that can seamlessly call the ORCHESTRA geochemical code to model chemical attack as well as carbonation, oxidation, and leaching of cementitious materials. THAMES is being developed to describe cementitious binder microstructures and calculate important engineering properties during hydration and degradation. Through the CBP, conceptual models and computational tools will be developed or modified to improve the assessment of long-term structural, hydraulic, and chemical performance of cementitious materials.

Characterizing properties and understanding the mechanistic behavior of cementitious barriers is necessary to evaluate and improve system designs. Uncertainty reductions require coupling multi-scale and multi-physics processes, including physical-chemical evolution and transport phenomena applied to heterogeneous materials with changing boundary conditions. The selected codes will be coupled using a GoldSim probabilistic simulation framework. Uncertainty evaluation will be included with simulations at both the phenomenological and integrated system level.

## 1 INTRODUCTION

The purpose of this document is to summarize the state-of-the-art models selected for use in the CBP project. Each CBP model has been developed in different types of software for different purposes (e.g., research or commercial). Therefore, different design and documentation are available for the different tools. The basic descriptions for the software tools are summarized.

### 1.1 Common Elements of Software Development<sup>1</sup>

All software requires understandable documentation to be useful and maintainable. All phases of software design, development, and maintenance should be accompanied by suitable documentation. The following is a list of documents recognized as being useful during a software development project:<sup>2</sup>

- **Software Quality Assurance Plan.** This plan contains details on how the quality of the development will be monitored, measured, and maintained throughout the project.
- **Software Development Plan.** This plan contains details of the methods and techniques to be developed together with task breakdowns, time scales, and dependencies. It should also contain details on any standards being adopted by the project and details of any specific methods/techniques being used in the project.
- **Software Configuration Management Plan.** This plan details how control of the software and its associated documents will be managed. Use of a document repository and code management systems are detailed as well as processes of update and changing documents together with how the software will be released and maintained.
- **Software Verification and Validation Plan.** This plan will contain details on the approach to testing. It should cover methods, documentation, and approaches to unit testing, integration testing, and system testing.
- **User Requirements Document.** This document will contain a detailed description of the functional and environment requirements of the project. This is a high level description of the objectives of the project and may contain information on system constraints, user interfaces, performance, and use of external or existing software.
- **Software Requirements Document.** This document will contain details on the algorithms and techniques to be used but also system and environmental requirements or constraints. There may be details on the libraries to be used or software to be re-used, requirements on the implementation language and the target hardware.
- **Architectural Design Document.** This document is a large scale overview of the “look and feel” of the system. Elements such as implementation language, external systems, software structure, general module descriptions, and data structures are described. Many of these descriptions will relate back to the **Software and User Requirements Documents**.
- **Detailed Design Document.** This document will contain the detailed specification of the software modules or routines. It should contain not only how the modules will be written but also how they should be tested. In many cases, the

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<sup>1</sup> This information was distilled from that given at:  
<http://www.sesp.cse.clrc.ac.uk/Publications/BestPractice/SoftwareDevelopmentPractices-v6/node19.html>.

<sup>2</sup> In general, a **Plan** will drive or direct part of the process and **Documents** will generally be an output describing the results of a particular development, testing, or maintenance phase.

documentation of the design can be integrated into internal software documentation.

- **User Manual.** The manual will contain a complete description of the purpose and functionality of the system together with detailed instructions on how to use the program. It should have both a reference section giving details on each option available to the user and some form of walk-through tutorial covering the main elements of the systems usage. It should also contain suitable (often high-level) information on the algorithms being used and their implementation.
- **Installation and System Summary Document.** This document will contain a complete description of the components of the system and external dependencies together with details on how the system is installed and tested on target systems.
- **System Documentation.** This document contains a detailed description of all elements of the system. It brings together how the user and system requirements have been implemented via the architecture and detailed designs. It includes details of the software architecture, call trees, external dependencies, and algorithms used with a detailed description of the implementation.
- **Project Web Site.** The Web is now the primary method of informing the scientific community about software and scientific results. As part of the documentation of a software system, information should be posted on the Web in a variety of formats. The web pages can contain information on bug reporting and release developments as well as points of contact.

Some of the above documents are the result of the software development process and others drive the necessary development. The manner in which these documents are developed will vary based on the type

of software and its intended application (e.g., research or commercial). For example, the **User Requirements Document** is typically the result of the initial information gathering process and details the purpose of the development. The **Software Verification and Validation Plan** should drive the testing and validation phases.

A report entitled “Quality Assurance Program: Cementitious Barriers Partnership (CBP)” has been issued by the Savannah River National Laboratory (SRNL) on behalf of the CBP and is available at <http://cementbarriers.org>. The information required during the CBP software development, testing, and maintenance phases (as needed) is described in the aforementioned CBP QA requirements report. The QA requirements for CBP software development are based on the ASME NQA-1 Software QA requirements (ASME 2000).

## 2 ELEMENTS OF THE SOFTWARE DESCRIPTIONS FOR THE CBP

The previous section describes the various documents that typically form the basis for assuring the quality of the software developed, modified, and used by the CBP. However, the voluminous nature of the reports enumerated above can prove cumbersome. The information generated during design, implementation, testing, and maintenance phases has been distilled into more accessible descriptions of the state-of-the-art tools in the chapters to follow<sup>3</sup>. The following information is provided in detail for the selected software:

- **Overview.** This section outlines in a high-level fashion the software tool including primary uses,

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<sup>3</sup> The descriptions here are not meant to be exhaustive but instead to convey the types of information provided to describe the CBP tools. Much of the information contained in these sections is readily available from an adequately designed, implemented, and maintained software system.

significant limitations<sup>4</sup>, conceptual model(s), general computational algorithms and methods, primary modules, and user interface(s). The program elements outlined in this section are typically described in greater detail in the sections to follow.

- **Explanation of Conceptual Models and Theory.** The primary conceptual models used as the solution basis(es) for the tool are described including pertinent formulae and references<sup>5</sup>. The concepts are described in sufficient detail so that a highly knowledgeable researcher could connect the critical concepts and theories to the implementation. For complex codes, these descriptions can be combined with the descriptions of program elements (or entities<sup>6</sup>) as described below.
- **Hardware and Software Requirements.** The hardware and software requirements for developing<sup>7</sup> (if needed), executing, and maintaining the code are described to assure the tool or code satisfies CBP requirements.
- **Program Execution Mode(s) and User/Program Interface Information.** Programs often run either interactively (e.g., using a Graphical User Interface or GUI) or in batch mode after initial values and settings have been defined (using a user interface, input database(s), or input file(s)). Some programs (e.g., STADIUM®) can either be run interactively or using a command line operation.
- **System Performance.** An indication of the general performance of the tool is useful to evaluate system performance including potential impacts during integration. Performance indications are machine-dependent and the characteristics of the hardware/software combination and specific benchmark conditions are specified.
- **Input Data Description.** A description of the input data and boundary conditions needed to solve problems pertinent to the CBP is provided. An example of an input data description is provided in Table 1 for STADIUM®. Because of implications when coupling codes, any temporally or spatially varying boundary conditions, material properties, and other input data are identified so that potential interactions and conflicts can be addressed as early as possible in the development, improvement, and integration processes.
- **Output Descriptions.** A description of the output results is provided. The description may provide output file or database specifications as well as other information needed to interact with the output file, database, and/or stream. An example of such a specification is provided in the section entitled **Outputs Generated by STADIUM®**.
- **Detailed Example(s).** A set of examples (including input variables and boundary conditions) is provided that is pertinent to the CBP. These examples may be based on the reference cases (Langton et al. 2009) to the extent possible and can later be used to develop benchmarks for performance testing.
- **Program Structure.** The *basic structure* of the system is described (e.g., object-oriented, modular, or procedural) and may include a *diagram* or *diagrams* illustrating how program

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<sup>4</sup> The descriptions of the primary uses and limitation of the software tool includes information specific to intended CBP use and integration.

<sup>5</sup> Important considerations of time and scale and any resulting limitations or significant abstractions and simplifications are addressed.

<sup>6</sup> In IEEE software design parlance, these elements are referred to as *entities*, which are elements or components of a design that are structurally or functionally distinct and can be separately named and referenced (IEEE 1998a). Entities can exist as systems, subsystems, data stores, modules, programs, or processes (IEEE 1990).

<sup>7</sup> Development consists of planning, analysis, and implementation (IEEE 1998a).

elements are linked. A general description of element interfaces (i.e., linkages and information transfers) including those to and from external files and databases may be provided. This information may be provided in the sections describing the program elements or entities.

- **Detailed Explanation of Computational Algorithms and Methods.** The primary *computational algorithms* and *methods* implemented in the program are described with examples and references, when appropriate, and may be provided on an entity-specific basis.
- **Detailed Explanations of Program Elements or Entities.** Each major program element or entity (e.g., procedure, module, class, or data store) is described including identification of underlying models and significant assumptions. One standard practice that is used in the chapters to follow is to define the following attributes for each major program element or entity (IEEE 1998a):<sup>8</sup>
  - **Identification.** The *name of the entity* is uniquely selected to characterize the nature of the entity.
  - **Type.** A *description of the type of entity* (e.g., subprogram, module procedure, process, data store, or object).
  - **Purpose.** This describes *why the entity exists* including the *specific functional and performance requirements* for the entity (IEEE 1998b).
  - **Function.** This describes *what the entity does*. This attribute describes the transformation applied to inputs to produce the desired output or, in the case of data, the type (and structure, if applicable) of information stored or transmitted. *Relevant uncertainties in input information and the transformation* (e.g., modeling or numerical) are considered.
  - **Subordinates.** Any *major entities composing the entity* are identified to trace design requirements and identify parent/child relationships.
  - **Dependencies.** The *relationships of the entity to others* are often identified graphically using charts, data flow diagrams, and/or transaction diagrams (IEEE 1990). The nature of any significant interactions including *timing* and *conditions* are identified (and may involve initiation, execution order, data sharing, creation, usage, storage, or garbage collection).
  - **Interface.** A description of *how other major entities interact with this entity* is provided. The *methods* and *rules* for interacting are described. Methods may include mechanisms for invoking or interrupting the entity, for communicating through parameters, common data areas or messages, and for direct access to internal data. Rules may include the communications protocol, data format, acceptable values, and meanings of values.
  - **Resources.** The *primary external elements used* are described. Interaction rules and methods for resource allocation are specified where appropriate.
  - **Processing.** The *rules by which the entity achieves its functionality*, which is a refinement of the function description, are described. The algorithm used to perform the specific task is described including any significant contingencies and references.
  - **Data.** The *data elements internal to the entity* are described including methods of representation, initial values, uses, and acceptable values. These data elements may be restricted to those pertinent for CBP use (e.g., describing inputs and boundary conditions).

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<sup>8</sup> An equivalent standard or standards can be substituted for the IEEE standards used here.

In general, the conceptual models and significant assumptions underlying the computational methods and algorithms are described in sufficient detail for a highly knowledgeable researcher to connect the critical concepts and theories to the implementation. Module interfaces, message passing, or calling specifications are described referencing the system architecture to begin to provide the basis for future integration activities.

- **Descriptions of Required External Databases and Programs.** The primary external thermodynamic databases and other programs are resource entities that are described in the previous section. However, these elements are critical enough to the CBP activities that they are highlighted here.
- **System-Level Uncertainty Considerations.** Uncertainty considerations on an *entity*-specific basis are described in the *function* attribute. However, there are system-level uncertainty issues that should also be addressed. These considerations may be described in the **Verification and Validation** section below, but are also highlighted here because of their importance.
- **Verification and Validation.** It is vitally important to the CBP that verification and validation of any codes or data be demonstrated (IEEE 1990). The CBP shall define system level performance requirements as well as those for individual models.
- **Summary of Model Limitations.** The important conceptual and algorithmic limitations for employing the model and how these limitations may impact future coupling and integration of the model with other state-of-the-art models are identified.
- **Data Dictionary.** A collection of the names of all data items used in the software system including relevant properties (e.g., length of data item or representation).

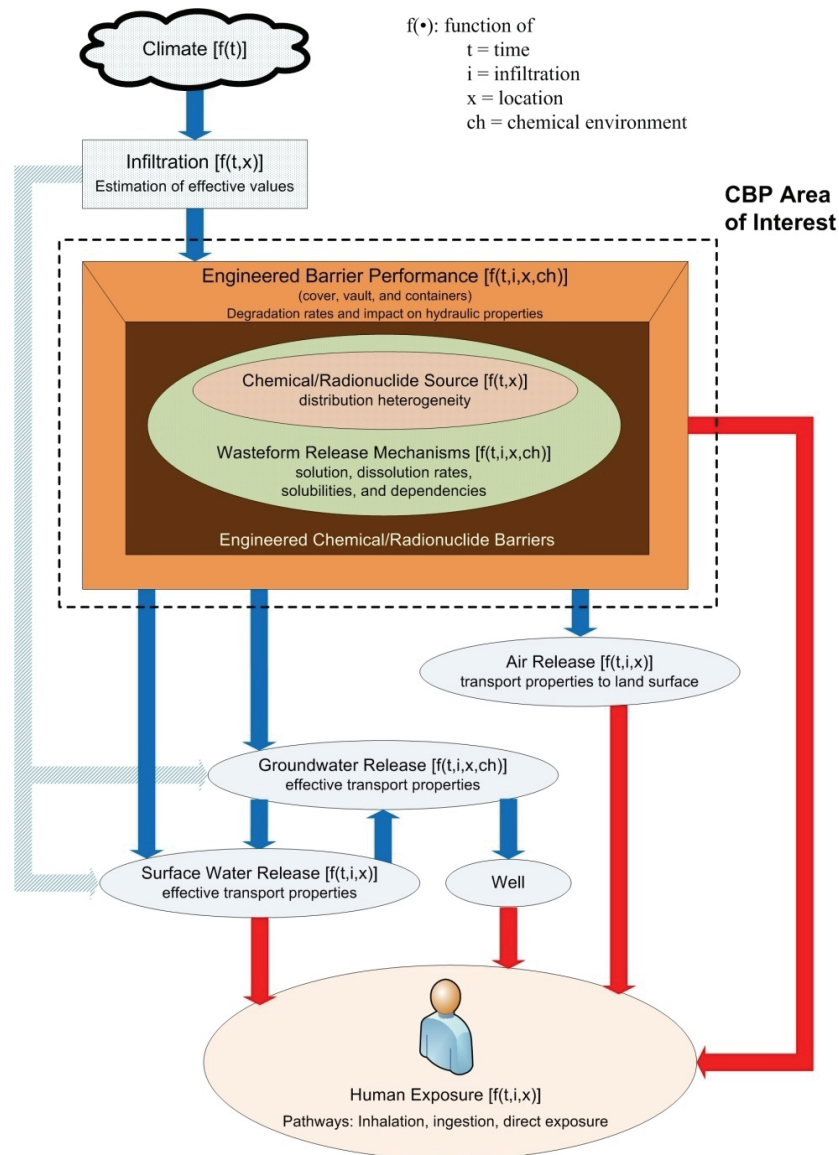
- **Bibliography.** A list of the works referred to in the chapter; additional supporting citations may also be provided.

### 3 PERFORMANCE ASSESSMENTS AND THE CBP

The relationship between a performance assessment (PA) and cementitious barrier (denoted “engineered barrier”) is illustrated in Figure 1. Conceptually, the barrier—and perhaps the materials contained within the barrier—can be segregated from the environment (and thus PA calculations) by an imaginary boundary across which input information from the PA enters and output information representing the calculated responses exits (e.g., constituent releases or hydraulic properties) making the development of a stand-alone cementitious barrier tool feasible. The level of detail required of the cementitious barrier responses will depend on the specific needs of the application. A review of PA analyses is provided in *Overview of the U.S. Department of Energy and Nuclear Regulatory Commission Performance Assessment Approaches (Volume I and II)*, and the CBP modeling capabilities will be developed to ultimately satisfy PA modeling requirements (and may be extended to other calling programs) and in response, return those properties and performance parameters in a manner consistent with the needs of the calling program (e.g., point values, spatially and temporally averaged values, or time series).

Another way to conceptualize how the CBP model will fit into the performance assessment universe is depicted in Figure 2. There are a number of potential applications employing concrete barriers that must be abstracted and simplified to be represented by predictive models and evaluated using performance assessment tools over long periods of time. The CBP models will fill several critical roles for performance

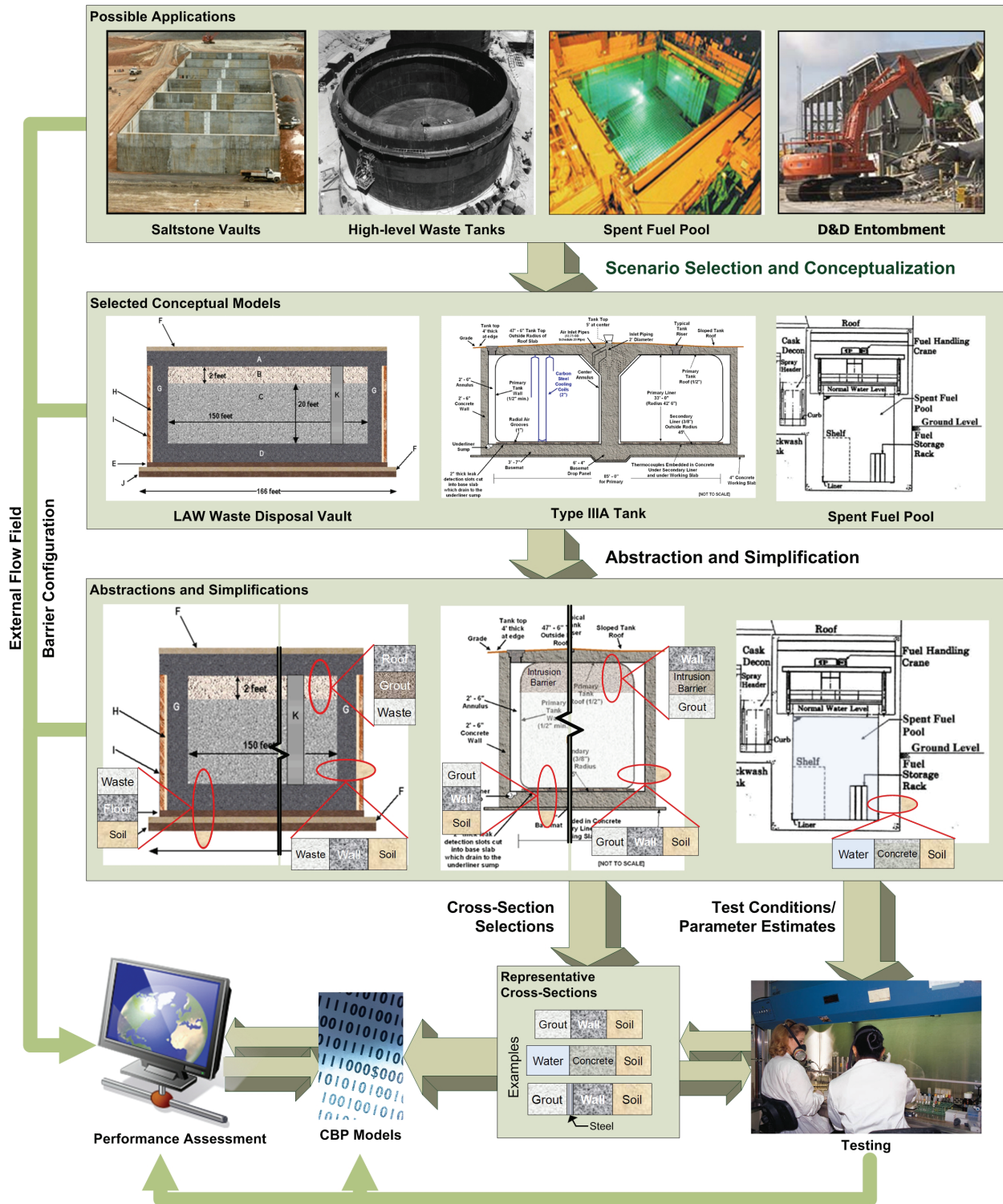




**Figure 1. Generalized Performance Assessment Conceptualization (adapted from a diagram by Philip and Nicholson (2006))**

assessment. The first role is in understanding barrier performance from a phenomenological perspective where individual models have been used to study and predict important degradation and release phenomena. The second role, which is unique to the

CBP, will be to couple these state-of-the-art phenomenological models into an integrated framework that will be used to provide the source term and hydraulic properties needed to study overall barrier system performance.



## **4 SUMMARIES OF THE STATE-OF-THE-ART TOOLS SELECTED FOR THE CBP**

A set of state-of-the-art phenomenological tools is available from or proposed by members of the CBP that describe important phenomena needed for individual use as well as in the CBP integrated framework. These tools often require a significant amount of physical and chemical data as input, may involve a detailed computational grid as part of the solution, and describe a specific behavior of the cementitious barrier. Detailed descriptions of the selected tools are provided in the chapters to follow<sup>9</sup>; however, brief descriptions including important information for the tools (i.e., overview, conceptual models, inputs, outputs, external databases, and development needs for integration) are provided in this overview section.

### **4.1 LeachXS™/ORCHESTRA**

LeachXS™ is a database/expert decision support system for characterization and environmental impact assessment based on estimated contaminant release as derived from leaching tests<sup>10</sup>. Databases used by LeachXS™ include leaching for 600+ materials, scenarios, and regulations to allow comparisons of test data versus specific utilization or disposal conditions. The expert decision system assists in evaluation and laboratory guidance, data management and evaluation, source term description, impact evaluation, and decision analysis. Applicable

materials for assessment using LeachXS™ include:

- |                               |                                   |
|-------------------------------|-----------------------------------|
| • Treated Wastes              | • Sludge                          |
| • Stabilized Waste            | • Compost                         |
| • Construction Materials      | • Sediments                       |
| • Cement Mortars and Concrete | • Municipal Wastes                |
| • Soils and Contaminated Soil | • Industrial and Hazardous Wastes |
|                               | • Mining Wastes                   |
|                               | • Preserved Wood                  |

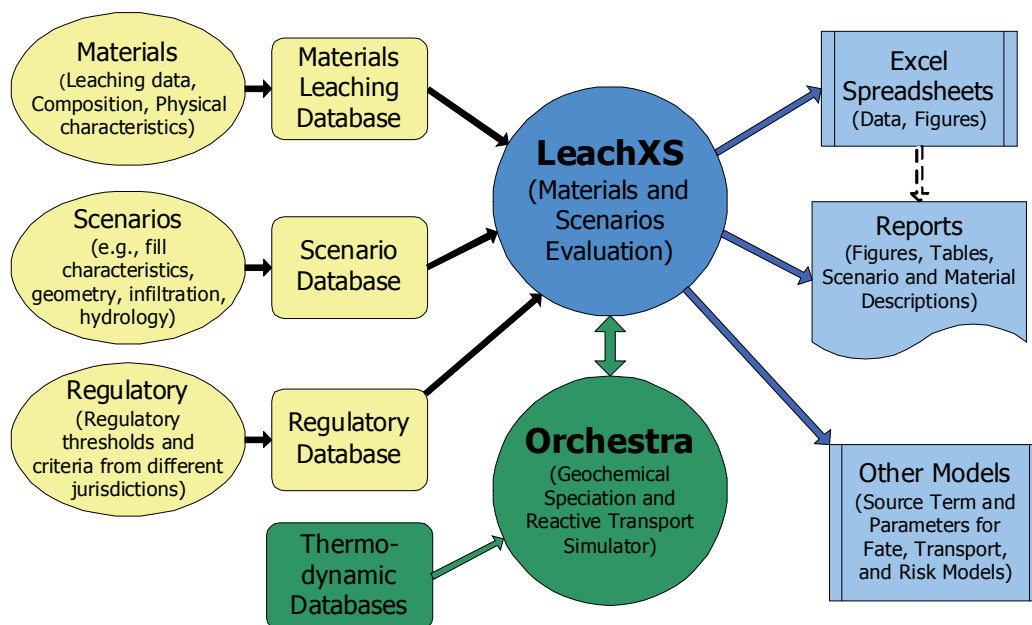
Geochemical speciation and chemical reaction/transport modeling capabilities are integrated into LeachXS™ using the ORCHESTRA (Objects Representing CHEmical Speciation and TRANsport) modeling environment as illustrated in Figure 3.

ORCHESTRA is a modeling framework for defining state-of-the-art geochemical equilibrium models and combining these models with mass transport (including diffusion, convection, etc.) for user-defined processes (Meeussen 2003). The ORCHESTRA chemical module can calculate chemical thermodynamic equilibrium in a similar way to well known speciation codes, but is internally organized very differently. Instead of defining all model equations within source code, equations are defined in a separate user accessible text file in ORCHESTRA. ORCHESTRA has been used in practice for a wide range of applications that include aqueous speciation, precipitation, different forms of surface complexation, ion exchange, diffusion (including radial and electroneutral), convection, solid solutions, colloid adsorption, and biota uptake.

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<sup>9</sup> The detailed information describing the LeachXS™/ORCHESTRA and STADIUM® tools contain both Proprietary Information and Background Intellectual Property and thus is not part of this report. Distribution of said detailed information must be approved by ECN, SIMCO Technology, Inc. and SRNS, where appropriate.

<sup>10</sup> From LeachXS™ flyer entitled “Leaching eXpert System: A new environmental impact assessment tool” (available at <http://www.leaching.org/LeachXSFlyer.pdf>; accessed April 2, 2009).



**Figure 3. Schematic of LeachXS™/ORCHESTRA Input and Output Functions and Databases**

#### 4.1.1 Description of Conceptual Models

The LeachXS™ system is based on evaluating the leaching behavior of materials using equilibrium-based information obtained from pH dependence leaching tests (e.g., EPA method 1313, CEN/TS 14405, CEN/TS 14497, or ISO/TS21268-4) and dynamic release information from a percolation type test (e.g., EPA method 1314 or CEN TS 14405) and monolith leach testing (e.g., EPA method 1315 or CEN TS 15683). The latter tests have a time dependent element in them, which is closely linked to the actual release under field conditions with the added complexity of different hydrological conditions and long term external influences on the material. The combination of these methods allows an evaluation of the long term release (see Kosson et al. (2002) and Van der Sloot et al. (2009)). A key aspect in the basic approach in LeachXS™ is the ability to display information from a variety of different tests over different scales in the same

graphical representation, which allows conclusions to be drawn on long term behavior.

LeachXS™/ORCHESTRA can be used to simulate different contaminant release situations. These include a number of common experimental test procedures that can be used to evaluate model performance under well-defined conditions. The same chemical and physical model components can also be used as part of the larger scale release scenario supporting environmental impact assessments.

The predefined LeachXS™/ORCHESTRA release models are:

- A model that calculates pH dependent element solubility in a batch system (pH-stat test),
- A model that calculates leaching of elements from a solid matrix by reaction-diffusion (Tank test),

- A model that calculates leaching of elements from a solid matrix by reaction-diffusion-convection (Column test), and
- A number of predefined release scenario models that make use of the same process sub-models (including reaction, (gas) diffusion, and convection) as the models above, but with a different system layout.

LeachXS™/ORCHESTRA also contains a special setup that assists users in the generation of a chemical model description for a given material. In this setup, a so-called SI run, pH dependent solubility data are used to calculate mineral saturation indices for a large set of minerals. These saturation indices can subsequently be used to select a set of mineral precipitation reactions that adequately describes observed leaching behavior. The input for this model setup is the set of pH dependent total element solubilities, dissolved organic carbon, and adsorbing surfaces; the output is a complete chemical model including a set of precipitation reactions (minerals). This chemical model can subsequently be used in any of the models mentioned above. Within LeachXS™ a number of generic models for different materials have been derived and are available.

For a number of material matrices, chemical speciation fingerprints (CSF) have been developed that, in generic terms including composition data, reactive surfaces, and set of minerals, can be used to describe the release from a given material under specified conditions. Such assemblages of composition data, reactive surfaces, and selected minerals can be developed based on calibration against experimental data (usually pH dependence leaching test results in combination with percolation test data to cover a wide range of pH and L/S conditions).

Materials, for which chemical speciation fingerprints have been assessed, can be modeled as a mixture assuming proportionality with the ratio of the constituent parts for composition and reactive surfaces. Any mixing ratio can be modeled, but experimental verification of adequate prediction is needed in specific instances to evaluate model performance.

#### **4.1.2 Inputs Required to Run and Outputs Generated by LeachXS™/ORCHESTRA**

The inputs required to run LeachXS™/ORCHESTRA depend on the type or types of leaching results (i.e., single material with pH dependent leaching test, single material with percolation or lysimeter test, or mixtures of materials with pH dependent leaching tests) that are available for the material.

##### **4.1.2.1 Input for the chemical models**

All models contain one (or more) chemical equilibrium modules that describe the chemical reactions and distribution of elements over different physical-chemical forms in a material. These chemical models require as input:

- A set of chemical equilibrium reactions representative for the material under consideration. LeachXS™ contains predefined sets for several typical materials (e.g., different soil types and cementitious materials) in the database; however, alternative sets may be provided by users.
- A set of total (or available) element concentrations (i.e., maximum leached concentrations) that can be estimated from total composition measurements or from pH dependent leaching test results.
- The amounts of adsorbing surfaces (including organic matter, hydrous ferric oxide, aluminum

hydroxide, and clay) that can be estimated by determining oxalate extractable Fe and Al.

- Liquid to solid ratio (L/S).

#### *4.1.2.2 Output of the chemical models*

The main result of a chemical equilibrium calculation is the distribution of elements over all the different physical and chemical forms (including different dissolved, adsorbed, precipitated, and gaseous species) according to a set of thermodynamic equilibrium reactions given as input. For each element, the distribution over all possible forms is calculated. Other generated outputs are:

- pH,
- REDOX potential,
- Ionic strength, and
- Electrical conductivity.

The ORCHESTRA model generates the basic numerical output of these calculations, while LeachXS™ processes this output and presents data in graphical form.

For a reactant of interest, the following general model data can be displayed graphically:

- pe as function of pH,
- Dissolved Humic Acid (HA) as function of pH,
- Conductivity as function of pH,
- Acid/Base neutralization capacity as function of pH, and
- REDOX capacity as function of pH.

The geochemical speciation results from ORCHESTRA can be viewed and exported. These results include:

- **Solubility prediction results.** These provide a comparison of measured test results and

modeled solution composition (free + DOC associated).

- **Solid and liquid phase partitioning.** This allows visualization of partitioning of the constituent among free, DOC associated, clay-bound, Fe-oxide bound, solid organic matter (POM) bound, and mineral precipitate or incorporated in a solid solution.
- **A combination of solubility prediction and partitioning for a specific reactant in the selected reactant series.** Additional graphs including solid phase partitioning and liquid phase partitioning will be shown.

#### *4.1.2.3 Input for the physical transport models*

The transport modules calculate mass transport based upon the information provided by the chemical modules on the mobility of elements. These transport modules keep track of how much of each element is present as a function of time and space. The modules need to be initialized with the initial chemical conditions of the system at the start of the simulation. This is exactly the same information as required for a single chemical equilibrium calculation; however, it is also required for each material layer or cell in the transport system. Apart from the chemical information, the transport model also needs a set of physical input parameters of which the most important ones are:

- Physical dimensions of the system,
- Porosity of the material(s),
- Density of solid material(s),
- Effective tortuosity of the material(s),
- Flow rates (for column simulation),
- Refresh rates (for tank test),
- Water saturation/gas volume, and



- Chemical composition of each solid material and each solution that is used in the simulation, including amounts of adsorbing surfaces.

#### **4.1.2.4 Output of the transport models**

The reactive transport models generate the chemical composition that is basically the same output as that for a single chemical equilibrium reaction, but now as a function of time and space. Outputs include:

- Chemical composition of the system as a function of time and space (i.e., concentration profiles) including distribution of elements (over mineral, aqueous, gaseous, and other phases), pH, and REDOX conditions and
- Total fluxes of elements over chosen internal or external system boundaries.

As in the case of a single chemical equilibrium calculation, the numerical output data are generated by ORCHESTRA, while LeachXS™ uses these data to generate output in graphical form.

For a reactant of interest, the following general model data can be displayed graphically (ECN 2007):

- pH as a function of liquid to solid ratio (L/S),
- pe as a function of L/S,
- Dissolved Humic Acid (HA) as a function of L/S,
- Conductivity as function of L/S,
- Acid/Base neutralization capacity as a function of L/S, and
- REDOX capacity as a function of L/S.

For the percolation or lysimeter test results, geochemical speciation results from ORCHESTRA can be viewed and exported including:

- **Leachate concentrations.** The measured percolation or lysimeter test concentrations and

the predicted concentrations are graphed as functions of L/S as well as the concentrations predicted for the collected fractions.

- **Cumulative release.** The cumulative leached amount (as derived from the percolation or lysimeter test data) is compared with the predicted cumulative release as a function of L/S.
- **Concentration profiles at a specified time.** The partitioning between dissolved and solid phases is represented as a function of the depth in the column at the specified time.
- **Concentration profiles at a specified depth.** The partitioning between dissolved and solid phases is represented at a specified depth in the column as a function of time.
- **Animated time profiles for a single reactant.** An animation can be generated of the partitioning of a constituent between dissolved and solid phases as a function of depth in the column over the time span of the percolation test.

### **4.1.3 Embedded Databases and Systems Including ORCHESTRA**

LeachXS™ relies on various external databases and a geochemical code (i.e., ORCHESTRA) to estimate contaminant release from the results of leaching tests. The databases and ORCHESTRA are described in the following sections.

#### **4.1.3.1 Materials Leaching Database**

The materials leaching database contains results of laboratory leaching tests, lysimeter tests, and field data from more than 600 materials and wastes. In some cases, interrelated laboratory, lysimeter, and field scale data are available for the same material. A set of tools is also available for importing additional materials into the LeachXS™ materials database. Leaching tests are interpreted using an expert system to provide estimates of the short and long term

release of constituents of interest. These capabilities make LeachXS™ a unique tool to study the release behavior of different materials for use, recycling, or landfilling.

#### **4.1.3.2 Regulatory Database**

A regulatory database allows comparison of test results against criteria for specific utilization or disposal conditions. Constituents included comprise virtually all inorganic constituents as well as a selection of organic components. The system will also be suitable for radionuclides. At present, the database system covers leaching/extraction test data, field data, and composition data.

#### **4.1.3.3 ORCHESTRA and the Thermodynamic Database**

Geochemical speciation and chemical reaction/transport modeling capabilities are integrated into the LeachXS™ system using the ORCHESTRA modeling environment (Meeussen 2003). The geochemical modeling includes mineral solubility (extended MINTEQ database), sorption on Fe-oxide, Al-oxide, dissolved organic carbon, and particulate organic carbon interaction. Graphical and tabular output is generated in files that can be opened by standard spreadsheet applications.

ORCHESTRA employs an object-oriented structure for chemical equilibrium calculations (Meeussen 2003)<sup>11</sup>. In contrast to standard chemical equilibrium algorithms (e.g., MINEQL, MINTEQA2, PHREEQC, or ECOSAT), model equations are not hardcoded in the source code, but instead all equations are defined in text format and read by the ORCHESTRA calculation kernel at run time. This makes model definitions easily accessible and

extendible and results in a very compact and efficient calculation kernel that can be used as a submodel within mass transport or kinetic models. Finally, the object-oriented structure of the chemical model definitions makes it possible to implement a new object-oriented framework for implementing chemical models. The framework consists of three basic object types (i.e., entities, reactions, and phases) that form the building blocks from which chemical models are comprised. The hierarchical approach also ensures consistent and compact model definitions including, for example, aqueous complexation, activity correction, precipitation, surface complexation, ion exchange, electrostatic interactions, NICA, and CDMUSIC.

#### **4.1.4 Potential Development Needs for Integration**

As indicated above, any potential issues related to integration and coupling must be considered early in the project and focused on throughout the project. The most recent version of LeachXS™ (which communicates with the ORCHESTRA chemical equilibrium code using text files) has several advantages from an integration perspective:

- LeachXS™/ORCHESTRA can export results to files that can be opened by standard spreadsheet or compatible programs.
- LeachXS™/ORCHESTRA provides a wealth of information concerning the leaching behavior of cement and concrete systems that can be used by the CBP.
- ORCHESTRA includes command line execution (typically using batch files); the ORCHESTRA calculation kernel can be used as a submodel within mass transport or kinetic models—either mode may allow probabilistic or sensitivity

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<sup>11</sup> The ORCHESTRA framework is available electronically from <http://www.ecn.nl/orchestra/>.



analysis using an appropriate shell program or integration with CBP framework program.<sup>12</sup>

There are also features of LeachXS™/ORCHESTRA that present potential development needs for integration purposes:

- The current version of LeachXS™ does not appear conducive to coupling with the framework program without some modification (although communication via output files may be possible). For example, there is no command line access to the LeachXS™ program. The addition of such an option (based on input text files) in conjunction with existing ORCHESTRA templates could be used to provide a simple method to couple LeachXS™/ORCHESTRA to the framework program.
- The current standard method of selecting mineral phases for a new material being tested for leaching behavior is interactive, requires expert input, and may be difficult to automate. The option to select from predefined generic sets of minerals that are suitable for the type of material under consideration needs to be made operational.
- Limited probabilistic or sensitivity capabilities are currently available in LeachXS™/ORCHESTRA<sup>12</sup>.

## 4.2 STADIUM®

SIMCO Technologies, Inc. developed a numerical model called Software for Transport and Degradation in Unsaturated Materials (STADIUM®)

that can be used to predict the transport of ions and liquids in reactive porous media (Marchand et al. 2002; SIMCO 2008)<sup>13</sup>. The model has been used to predict the degradation of unsaturated concrete structures exposed to chemically aggressive environments. The results provided by STADIUM® have been validated on the basis of laboratory test results and field exposure observations. The model has been used to predict the behavior of numerous existing structures exposed to various forms of chemical degradation phenomena.

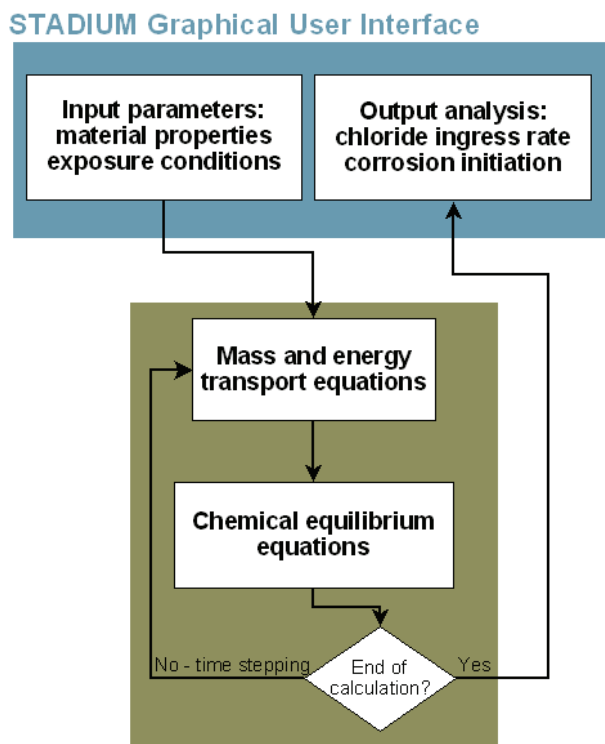
### 4.2.1 Description of STADIUM® Including Conceptual Models

The calculations in the STADIUM® model are divided into two primary modules as illustrated in Figure 4. The first module accounts for coupled transport of ions and water without considering chemical reactions (e.g., dissolution, precipitation, etc.). Transport is modeled with a volume-averaged version of the extended Nernst-Planck equation, which accounts for the electrical coupling between the ions as well as for the chemical activity of the species in solution. Terms are added to consider the impact of fluid flow and temperature gradients on ionic fluxes. The transport equations are coupled to Poisson's equation, which gives the electrical potential in the material as a function of the ionic profiles distribution. Coupling with moisture conservation and heat conduction equations is also taken into account.

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<sup>12</sup> Based on a personal communication from Meeussen, probabilistic capabilities are being added to ORCHESTRA.

<sup>13</sup> This section was taken from "More Details About STADIUM<sup>SM</sup>," available at [http://www.simcotechnologies.com/case\\_studies/pdf/More\\_Detail.pdf](http://www.simcotechnologies.com/case_studies/pdf/More_Detail.pdf) (accessed February 6, 2009) and the STADIUM® User Guide (SIMCO 2008).



**Figure 4. General Overview of STADIUM®**

The second STADIUM® module is a chemical equilibrium code. After each transport step, this module equilibrates the concentrations at each node of the finite element mesh with the phases of the hydrated cement paste. Solid phases can also be formed as a result of the penetration of aggressive species into the porous network of the material. The variation of solid phases will lead to local variations in porosity. These variations will likely affect the transport properties of the material locally. STADIUM® takes this locally varying phenomenon into account in the transport module described above.

#### 4.2.2 Inputs Needed to Run STADIUM®

The input information needed to run STADIUM® consists of the following (SIMCO 2008):

- Geometry and Time.** STADIUM® performs separate sets of calculations for ionic transport and chemistry. The ionic transport model consists of a set of partial differential equations that are solved by using a finite element method. The user must thus provide the space and time discretization parameters needed for the numerical algorithm.
- Material Properties.** The characteristics of the material to be modeled, some of which can be modified by the user, are entered via a set of interactive windows (although STADIUM® can be run via the command line). The properties to be entered for the material fall into the following categories: mixture proportions, transport properties, binder chemical composition, and initial state. Each category consists of numerous parameters to be entered. For example, the material transport properties are listed in Table 1.

- **Exposure Conditions (Boundary Conditions).** STADIUM® can simulate many different types of exposure conditions for concrete structures. The exposure conditions include information describing the ionic species and temperature and humidity boundary conditions. The user can modify some parameters (e.g., average temperature and relative humidity of the environment, the salinity of seawater, or the concentration of the ionic contaminant). When sulfate attack is selected, the user enters the external sulfate concentration. Boundary conditions associated with chlorides must be considered—the composition of the solution at the surface is entered.
- **Initial Values.** Initial values are provided for each variable in the model including data on the initial composition of the hydrated cement paste. The initial values are divided into three main sections: moisture and temperature, concentration, and solid phases. In the Moisture and Temperature section, the user provides the initial degree of the material saturation and the initial temperature of the material at the beginning of the simulation. In the Concentration section, the user provides the initial (neutral) composition of the pore solution. Finally, the initial content of the solid phases forming the hydrated cement paste of the material are entered.
- **Corrosion and Printing Options.** These options control how various output files will be generated. The output frequency (step) is defined. How and where corrosion results are to be computed are also defined. A frequency and number of rebar positions to be analyzed are entered. The model calculates total chloride content and the chloride/hydroxide ratio in the pore solution at each rebar position at the defined frequency.

**Table 1. STADIUM® Material Transport Input Parameters (SIMCO 2008)**

| Input Property        | Meaning  | Other Information (if Needed)  |
|-----------------------|--|--|
| Reference temperature | The temperature measured in the laboratory where the material characterization testing is conducted. | None   |
| Water/binder ratio    | The water/binder ratio of the concrete mixture.  | None   |
| Total Binder          | The total amount of binder (i.e., cement and any supplementary cementitious materials (SCMs)).       | None   |
| Total Aggregates      | The total amount of aggregates (fine and coarse) in the mixture.                                     | None   |
| Specific gravity      | A measure of the binder density.   | Typically 3.15 (3150 kg/m <sup>3</sup> ) for normal Portland cement and lower for mixtures with SCMs.  |
| Porosity              | The total porosity of the material, expressed as the percentage of void volume in the material.      | This parameter can be evaluated using ASTM C642 Standard Test Method.  |
| Cement type           | The type of Portland cement used in the concrete mixture.  | In the 1-D version, one of six cement types can be selected: 1) ASTM Type I or CSA Type 10, 2) ASTM Type II or CSA Type 20, 3) ASTM Type I/II, 4) ASTM Type V or CSA Type 50, 5) Pre-Blended binary, or 6) Pre-blended ternary cement. |
| SCM                   | The supplementary cementitious materials used in the concrete mixture.                               | The 1-D version allows the selection among four types of cementitious materials: Fly Ash type (C), Fly Ash type (F), Slag and Silica Fume.   |

**Table 1. STADIUM® Material Transport Input Parameters (Contd)**

| Input Property                        | Meaning   | Other Information (if Needed)   |
|---------------------------------------|---|---|
| OH- diffusion coefficient             | Hydroxide diffusion coefficient   | SIMCO developed a procedure to evaluate the tortuosity of the material based on the results of a migration test. When tortuosity is known, diffusion coefficients are calculated using the freewater diffusion coefficients. Accordingly, only the OH- diffusion coefficient is entered in the input file.          |
| Water diffusivity parameters          | The moisture transport parameters are the permeability and two parameters that characterize the water retention function of the material.   | Evaluated from the results of a SIMCO drying test. The software required to evaluate the moisture transport parameters from the drying test results is under development. When a simulation is performed in saturated conditions, these values are not considered in the calculations.                              |
| Initial hydration                     | The age of the concrete when first exposed to the environment.  | This feature was implemented to address precast materials, which may spend several weeks in storage before being exposed to the environment.  |
| Age of testing (days)                 | The age of the material when the transport properties were measured.  | None  |
| Hydration parameters $a$ and $\alpha$ | Parameter $a$ represents the fraction of the transport properties values when hydration is complete compared to actual values. Parameter $\alpha$ is the rate at which the transport properties decrease over time. | Typically $a$ is in the 0.2 – 0.8 range and $\alpha$ is in the 0.001 – 0.01 s <sup>-1</sup> range. Transport properties tend to decrease with time as hydration increases. While this can usually be neglected for high water-to-cement ratios, it is an essential feature of high performance concrete durability. |
| Thermal conductivity                  | The thermal conductivity value of the material.   | Typical values for concrete are between 1 and 5 W/m <sup>2</sup> /K. Simulation results have shown a weak sensitivity to this parameter.  |
| Specific heat                         | The specific heat value of the material.  | Typical values for concrete are between 800 and 1300 J/kg/K. Simulation results have shown a weak sensitivity to this parameter.  |

#### 4.2.3 Outputs Generated by STADIUM®

Three series of results are generated by STADIUM® (SIMCO 2008):

- Content versus depth (i.e., solution over the thickness as a function of time),
- Content versus time (i.e., corrosion related quantities, in total chloride or chloride/hydroxide ratio at specific rebar locations as a function of time), and
- Corrosion initiation results.

At the end of a calculation, output text files are created containing the simulation results. It is

possible to generate graphs from the main output file of the STADIUM® GUI using most plotting software.

#### 4.2.4 STADIUM® Embedded Databases

STADIUM® includes both materials properties and exposure conditions databases to enable data input of materials and exposure conditions by structure type.

##### 4.2.4.1 Material Properties Database

As part of a separate research program, a database of concrete transport properties was assembled to provide data for STADIUM®. A total of 24 concrete mixtures were prepared. Different types of cement

and supplementary cementitious materials were used. The following properties were evaluated at several time intervals in order to evaluate the effect of hydration on the transport parameters: porosity, diffusion coefficients, and water transport properties. The database also includes the initial pore solution of the materials as well as the chemical composition of the hydrated paste (i.e., portlandite, C-S-H, monosulfate, hydroxy-AFm, and ettringite content).

Three series of concrete mixtures were prepared. In each series, concrete batches were prepared at two different water-to-cement ratios: 0.35 and 0.45. The first series was dedicated to materials without supplementary cementitious admixtures. In the second series, supplementary cementitious materials were substituted for a fraction of the cement. The third series consisted in concretes prepared with corrosion inhibitors or shrinkage reducing admixtures.

#### 4.2.4.2 Exposure Conditions Database

STADIUM® contains a database of exposure conditions, continually updated, that depend on the structure and structural element type:

- Bridge
- Marine Structures
- Parking
- Road
- Commercial - Residential - Industrial
- Testing Laboratory

When an exposure condition includes sodium sulfate ( $\text{Na}_2\text{SO}_4$ ), the user selects the sulfate exposure category (i.e., *Mild*, *Moderate*, *Severe*, or *Very Severe*) and the concentration.

#### 4.2.5 STADIUM® Potential Development Needs for Integration

One purpose of the CBP is to develop an integrated set of tools to allow prediction of the performance of cementitious barriers impacted by several different phenomena over extended periods of time. The ability to integrate either the CBP tools or the capabilities of the tools is critical to the CBP. Thus issues related to integration and coupling must be considered early in the project and focused on throughout the project.

The current implementation of STADIUM® appears to have several advantages from an integration perspective:

- 1-D and 2-D versions of STADIUM® are available including a command line version.
- Detailed descriptions of underlying conceptual models are available (Marchand et al. 2002; SIMCO 2008).
- Results are saved to text files which can be opened and analyzed using standard spreadsheet or compatible applications.
- Limited probabilistic capabilities are available<sup>14</sup> that could be extended to non-financial parameters of interest.
- Testing results and methods are available that relate directly to model predictions and validation (Marchand et al. 2002; SIMCO 2008).

There are also features of STADIUM® that present potential development needs for integration:

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<sup>14</sup> The usefulness of the probabilistic approach in STADIUM® appears limited by the ability to only sample from the financial input variables (i.e., inflation and interest rates). Perhaps, this capability could be extended to other input parameters (e.g., material property, boundary conditions, etc.).

- A finite element (FE) mesh is built into STADIUM® code and solution routines; conceptual and algorithmic complications may arise from potential interactions of temporally- and spatially-varying boundary conditions among STADIUM®, the integration framework, and external PA model.
- Probabilistic capabilities are restricted to financial parameters for Net Present Value (NPV) calculation<sup>15</sup>.
- No sensitivity analysis capabilities are currently available.

### 4.3 THAMES

The Thermodynamic Hydration And Microstructure Evolution Simulator (THAMES) is in the beginning stages of development<sup>16</sup>. THAMES leverages thermodynamic predictions of equilibrium phase assemblages in aqueous geochemical systems to construct 3-D virtual microstructures of a cementitious binder at different times during the hydration process or during degradation phenomena. These virtual microstructures can then be used directly to calculate important engineering properties of a concrete made from that binder at prescribed times. In this way, THAMES will calculate the time evolution of important material properties such as elastic stiffness, compressive strength, effective DC conductivity, and permeability.

THAMES is being built around a thermodynamic engine, which rapidly predicts bulk mineral phase volumes as a function of time in cement paste microstructures evolving by hydration or degradation phenomena. However, the bulk information alone is

insufficient to make accurate predictions of transport properties and mechanical properties—microstructure information is also required. A model must predict not only the overall phase quantities, but also how these phases are distributed in space. As illustrated in Figure 5, THAMES ultimately will include 1) a module for generating a representative 3-D initial microstructure of cementitious particles in water (GENMIC), 2) a module for simulating microstructure changes (THAMES) guided by the thermodynamic calculations (e.g., GEMS), and 3) a module for calculating the elastic moduli, DC conductivity/diffusivity, and permeability on the predicted cement paste and mortar/concrete microstructure (CONCPROPS). A detailed description of THAMES is provided in the chapter entitled *CBP Software Description Chapter: THAMES*.

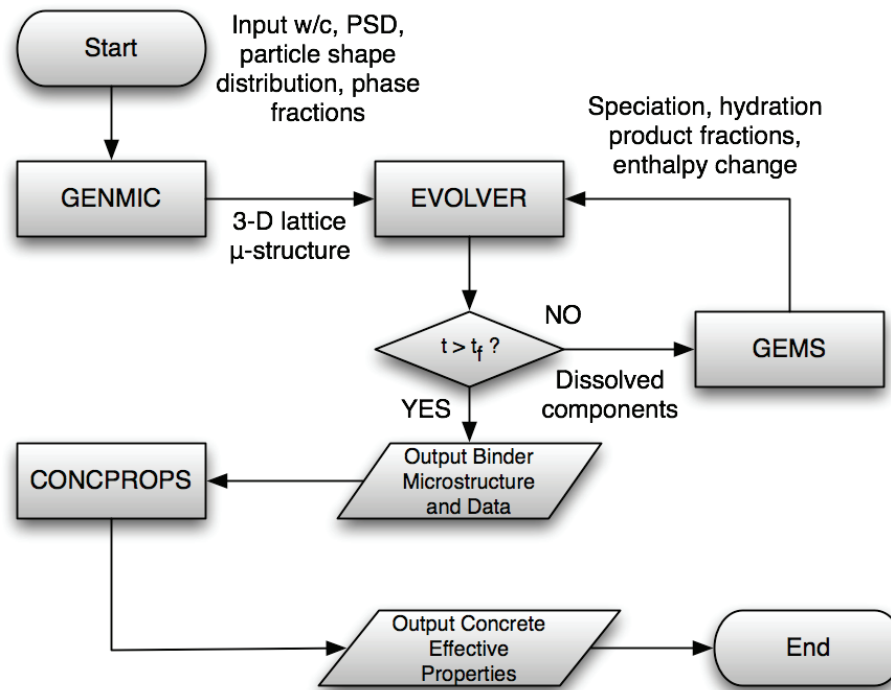
#### 4.3.1 Description of THAMES Including Conceptual Models

The overarching conceptual model in THAMES is the abstraction of the 3-D microstructure of a cementitious material as a scalar function  $M(\mathbf{r},t)$  of  $\mathbf{r}$ , the position vector relative to an arbitrary origin of space and  $t$ , the time relative to an arbitrary origin of time. For any given  $\mathbf{r}$  and  $t$ , the function  $M$  gives an integer identifying the phase occupying that point in space and time. A THAMES simulation begins with input of statistical data describing the mass fractions and spatial distribution of phases within the microstructure. The input is sufficiently detailed to enable the creation of a representative volume element (RVE) of an initial microstructure,  $M(\mathbf{r},0)$ ,

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<sup>15</sup> STADIUM® includes a Life Cycle Cost Analysis (LCCA) module that can be used to perform probabilistic analyses based on the Monte Carlo method (SIMCO 2008). The Net Present Value (NPV) is the risk indicator of choice in STADIUM®. The risk analysis approach uses random sampling from probabilistic descriptions of uncertain input variables (i.e., inflation and interest rates) to generate a probabilistic description of results for various scenarios. Results are captured for later statistical analysis.

<sup>16</sup> The information in this section is a summary of *CBP Software Description Chapter: THAMES*.



**Figure 5. Flow chart showing THAMES structure and relationship of GENMIC, GEMS, and EVOLVER modules.**

that is consistent with the input data. A module called GENMIC accomplishes this task, discretizing the RVE onto a 3-D cubic lattice using random parking of digitized particle shapes and a Gaussian filter to distribute the clinker phases.

Generally, an initial microstructure,  $M(\mathbf{r}, 0)$ , contains a collection of mineral phases that are not at thermodynamic equilibrium with the aqueous solution in the capillary pores. As a result, interactions between the solution and the solid phases will take place, with some phases partially dissolving and other phases precipitating as the system tends toward equilibrium. The goal of THAMES is to capture the trajectory of microstructural changes and determine the  $M(\mathbf{r}, t)$  function during this process. The GEMS module identifies a particular subspace of the range of

$M(\mathbf{r}, t \rightarrow \infty)$  to which the equilibrium state of a collection of components must belong. However, this thermodynamic constraint neither specifies the spatial distribution of phases nor indicates how the initial microstructure changes continuously along a path toward the equilibrium state.

THAMES assumes that the path toward equilibrium can be partitioned into a sequence of quasi-static changes in microstructure subject to time-dependent boundary conditions on the chemical composition of the pore solution. The sequence is constructed by assuming that, during a suitably small time interval  $\Delta t$ ,

- a) each phase that is unstable with respect to dissolution will dissociate according to a prescribed rate law;

- b) the partial dissolution of the unstable phases establishes an initial condition on the solution composition for that time interval;
- c) subject to the initial condition from (b), a thermodynamic calculation determines the solution speciation and the mass fractions of solid phases that are in equilibrium with the pore solution at the end of the time interval  $\Delta t$ ; and
- d) a set of customized rules for each phase, based on real microstructure formation and known physics, determines how to add or subtract phase volumes from the microstructure to obtain realistic spatial distributions of those phases that are consistent with experimental observation.

The new state of microstructure,  $M(\mathbf{r}, t+\Delta t)$ , then serves as the starting microstructure for the next time interval, and the process is repeated until a desired end time is reached.

One key tenet of materials science is that structure, together with chemistry, determines the properties of any material. If the microstructure of a cementitious material is resolved with sufficient accuracy, then that structure can be used to estimate engineering properties of the material using computational mechanics and composite theory. In THAMES, therefore, the output of the microstructure at any time can be used to estimate properties including linear elastic moduli, DC conductivity, and permeability of the material using established algorithms developed and validated at NIST. This collection of models for calculating engineering properties comprises the CONCPROPS module of the THAMES software, which works at the cement paste and mortar/concrete levels.

#### **4.3.2 Inputs Needed to Run THAMES**

The data required to begin a THAMES simulation are the set of statistical parameters and functions needed to create a 3-D approximation of the initial microstructure. Generally, the inputs will include:

- (1) the frequency with which to output the state of the lattice microstructure and to calculate selected properties;
- (2) the particle size distribution of each distinct component (including cement, gypsum, and fly ash) tabulated as a probability density function;
- (3) the shape distribution of each distinct component, catalogued in a database of spherical harmonic coefficients for individual particles;
- (4) the mass fractions of each phase, including pore solution, in the initial microstructure;
- (5) the surface area fractions of each solid phase;
- (6) a two-point correlation function for each solid phase in the cement clinker; and
- (7) a database of thermodynamic functions and thermophysical properties of cementitious phases. This database can be embedded in the GEMS module and thus may not be considered an input.

For simulating mortar or concrete, additional input parameters are required including:

- (8) the aggregate mass fraction;
- (9) the aggregate grading, which is the mass fraction of aggregate particles retained in each of a stack of sieves; and
- (10) the aggregate shape distribution, catalogued in the same way as for cement particles.

To calculate engineering properties in the CONCPROPS module, the relevant physical properties for each phase in the microstructure are required, including:



- (11) the bulk modulus of each phase,
- (12) the shear modulus of each phase,
- (13) the effective diffusivity of ions through the phase relative to their diffusivity in bulk pore solution, and
- (14) the liquid or gas permeability of each phase.

As part of the continued development of THAMES, the software will be extended to allow changes to be made to the pore solution composition at prescribed times to simulate the influence of the ingress of external agents, such as sulfates and chlorides. Additional input will be required in the form of a table of time-dependent boundary conditions on the pore solution chemistry, specifically the elemental molal concentrations of certain components.

Specific inputs for each module of THAMES are listed in tabular form in the detailed description of those modules in the chapter entitled *CBP Software Description Chapter: THAMES*.

#### **4.3.3 Outputs Generated by THAMES**

The output of the THAMES software consists of (a) the 3-D state of the lattice approximation to the microstructure RVE, given by the integer phase identification number at each lattice site, which may be prescribed by the user and (b) values of selected properties prescribed by the user. These outputs are in the form of regular ASCII text files.

#### **4.3.4 Embedded Databases**

The spherical harmonic (SH) coefficients of hundreds of real-shaped particles for a given cement are generally stored in a folder on the computer running the GENMIC module. The external resources for the GEMS module, originally

developed for environmental geochemistry applications, consist of thermodynamic databases supplemented with a cementitious material database called *cemdata07*, which contains thermodynamic data on important cementitious phases that are missing from the standard databases.

#### **4.3.5 Potential Development Needs for Integration**

As indicated above, any issues related to integration and coupling must be considered early and focused on throughout the project. Because THAMES is in the initial stages of development, the needs for efficient integration will be the focus. These include:

- Command line execution is needed to allow probabilistic or sensitivity analysis using an appropriate shell program as well as integration with the CBP framework program.
- Complete source code should be made available so that subroutines may be called from a Dynamic Link Library (DLL), if needed.
- The program should save results to ASCII text files that can be opened by standard spreadsheet or compatible programs.
- Thermodynamic data should be accessible via an external database to maintain consistency with the other codes in the integrated framework.

### **4.4 GoldSim**

GoldSim (Version 10) is a graphical, object-oriented computer program that runs under Microsoft Windows for executing dynamic, probabilistic simulations<sup>17</sup>. Simulation as defined here is the process of creating a model (i.e., an abstract representation) of a system to identify and understand those factors which control the system

---

<sup>17</sup> The information in this section summarizes Chapter III entitled *Detailed Description of the Integrating Platform Selected for the CBP Project – GoldSim*.

and/or to predict future behavior (GTG 2009a). As illustrated in Figure 6, GoldSim is a "visual spreadsheet" allowing the user to visually create and manipulate data and equations, including links to external programs and databases (GTG 2009a). Although GoldSim can be run deterministically, one of its key features is to quantify and assess uncertainties through the use of probabilistic analysis.

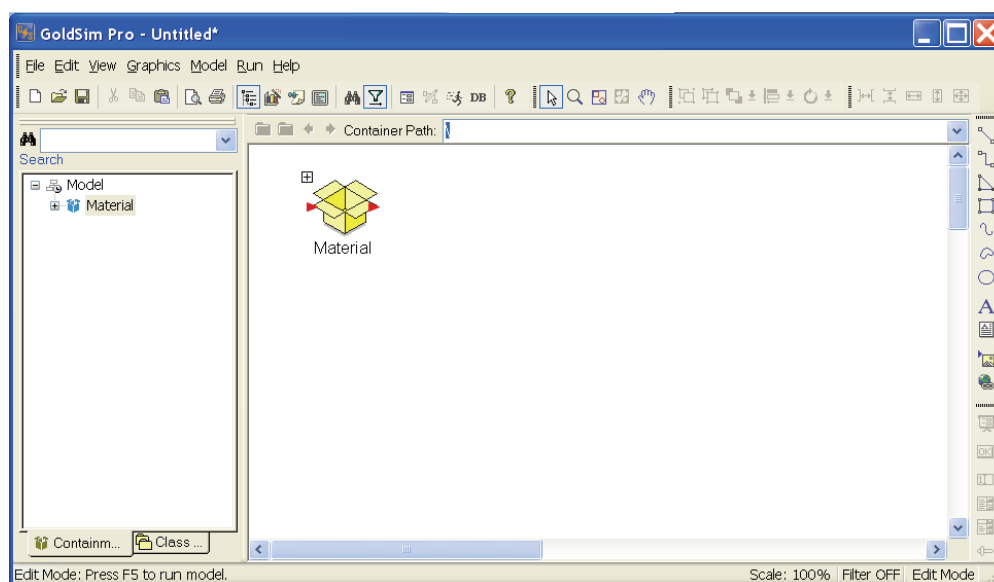
GoldSim was designed to be flexible and has been used to simulate various types of systems including Strategic Planning, Ecology, Environment, Reliability Engineering, and Manufacturing (GTG 2009a). GoldSim was also designed to readily incorporate additional modules (i.e., extension modules) to address specialized problems. These extensions include Financial, Contaminant Transport, Radionuclide Transport, Reliability, Dashboard Authoring, and Distributed Processing modules (GTG 2009a).

Although GoldSim was designed to be a flexible tool to simulate systems, there are limitations related to

how the program is used. Only certain types of functionality are built into GoldSim (e.g., input, expression, stock and delay, and linking) and its extension modules. As examples, the transport functions available in the GoldSim extension modules are one-dimensional in nature, and sensitivity analysis features are limited to one-at-a-time type analyses. A user may create additional functionality using built-in functional forms or calling external programs. However, user-supplied external functions may not fully integrate with built-in features of GoldSim. For example, if external programs related to transport are used, then the overall system material balance must be maintained by the user externally as with any such program.

#### **4.4.1 Description of GoldSim Including Conceptual Models**

A simulation is an abstract representation of a system including simplifications based on those aspects assumed to be important and omitting those considered nonessential so as to obtain predictions in



**Figure 6. A Screenshot of the GoldSim Graphical User Interface (GUI)**

an efficient manner (GTG 2009b). For real world systems, there will also be significant uncertainties regarding controlling processes and the parameter values needed to describe those processes. The most important factor impacting the accuracy is the degree to which the conceptual model captures reality and the degree to which uncertainty in the system has been represented (GTG 2009b).

The various objects with which a GoldSim model is constructed are referred to as *elements*. *Elements* represent the basic building blocks of the simulation. Elements provide mechanisms for entering data into the model; there are also functional elements that operate on one or more inputs to produce outputs. Stock and delay elements are critical for representing dynamic behavior. Detailed descriptions of the elements available in GoldSim are provided in the chapter entitled *Detailed Description of the GoldSim Integrating Platform Selected for the CBP Project*.

#### **4.4.2 Inputs Needed to Run GoldSim**

Input elements are used to provide the basic inputs to a GoldSim model. Three basic types of input elements are available (GTG 2009a):

- A Data element allows a single scalar value or an array of values with the same units to be specified.
- A Time Series element allows a time series to be specified for a parameter.
- A Stochastic element allows an uncertain parameter to be represented by defining its probability distribution.

GoldSim can also import data from spreadsheets (using a Spreadsheet element), or input elements can be linked directly to an ODBC-compliant database (GTG 2009a). GoldSim can be instructed to download the data at any time and will internally record the time and date at which the download occurred, providing a mechanism for quality control of input data. User-supplied Dynamic Link Libraries

(DLL's) can also be used to provide input information to the GoldSim simulation.

#### **4.4.3 Outputs Generated by GoldSim**

Some elements have a single output and others, such as the Stochastic element, have multiple outputs (GTG 2009a). One of the outputs is usually denoted the primary output, and the other outputs are referred to as secondary outputs. The name of the primary output for an element is the same as the name of the element itself. Therefore, output names are important because links are created by referencing the name of the output of one element in an input field of another element.

All element outputs in GoldSim have three output attributes (GTG 2009a):

- **Type.** The type can be either a value or a condition where values can be any real number and conditions are either true or false.
- **Order.** The order of an output can be scalar, vector, or matrix.
- **Dimensions.** Outputs (of values) can be assigned dimensions that can be displayed in any units.

Output attributes are important because GoldSim also uses them to ensure dimensional consistency between inputs and outputs when elements are linked.

Typically information is transferred between GoldSim elements (via links) continuously. However, to propagate discrete events (and consequences) between model elements, it is necessary to send information between elements intermittently (GTG 2009a). GoldSim allows certain elements to emit and receive discrete signals.

GoldSim Result elements provide a mechanism to collect and display simulation results for subsequent analysis. In some cases, rather than using the plotting and post-processing capabilities provided by

GoldSim, it may be useful to plot, analyze, or store results using a separate program, such as a spreadsheet, a database, or statistical analysis package. GoldSim provides three methods for exporting results in an ASCII or binary file, an MS-Excel file, or an Access database file:

- Exporting results to a text file, binary file or database,
- Exporting time histories from a Time History Result element, or
- Exporting results using a Spreadsheet element.

#### **4.4.4 Embedded Databases**

GoldSim allows the user to create and manipulate data and equations including linking to external programs and databases (GTG 2009a). Although GoldSim can interact with worksheets and external databases, no databases are *required* for a GoldSim model. For example, no databases are required for a GoldSim Lookup Table element; however, data can be imported into either a 1-D or 2-D table function from an external database denoted a “Yucca Mountain Database” as described in the chapter entitled *Detailed Description of the GoldSim Integrating Platform Selected for the CBP Project*. A “Yucca Mountain Database” is one of several database structures supported by GoldSim, but the only one that supports Lookup Table elements. A “Yucca Mountain Database” is also required for a GoldSim File element when it is used to ensure that support files that are stored on a network are accessed for use in a simulation and to provide an “audit trail” of the file transfer.

Additional information for linking GoldSim to external databases is provided in the chapter entitled *Detailed Description of the GoldSim Integrating Platform Selected for the CBP Project*.

#### **4.4.5 Potential Development Needs for Integration**

The GoldSim program uses various types of built-in elements as well as those available in “add-in” or extension modules. The most important elements in the context of the CBP are those that can be used to couple GoldSim to external codes including the Lookup Table, Spreadsheet, and External (or DLL) elements. The primary sources for these descriptions are Volumes 1 and 2 of the GoldSim User’s Guides (GTG 2009a; GTG 2009b).

Each of the GoldSim elements that can be used to couple external codes to GoldSim may, in general, have the following uses:

- **Lookup Table element.** If running an external code is not sufficiently efficient (e.g., for uncertainty analysis), then a surrogate may be developed for the code and implemented using a Lookup Table element.
- **Spreadsheet element.** Custom Visual Basic for Applications (VBA) code (in Microsoft Excel) may be used to create input, run the external code, and collect results for transfer to GoldSim using a Spreadsheet element.
- **External element.** The most efficient and strongest coupling may be created using Dynamic Link Libraries (DLL) using External elements; however, these elements require the most expertise to develop and maintain.

An example for each of these types of coupling between GoldSim and the PHREEQC geochemical code is provided on the GoldSim website (<http://www.GoldSim.com>) and briefly described in the chapter entitled *Detailed Description of the GoldSim Integrating Platform Selected for the CBP Project*.

## 5 SUMMARY AND CONCLUSIONS

A number of important transport processes (e.g., diffusion and advection through aqueous and vapor phases) and degradation phenomena (e.g., sulfate and chloride attack, carbonation, REDOX changes, and cracking) must be modeled to adequately describe the performance of a cementitious material over time. State-of-the-art computer codes have been selected that collectively represent much of the needed functionality for CBP modeling. However, these codes are presently not linked and do not contain all needed functionality to model cementitious materials over the long times necessary. Thus these codes or their functionality will need to be enhanced and coupled to provide the set of needed CBP tools.

Coupling of independent computer codes has been addressed by national laboratories, universities, and others using a variety of approaches driven by numerical stability and software considerations. One method is tight coupling by advancing and iterating all codes at each time step using grid mapping techniques to relate the response from one calculation onto the domain of another. The high volume of inter-code communication often required by this methodology typically requires significant interface development and computing resources and may lead to long run times. An alternative is a coarsely distributed parallel construct based on object-oriented programming principles. This latter alternative, which is related to more modern integrating methodologies, is likely to be more attractive for the proposed CBP model. Here inter-code communication occurs less frequently and may be accomplished through a variety of information exchange options, such as shared data files. The GoldSim software can be used to couple separate codes through Lookup Table, Spreadsheet, and External (or DLL) elements. The latter provides the

most flexible mechanism and a feasible means to tightly couple external codes.

The selected codes are excellent for their intended purposes and possess a number of features that lend themselves to integration using GoldSim. However, to couple these computer codes in the CBP framework, some changes will be needed. For example, LeachXS™/ORCHESTRA will likely need a command line option with the ability to define conditions and mineral species separately from the GUI. The STADIUM® computational core can already be accessed from the command line; however, like the other selected codes, conceptual and algorithmic complications may arise from interactions of temporally- and spatially-varying boundary conditions among STADIUM®, the integration framework, and external PA model. The THAMES model is under development and capabilities must be added for access to the code from the integration framework (e.g., command line or direct access via a Dynamic Link Library). These changes will provide the ability to integrate these existing codes in a framework to provide a set of tools for long-term prediction of the performance of cementitious materials.

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# **CBP DETAILED SOFTWARE DESCRIPTION CHAPTER: THAMES**

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## **LIST OF ACRONYMS AND ABBREVIATIONS**

|        |  |
|--------|--|
| ASCII  | American Standard Code for Information Interchange             |
| ASR    | Alkali-silicate reactions                                      |
| CBP    | Cementitious Barriers Partnership                              |
| DC     | Dependent Component  |
| GCC    | GNU Compiler Collection  |
| GUI    | Graphical User Interface                                       |
| GGBFS  | Ground Granulated Blast Furnace Slag                           |
| IC     | Independent Component  |
| MPI    | Message Passing Interface                                      |
| NIST   | National Institute of Standards and Technology                 |
| OPC    | Ordinary Portland Cement                                       |
| RVE    | Representative Volume Element                                  |
| SS     | Solid Solution   |
| SH     | Spherical Harmonic   |
| STL    | Standard Template Library                                      |
| THAMES | Thermodynamic Hydration And Microstructure Evolution Simulator |
| VCCTL  | Virtual Cement and Concrete Testing Laboratory                 |

# CBP Detailed Software Description Chapter: THAMES

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The goal of the Cementitious Barriers Partnership (CBP) is to develop a reasonable and credible set of tools to predict the structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over extended time frames (e.g., >100 years for operating facilities and >1000 years for waste management). The simulation tools will be used to evaluate and predict the behavior of cementitious barriers used in near surface engineered waste disposal systems including waste forms, containment structures, entombments, and environmental remediation. These cementitious materials are exposed to dynamic environmental conditions that cause changes in material properties via (i) aging, (ii) chloride attack, (iii) sulfate attack, (iv) carbonation, (v) oxidation, and (vi) primary constituent leaching. A set of state-of-the-art software tools has been selected as a starting point to capture these critical aging and degradation phenomena. One of these tools, THAMES, is being developed to describe cementitious binder microstructures and calculate important engineering properties during hydration and degradation. Through the CBP, computational tools will be developed or modified to improve the assessment of long-term structural, hydraulic, and chemical performance of cementitious materials.

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## 1 OVERVIEW

THAMES<sup>1</sup> software is in the beginning stages of development. It leverages thermodynamic predictions of equilibrium phase assemblages in aqueous geochemical systems to construct 3-D virtual microstructures of a cementitious binder at different times during the hydration process or, with further development, during degradation. These virtual microstructures can then be used to calculate important engineering properties of a concrete made from that binder at prescribed times. In this way, the THAMES model will provide a way to calculate the

time evolution of important material properties such as elastic stiffness, compressive strength, effective DC conductivity, and permeability.

The basic idea in using *equilibrium* thermodynamics to guide the *non-equilibrium* development of microstructure is to approximate changes in the system as a sequence of quasi-static (i.e., reversible) changes of state during “small” time intervals. In mature concrete, dissolution of the initial cement phases is so slow—due to decreased surface area and

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<sup>1</sup> THAMES is an acronym for Thermodynamic Hydration And Microstructure Evolution Simulator.

diffusion barriers set up by hydration products—that a good estimate of the solution composition can be obtained by assuming the solution to be in equilibrium with all of the hydration product phases that are present at the time. This calculation of multiphase chemical equilibrium is readily accomplished using any of a number of environmental geochemistry programs such as PHREEQC (PHREEQC 2008), CHESS (CHESS 2008), GEMS (GEMS 2008) or ORCHESTRA (Meeussen 2003), although there can be differences among programs and errors in the programs. The equilibrium solution composition and number of moles of each solid phase represents the initial conditions for the system. The driving force for subsequent state changes are small excursions of the pore solution composition from equilibrium with the existing phases, due to continuous but slow dissolution of cement phases, by the exchange of ions with external groundwater, by gradual changes in temperature, and/or by degradation reactions. Even relatively fast changes, like a sudden ingress of external sulfate ions, often can be well-approximated by an assumption of thermodynamic control on the formation of reaction products (Lasaga 1981; Lothenbach and Winnefeld 2006).

The feasibility of this idea already has been demonstrated for simulating the hydration of cement paste (Lothenbach and Wieland 2006; Lothenbach and Winnefeld 2006; Guillon 2008). A number of physical parameters of the initial paste, such as solid surface area, phase composition, and water-solid mass ratio, are used to generate a semi-empirical description of the rate of dissociation of each cement clinker phase (Parrott and Killoh 1984; Tomosawa 1997). These dissolution rates make it possible to determine the (non-equilibrium) solution composition at any time, which in turn is used to compute the new equilibrium solution composition and the change in number of moles of each hydration

product phase. Predictions of solution composition, pH, mole fractions of hydration product phases, and total capillary porosity have been validated against experimental results for several different cement compositions (Lothenbach and Wieland 2006; Lothenbach and Winnefeld 2006).

THAMES is being built around a thermodynamic engine that predicts the bulk phase volumes in cement paste microstructures that occur through hydration or degradation phenomena. However, the bulk information alone is insufficient to make accurate predictions of transport properties and mechanical properties; microstructural information is also required. That is, a successful model must predict not only the overall phase quantities, but also how these phases are distributed in space. Therefore, the complete THAMES software will include a module for generating a representative 3-D initial microstructure (GENMIC), a module for simulating microstructure changes (THAMES) guided by the thermodynamic calculations (e.g., GEMS), and a module for calculating the elastic moduli, DC conductivity/diffusivity, and permeability on the predicted cement paste and mortar/concrete microstructure (CONCPROPS). The following sections describe the conceptual models, limitations, validation requirements, and potential development opportunities for these modules.

## **2 EXPLANATION OF CONCEPTUAL MODELS AND THEORY**

The overarching conceptual model of THAMES is the abstraction of the 3-D microstructure of a cementitious material as a scalar function  $M(\mathbf{r},t)$  of  $\mathbf{r}$ , the position vector relative to an arbitrary origin of space and  $t$ , the time relative to an arbitrary origin of time. For any given  $\mathbf{r}$  and  $t$ , the function  $M$  gives an integer identifying the phase occupying that point in

space and time. A THAMES simulation begins with input of statistical data on the mass fractions and spatial distribution of phases within the microstructure that is sufficiently detailed to enable the creation of a representative volume element (RVE) of an initial microstructure,  $M(\mathbf{r},0)$ , that is consistent with the input statistical data. A module called GENMIC accomplishes this task, discretizing the RVE onto a three-dimensional cubic lattice, using random parking of digitized particle shapes and a Gaussian filter to distribute the clinker phases.

Generally, an initial microstructure  $M(\mathbf{r},0)$  contains a collection of mineral phases that are not at thermodynamic equilibrium with the aqueous solution in the capillary pores. As a result, interactions between the solution and the solid phases will take place, with some phases partially dissolving and other phases precipitating as the system tends toward an equilibrium state. The goal of THAMES is to capture the trajectory of microstructural changes and determine the  $M(\mathbf{r},t)$  function during this process. For any collection of components and a sufficiently comprehensive thermodynamic database, one can determine a particular subspace of the range of  $M(\mathbf{r},t \rightarrow \infty)$  to which the equilibrium state must belong, i.e., the equilibrium mass fractions of each phase. The role of the GEMS module (see description below) is to identify that subspace. However, this thermodynamic constraint does not specify the spatial distribution of those phases, nor does it indicate how the initial microstructure changes continuously along a path toward that equilibrium state.

Therefore, the THAMES software assumes that the path toward equilibrium can be partitioned into a sequence of quasi-static changes in microstructure subject to time-dependent boundary conditions on the chemical composition of the pore solution. This

sequence is constructed by assuming that, during a suitably small time interval  $\Delta t$ , (a) each phase that is unstable with respect to dissolution will dissociate according to a prescribed rate law; (b) the partial dissolution of those phases establishes an initial condition on the solution composition for that time interval; (c) subject to that initial condition, a thermodynamic calculation determines the solution speciation and the mass fractions of solid phases that are in equilibrium with the pore solution at the end of the time interval  $\Delta t$ ; and (d) a set of customized rules for each phase determines how to add or subtract phase volumes from the microstructure to obtain realistic spatial distributions of those phases that are consistent with experimental observation. The new state of microstructure,  $M(\mathbf{r}, t+\Delta t)$ , then serves as the starting microstructure for the next time interval, and the process is repeated until a desired end time is reached.

One of the key tenets of materials science is that structure, together with chemistry, determines the properties of any material. If the microstructure of a cementitious material is resolved with sufficient accuracy, that structure can be used to calculate engineering properties of the material using computational mechanics and composite theory. In the THAMES software, the output of the microstructure calculations at any time, i.e., the 3-D lattice approximation of  $M(\mathbf{r},t)$ , can be used to generate a finite element or finite difference mesh to estimate properties including linear elastic moduli, DC conductivity, and permeability of the material using established algorithms developed and validated at the National Institute of Standards and Technology (NIST). This collection of models for calculating engineering properties comprises the CONCPROPS module of the THAMES software that works at the cement paste and mortar/concrete levels.

### 3 HARDWARE AND SOFTWARE REQUIREMENTS

THAMES is composed of software modules written in the C and C++ programming languages. Theoretically, it can be compiled and run on any platform with a C/C++ compiler. The development version of THAMES has been used with Unix/Linux<sup>2</sup> and Mac OS X, both of which have the GNU GCC compiler (GNU 2009). MS Windows platforms furnished with a Linux virtual machine or a commercial C/C++ compiler also could be viable, although it has not been verified.

Several of the programs within the CONCPROPS module are available in both serial and parallelized versions, with the remainder and all the programs in the other modules only available in serial form. Parallelizing the programs, which enables much larger microstructures to be simulated, requires libraries for the Message Passing Interface (MPI) protocol to be installed. In the latter case, the parallelized version requires multiple processors or multi-core processors, linked via Ethernet or higher-speed network (e.g., myrinet) connections.

### 4 PROGRAM EXECUTION MODE(S) AND USER/PROGRAM INTERFACE INFORMATION

Currently, the development version of the THAMES software operates exclusively in command-line mode. A graphical user interface (GUI), probably based on Java applets, could be developed at some point during the CBP project if necessary.

### 5 SYSTEM PERFORMANCE

On a computer with a 2.33 GHz 2-core processor, the GENMIC module can create a  $100\text{ }\mu\text{m}^3$  volume of cement paste ( $10^6$  pixels) in about 20 minutes. Simulating 3 years of hydration of this microstructure with the THAMES and GEMS modules requires about one or two hours. Calculating concrete properties, such as effective elastic moduli, with the CONCPROPS module currently requires less than an additional hour of computational time. Larger cement paste volumes require proportionally longer computational times, scaling roughly linearly with system volume.

### 6 INPUT DATA DESCRIPTION

The input data required to begin a simulation with THAMES are the set of statistical parameters and functions that are sufficient to create a 3-D approximation of the initial microstructure on a cubic lattice. Generally, the input requirements will include (1) the frequency with which to output the state of the lattice microstructure and to calculate selected properties; (2) the particle size distribution of each distinct component (cement, gypsum, fly ash, etc.) tabulated as a probability density function; (3) the shape distribution of each distinct component, catalogued in a database of spherical harmonic coefficients for individual particles; (4) the mass fractions of each phase, including pore solution, in the initial microstructure; (5) the surface area fractions of each solid phase; (6) a two-point correlation function for each solid phase in the cement clinker; and (7) a database of thermodynamic functions and thermophysical properties of

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<sup>2</sup> Certain computer programming languages and operating systems, either commercial or open source, are identified to adequately specify program compilation procedures. In no case does such identification imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the items identified are necessarily the best available for the purpose.



cementitious phases. This database can be embedded in the GEMS module and, therefore, may not be technically considered as an input. For simulating mortar or concrete, additional input parameters are required including (8) the aggregate mass fraction; (9) the aggregate grading, which is the mass fraction of aggregate particles retained in each of a stack of sieves; and (10) the aggregate shape distribution, catalogued in the same way as for cement particles. To calculate engineering properties in the CONCPROPS module, one must also input the relevant physical properties of each phase in the microstructure, including (11) bulk modulus of each phase, (12) the shear modulus of each phase, (13) the effective diffusivity of ions through the phase relative to their diffusivity in bulk pore solution, and (14) the liquid or gas permeability of each phase. More detailed descriptions of many of these parameters are given in the following sections.

As part of the development of THAMES during the lifetime of the CBP project, the software will be extended to allow the possibility to make changes to the pore solution composition at prescribed times. This will be done to simulate the influence of the ingress of external agents, such as sulfates and chlorides. When this is accomplished, additional input will be required in the form of a table of time-dependent boundary conditions on the pore solution chemistry, specifically the elemental molal concentration of certain components.

Specific inputs for each module of THAMES will be listed in tabular form in the detailed description of the modules.

## **7 OUTPUT DESCRIPTIONS**

The output of the THAMES software consists of (a)

the three-dimensional state of the lattice approximation to the microstructure RVE, given by the integer phase identification number at each lattice site, at times prescribed by the user and (b) values of selected properties prescribed by the user. Both of these outputs are in the form of regular ASCII text files.

## **8 DETAILED EXAMPLE(S)**

No detailed examples are available at this time because the development of the THAMES model is not yet finished.

## **9 PROGRAM STRUCTURE**

THAMES software is comprised of four interacting modules:

- (1) A generator for the initial 3-D microstructure of a cementitious paste (GENMIC).
- (2) A Gibbs free energy minimizer (GEMS) including a thermodynamic database customized for cementitious phases.
- (3) A lattice-based model for simulating the microstructure state as a function of time (EVOLVER).
- (4) A module for calculating the mechanical and transport properties of cement paste, mortar, or concrete based on the cement paste microstructure and constituent phase properties (CONCPROPS).

The relationship among these modules is shown schematically in Figure 1. In the following subsections, the conceptual models, and the required inputs and outputs of each module, are enumerated.

## 10 DETAILED EXPLANATION OF COMPUTATIONAL ALGORITHMS AND METHODS

THAMES is composed of four primary modules. Interactions among the modules are shown in Figure 1. A discussion of the algorithms and methods is deferred until the next section, which explains the details of each of these four computational modules.

## 11 DETAILED EXPLANATIONS OF PROGRAM MODULES

### 11.1 Program Element 1: GENMIC

#### 11.1.1 Identification

The name of the element is GENMIC, which is

descriptive of its purpose of generating initial 3-D microstructures on a computational lattice.

#### 11.1.2 Type

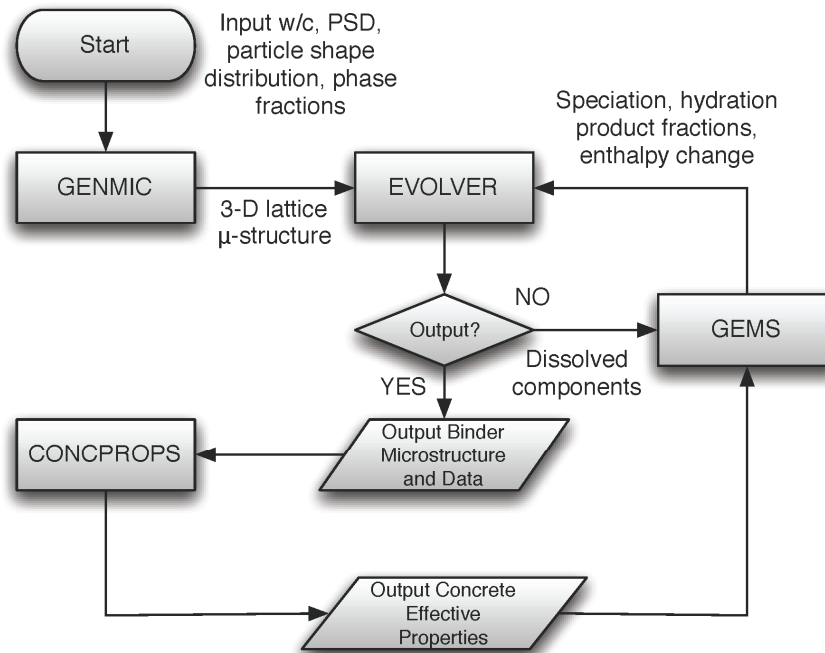
GENMIC is one of four modules in THAMES.

#### 11.1.3 Purpose

GENMIC is used to create a realistic representation of a 3-D cementitious paste microstructure on a computational lattice.

#### 11.1.4 Function

The GENMIC module uses random parking algorithms to populate a 3-D lattice with particles that follow the prescribed particle size distribution. The particles can assume shapes taken from a database of shapes obtained by spherical harmonic (SH) analysis of tomographic images of real



**Figure 1. Flow chart showing THAMES structure and relation of GENMIC, GEMS, and EVOLVER modules**

particles. After the particles have been placed to achieve a desired mass fraction of solids, a Gaussian filter is used to distribute the major clinker phases among the particles using two-point correlation functions obtained on segmented micrographs of the cement powder. The difference between the target and actual volume fraction of phases is typically less than 0.01. The uncertainty in the surface area fractions of each clinker phase is generally 0.001.

### 11.1.5 Subordinates

GENMIC is a self-contained module, consisting of a number of subroutines for accomplishing the separate tasks of particle placement (subroutine `create`), clinker phase distribution (subroutine `distrib3d`), and surface area adjustment (subroutine `sinter3d`).

### 11.1.6 Dependencies

GENMIC is used once to generate an initial microstructural state for a simulation. It has no dependencies on the other THAMES modules.

### 11.1.7 Interface

GENMIC requires input of mix formulation parameters, including volume fraction of solids, volume fractions of clinker phases, gypsum, etc., and autocorrelation functions to use for distributing the clinker phases in 3-D space among the cement particles. All of these data are contained in ASCII text files. The program can be executed from the command line.

### 11.1.8 Resources

There are no primary external resource elements for GENMIC.

### 11.1.9 Processing

The GENMIC module uses the input value of the target volume fraction of solids, together with an input probability density function for the particle size distribution, and uses a random parking algorithm with no overlaps to place particles according to the size distribution until the target volume fraction is reached. If the particles are to have realistic shapes, the spherical harmonic (SH) coefficients for a representative ensemble of particle shapes must be available. The SH coefficients for each particle are stored in separate ASCII text files that are read by GENMIC and used to place the shape with specified volume and arbitrary orientation. After the particles are placed, the input autocorrelation functions are used to partition the structure into silicates and aluminates. After this, the partitioning is refined to the individual four major clinker phases of Portland cement. After the partitioning of phases, the surface areas of each phase are adjusted using a sintering algorithm that conserves volume but changes the shape of the phase domains. Further details may be found in Bentz (1997). The required input data are summarized in Table 1. At the conclusion of GENMIC, the lattice is stored as a 3-D array, with an integer identification number at each lattice site to specify the phase located there.

### 11.1.10 Data

There are no major internal data elements in GENMIC.

### 11.1.11 Descriptions of Required External Databases and Programs

The SH coefficients of hundreds of real-shaped particles for a given cement are generally stored in a folder on the computer running the GENMIC module. Other than the input files already described, no external databases or programs are required.

**Table 1. Input parameters for GENMIC module**

| Input Property  | Meaning   | Other Information   |
|---|---|---|
| Lattice dimensions  | x, y, z (number of lattice sites in each dimension)   | None  |
| Lattice spacing   | Physical distance between lattice points  | Units of $\mu\text{m}$  |
| Unsigned integer values representing phases   | Phases: Pore solution, alite, belite, tricalcium aluminate, etc.  | Typical values 0, 1, 2, ..., catalogued in a phase database (db) file                           |
| Density of each phase   | Mass per unit volume  | Units of $\text{g}/\text{cm}^3$ , catalogued in a phase db file; value from cemdata07 GEMS db   |
| Molar volume of each phase  | Volume occupied by one mole of phase  | Units of $\text{cm}^3/\text{mol}$ , catalogued in a phase db file; value from cemdata07 GEMS db |
| Particle size distribution  | Probability density function  | Two-column ASCII file   |
| Particle shape distribution   | Pointer to collection of SH coefficients for different shapes   | SH coefficients for each shape stored in separate ASCII file                                    |
| Target mass fractions of cement clinker minerals  | Masses of alite, belite, tricalcium aluminate, and ferrite phases per unit mass of clinker                | Sum normalized to 1   |
| Target surface area fractions of cement clinker minerals  | Surface areas of alite, belite, tricalcium aluminate, and ferrite phases per unit surface area of clinker | Sum normalized to 1   |
| Two-point correlation functions for each clinker phase  | Separate functions for alite, belite, tricalcium aluminate, and ferrite phases                            | Two-column ASCII file, assumes isotropic homogeneous medium                                     |
| Target mass fraction of calcium sulfate in cement   | Masses of gypsum, bassanite, and anhydrite per unit mass of cement  | None  |
| Target mass fractions of supplementary cementitious materials (e.g., silica fume, slag, fly ash, limestone) | Mass of supplementary cementitious material per unit mass of cementitious material                        | None  |
| Target mass fractions of fly ash constituents   | Masses of aluminosilicate glasses, tricalcium aluminate, etc. per unit mass of fly ash                    | Sum normalized to 1 (fly ash only)  |
| Target mass fraction of water   | Mass of water in cement paste per unit mass of cement paste   | Can be inferred from water-cement mass ratio  |
| Flocculation parameter  | Number of particle agglomerates in microstructure   | None  |

### 11.1.12 Verification and Validation

The ability of GENMIC to accurately reproduce desired water-to-cement ratio (w/c), cement phase volume fraction, surface area fraction, spatial

distribution, and cement particle size and shape distribution has been extensively verified and validated in the literature (Bentz and Stutzman 1994; Bentz 1997; Bullard and Garboczi 2005; Bentz et al 2006). Further verification and validation is needed

for cements containing fly ash or other waste-stream materials to ensure that the simulated distributions of phases in those materials are sufficient to accurately describe subsequent hydration and property development. Experimental characterization of waste-stream materials needs to be developed to serve as input to improved versions of GENMIC.

## **11.2 Program Element 2: GEMS**

### **11.2.1 Identification**

The name of the element is GEMS.

### **11.2.2 Type**

GEMS is one of four modules in THAMES.

### **11.2.3 Purpose**

GEMS is used to make calculations of equilibrium solution compositions and phase assemblages in cementitious microstructures. These calculations are used to determine how the 3-D microstructure should be modified at each time increment of hydration to be consistent with thermodynamic calculations.

### **11.2.4 Function**

The GEMS module is basically identical to the GEMIPM2K standalone version of the GEMS application developed by Dmitrii Kulik (Kulik and Kersten 2001; Kulik and Kersten 2002). It is being embedded in THAMES as a module that can be called by the EVOLVER module and which can return calculated phase assemblages in tabular form to the EVOLVER module.

### **11.2.5 Subordinates**

The GEMS module has no major subordinate entities.

### **11.2.6 Dependencies**

The GEMS module depends on the EVOLVER module for prescribing the boundary conditions on the solution composition at each time increment for which a thermodynamic calculation is required.

### **11.2.7 Interface**

The GEMS module has no user interface. All of its calculations are internal to the THAMES program.

### **11.2.8 Resources**

Originally developed for environmental geochemistry applications, the external resources for GEMS consist of thermodynamic databases, supplemented with a cementitious material database, called cemdata07, which contains thermodynamic data on important cementitious phases that are missing from the standard databases, e.g., SUPCRT.

### **11.2.9 Processing**

The GEMS module is based on the GEMIPM2K program for minimizing the Gibbs free energy of multicomponent, multiphase aqueous systems (GEMS 2008). The GEMS module requires input of the equivalent oxide mass fractions in the cement, as well as the elemental mass fractions of the capillary pore solution. After minimizing the free energy of the system subject to these boundary conditions, the GEMS module outputs the volume and mass fractions and compositions of each phase in the microstructure, the enthalpy change, and the speciation of the pore solution. The volume fractions are used as input to EVOLVER for the next time step of microstructure development. The inputs required by the GEMS module are given in Table 2.

### 11.2.10 Data

There are no major internal data elements in GEMS.

### 11.2.11 Descriptions of Required External Databases and Programs

No external databases or programs are required besides those listed in the Resources section.

**Table 2. Input parameters for GEMS module**

| Input Property  | Meaning  | Other Information  |
|---|--|--|
| Temperature   | System temperature   | Units of °C  |
| Pressure  | System hydrostatic pressure  | Units of bars  |
| Number of independent components (ICs)                    | Maximum number of components that form the basis set for describing all phases in the system | Typically between 4 and 8. Used for memory allocation  |
| Number of dependent components (DCs)                      | Maximum number of DCs, i.e., the individual phases and pore solution species                 | Typically between 20 and 30. Used for memory allocation  |
| Number of phases  | Maximum number of phases that can coexist  | Typically between 10 and 20. Used for memory allocation  |
| Number of solid solution (SS) phases                      | Maximum number of SS phases that can coexist   | Must be less than the number of phases. Typically between 4 and 8. Used for memory allocation  |
| Number of DCs in SS phases                                | Maximum number of DCs needed to characterize SS phase compositions                           | Must be less than the number of DCs. Typically between 15 and 20. Used for memory allocation   |
| Names of ICs  | Text identifying ICs   | Character strings in single quotes, separated by a space   |
| Molar masses of ICs                                       | Molar masses of ICs  | Real-valued, separated by a space; units of g/mol  |
| Names of phases   | Text identifying phases  | Character strings in single quotes, separated by space   |
| Number of DCs in each phase                               | Minimum number of DCs required to characterize the composition of each phase                 | Vector of unsigned integers, separated by a space  |
| Stoichiometry matrix for ICs                              | Matrix that specifies the composition of each IC   | One column for each IC, one row for each DC. Each element $ij$ is the molar stoichiometric coefficient of the $i$ -th DC in the $j$ -th IC |
| Molar volumes of DCs                                      | Molar volume of each DC, including solutes   | Units of J/bar   |
| Molar Gibbs free energy function coefficients for each DC | Molar Gibbs free energy of each DC, including solute species, at reference temperature       | Units of J/mol   |

### 11.2.12 Verification and Validation

The GEMS module and database have been carefully verified and validated in the literature for regular OPCs (Lothenbach and Winnefeld 2006; Lothenbach and Matschei 2008), sulfate-resisting OPCs (Lothenbach and Wieland 2006), OPC/limestone blends (Lothenbach and LeSaout 2008), certain alkali-activated slags (Gruskovnjak, Lothenbach, and Holzer 2006), and super-sulfated slag cements (Gruskovnjak, Lothenbach, and Winnefeld 2008). Further verification and validation are needed for cements containing additions of slag, fly ash, or other chemicals/minerals, such as those often found in Saltstone waste forms.

### 11.2.13 Summary of Model Limitations

The cemdata07 database in GEMS contains very limited data on the calcium silicate hydrate (C–S–H<sup>3</sup>) gel formed in the presence of pozzolans and on the binding of alkali and transition metal cations. These are subjects of ongoing research at EMPA and the Paul Scherrer Institute, Swiss institutions where the cemdata07 database and C-S-H solid solution model, respectively, were developed.

The current kinetic module for cement hydration was originally developed by Parrott and Killoh for ordinary Portland cement (OPC) pastes (Parrott and Killoh 1984) and provides empirical equations for the rate of dissolution of the major clinker phases as a function of the mass water-to-cement ratio (w/c), cement fineness as measured by the Blaine air permeability test, and temperature. This kinetic model will not be applicable in cement blends containing ground granulated blast furnace slag (GGBFS) or fly ash. Currently there is no reliable kinetic model for blended cements, so developing

one will be an important subject of research.

## 11.3 Program Element 3: EVOLVER

### 11.3.1 Identification

The name of the element is EVOLVER, which is descriptive of its task of simulating the evolution of 3-D microstructure of cementitious concrete binders.

### 11.3.2 Type

EVOLVER is one of four modules in THAMES.

### 11.3.3 Purpose

The EVOLVER module operates directly on the 3-D lattice that is output by the GENMIC module, as depicted in Figure 1. It modifies the lattice sequentially by changing the value of the phase identification number of selected lattice sites to simulate growth or dissolution of phases consistent with the calculations of the GEMS module for that time increment.

### 11.3.4 Function

The EVOLVER module keeps a running record of the volume fraction of each phase and an updated list of all lattice sites that lie on an interface between phases. The different interfaces are categorized by the phases that they separate. During a given time increment, EVOLVER uses kinetic equations (Parrott and Killoh 1984) to determine the boundary conditions on the pore solution elemental composition. These boundary conditions are passed to the GEMS module, which returns a list of target volume fractions for the system at the end of that time increment. For each phase, EVOLVER compares the current volume fraction with the target

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<sup>3</sup> Conventional cement chemistry notation is used here, e.g., C = CaO, S = SiO<sub>2</sub>, and H = H<sub>2</sub>O.

volume fraction calculated by the GEMS module for that same time increment. The volume fractions are adjusted accordingly by modifying the phase identification numbers at selected points along the interface of each phase to simulate either growth or dissolution of the phase.

### 11.3.5 Subordinates

EVOLVER contains subroutines for sorting the lists of interface sites according to various criteria, generically termed affinities. It also contains subroutines for modifying the interface sites depending on whether growth or dissolution of a given phase is required. These subroutines are all internal to the EVOLVER module.

### 11.3.6 Dependencies

The EVOLVER module depends on the GEMS module to provide a list of phase volume fractions during each time increment subject to the boundary conditions on the elemental composition of the pore solution that the EVOLVER module provides to the GEMS module.

### 11.3.7 Interface

The EVOLVER module has no user interface. It accesses the GEMS module during each time increment to retrieve an updated list of phase volume fractions, but this is internal to the program.

### 11.3.8 Resources

EVOLVER requires no external resources. It requires an input file, as ASCII text, that provides information on the growth morphology of each phase, which is used to determine the rules for modifying the phase identification numbers at interface sites to achieve different morphologies.

### 11.3.9 Processing

The EVOLVER module operates directly on the 3-D lattice that is output by the GENMIC module, as depicted in Figure 1. During each time step, EVOLVER computes the surface area of each phase, degree of saturation of the capillary pore volume, and the local environment of each lattice site (i.e., the phases occupying itself and its nearest neighbors) to generate a list of interfaces and a list of potential growth and dissolution sites of each phase sorted by the affinity of the site, which depends on the phase and the local environment of the interface site. The interface sites are stored as vectors, which are standard containers in the C++ Standard Template Library (STL). Microstructure evolution is accomplished by changing the state (phase) of selected lattice sites according to the sorted lists of growth/dissolution sites. A degree of random deviation from the sorted list is allowed for each phase. That is, each growing phase has a finite probability that it may grow at a site other than that at which it attains maximum affinity. As mentioned earlier, the affinity at each interface site is determined from user-specified growth morphology types. The possible morphology types are:

- (1) Driven by decreasing mean curvature; dissolution occurs at sites of highest mean curvature and growth occurs at sites of lowest mean curvature. This produces compact, equiaxed growth morphologies.
- (2) Random; growth or dissolution occurs with equal probability at any location along the existing interface. This produces a compact morphology with considerable surface roughness.
- (3) Driven by increasing mean curvature. This produces compact but non-equiaxed shapes and can be tailored to produce either acicular or tabular morphologies.



The inputs required by the EVOLVER module are given in Table 3.

### 11.3.10 Data

There are no major internal data elements in EVOLVER.

### 11.3.11 Descriptions of Required External Databases and Programs

No external databases or programs are required besides those listed in the Resources section.

**Table 3. Input parameters for EVOLVER module**

| Input Property                     | Meaning  | Other Information  |
|------------------------------------|--|--|
| Initial microstructure file        | 3-D cubic lattice populated with integers identifying the phases   | Output from GENMIC module, header contains the x, y, and z dimensions of the lattice and the lattice spacing                           |
| Lattice spacing                    | Physical distance between lattice points   | Units of $\mu\text{m}$   |
| List of phase IDs                  | Phases: Saturated porosity, alite, belite, tricalcium aluminate, etc.  | Typical values 0, 1, 2, ..., catalogued in a phase database (db) file, must coincide with values used to create initial microstructure |
| Phase densities                    | Mass per unit volume   | Units of $\text{g}/\text{cm}^3$ , catalogued in a phase db file; value from cemdata07 GEMS db  |
| Phase molar volumes                | Volume occupied by one mole of phase   | Units of $\text{cm}^3/\text{mol}$ , catalogued in a phase db file; value from cemdata07 GEMS db  |
| Growth “templates” for each phase  | A list of phases (integer IDs) upon which a precipitating phase can favorably grow   | Used for determining nucleation sites for new phases; catalogued in a phase db file  |
| Affinities for each pair of phases | Empirical integer factors; represents rankings of interface free energies  | Catalogued in a phase db file  |
| Random growth factor               | Real-valued parameter that gives probability that a growing phase can grow at a site other than the site having maximum affinity for the phase | Real number on [0,1]   |
| Target volume fractions            | Output from GEMS module at each time step, gives the equilibrium volume fraction of each phase at a given time step                            | Used to determine how many lattice sites need to change state to cause updated microstructure to agree with target volume fractions    |
| Output frequency                   | How often to output the microstructure lattice in the form of an ASCII file  | Units of hours   |

### 11.3.12 Verification and Validation

The THAMES module is used to simulate the development of microstructure in a hydrating cement paste. It has not been verified or validated at any

significant level. However, the verification and validation procedure for THAMES on OPCs will be identical to that used for verifying and validating NIST’s CEMHYD3D model (Bentz 1997). The experimental data used to validate CEMHYD3D are

extensive and cover a wide range of OPCs with differing phase distributions, alkali contents, w/c ratios, powder finenesses, and curing conditions (Bentz 1995, Bentz 1997; Bentz and Remond 1997; Bentz, Snyder and Stutzman 1997; Bentz and Feng 2000; Bentz 2005; Bentz 2006; Bullard and Stutzman 2006). These same data sets will be used to systematically verify and validate the THAMES module on OPCs. Further validation work will be needed for cements containing slag, fly ash, or Saltstone. Such testing may reveal that modifications are required in the code to better capture the growth morphology of hydration products, but most of the anticipated modifications will need to be made in the thermodynamic database for the GEMS module.

### 11.3.13 Summary of Model Limitations

EVOLVER currently simulates only hydration and microstructure evolution of ordinary Portland cement binders. It is not yet able to simulate the effects of slag, fly ash, or other waste stream materials on the hydration and microstructure development, although this limitation is due primarily to limitations in the cemdata07 database used by GEMS. At this time, EVOLVER cannot directly simulate degradation mechanisms such as alkali-silicate reactions (ASR), sulfate attack, chloride ingress, or freeze-thaw cycling, nor the initiation/evolution of damage associated with those degradation phenomena. However, it could be extended to capture these phenomena with sufficient research and development.

EVOLVER has no intrinsic limitations on the size or resolution of its computational domain, i.e., the lattice. These limitations are set by the memory capacity of the computer. On a single processor desktop computer, cement paste microstructures with

up to 500 lattice sites in each dimension can typically be simulated, although the execution time will scale with the number of lattice sites to the 2/3 power. Parallel versions of THAMES, which have not yet been developed, could work with larger systems and/or have significantly faster run times.

The current kinetic module for cement hydration was originally developed by Parrott and Killoh for OPC pastes (Parrott and Killoh 1984) and provides empirical equations for the rate of dissolution of the major clinker phases as a function of water-cement mass ratio (w/c), cement fineness as measured by the Blaine air permeability test, and temperature. This kinetic model will not be applicable in cement blends containing ground granulated blast furnace slag (GGBFS) or fly ash.

## 11.4 Program Element 4: CONCPROPS

### 11.4.1 Identification

The name of the element is CONCPROPS, which is descriptive of its task of calculating the resultant properties of concrete materials.

### 11.4.2 Type

CONCPROPS is one of four modules in THAMES.

### 11.4.3 Purpose

The CONCPROPS module operates directly on the 3-D lattice that is output by the EVOLVER module at prescribed times, as depicted in Figure 1. It calculates engineering properties, such as linear elastic moduli, compressive strength, and DC conductivity of concrete materials made from the cementitious binders simulated by the THAMES program.

#### 11.4.4 Function

The CONCPROPS module is a collection of models developed at NIST for calculating the effective (composite) mechanical and transport properties of cement paste, mortar, or concrete, based on the microstructure of the cement paste binder. Using the 3-D lattice microstructure output from EVOLVER at a particular age, the CONCPROPS module adopts the same lattice as a finite element/finite difference mesh to calculate the effective linear elastic moduli,

compressive strength, or effective DC conductivity/diffusivity. The finite element models use a conjugate gradient method to minimize energy of the lattice subject to imposed boundary conditions, e.g., applied strain or concentration gradient, and then uses computation of the mean values of the material response, e.g., elastic stress field or diffusive flux, to infer the effective linear property of the composite. Table 4 lists the input parameters required by the CONCPROPS module.

**Table 4. Input parameters for CONCPROPS module**

| Input Property                      | Meaning   | Other Information  |
|-------------------------------------|---|--|
| Cement binder microstructure        | 3-D lattice of hydrated cement microstructure output from THAMES module.  | ASCII text file  |
| List of phase IDs                   | Phases: Pore solution, alite, belite, tricalcium aluminate, etc   | Typical values 0, 1, 2, ..., catalogued in a phase database (db) file, must coincide with values used to create initial microstructure |
| Phase elastic moduli                | File listing the bulk and shear modulus of each phase in the hydrated cement paste  | ASCII text file. All moduli given in GPa units   |
| Phase relative conductivities       | File listing the DC conductivity of each phase in the hydrated cement paste, normalized to the conductivity of bulk pore solution | ASCII text file. All quantities are dimensionless  |
| Fine aggregate grading              | Given as a sieve distribution, between 0.01 mm and 4.5 mm, in terms of mass fraction retained at each size.                       | Two-column ASCII text file, with first column as a sieve opening in mm, and the second column as the mass fraction retained            |
| Coarse aggregate grading            | Given as a sieve distribution, between 4.75 mm and 100 mm, in terms of mass fraction retained at each size.                       | Two-column ASCII text file, with first column as sieve opening in mm, and the second column as the mass fraction retained              |
| Fine aggregate elastic moduli       | Bulk and shear modulus of the aggregate particles   | GPa units  |
| Coarse aggregate elastic moduli     | Bulk and shear modulus of the aggregate particles   | GPa units  |
| Fine aggregate shape distribution   | Pointer to collection of SH coefficients for different shapes   | SH coefficients for each shape stored in a separate ASCII file   |
| Coarse aggregate shape distribution | Pointer to collection of SH coefficients for different shapes   | SH coefficients for each shape stored in a separate ASCII file   |

### 11.4.5 Subordinates

The CONCPROPS module consists of several subordinate programs, each of which is responsible for calculating a different engineering property. The program `elastic` calculates the effective linear elastic moduli and compressive strength of the concrete. It uses a finite element model of the cement binder microstructure (subroutine `cpelas`) to compute the linear elastic moduli of the binder. These moduli are then used in a calculation (subroutine `concelas`) based on differential effective medium theory (D-EMT) to compute the linear elastic moduli of the concrete (including coarse and fine aggregate components as well as air voids). The linear elastic moduli of the concrete are used to estimate the compressive strength of a cube of the material using an empirical relation (Neville 1973).

The program `dc3d` calculates the effective DC conductivity of the cement paste binder, relative to the conductivity of bulk solution of the same composition. The program solves the Laplace equation using a finite difference method. It requires input of the transport factor (i.e., the inverse of the formation factor) of each phase present in the cementitious binder.

For calculations of cement paste permeability, a Stokes solver called `Permsolver` reads the 3-D digital image of the hydrated microstructure and calculates the flow response to a fluid pressure head as a boundary condition. The program requires input of the permeability of each phase present in the cementitious binder.

### 11.4.6 Dependencies

The CONCPROPS module has no dependencies on any other module in THAMES.

### 11.4.7 Interface

The CONCPROPS module currently is operated as a collection of separate programs, each of which is executed from the command line.

### 11.4.8 Resources

CONCPROPS requires no external resources.

### 11.4.9 Verification and Validation

The CONCPROPS module incorporates a number of models developed at NIST, many of which have been extensively validated on OPCs in recent years (Garboczi and Bentz 1992; Christensen, Mason, Bentz, and Garboczi 1992; Bentz, Detwiler, et al 1997; Bentz, Garboczi, Haecker, and Jensen 1999; Bentz, Jensen, Coats, and Glasser 2000; Garboczi and Berryman 2000; Haecker et al 2005). These models have not been systematically validated on blended cements with waste-stream materials. Such validation will need to be made.

### 11.4.10 Summary of Model Limitations

The CONCPROPS module for calculating cement and concrete properties currently is limited to calculations of linear elastic moduli (for cement paste, mortar, or concrete), thermal expansion coefficients (for cement paste, mortar, or concrete), compressive strength (semi-empirical estimates for mortar or concrete), DC conductivity/diffusivity (for cement paste, mortar or concrete), and permeability (for cement paste only). When new materials (e.g., fly ash, slag, or other waste stream materials) are added to cementitious binders, their individual elastic moduli will need to be measured experimentally before the CONCPROPS module can make accurate calculations using them.

## 12 SUMMARY AND CONCLUSIONS

Both the current state and development needs of THAMES have been described. The complete THAMES software includes a module for generating a representative 3-D initial microstructure (GENMIC), a module for simulating microstructure changes (THAMES) guided by thermodynamic calculations (GEMS), and a module for calculating the elastic moduli, compressive strength, DC conductivity/diffusivity, and permeability on the predicted cement paste and mortar/concrete microstructure (CONCPROPS).

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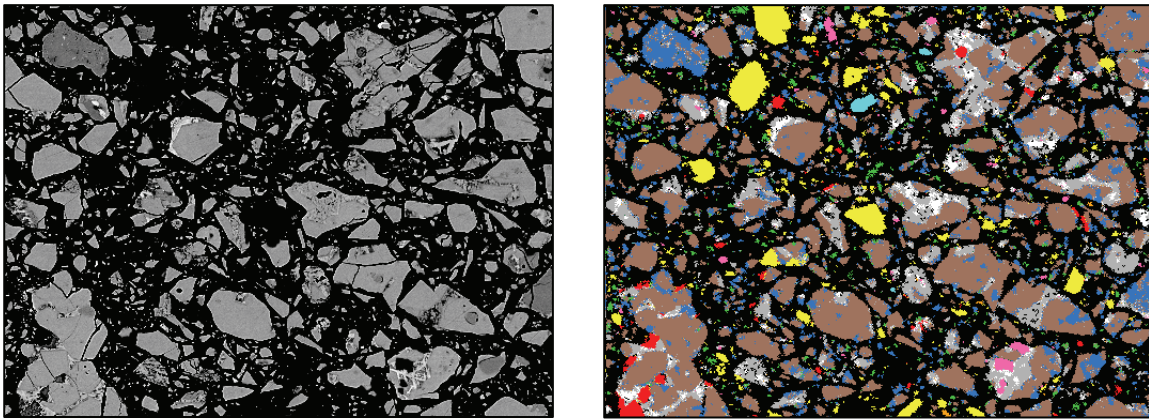
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## APPENDIX A. NECESSARY MATERIAL CHARACTERIZATION TECHNIQUES

Although not technically within the scope of a detailed description of the THAMES modeling software, reference is briefly made to the important experimental measurements and characterization techniques required to obtain the necessary input for the GENMIC and CONCPROPS modules.

The usual methods of cement mineralogy characterization involve oxide analysis via X-ray fluorescence and then estimation of phase abundance via the Bogue calculations (Taylor 1997). The Bogue calculations are notoriously inaccurate, especially for the minor clinker phases. Fortunately, these methods are gradually being supplemented with quantitative X-ray diffraction techniques based on the Rietveld method (Stutzman & Leigh 2007). However, even the quantitative XRD techniques do not give any information about how the phases are arranged in each particle, only bulk averages. Therefore, particle-level characterization of cements (Stutzman & Leigh 2000; Bentz & Stutzman 1994; Stutzman 2004) is also required because the average spatial distribution of different clinker phases affects their reaction rates. Fly ashes and other multi-phase mineral admixtures need to be characterized in this way as well (Chancey et al. 2008; Williams et al. 2005). To understand how different mineral admixtures react together with cement over time, in hydration, and in degradation, it is very important to have detailed characterization of their mutual reactions (Feng et al. 2004). This particular interaction will be important to obtain at later ages in the CBP work, as well as more general mineral interactions over lifetimes of 100 years to 1000 years.



**Figure 2.** A polished back-scattered scanning electron micrograph of cement particles embedded in epoxy (left). The false colors in the image at the right are added based on analysis of the X-ray signals given off in the back-scattered electron process. Each color (except black) corresponds to a different mineralogical phase. Some examples are yellow = gypsum, brown = tricalcium silicate, and blue = dicalcium silicate.

There is no standard method of cement particle shape analysis, though some recent work addresses this issue (Bentz et al. 2006, Garboczi 2002; Taylor et al. 2006, Holzer et al. 2008; Erdoğan et al. 2008). Cement particle shape is probably not very important at later ages, where most of the cement has already dissolved and

reacted (Garboczi & Bullard 2004; Bullard & Garboczi 2005). Aggregate shape and chemistry, however, significantly affect concrete properties. Aggregate shape plays a major role in fresh concrete rheology and early age mechanical properties (Douglas & Garboczi 1995), and at later ages, aggregate chemistry plays a major role in the resistance to degradation processes such as alkali-silica reactions. Both shape and chemistry need to be characterized, and the current characterization tests (e.g., ASR) are inadequate in that they often cannot distinguish between “good” performers and “bad” performers at fairly early ages (before six months). At the kind of ages required in the CBP work, 100 years to 1000 years, it is possible that aggregates that pass the usual earlier-age tests will still cause ASR problems at these long ages because they are exposed to different ionic species from the contained waste material. The proposed THAMES model does not address aggregate reactions. But the CBP concrete modeling, which will derive from THAMES, must be able to handle aggregates in some way, although not necessarily in a full 3-D manner. Some of the reference cases that will be addressed by the CBP work do not necessarily have aggregates, i.e., waste forms and grout.

## **APPENDIX B. HISTORICAL DEVELOPMENT OF CONCRETE MICROSTRUCTURE MODELS**

This Appendix is presented to provide a better appreciation of the importance of accounting for the microstructure of cement-based materials using a brief historical account of the microstructure modeling of concrete. In particular, this Appendix highlights the theoretical foundations of microstructure modeling and the important breakthroughs in understanding and performance prediction that have been made possible by microstructure modeling approaches.

The first computer model of cement hydration and chemistry was described in an article entitled “The Mathematical Simulation of Chemical, Physical and Mechanical Changes Accompanying the Hydration of Cement” (Frohnsdorff et al. 1968). In this first effort, there was an attempt to very carefully model kinetics, but there was no 3-D microstructural information and no property prediction. A more successful model of this type, with a more diligent effort to empirically predict a wide range of properties but still including no 3-D microstructure calculation, has been extensively described (Parrott 1989).

While Parrott’s model was in the final development stage, efforts turned to the problem of how to model the complex 3-D microstructural formation of cementitious materials. In 1981, Frohnsdorff at NIST led a successful effort to secure internal, multi-year funding for cement hydration and eventually concrete modeling research. This team effort resulted in a tricalcium silicate-only model (where tricalcium silicate is the main constituent of Portland cement) that could generate a 3-D microstructure upon which a limited number of property calculations could be made (Jennings & Johnson 1986). This model, however, contained almost no thermodynamics and kinetics. Particles of various sizes that followed a real cement particle size distribution were dispersed randomly in 3-D. Various rules were applied to these continuum spherical particles to simulate the dissolution of cement and the growth of hydration products. This model has inspired other work in the Netherlands (Ye, van Bruegel & Fraai 2003), Japan (Maekawa, Ishida & Kishi 2003), and Switzerland (Navi & Pignat 1991; Bishnoi & Scrivener 2008). The model is based on a continuum description of particles (e.g., spheres), so inherently it can do only a limited job of modeling the real, random, complex nature of cement paste microstructure. Overcoming these limitations to accommodate more realistic chemistry, microstructure, and property computations required a different point of view and had three intellectual roots.

The work on the structure of amorphous semiconductors like silicon and germanium in the 1960’s and 1970’s was the first root. Physicists had previously developed crystal physics to a high degree and had even allowed for crystal defects like dislocations. However, the problem of amorphous semiconductors, or of glass, was entirely different—there was no underlying crystal lattice. How was it possible to do any calculations at all? Analytical approximations were tried, with only a limited degree of success (Zallen 1983). Then models were built with several hundred atoms linked into a random network, pushing the limits of computing power at the time (Dean 1972). Algorithms were applied to these models to compute properties, which were then compared to experimental results in an attempt to explain the results.

The second root occurred in the 1980’s. In 1984 and 1985, Wittmann, Roelfstra, and Sadouki published two important papers on the numerical simulation of the structure and properties of concrete in 2-D (Wittmann,

Roelfstra & Sadouki 1984; Roelfstra, Sadouki & Wittmann, 1985). In these papers, 2-D models were developed for simulating the shape and arrangement of aggregates in concrete with finite elements applied to compute properties like thermal conductivity and elastic moduli.

The third root of the new modeling point-of-view was a paper showing how a random walk algorithm could be applied to models of porous materials to compute electrical and diffusive transport (Schwartz & Banavar 1989). The combination of the ideas of random walks, digital images, the application of finite elements to random structures, and the existing cement paste hydration microstructure development model (Jennings & Johnson 1986) led directly to the first NIST digital-image-based cement paste hydration model, which eventually became CEMHYD3D (Bentz 1997). Since CEMHYD3D was built on a digital lattice, almost any finite element or finite difference algorithm could be readily applied to it, so that almost any physical property could be simulated and compared to experimental results. Having a 3-D model with some chemistry and a 3-D microstructure, and being able to realistically compute properties, gave rise to the computational materials science of concrete.

The current state of computational materials science of concrete at NIST, which involves the computation of many other properties including microstructure formation via cement hydration, is embodied in the Virtual Cement and Concrete Testing Laboratory (VCCTL) (Bentz et al. 2006), which is being developed at NIST with the active cooperation of leading corporations and associations in the concrete field. Computer power and model effectiveness have grown together over the years so that this large, integrated software package can be designed to mimic a complete physical testing laboratory, with databases of cement and aggregates instead of bins and hoppers, material combination and concrete curing models instead of mixers and molds, a software interface instead of a cart to take materials and samples around the laboratory, and accurate models for performance prediction instead of instrumented testing machines.

# **DETAILED DESCRIPTION OF THE GOLDSIM INTEGRATING PLATFORM SELECTED FOR THE CBP PROJECT**

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## **LIST OF ACRONYMS AND ABBREVIATIONS**

|           |   |
|-----------|---|
| ASCII     | American Standard Code for Information Interchange            |
| BLT-MS    | Breach, Leach, and Transport-Multiple Species                 |
| BNL       | Brookhaven National Laboratory                                |
| CBP       | Cementitious Barriers Partnership                             |
| CT        | Contaminant Transport   |
| DUST-MS   | Disposal Unit Source Term-Multiple Species                    |
| DLL       | Dynamic Link Library  |
| D&D       | Decontamination and Decommissioning                           |
| GTG       | GoldSim Technology Group                                      |
| GUI       | Graphical User Interface                                      |
| LHS       | Latin Hypercube Sampling                                      |
| LLW       | Low-Level radioactive Waste                                   |
| NRC       | U.S. Nuclear Regulatory Commission                            |
| ODBC      | Open Database Connectivity                                    |
| ORCHESTRA | Objects Representing CHEmical Speciation and TRANsport models |
| PPA       | Probabilistic Performance Assessment                          |
| RT        | Radionuclide Transport  |
| SNL       | Sandia National Laboratories                                  |
| VB        | Visual Basic  |

# Detailed Description of the Integrating Platform Selected for the CBP Project – GoldSim

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The goal of the Cementitious Barriers Partnership (CBP) is to develop a reasonable and credible set of tools to predict the structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over extended time frames (e.g., >100 years for operating facilities and >1000 years for waste management). The simulation tools will be used to evaluate and predict the behavior of cementitious barriers used in near surface engineered waste disposal systems including waste forms, containment structures, entombments, and environmental remediation. These cementitious materials are exposed to dynamic environmental conditions that cause changes in material properties via (i) aging, (ii) chloride attack, (iii) sulfate attack, (iv) carbonation, (v) oxidation, and (vi) primary constituent leaching. A set of state-of-the-art software tools has been selected as a starting point to capture these critical aging and degradation phenomena. Through the CBP, conceptual models and computational tools will be developed or modified to improve the assessment of long-term structural, hydraulic, and chemical performance of cementitious materials.

Characterizing properties and understanding the mechanistic behavior of cementitious barriers is necessary to evaluate and improve system designs. Uncertainty reductions require coupling multi-scale and multi-physics processes, including physical-chemical evolution and transport phenomena applied to heterogeneous materials with changing boundary conditions. The selected codes will be coupled using a GoldSim probabilistic simulation framework. Uncertainty evaluation will be included with simulations at both the phenomenological and integrated system level.

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## 1 OVERVIEW

GoldSim (Version 10) is a graphical, object-oriented computer program running under Microsoft Windows for executing dynamic, probabilistic

simulations<sup>1</sup>. GoldSim is a "visual spreadsheet" allowing the user to visually create and manipulate data and equations including links to external

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<sup>1</sup> Simulation is defined here as the process of creating a model (i.e., an abstract representation) of a system to identify and understand those factors which control the system and/or to predict future behavior (GTG 2009d).

programs and databases (GTG 2009d). Although GoldSim can be run deterministically, one of its key features is to quantify and assess uncertainties through the use of probabilistic analysis.

GoldSim was designed to be flexible and has been used to simulate various types of systems including (GTG 2009d):

- **Strategic Planning:** Simulate the implementation of a complex undertaking by describing the tasks involved, precedents, durations and costs, and events that could impact the process. The output might be the probability of success, and the results could be used to identify potential problems that might arise and to design contingency plans.
- **Ecology:** Simulate the growth of a group of animals by describing the initial number of animals, the birth and death rates, the migration rate, etc. The output would be the number of animals in the group as a function of time and could be used to better manage the system to stabilize or increase the population.
- **Environment:** Simulate the performance of a hazardous waste site by describing initial conditions and the processes acting on the system. The output would be the contaminant concentrations around the site as a function of time and could be used to design remedial measures to minimize environmental impacts.
- **Reliability Engineering:** Simulate the reliability of a proposed satellite system by describing the components of the system and the processes and events which could compromise the system's integrity and lead to downtime or failure. The outputs, which include the predicted reliability of the system and the probabilities and consequences of failures, could be used to modify the design to maximize reliability and to minimize the probabilities and/or consequences of failures.
- **Manufacturing:** Simulate the coupled dynamics of a manufacturing supply chain by defining the "links" in the chain and how these links interact. The output would be the movement of materials through the supply chain and could be used to identify ways in which the system could be modified to operate more efficiently.

GoldSim was also designed to readily incorporate additional modules (i.e., extension modules) to address specialized problems. These extension modules are (GTG 2009d):

- **Financial Module:** Simulates financial systems including accounts and funds, investments, options, projects, or undertakings with specified cash flows and insurance policies.
- **Contaminant Transport Module:** Consists of ten specialized elements representing contaminant species, transport media, transport pathways, contaminant sources, and receptors and the coupled differential equations describing these systems.
- **Radionuclide Transport Module:** A premium version of the Contaminant Transport Module that contains additional specialized features (e.g., first-order decay with daughters and source term elements) designed to facilitate simulation of radioactive waste disposal facilities and the fate and transport of radionuclides in the environment (GTG 2009a).
- **Reliability Module:** Simulate the reliability of complex engineered systems over time by providing the ability to model the interdependence of components through requirements and fault trees and to define multiple independent failure modes for each component.
- **Dashboard Authoring Module:** Allows the user to design and construct interfaces to look like "dashboards" or "control panels" with buttons, gauges, sliders, and display panels.



- **Distributed Processing Module:** Allows multiple computers to be used (linked over a network such as a LAN or even the Internet) to carry out probabilistic simulations of a system.

Although GoldSim was designed to be a flexible tool to simulate systems, there are limitations depending on how the program will be used. Only certain types of functionality are built into GoldSim (e.g., input, expression, stock and delay, and linking) and its extension modules. As examples, the transport functions available in the GoldSim extension modules are one-dimensional in nature, and sensitivity analysis features are limited to one-at-a-time type analyses. The user may create their own functionality by using built-in functional forms or calling external programs. However, user-supplied external functions may not fully integrate with built-in features of GoldSim. For example, if external programs related to transport are used, then the ability to assure that the system material balance is maintained may be compromised.

The various objects with which a GoldSim model is constructed are referred to as *elements*. *Elements* represent the basic building blocks of the simulation. Some elements provide mechanisms for entering data into the model as illustrated in Table 1. Functional elements operate on one or more inputs to produce outputs as presented in Table 2. The stock and delay elements that are critical for representing dynamic behavior are provided in Table 3.

A special set of function elements (as shown in Table 4<sup>2</sup>) can be used to link GoldSim models to external applications including Microsoft Excel spreadsheets and other applications outside of GoldSim using Dynamic Link Libraries (DLL's) (GTG 2009d). Because much of the functionality needed for the

CBP tools is available in existing codes (including ORCHESTRA, LeachXS™, STADIUM®), the ability to link a GoldSim model to external codes using the function elements in Table 4 is likely to be critical. These elements are described in additional detail in the sections to follow.

Another special set of function elements is available to superimpose the occurrence and impacts of discrete events onto continuously varying systems (GTG 2009d). These elements are enumerated in Table 5. Delay elements (as shown in Table 6) provide the ability to impart inertia and memory to a system by delaying (and optionally dispersing) continuous and discrete signals or flows (GTG 2009d).

The result elements shown in Table 7 provide a mechanism to collect and display simulation results for subsequent analysis (GTG 2009d).







## **1.1 Contaminant Transport/ Radionuclide Transport Module**

The Contaminant Transport (CT) and Radionuclide Transport (RT) Modules provide specialized elements (as summarized in Table 8) for representing contaminant species, transport media, transport pathways, contaminant sources, and receptors as well as the coupled sets of differential equations underlying these systems. By linking these environmental elements together (and integrating them with GoldSim's basic elements), both simple and complex contaminant transport simulations can be developed. The RT Module is a premium version of the CT Module and contains additional, specialized features including first-order decay with daughter products and Source term elements.



















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<sup>2</sup> One additional GoldSim element that provides external linking capability, the External\_Pathway, is summarized in Table 8. This element is only available if the Reliability Module is included.

**Table 1. Overview of GoldSim Input Elements (GTG (2009d))**





| Input Element      | Default Symbol  | Browser Icon  | Function   |
|--------------------|---|---|--|
| Data               |  |  | Defines scalar, vector, or matrix data.                                |
| Time Series $f(t)$ |  |  | Accepts time histories of data and converts them for use in the model. |
| Stochastic         |  |  | Defines uncertain data using probability distributions.                |

**Table 2. Overview of Selected GoldSim Function Elements (GTG (2009d))**







| Function Element* | Default Symbol  | Browser Icon  | Function   |
|-------------------|---|---|--|
| Expression        |    |    | Defines mathematical or logical expressions.   |
| Previous Value    |   |   | Returns the value of the specified input from the previous model update.                         |
| Extrema           |  |  | Calculates the highest or lowest value for the specified input.                                  |
| Selector          |  |  | Defines expressions with nested if...then...else type logic.                                     |
| Splitter          |  |  | Splits the incoming signal into multiple outputs based fractions specified by the user.          |
| Allocator         |  |  | Allocates an incoming signal into multiple outputs given user-specified demands and priorities.  |
| Lookup Table      |  |  | Defines a one-, two-, or three-dimensional lookup table (e.g., representing a response surface). |
| Convolution       |  |  | Solves a convolution integral.   |
| History Generator |  |  | Generates stochastic time histories based on specified statistics.                               |

\* Function elements are also available in GoldSim to facilitate summation operations (i.e., Sum element) and perform logical operations (i.e., AND, OR, and NOT elements).















**Table 3. Overview of GoldSim Stock Elements (GTG (2009d))**

| Stock Element | Default Symbol  | Browser Icon  | Function   |
|---------------|---|---|--|
| Reservoir     |  |  | Integrates flows of materials (while conserving mass) within specified upper and lower bounds. |
| Integrator    |  |  | Integrates values.   |



**Table 4. Overview of GoldSim External Linking Elements (GTG (2009d))**

| External Linking Element | Default Symbol   | Browser Icon  | Function   |
|--------------------------|--|---|--|
| External (DLL)           |   |  | Dynamically links to a user-specified external function (compiled as a Microsoft Windows Dynamic Link Library or DLL). |
| Spreadsheet              |   |  | Dynamically links to an Excel spreadsheet.   |
| File                     |  |  | Dynamically copies a file to a specified directory (for use by External elements).                                     |









**Table 5. Overview of GoldSim Discrete Event Elements (GTG (2009d))**

| Discrete Event Element | Default Symbol  | Browser Icon  | Function   |
|------------------------|---|---|--|
| Timed Event            |  |  | Generates discrete event signals using the specified rate of occurrence regularly, or randomly according to a specified distribution.          |
| Triggered Event        |  |  | Generates discrete event signals using one or more specified conditions.   |
| Decision               |  |  | Generates one of up to three defined discrete event signals using user-specified conditions.   |
| Random Choice          |  |  | Generates a user defined discrete event signal using specified probabilities.  |
| Milestone              |  |  | Records the simulation time at which a particular event or specified condition(s) occurs.  |
| Status                 |  |  | Generates a condition (i.e., True or False) in response to particular events or specified conditions.  |
| Discrete Change        |  |  | Generates a discrete change signal (i.e., a value) that can discretely modify the values of other elements (e.g., Integrators and Reservoirs). |









**Table 5. Overview of GoldSim Discrete Event Elements (Contd)**

| Discrete Event Element | Default Symbol  | Browser Icon  | Function   |
|------------------------|---|---|--|
| Interrupt              |  |  | Interrupts a simulation when a specified event or condition occurs and displays a user-defined message and/or writes the message to the run log. |

**Table 6. Overview of GoldSim Delay Elements (GTG (2009d))**

| Delay Element         | Default Symbol  | Browser Icon  | Function   |
|-----------------------|---|---|--|
| Material Delay        |  |  | Delays (and optionally disperses) material flows.                              |
| Information Delay     |  |  | Delays (and optionally disperses) a signal.                                    |
| Event Delay           |  |  | Delays a discrete event signal (Table 5). Can also be used to simulate queues. |
| Discrete Change Delay |  |  | Delays a discrete change signal (Table 5).                                     |

**Table 7. Overview of GoldSim Result Elements (GTG (2009d))**

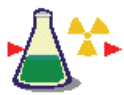













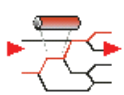


| Result Element      | Default Symbol  | Browser Icon  | Function   |
|---------------------|---|---|--|
| Time History Result |  |  | Displays time history results.   |
| Result Distribution |  |  | Displays probability distributions.  |
| Multivariate Result |  |  | Displays multivariate results (i.e., scatter plots, correlation tables, and raw data). |
| Array View          |  |  | Displays vectors and matrices of results.  |

## 1.2 Reliability Module



The Reliability Module is an extension to GoldSim that allows the probabilistic simulation of the reliability and performance of complex engineered systems over time (GTG 2009c). The primary

outputs are predicted reliability metrics (e.g., reliability and availability) for the overall system as well as for components within the system. The probabilities for specific consequences that are often needed to support risk analysis can be predicted. The specific elements included with the Reliability Module are provided in Table 9.

**Table 8. Overview of Contaminant/Radionuclide Transport Elements (GTG 2009a; GTG 2009d)**

| CT/RT Element              | Default Symbol  | Browser Icon  | Function  |
|----------------------------|---|---|---|
| Species                    |    |    | Describes the chemical constituents that may undergo chemical reactions and transport. Species can behave independently or either as part of a reaction/decay chain or as isotopes of the same chemical element.  |
| Fluid                      |    |    | Describes one of the two environmental media available in GoldSim. By default, water is included as the Reference Fluid. Other fluids can be added by specifying diffusivities and either solubilities or partition coefficients for the species in the model.  |
| Solid                      |    |    | Describes the other environmental medium available in GoldSim. Properties include bulk density, porosity, tortuosity, and partition coefficients.   |
| Cell_Pathway               |    |    | Represents partitioning, solubility limits, and mass transport (i.e., advection, diffusion, direct transfer, treatment, and precipitate removal) processes* in what is mathematically equivalent to a mixing cell.  |
| Pipe_Pathway               |    |    | Represents a feature that behaves as a fluid conduit. Unlike Cell pathways, Pipe pathways can contain only a single fluid medium; however, they contain solid media that impact transport (e.g., by modifying porosity and/or acting to sorb and retard species).**   |
| External_Pathway           |  |  | Provides a mechanism by which external contaminant transport modules (e.g., analytical, finite element model, or finite difference model) can be directly integrated into GoldSim. These modules are linked into GoldSim as DLL's (Dynamic Link Libraries) at run time.   |
| Network_Pathway            |  |  | Provide a computationally efficient way to simulate large, complex networks of one-dimensional conduits to describe contaminant transport through fractured systems†. A Network pathway is composed of multiple “pipes” where each pipe has the features and capabilities of Pipe pathways.   |
| Fracture_Set               |  | <b>fs</b>   | Identifies the transport properties (e.g., infill material, coating material, properties of matrix diffusion zones) of the pipes in a Network pathway.  |
| Source<br>(RT Module Only) |  |  | Provides one means of introducing mass into the system. Properties consist of 1) the failure rate of any barriers (e.g., drums or boxes) which must fail before species are released and 2) the degradation rate of any matrix (e.g., cement or grout) in which contaminants are bound, which must degrade before the species are released. |

**Table 8. Overview of Contaminant/Radionuclide Transport Elements (Contd)**





| CT/RT Element | Default Symbol  | Browser Icon  | Function   |
|---------------|---|---|--|
| Receptor      |  |  | Computes impact of contaminants on specific receptors (e.g., humans, wildlife, flora, etc.) by multiplying concentrations in environmental media (e.g., water, soil, air) by user-defined impact conversion factors. |

\* When multiple Cell elements are linked via advective and diffusive transport, the behavior of the resulting network, which is equivalent to a finite difference network of nodes, is mathematically described using a coupled system of differential equations. The coupled system is solved numerically as a function of time (GTG 2009a).

\*\* A Laplace transform approach is used to analytically solve a broad range of advectively-dominated transport problems involving one-dimensional advection, longitudinal dispersion, retardation, decay and ingrowth, and exchanges with immobile storage zones (e.g., matrix diffusion) (GTG 2009a).

† GoldSim uses a Laplace transform algorithm to solve complex fracture networks efficiently.

**Table 9. Overview of GoldSim Reliability Elements (GTG 2009c; GTG 2009d)**

| Reliability Element | Default Symbol  | Browser Icon  | Function   |
|---------------------|---|---|--|
| Function_Element    |   |   | Used to model components (e.g., pumps, engines, etc.) that operate continuously once turned on.                  |
| Action_Element      |  |  | Used to represent components (e.g., switches, relays, etc.) that must respond to a control command or condition. |

## 2 EXPLANATION OF CONCEPTUAL MODELS AND THEORY

A simulation is an abstract representation of a system including simplifications based on those aspects assumed to be important and omitting those considered nonessential so as to obtain predictions in an efficient manner (GTG 2009e). For real world systems, there will also be significant uncertainties regarding controlling processes and the parameter values needed to describe those processes. The most important factor impacting the accuracy is the degree to which the conceptual model captures reality and the degree to which uncertainty in the system has been represented (GTG 2009e).

In real world systems, uncertainties in predictions that result from uncertainties in processes and parameters will likely be far greater than inaccuracies introduced by the numerical solution method. As a result, it is generally more worthwhile to spend time ensuring that the model captures the key aspects of the system rather than evaluating the numerical accuracy of the solution methods (GTG 2009e).

However, it is important to understand the nature of inaccuracies that can arise from the numerical approximations used to ensure that these remain relatively small. The primary numerical factors

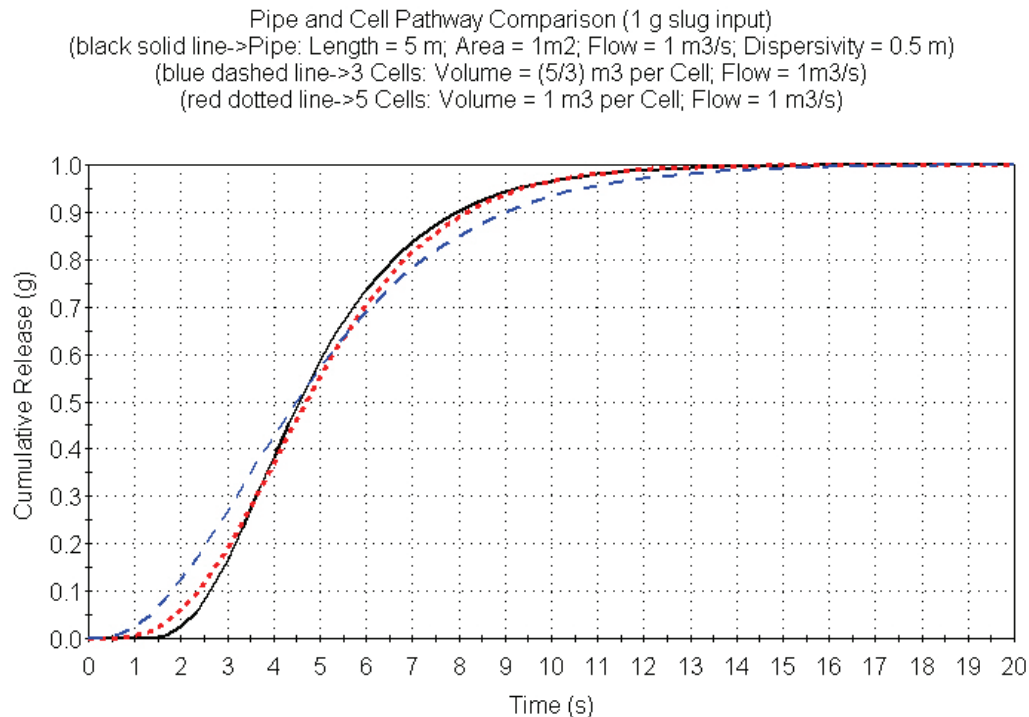
affecting the accuracy of GoldSim models are (GTG 2009e):

- **Integrating Differential Equations:** GoldSim solves differential equations by numerically integrating them (via Stock and Delay elements). This numerical integration is the largest potential source of numerical inaccuracies in a model.
- **Solving Coupled Equations:** A model may include coupled equations or coupled differential equations, which can be computationally-intensive to solve. GoldSim provides fast and accurate solution techniques for certain types of coupled systems (e.g., Cell elements linked via advective and diffusive transport mechanisms) (GTG 2009a). In other cases, coupled equations must be solved approximately using Previous Value elements, which can introduce numerical approximations on the same order as those

introduced from numerical integration of ordinary differential equations.

- **Representing Discrete Events:** Discrete events may occur that impose discontinuous changes onto the system. Superimposing discontinuities onto a continuously-varying system that must be discretized in time can introduce inaccuracies. GoldSim provides a powerful time-stepping algorithm for accurately representing these systems (GTG 2009a).

Other numerical approximations may arise when GoldSim elements are used to create a discrete analogue to a continuous system. For example, a string of Cell elements can be used to approximate solute transport in a continuum that could otherwise be represented using a Pipe element as illustrated in Figure 1. The series of Cell elements is equivalent to



**Figure 1. Comparison of breakthrough curves for a simple one-dimensional pathway using both a single Pipe and series of Cell elements**



a finite difference numerical scheme and exhibits similar numerical dispersion. However, these numerical approximations are managed outside the GoldSim computational kernel itself (although using built-in elements) and are a function of how the modeler uses GoldSim to abstract a physical process.

## **2.1 Primary Numerical Approximations in GoldSim**

Two of the more influential types of errors will be examined as examples of how these errors can be managed in GoldSim. These errors are those introduced using the built-in GoldSim integration method and the errors introduced by approximations needed to solve coupled equations.

### **2.1.1 Numerical Integration Algorithm**

The integration method used in GoldSim is referred to as *Euler integration* (GTG 2009e), which is the simplest and most common numerical integration method for a dynamic process. The key assumption is that the rate is constant over a timestep, which is reasonable if the timestep is sufficiently small<sup>3</sup>. An example of the integration error as a function of the selected timestep is illustrated in Figure 2 for first-order decay (that requires use of a Previous Value element as described in Table 2). As can be seen, the method is reasonably accurate for smaller timesteps. An integration error of several percent may be acceptable when compared to uncertainties in initial conditions, parameters, and conceptual model. Generally, a timestep should be selected that is 1/3 to 1/10 of the timescale of the fastest process simulated in the model (GTG 2009e).

Although the Euler integration method is simple and often used, other more computationally efficient methods are available that can achieve better accuracy with a larger timestep (e.g., Runge-Kutta or variable timestep methods) (GTG 2009e). These methods are not used in GoldSim because:

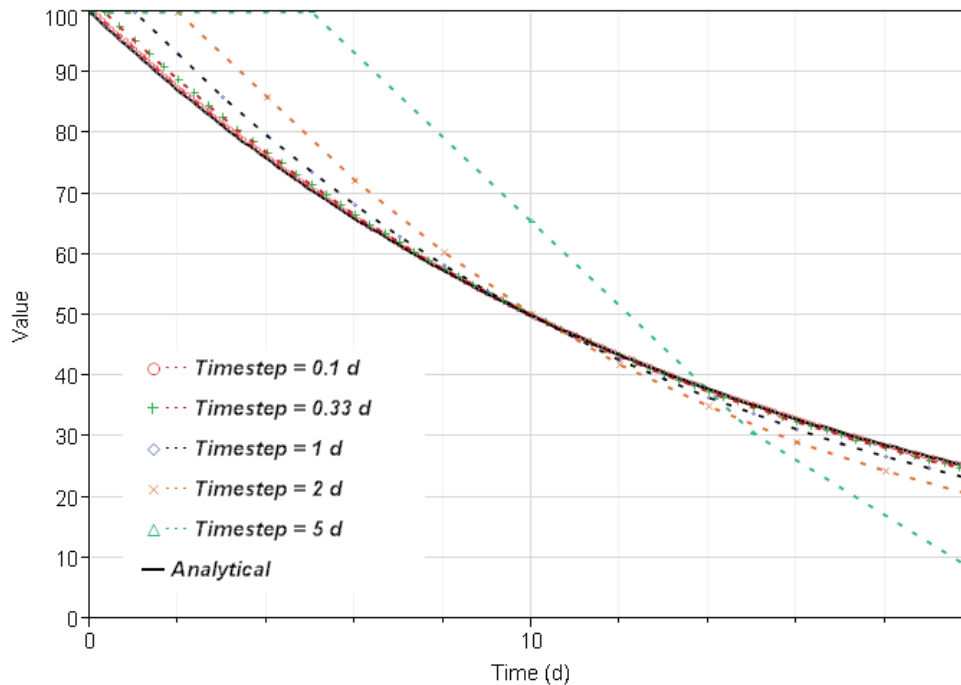
- Higher-order methods are most useful when simulating systems in which the mathematical model, initial conditions, and input parameters are precisely known and small integration errors can be problematic. Often the kinds of systems simulated using GoldSim can be handled effectively using Euler integration (GTG 2009e).
- Higher-order methods work best for continuously-varying systems but are less appropriate for systems impacted by discontinuities. GoldSim provides algorithms for accurately superimposing discontinuities onto a continuously-varying system that are incompatible with higher-order integration methods (GTG 2009e).
- For some systems, GoldSim has algorithms to accurately solve nonlinear coupled differential equations by dynamically adjusting the timestep during the simulation (GTG 2009e). These algorithms are incompatible with higher-order integration methods.

In cases where a small timestep is required to maintain accuracy, Containers with Internal Clocks can be used to locally define a much smaller timestep (than elsewhere in the system) in a computationally efficient manner.

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<sup>3</sup> The magnitude of the integration error depends on the model itself (GTG 2009e). In stable models dominated by negative feedback (and thus tend to equilibrium), errors tend to decrease with time. However, unstable systems that increase exponentially or oscillate with no damping tend to accumulate errors over time. For these latter systems, a very small timestep may be required to accurately simulate the system.





**Figure 2. GoldSim Integration Error for First-Order Decay as a Function of Time for Selected Timesteps (after GTG (2009e))**

### 2.1.2 Approximate Solutions to Coupled Equations

In some situations, there may be static or dynamic processes in which the variables are coupled such that they respond to each other with no time lags. In GoldSim, these interactions can be handled in one of two ways. The system of equations can be solved directly either prior to running the model (via substitution) or dynamically while running the model (e.g., using an External element). However, for many complex models, the solution could be very computationally intensive. GoldSim offers the alternative of solving the system approximately and iteratively using Previous Value elements (GTG

2009e)<sup>4</sup>.

## 3 HARDWARE AND SOFTWARE REQUIREMENTS

GoldSim runs on personal computers using either 32-bit or 64-bit Microsoft Windows operating systems (i.e., Windows 2003 Server, Windows XP, or Windows Vista) (GTG 2009e). The user must have Administrative Privileges. A minimum of 200 MB of disk space is required during installation with 100 MB in the target directory and 40 MB of free space in Common Files folder. A minimum of 16-bit color depth is required (although 32-bit is recommended).

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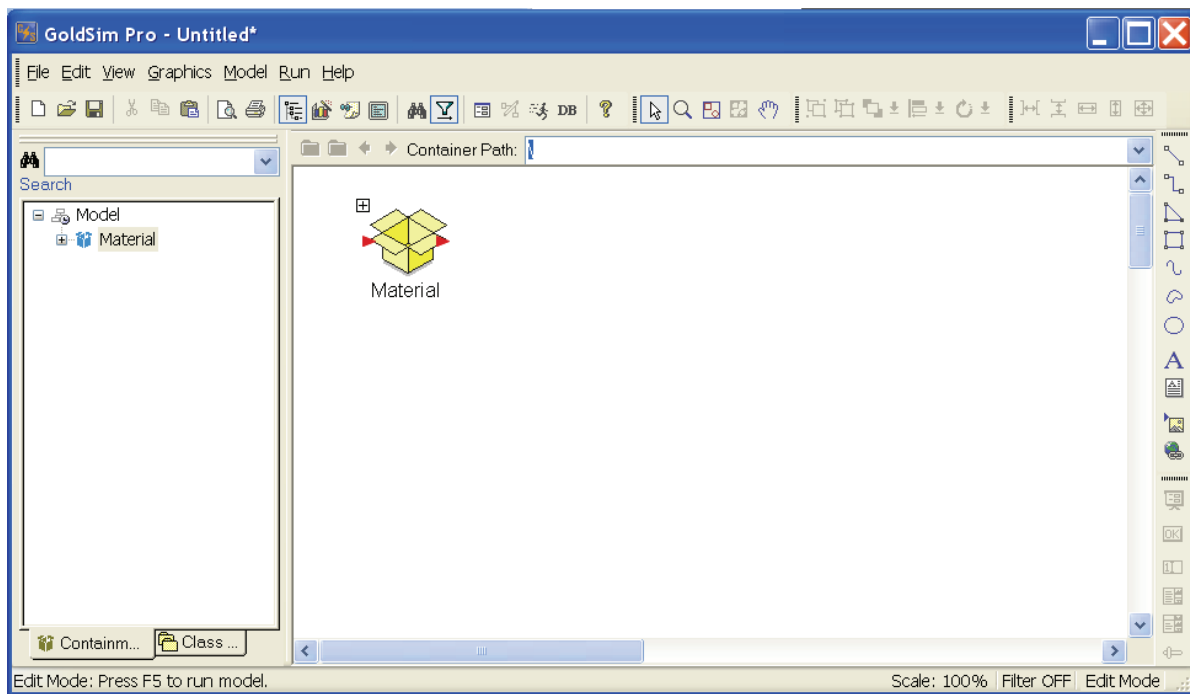
<sup>4</sup> A Previous Value element allows referencing the previous value of an output from the previous timestep.

## 4 PROGRAM EXECUTION MODE(S) AND USER/PROGRAM INTERFACE INFORMATION

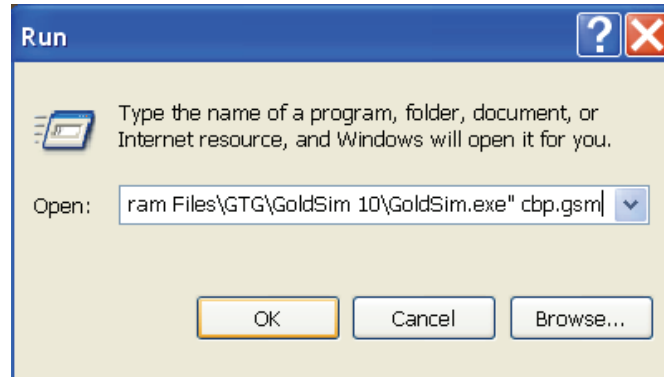
GoldSim can be operated both using its Graphical User Interface (GUI) and via the command line. The primary GoldSim user interface is shown in Figure 3. The graphics pane, which occupies the largest area of the screen, is where the model is depicted graphically and, for most users, is where most model building and manipulation is executed (GTG 2009d). The browser displays the GoldSim model either hierarchically (by containment) or by element type. The menu bar provides menus from which most GoldSim operations can be performed. The toolbars

provide buttons for common GoldSim actions and for adding graphical images to your models. The appearance of the interface can be customized by the user.

While GoldSim models are typically constructed, tested, and executed using the graphical interface shown in Figure 3, models can also be executed from the command line. This execution is done by selecting **Run** from the Windows **Start** menu as shown in Figure 4 (GTG 2009d). The primary reason for running GoldSim in this manner is to take advantage of specific command line parameters, placed after the filename, that control GoldSim execution. Selected command line parameters are described in Table 10.



**Figure 3. The GoldSim Graphical User Interface (GUI)**



**Figure 4. Running GoldSim from the Command Line**

**Table 10. Selected GoldSim Command Line Parameters and Typical Uses (GTG 2009d)**

| Parameter | Description  | Comments   |
|-----------|--|--|
| -c <name> | Opens the GoldSim application and jumps to the Container specified by <name>.            | Used to immediately display the contents of a specific Container (other than the Root Container) when opening. |
| -r        | Opens the GoldSim model and immediately runs the simulation.                             | GoldSim automatically skips the “Ready” state and starts the simulation.                                       |
| -rx       | Opens GoldSim, immediately runs the simulation, saves the GoldSim file, and then closes. | This mode is useful if you want to “stack” a set of simulations in a batch file.                               |
| -s        | Opens the GoldSim model in Slave Mode.   | Used when running models over a network using GoldSim’s distributed processing features (GTG 2009b).           |

## 5 SYSTEM PERFORMANCE

The performance of a GoldSim model is a function of the complexity of the model itself including interactions, number of realizations, external calls, network processing, and the capabilities of the host computer(s). GoldSim does supply a number of features to improve the efficiency of models including (GTG 2009d):

- a dynamic time-stepping algorithm to accurately solve non-linear, coupled differential equations

(e.g., those associated with mass and heat transport),

- an importance sampling algorithm to modify the conventional Monte Carlo approach to sample high-consequence, low-probability outcomes at a higher frequency, and
- the capability to use multiple computers linked via a network to perform probabilistic simulations, which greatly facilitates the evaluation of highly complex systems (GTG 2009b).

## **6 INPUT DATA DESCRIPTION**

Input elements are used to provide the basic inputs to a GoldSim model. Three basic types of input elements are available (GTG 2009d):

- A Data element allows a single scalar value or an array of values with the same units to be specified.
- A Time Series element allows a time series to be specified for a parameter.
- A Stochastic element allows an uncertain parameter to be represented by defining its probability distribution.

Additional information for the input elements was provided in Table 1.

GoldSim can also import data from spreadsheets (using a Spreadsheet element) or input elements can be linked directly to an ODBC-compliant database (GTG 2009d). GoldSim can be instructed to download the data at any time and will internally record the time and date at which the download occurred, providing a mechanism for quality control of input data. User-supplied Dynamic Link Libraries (DLL's) can also be used to provide input information to the GoldSim simulation.

## **7 OUTPUT DESCRIPTIONS**

Some elements have a single output and others, such as the Stochastic element, have multiple outputs (GTG 2009d). One of the outputs is usually denoted the primary output for the element, and the other outputs are referred to as secondary outputs. The name of the primary output for an element is the same as the name of the element itself. Therefore, output names are important because links are created

by referencing the name of the output of one element in an input field of another element.

All element outputs in GoldSim have three output attributes (GTG 2009d):

- Type: The type can be either a value or a condition where values can be any real number and conditions are either true or false.
- Order: The order of an output can be scalar, vector, or matrix.
- Dimensions: Outputs (of values) can be assigned dimensions that can be displayed in any units.

Output attributes are important because GoldSim also uses them to ensure dimensional consistency between inputs and outputs when elements are linked together. For those with programming experience, this would be analogous to a programming language which is strongly-typed (GTG 2009d).

Typically, information is transferred between GoldSim elements (via links) continuously. However, to propagate discrete events (and consequences) between model elements, it is necessary to send information between elements intermittently as a "spike" or discrete "packet" of information (GTG 2009d). GoldSim allows certain elements to emit and receive discrete signals (Table 5), which are a special category of outputs that emit information discretely rather than continuously. The result elements shown in Table 7 provide a mechanism to collect and display simulation results for subsequent analysis.

In some cases, rather than using the plotting and post-processing capabilities provided by GoldSim (Table 7), it may be useful to plot, analyze, or store results using a separate program, such as a spreadsheet, a database, or statistical analysis package. GoldSim provides three methods for exporting results in an ASCII or binary file, an MS-Excel file, or an Access database file:

- **Exporting Results to a Text File, Binary File or Database.** The Results Export Wizard can be used to export results (i.e., timesteps, realizations, and elements) to one of three formats (an ASCII file, a binary file, or an Access database file).
- **Exporting Time Histories from a Time History Result Element.** Outputs including time history data and probability histories that are specified within a Time History Result can be exported to an MS-Excel spreadsheet file or an ASCII text file. The export can be set to occur automatically at the end of a simulation or manually while in Result Mode.
- **Exporting Results Using a Spreadsheet Element.** Any output can be exported to an MS-Excel spreadsheet using a Spreadsheet element. Using the built-in capabilities of the Spreadsheet elements, time histories and/or multiple realizations can be output automatically during the simulation.

## 8 DETAILED EXAMPLE(S)

GoldSim is commercial Monte Carlo simulation software for dynamically modeling complex systems (GTG 2009d; GTG 2009e). The GoldSim software has been used in many applications including modeling environmental, business, and engineered systems<sup>5</sup>. 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. Detailed examples for both types of models were provided in

*Survey of Integrating Programs and Code Structures Previously Applied to Environmental Assessments.*

The examples provided in this section relate to the external linking abilities of GoldSim, which are considered crucial to the use of GoldSim for the CBP.

### 8.1 SNL Coupled GoldSim-BLT-MS Software Package

GoldSim can be used as an integrating framework from which existing, external programs can be called and their results dynamically coupled into a 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) 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<sup>6</sup>. The BLT-MS code (which provides point-value estimates) was coupled with GoldSim to create a framework for

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<sup>5</sup> Examples of the types of problems to which GoldSim has been applied are listed at <http://www.goldsim.com/> (accessed October 1, 2008).

<sup>6</sup> 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).

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 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 allow the code to be coupled with GoldSim (Mattie, Knowlton & Arnold 2007).

Figure 5 illustrates a highly simplified conceptual model describing how a point-value relationship (or, in this case, the BLT-MS model) can be 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<sup>7</sup>.

The conceptualization illustrated in Figure 5 typically oversimplifies the analysis of uncertainties in predicted human health risks because (Brown 2008):

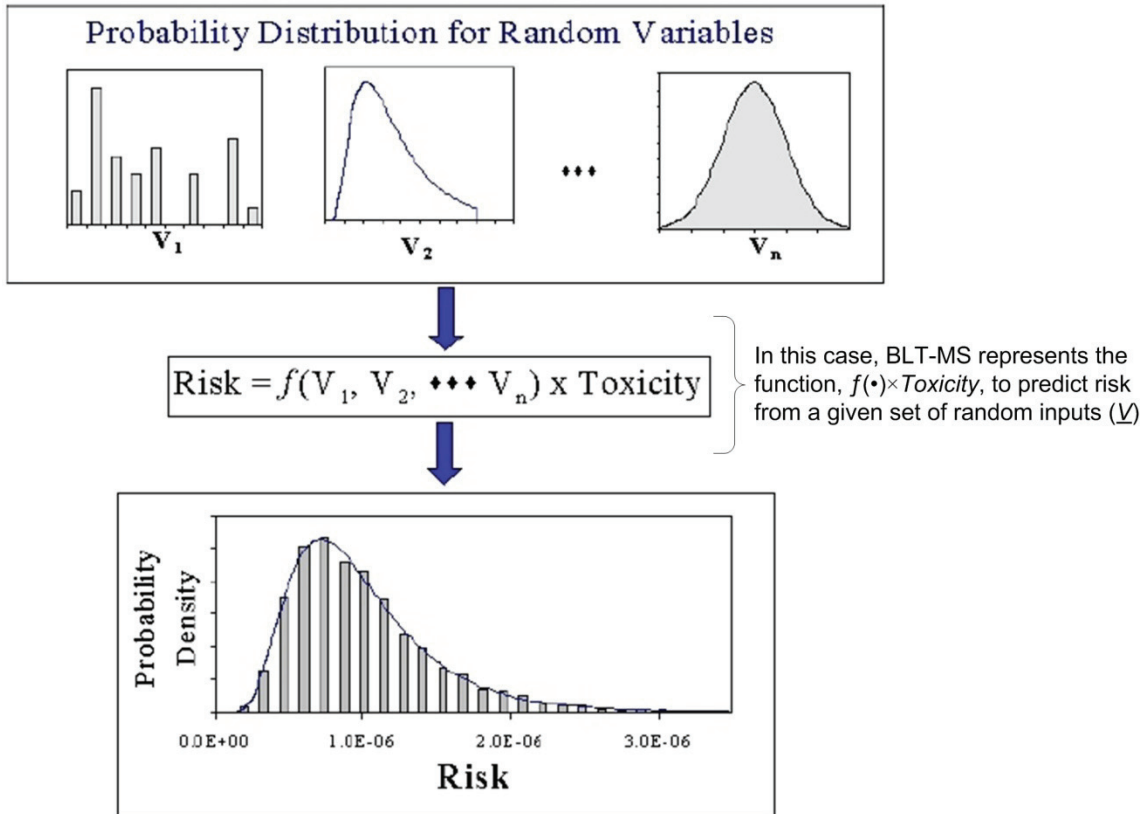
- Probabilistic exposure analysis is performed (i.e., toxicity is fixed and is often overly conservative<sup>8</sup>), not probabilistic risk analysis.
- To be more accurate, uncertain parameters should be separated into those that are stochastic and those that are variable, and then a two-dimensional Monte Carlo simulation should be 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 risk distribution estimates.

The parameters that are considered fixed versus those that are considered uncertain in the GoldSim-BLT software package are listed in Table 11.

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<sup>7</sup> Haldrar 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 standard Monte Carlo analysis (GTG 2009d; GTG 2009e).

<sup>8</sup> 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 5. Conceptual model of a Monte Carlo risk analysis (reproduced from USEPA (2001)). Random variables ( $V_1, V_2, \dots, V_n$ ) are characterized by probability distributions. A point-value risk is predicted for each set of random values—in this case, the BLT-MS code is used. Repeated sampling results in the distribution of risk.**

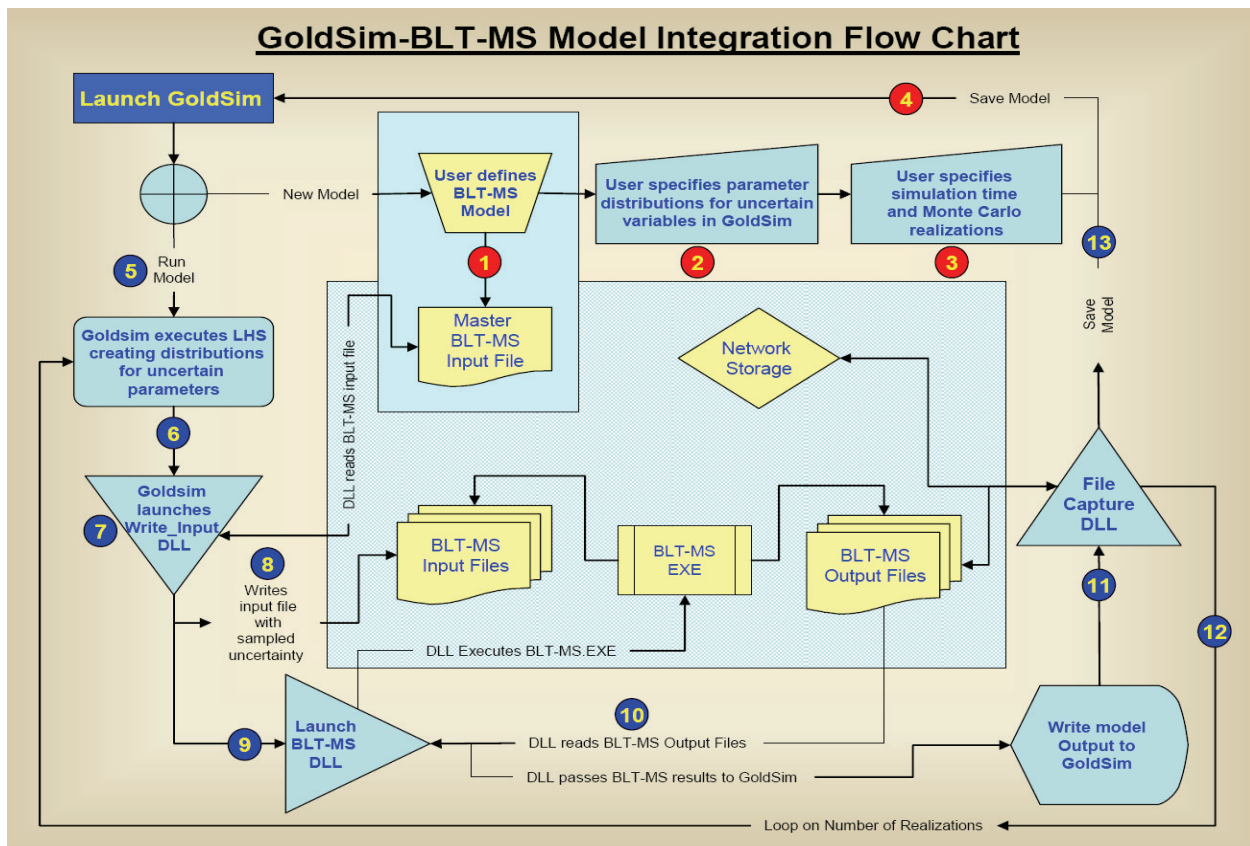
**Table 11. Examples of fixed and uncertain parameters in the GoldSim BLT-MS Integrated Software Package (Mattie, Knowlton & Arnold 2007)**

| 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 (BCs) 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  |   |



A conceptual model of how to apply Monte Carlo to risk analysis was illustrated in Figure 5. The manner in which the BLT-MS program is coupled with GoldSim to provide probabilistic risk analysis for candidate low-level waste (LLW) disposal sites is summarized in Figure 6 (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 6). Then in GoldSim, the user (2) specifies the uncertain parameters, 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



**Figure 6. Flow Chart for GoldSim/BLT-MS Integration Model (reproduced from Mattie et al. (2007)).**



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 2009b), 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.

This example demonstrates a successful integrated software solution using the external model linkage capabilities in the GoldSim software and the techniques used to facilitate this process using legacy applications, including Breach, Leach, and Transport-Multiple Species (BLT-MS) (Mattie, Knowlton & Arnold 2007). The subsurface low-level waste disposal facility used in the original example was meant for the preliminary assessment of potential low-level waste repository sites in Taiwan. However, the software can be modified to model site specific conditions for assessments of other potential low-level radioactive waste repositories (Mattie, Knowlton & Arnold 2007).

## **8.2 Linking Geochemical Codes to GoldSim**

Many environmental applications, including those related to the CBP, may involve consideration of complex geochemical processes. Although GoldSim can be used to solve mass transport equations and model simple chemical reactions, GoldSim cannot solve complex geochemical problems using built-in functionality. However, it is possible to link GoldSim to geochemical equilibrium codes (such as PHREEQC (Parkhurst & Appelo 1999)) to achieve

this effect<sup>9</sup>. Situations where linking GoldSim to a geochemical model may be useful include (Eary 2007c):

- **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.

Four examples will be provided that illustrate the various manners in which GoldSim can be linked to PHREEQC to solve problems involving complex geochemical processes.

### **8.2.1 Indirect Linkage between GoldSim and PHREEQC using a Lookup Table Element**

This example shows an approach to linking a GoldSim model to a geochemical model (PHREEQC) through an indirect method using a GoldSim "Lookup Table" element as illustrated in Figure 7 (Eary 2007a). A Lookup Table element (which acts as a response surface or surrogate model in one, two, or three independent variables (GTG 2009d)) is initially constructed using results from a series of PHREEQC model runs covering the expected range of compositions. The Lookup Table can be constructed manually in GoldSim, or, for a 3-D table, the information can be directly imported as a text file.

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<sup>9</sup> Please refer to <http://www.goldsim.com/Content.asp?PageID=505> (accessed on July 1, 2009).

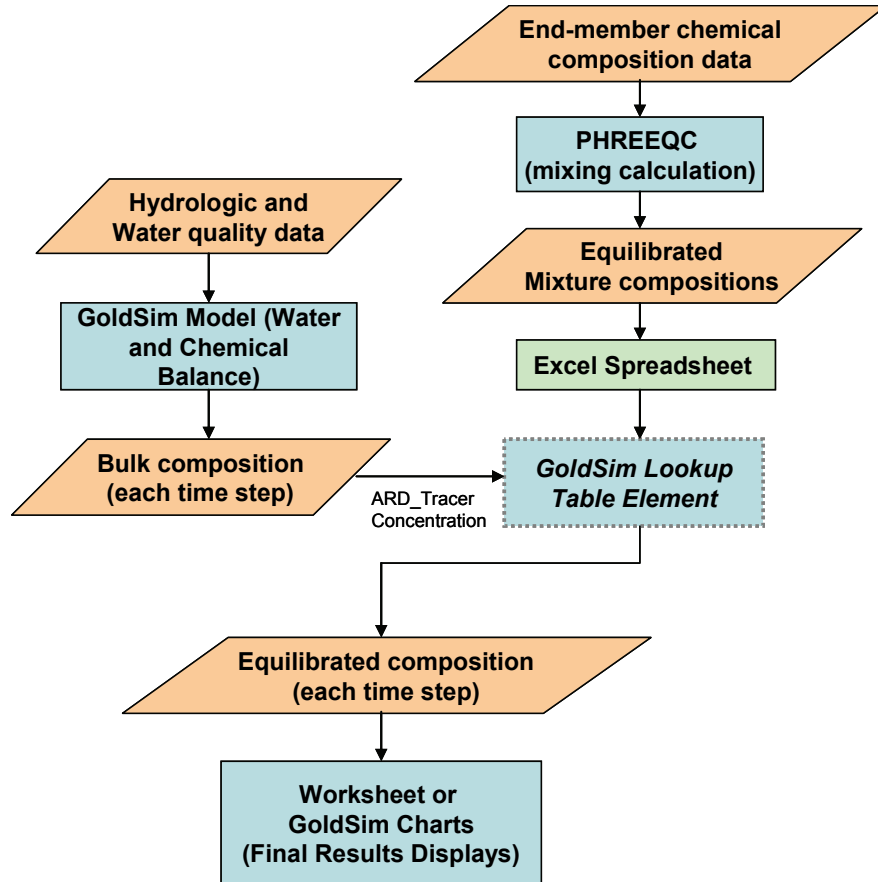
This method provides a starting point for creating more complex GoldSim models where linkage to a geochemical model is needed. This approach requires more time at the start because of the need for a detailed conceptualization of the geochemical processes and the development of the surrogate model. However, the approach is simple and fast computationally.

The mixture in the GoldSim model is not at equilibrium with respect to various geochemical reactions (Eary 2007a). The PHREEQC geochemical

model is used to equilibrate the mixture external to GoldSim by making a PHREEQC model run that produces equilibrated chemical compositions as a function of the fraction of a fixed input stream. These results are imported into an Excel spreadsheet file that is referenced in GoldSim Lookup Table element.

The approach can be summarized as follows (Figure 7) (Eary 2007a):

- 1) Compositions are defined for the necessary end-



**Figure 7. Schematic of data flow for the Lookup Table element method of indirect linkage between GoldSim and PHREEQC (reproduced from Eary (2007a)).**

member solutions. These compositions must be charge-balanced, which can be performed with PHREEQC.

- 2) The PHREEQC model is run for the range of mixture composition and set of desired equilibrium parameters. One method for defining the set of compositions that need to be evaluated to construct the Lookup Table (or response surface) is the use of orthogonal Latin hypercube (Ye 1998) or optimal, symmetric Latin hypercube designs (Ye, Li & Sudjianto 2000).
- 3) The PHREEQC results are then either 1) imported in an Excel spreadsheet referenced by the Lookup Table element or 2) copied directly into the Lookup Table element within the GoldSim model. Defining end-member solutions for either two- or three-dimensional solutions is straightforward; however, the system may have to be separated into parts adding some complexity.
- 4) The water balance model is constructed in GoldSim.
- 5) The chemical balance model is constructed using charge-balanced compositions for the end-member solutions using a GoldSim Cell element to mix the inflowing end-member solutions.

Advantages of linking PHREEQC to GoldSim using a Lookup Table include (Eary 2007a):

- This approach is applicable to both open and closed chemical systems.
- This approach is suitable for problems where two or more solutions are mixed in known fractions, which produces a new solution. It may also be applied to simple solubility-limited systems where a table of solubilities as a function of pH or other key component can be

defined.

- This approach provides the ability to model the effects of a large number of different types of chemical processes on solution compositions on a per time-step basis.
- This approach to describe equilibrium chemistry provides fast GoldSim models when compared to other approaches<sup>10</sup>.

The disadvantages of the approach include (Eary 2007a):

- It may require a large amount of time to develop a geochemical model that adequately represents all the processes potentially affecting solution compositions.
- It may require substantial effort to define the appropriate end-member solution compositions, especially if the compositions are time-dependent.
- An excellent working knowledge of PHREEQC is required.
- If more than three end-member solutions are needed (which can be directly represented using a GoldSim Lookup Table element), it may be a complicated task to divide the system into sub-parts that can be represented as mixtures of two or three end-member solutions.

### **8.2.2 Direct Linkage between GoldSim and PHREEQC through a Spreadsheet Element**

This example demonstrates linking a GoldSim model directly to a geochemical model (i.e., PHREEQC) through a GoldSim “Spreadsheet” element (Eary 2007b). This example provides a starting point for creating more complex GoldSim models where

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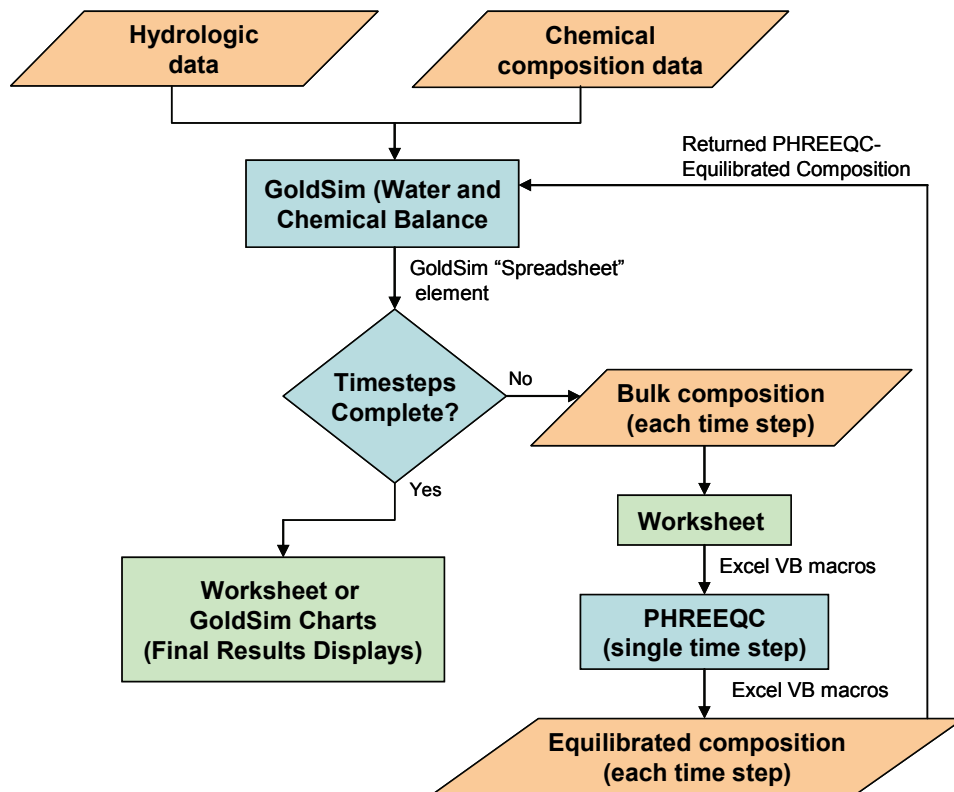
<sup>10</sup> The solution using a Lookup Table element for a five-year simulation with a daily step takes approximately 2 seconds of execution time compared to 10 minutes for the Direct-link Library (DLL) method described in the section entitled *Direct Linkage between GoldSim and PHREEQC using a DLL Element* on a laptop with a Pentium R 1.7 GHz processor with 515 MB RAM.

linkage to a geochemical model is needed. Data transfer among three applications (i.e., GoldSim, Excel, and PHREEQC) is illustrated in Figure 8.

The bulk solution in GoldSim is not in chemical equilibrium, and PHREEQC is again used to equilibrate the solution. This process is accomplished using an Excel spreadsheet as an intermediary between GoldSim and PHREEQC where the bulk chemical composition is sent to a spreadsheet through a Spreadsheet element at each time step (Eary 2007b). In the spreadsheet, custom code recognizes the event triggered by the export of data from GoldSim, and the event triggers the following sequence (Eary 2007b):

- 1) A new PHREEQC input file is created that contains the bulk chemical composition and user-defined equilibration parameters.
- 2) An asynchronous PHREEQC process is executed.
- 3) The operating system is polled to determine when the PHREEQC process has completed.
- 4) After the PHREEQC process executes, the PHREEQC results are imported into an Excel worksheet.
- 5) The resulting equilibrated composition is transferred to GoldSim through the Spreadsheet element.

Advantages of linking PHREEQC to GoldSim using



**Figure 8. Schematic of data flow for the Spreadsheet element method of direct linkage between GoldSim and PHREEQC (reproduced from Eary (2007b)).**

a Spreadsheet element include (Eary 2007b):

- The approach is applicable to open and closed chemical systems.
- This approach provides the ability to model the effects of a large number of different types of chemical processes on solution compositions on a per time-step basis.

The disadvantages of the approach include (Eary 2007b):

- The approach requires a large amount of time to define charge-balanced compositions if there are more than a few components.
- The approach requires a large amount of time to determine the most appropriate area in GoldSim to place the spreadsheet element used to communicate with PHREEQC.
- Times required to run the coupled model can be long because of the overhead associated with updating an Excel worksheet, creating a process to run PHREEQC, waiting for PHREEQC to execute, returning data to Excel from PHREEQC, and returning the equilibrated composition from Excel to GoldSim<sup>11</sup>.
- This approach has not been tested for models that require multiple links to PHREEQC per timestep or for real-world problems; thus the robustness of the method is still a question.

### **8.2.3 Direct Linkage between GoldSim and PHREEQC using a DLL Element**

This example involves coupling a complex geochemical code (in this case, PHREEQC) to GoldSim using the external linkage capability in GoldSim via a Dynamic Link Library (DLL)<sup>12</sup>. Figure 9 provides a schematic of how the PHREEQC

code can be coupled with GoldSim to perform geochemical calculations. Using this approach for other situations would require modification to the DLL and likely modification of the PHREEQC or other codes used for communication.

In running the GoldSim model, the bulk solution is not in chemical equilibrium, and the PHREEQC geochemical model is used to equilibrate the solution (Eary 2007c). The bulk compositions are transferred to PHREEQC via the DLL element as illustrated in Figure 9. The GoldSim DLL element takes the bulk composition and the PHREEQC input parameters stored in template file to build the necessary input file for PHREEQC. Routines in the DLL run PHREEQC, wait for its execution to complete, extract the equilibrated solution concentrations from the PHREEQC output, and transfer the solution concentrations back to GoldSim through the DLL element as a species vector (Eary 2007c).

Conceptually, this approach is similar to that used in the previous spreadsheet linkage example.

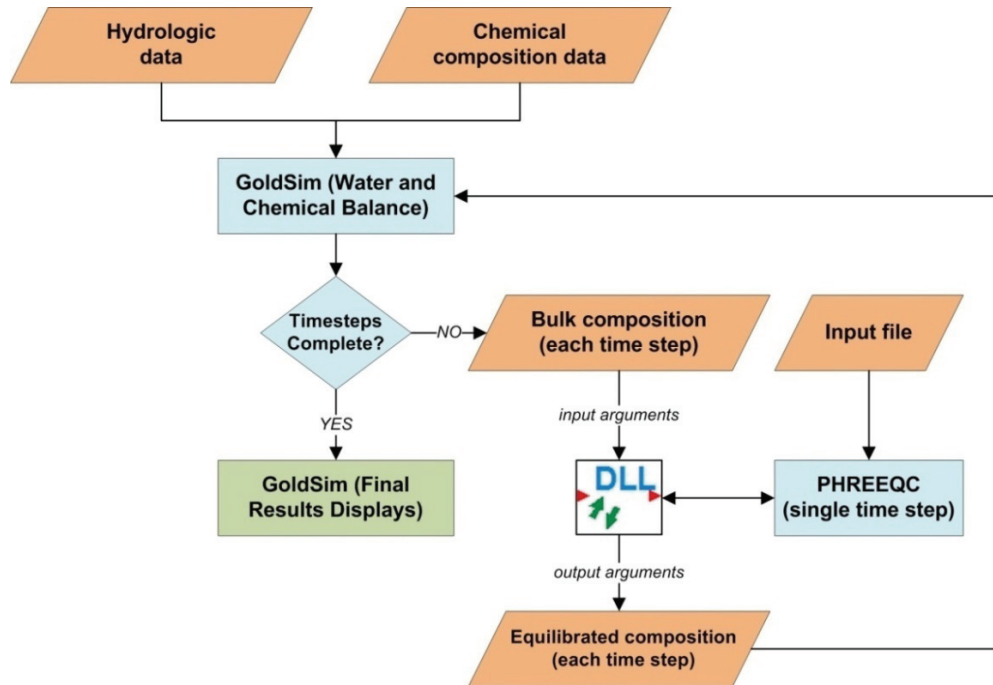
There are several considerations when determining whether or not a DLL should be used to couple a geochemical model to GoldSim for a particular modeling problem (Eary 2007c). Advantages of this approach include (Eary 2007c):

- applicability to multiple chemical systems with careful development of the conceptual model,
- the 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 because the need for a spreadsheet as an intermediary is eliminated.

---

<sup>11</sup> As a benchmark, on a laptop with a Pentium R 1.7 GHz processor with 515 MB RAM, a 1-year model run with a 1-day time step takes about 2 minutes (Eary 2007b).

<sup>12</sup> Other examples are provided at [www.goldsim.com](http://www.goldsim.com) coupling the PHREEQC geochemical code to GoldSim using either a Lookup table or spreadsheet.



**Figure 9. Schematic of data flow for the method of direct linkage between GoldSim and PHREEQC using a Dynamic Linked Library (DLL) (adapted from Eary (2007c)).**

Disadvantages of using a DLL to couple a geochemical code to GoldSim include (Eary 2007c):

- requiring 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
- requiring a working knowledge of C++ to modify and rebuild the DLL code for different modeling scenarios and species lists.

## 9 PROGRAM STRUCTURE

Complex models may require numerous subroutines or components (i.e., hundreds or thousands of elements in GoldSim terms). To organize such a model, it is often useful to group components into

modules or subsystems. In GoldSim a subsystem is simply a collection of elements in a Container, which is simply a "box" into which elements are placed (GTG 2009d).

Containers can be nested to any desired degree. The ability to organize a model hierarchically provides a powerful tool for creating "top-down" models where the level of detail increases as one drills down into the hierarchy (GTG 2009d). An example of a system that has been divided into a number of distinct subsystems using Containers is illustrated in Figure 10. The ability to create hierarchical models, coupled with GoldSim's powerful documentation and presentation capabilities, allows models to be developed and explained at appropriate levels of detail to different audiences (GTG 2009d).



## 10 DETAILED EXPLANATION OF COMPUTATIONAL ALGORITHMS AND METHODS

The primary elements and uses in the GoldSim software were summarized in the *Overview* Section, especially Table 1 through Table 9. Most of the computational methods underlying the elements (e.g., input, summation, allocation, results, etc.) are straightforward and do not require detailed explanations. The purpose of GoldSim in the context of the CBP is as an integration tool where existing codes or surrogate models for existing code will be coupled. Therefore, the primary features of GoldSim that will be used for CBP are the elements that allow coupling GoldSim to external codes (e.g., Lookup Table, Spreadsheet, DLL, File, and External\_Pathway elements). These are described in

detail in the next section.

However, there are a number of elements (i.e., Cell, Pipe, and Network Pathway in the Contaminant / Radionuclide Transport Modules) that may provide useful functionality when developing the CBP tools. The computational algorithms underlying these additional elements are described in detail in Appendix B of the *GoldSim Contaminant Transport Module User's Guide* (GTG 2009a).

## 11 DETAILED EXPLANATIONS OF PROGRAM ELEMENTS OR ENTITIES

The GoldSim program uses various types of built-in elements as well as those available in “add-in” modules. The most important elements in the context of the CBP are those that can be used to couple

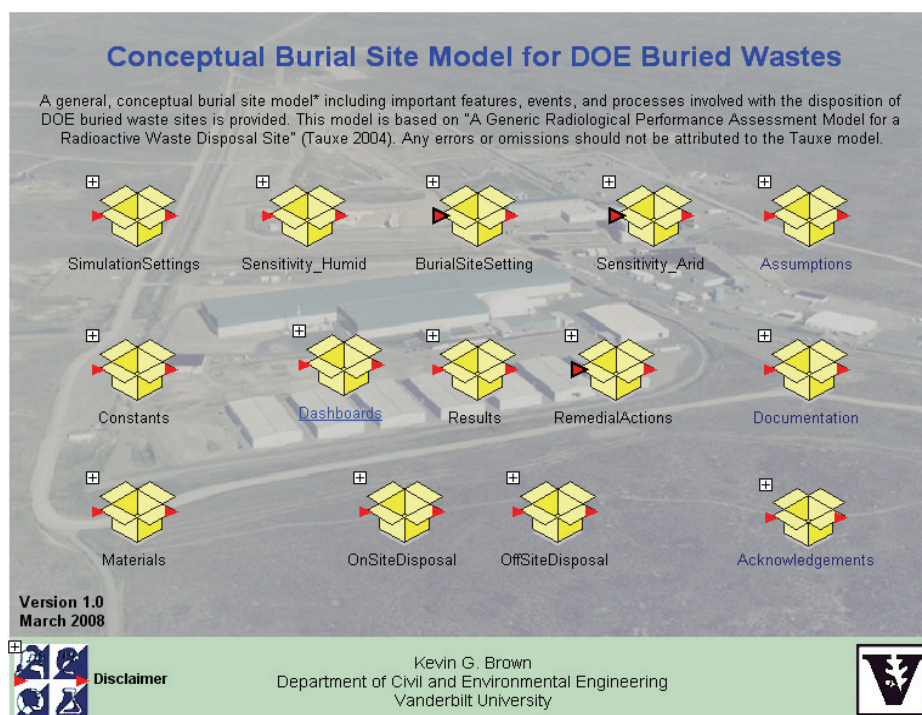
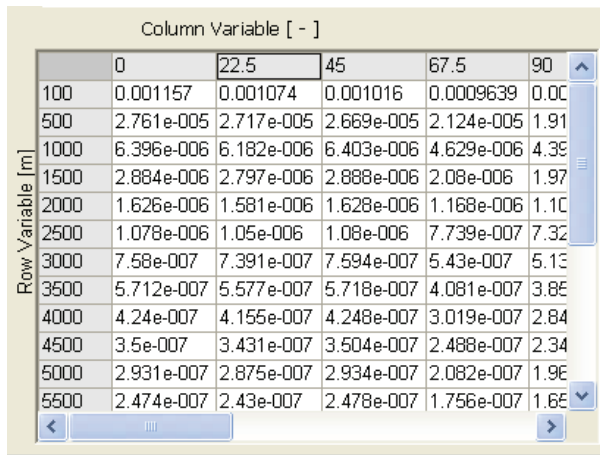


Figure 10. Example System divided into Distinct Sub-groups (Brown 2008)

GoldSim to external codes that include the Lookup Table, Spreadsheet, External (or DLL), and File elements; the primary sources for these descriptions are Volumes 1 and 2 of the GoldSim User's Guides (GTG 2009d; GTG 2009e). Two additional modules, namely the Contaminant/Radionuclide Transport Module (GTG 2009a) and Reliability Module (GTG 2009c), may provide useful functionality for the CBP and are also briefly described here.

## 11.1 Lookup Table Element

Lookup Table elements allow data to be defined and accessed in the form of a lookup table (which can be thought of as a response surface). The table is defined in terms of one, two, or three independent variables. An example of a two-dimensional Lookup Table is illustrated in Figure 11.



**Figure 11. Example Two-Dimensional GoldSim Lookup Table (Brown 2008)**

### 11.1.1 Identification

This element is uniquely identified as a Lookup Table, which can be considered a Class from which specific instances are created in the GoldSim model. Instances can be created locally in Containers or

globally. Global or local instances within the same Container must be uniquely identified.

Clones of an element can also be created. All clones are "equal" in that the original element (which becomes a clone) is no different than the clone which was created from it. Both are clones and a change to an input to one automatically changes the corresponding input to other clones. If clones are created at the same scope, GoldSim ensures that the names of the clones are unique by adding a number to the end of the new clone. If the clone is created at a different scope, then the cloned elements will have the same names.

### 11.1.2 Type

The Lookup Table is a GoldSim element (which can be considered a Class).

### 11.1.3 Purpose

Lookup Table elements allow data to be defined and accessed in the form of a lookup table (which can be considered a response surface).

### 11.1.4 Function

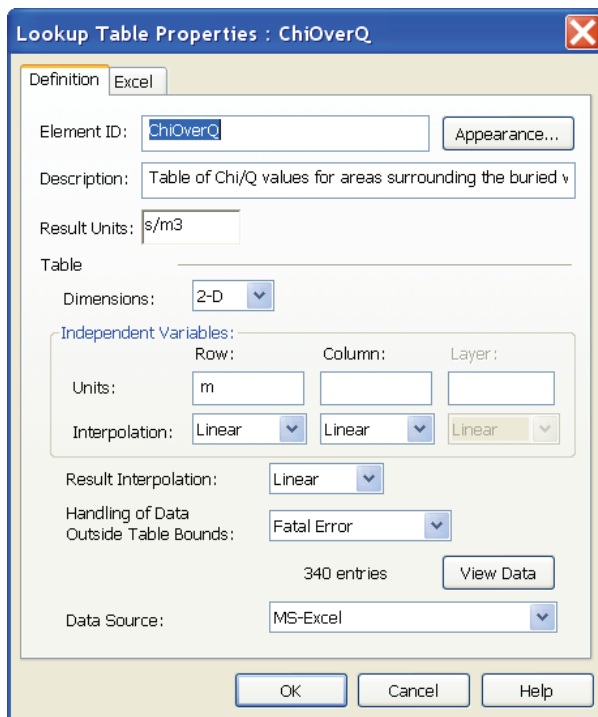
An instance of the Lookup Table element provides response surface data as a function of one, two, or three independent variables. GoldSim computes the value of the dependent variable for any given values of the independent variables by interpolating between data points in the table.

An instance of the Lookup Table element is created using the GoldSim dialog shown in Figure 12. The following steps are required to define a Lookup Table:

1. Dimensions (i.e., number of independent variables) must be specified. This list box provides three options: 1-D, 2-D or 3-D.



2. The Units are specified for each independent variable and the results (or dependent variable). For a 1-D Table, Row Units must be specified. For a 2-D table, the Row and Column Units are specified. For the 3-D Table, the Row, Column and Layer Units are defined.
3. The data representing the response surface are entered into the table. A dependent variable value is provided for each combination of independent variables. The data can be added manually, imported from a text file, or linked directly to an external data source (such as a spreadsheet file).
4. GoldSim computes the value of the dependent variable for a combination of independent variables by interpolating between the data in the table. The interpolation method (e.g., linear, log, next lower) and extrapolation condition are also specified.



**Figure 12. The GoldSim Dialog for creating a Lookup Table element**

### 11.1.5 Subordinates

There are no required subordinates or parents. However, if the Data Source used by the Lookup Table element is *MS-Excel*, then Microsoft Excel would be required. If a *Yucca Mountain Database* is specified, then an appropriate database would be required. The appropriate Dynamic Link Library is required if the Data Source type is *External DLL*.

### 11.1.6 Dependencies

Lookup Table elements do not have any significant dependencies or relationships to other elements.

### 11.1.7 Interface

Lookup Table elements are unique in that they are not referenced in the same manner that outputs of other elements are referenced. Instead, these elements are references in the same manner as a built-in function (GTG 2009d). That is, after defining a Lookup Table element, it is referenced in input expressions for other elements as if it were a custom function (denoted a *table function* in this case):

```
Equation
ChiOverQ(15m, 90)
```

The argument(s) to a table function are scalars and their dimensions must be the same as those of the independent variables with which the Lookup Table was originally defined (GTG 2009d). The dimensions of the table function are determined when the Lookup Table is defined. Table functions are referenced as follows:

- 1-D Tables: *Tablename*(Row Variable)
- 2-D Tables: *Tablename*(Row Variable, Column Variable)
- 3-D Tables: *Tablename*(Row Variable, Column Variable, Layer Variable)

The arguments to a table function can be either numbers or links from other elements.

#### 11.1.8 Resources

In addition to allowing data to be either input manually or imported from a text file, GoldSim also allows the data to be linked directly to an external data source. The three options for external linking are:

- A spreadsheet file,
- A database (although only 1-D and 2-D tables can be defined), or
- An external program (using a DLL) to output the data directly to the Lookup Table element.

#### 11.1.9 Processing

GoldSim computes the value of the dependent variable for values of the independent variables by interpolating between data points in the table. By default, interpolation is performed linearly with respect to independent variables. Other options are available for independent variables:

- **Linear:** This is the default that instructs GoldSim to linearly interpolate between table values.
- **Log:** GoldSim logarithmically interpolates between table values.
- **Next lower:** GoldSim returns the largest independent variable entry that is less than or equal to the input argument.
- **Exact only:** The Lookup table only accepts arguments that exactly match independent variable entries in the table. If there is not an exact match in the table, GoldSim issues a fatal error.

The only options available for Result Interpolation are **Linear** and **Log**.

When a Lookup Table is created, the manner in which references that are outside the bounds of the table will be handled is defined. GoldSim provides three options for 1-D Tables and two options for 2-D and 3-D Tables:

- **Fatal Error:** This is the default that displays a Fatal Error message during running the simulation.
- **Do Not Extrapolate:** GoldSim will not extrapolate but will instead compute the value for the dependent variable based on the values for the independent variables at the nearest portion of the defined region.
- **Extrapolate:** GoldSim extrapolates using the two closest data pairs. This option is only available for 1-D Tables.

#### 11.1.10 Data

A Lookup Table element is defined using the dialog shown in Figure 12. The inputs used to define an instance of the element include:

- **Element ID:** This is a text field describing the name of the instance, which may or may not be unique based on the scope. The default is the name of the element (in this case, Table) with an integer suffix to create a unique name depending on the scope.
- **Description:** This is an optional text field describing the instance. This field is empty by default.
- **Result Units:** This is a text field defining the units of the results. The default would be unitless.
- **Table Definition|Dimensions:** This is an option from a list box (with options 1-D, 2-D, or 3-D) defining the dimensions (i.e., number of independent variables) of the instance.
- **Independent Variables:**

- **Units:** This is a text field defining the units of the independent variable. The default would be unitless.
- **Interpolation:** This is an option from a list box (with options of Linear, Log, Next Lower, or Exact only) defining the manner in which interpolation may or may not be calculated. The default is Linear.
- **Result Interpolation:** This is an option from a list box (with options of Linear or Log) defining the manner in which interpolation is performed for results. The default is Linear.
- **Handling of Data Outside Table Bounds:** This is an option from a list box (with options of Fatal Error or Do Not Extrapolate for 1-D, 2-D, and 3-D tables and Extrapolate for 1-D tables) to define what to do with references that are outside the bounds of the table. The default is Fatal Error.
- **Data Source:** This is an option from a list box (with options of None, MS-Excel, Yucca Mountain Database, or External DLL) defining the data source for the table. The default is None.

#### **11.1.11 Descriptions of Required External Databases and Programs**

No databases are required for a GoldSim Lookup Table element; however, data can be imported into either a 1-D or 2-D table function from an external database denoted a “Yucca Mountain Database”. A “Yucca Mountain Database” is one of several database structures supported by GoldSim, but the only one that supports Lookup Table elements.

#### **11.1.12 System-Level Uncertainty Considerations**

There are no uncertainty considerations directly related to the Lookup Table elements.

#### **11.1.13 Verification and Validation**

No information is provided in the GoldSim documentation (GTG 2009a; GTG 2009b; GTG 2009c; GTG 2009d; GTG 2009e) that describes the verification and/or validation of the Lookup Table element.

#### **11.1.14 Summary of Model Limitations**

The Lookup Table element provides a response surface functionality that is restricted to three or fewer independent variables.

### **11.2 Spreadsheet Element**

A Spreadsheet element allows the dynamic exchange of data with a Microsoft Excel spreadsheet file (GTG 2009e). Data can be transmitted into specific spreadsheet cells, the spreadsheet recalculated, and the results copied back to the GoldSim model. A spreadsheet can also be used as a source of input data or as a repository for output results.

#### **11.2.1 Identification**

This is uniquely identified as a Spreadsheet element, which can be considered a Class from which specific instances are created in the GoldSim model. Instances can be created locally in Containers or globally. Global instances or local instances within the same Container must be uniquely identified.

Clones of an element can also be created. All clones are "equal" in that the original element (which becomes a clone) is no different than the clone which was created from it. Both are clones and a change to an input to one automatically changes the corresponding input to other clones. If clones are created at the same scope, GoldSim ensures that the names of the clones are unique. If the clone is

created at a different scope, then the cloned elements will have the same names.

### 11.2.2 Type

The Spreadsheet element is a GoldSim element (which can be considered a Class).

### 11.2.3 Purpose

Spreadsheet elements allow the dynamic exchange of data with a Microsoft Excel spreadsheet file.

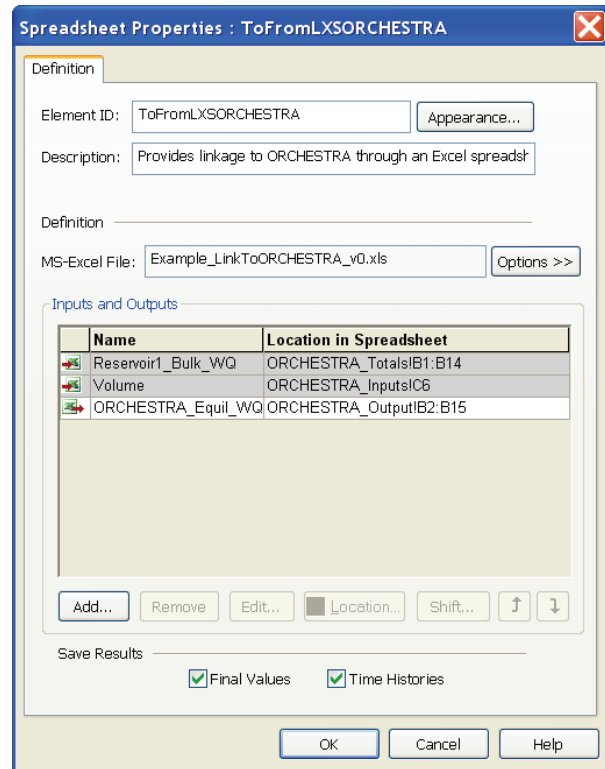
### 11.2.4 Function and Processing

An instance of the Spreadsheet element provides the ability to dynamically exchange data with an Excel spreadsheet file. An instance of the Spreadsheet element is created using the GoldSim dialog shown in Figure 13. The name of the file to be linked is selected using the **Options >>** button.

Spreadsheet elements can be used in one of three ways (GTG 2009e):

1. The spreadsheet can be used as a database where data are imported from the spreadsheet into GoldSim at the beginning of the simulation.
2. The spreadsheet can be used as a repository for results where data are exported from GoldSim to the spreadsheet throughout the simulation.
3. The spreadsheet can be used as a function by exporting data into specified cells in the spreadsheet, having the spreadsheet recalculate results, and then importing results back into the GoldSim model.

In all cases, at least one input to the spreadsheet element (i.e., those data exported from GoldSim to the spreadsheet) or one output from the spreadsheet (i.e., data imported from the spreadsheet into GoldSim) must be defined.



**Figure 13. The GoldSim Dialog for creating a Spreadsheet element**

### 11.2.5 Subordinates

Microsoft Excel is required. GoldSim supports both .xls (Version 98-2003) and .xlsx (Version 2007) file formats. For versions of Microsoft Excel prior to Office 2007, the Microsoft Office Compatibility Pack must be installed to read .xlsx files.

### 11.2.6 Dependencies

Spreadsheet elements dynamically exchange data with Microsoft Excel spreadsheets and thus the functionality of the spreadsheet elements depends on the availability and capabilities of Excel. If a Spreadsheet element is used, then there may be a

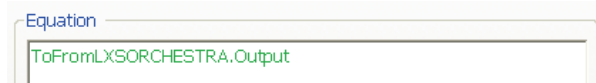
delay of several seconds at the start of a simulation as Microsoft Excel is loaded into memory. After loading, the simulation should progress without significant impact on performance.

Spreadsheet recalculations are managed in the following manner:

- Regardless of the Recalculate setting, Excel recalculates, by default, whenever cell values change. However, GoldSim will only retrieve updated data if **Recalculate in Excel during simulation** is selected. This setting can be changed in Excel (so it does not automatically recalculate) in the Calculation tab of Microsoft Excel's Options dialog.
- The **Recalculate in Excel during simulation** setting allows GoldSim: 1) to force Excel to recalculate and 2) to retrieve recalculated data. Thus if the Recalculate setting is off, GoldSim will not retrieve updated data from the spreadsheet even if cells have changed.

### 11.2.7 Interface

Spreadsheet elements are referenced in the same manner that outputs of other elements are referenced. This is typically done by right-clicking in the area that the output is needed and selecting **Insert Link....** A list is provided of the outputs available from the elements in the GoldSim model that can be selected. For example, if the Spreadsheet element is named *ToFromLXSORCHESTRA* and the output *Output*, then the resulting output link would be:



### 11.2.8 Resources

A Microsoft Excel spreadsheet is required to use the Spreadsheet element. The manner in which data are exchanged between GoldSim and the Excel spreadsheet (using the Spreadsheet element) is determined as illustrated in Table 12.

**Table 12. Determination of How Data Are Exchanged with the Spreadsheet Element (from GTG (2009e))**

| Type of Exchange Specified | Recalculate Setting | Offsets defined? | Results in GoldSim exchanging data with spreadsheet file when?  |
|----------------------------|---------------------|------------------|---|
| Export only                | Not available       | No               | Export all data at end of simulation  |
|                            | Not available       | Yes              | Export data from just before its offset changes*<br>Export all data at end of simulation  |
| Import only                | Not available       | No               | Import all data at beginning of simulation  |
|                            | Not available       | Yes              | Import all data at beginning of simulation<br>Import data when its offset changes   |
| Export and Import          | Off                 | No               | Import all data at beginning of simulation<br>Export all data at end of simulation  |
|                            | On                  | No               | Export and Import all data at beginning of simulation<br>Export and Import all data whenever an Export variable changes<br>Export all data at end of simulation |

\* The value that is exported when an export offset changes is the value from the update immediately before the offset changed.

**Table 12. Determination of How Data Are Exchanged with the Spreadsheet Element (Contd)**

| Type of Exchange Specified | Recalculate Setting | Offsets defined? | Results in GoldSim exchanging data with spreadsheet file when?   |
|----------------------------|---------------------|------------------|--|
| Export and Import (Contd)  | Off                 | Yes              | Export and Import all data at beginning of simulation<br>Export data from just before its offset changes*<br>Import data when its offset changes<br>Export all data at end of simulation   |
|                            | On                  | Yes              | Export and Import all data at beginning of simulation<br>Export and Import all data whenever an Export variable changes<br>Export data from just before its offset changes*<br>Import data when its offset changes<br>Export all data at end of simulation |

\* The value that is exported when an export offset changes is the value from the update immediately before the offset changed.

### 11.2.9 Data

A Spreadsheet element is defined using the dialog shown in Figure 13. The inputs used to define an instance of the element include:

- **Element ID:** This is a text field describing the name of the instance, which may or may not be unique based on the scope. The default is the name of the element (in this case, External) with an integer suffix to create a unique name depending on the scope.
- **Description:** This is an optional text field describing the instance. This field is empty by default.
- **MS-Excel File:** The name of a Microsoft Excel spreadsheet file must be named by selecting the **Options >>** button. This will provide options for either selecting an existing file or creating (and then selecting) a new spreadsheet file. There are additional options for:
  - **Lock onto selected file:** When selected, the following information regarding the referenced file is saved with the element: 1) file and path name, 2) date file was created, 3) date file was last modified, 4) file size, and 5) CRC signature. The CRC signature is a code that can be used to uniquely identify whether file contents have changed. When a model runs, GoldSim compares the CRC signature of the file with the original signature. If these are not identical, GoldSim displays an error message and stops. A file can be unlocked by clearing the **Lock onto selected file** item. If versioning is enabled, this information is logged with the version.
  - **Save MS-Excel File after simulation:** Selecting this option allows changes made to a spreadsheet (i.e., when GoldSim exports data to the spreadsheet) to be saved. Saving changes to a spreadsheet file and file locking are mutually exclusive.
  - **Recalculate in Excel during simulation:** This option helps control how recalculation is managed in GoldSim as described in Table 12.
- **Inputs and Outputs:**
  - **Name:** This is a text field defining the name of the input or output. For inputs, the default input will be Input $n$  where  $n$  is an integer. These names will be used to reference the inputs within GoldSim (as SpreadsheetElementName.Input $n$ ). For outputs, the default input is Output $n$ . These names are used to reference the outputs within GoldSim (as SpreadsheetElementName.Output $n$ ).

- **Location in Spreadsheet:** This field describes the location of the referenced cells in the MS-Excel file in the format of WorksheetName!CellReference(s). The size of the range specified in the spreadsheet must be consistent with the type (i.e., scalar, vector, or matrix) defined for the output. A scalar output must map to a single cell, a vector output must map to a single column or row range with the number of rows or columns matching the number of items in the vector, and a matrix output must map to a rectangular range with the number of rows and columns matching the dimensions of the matrix.

#### **11.2.10 Descriptions of Required External Databases and Programs**

No databases are required for a GoldSim Spreadsheet element.

#### **11.2.11 System-Level Uncertainty Considerations**

There are no uncertainty considerations directly related to Spreadsheet elements.

#### **11.2.12 Verification and Validation**

No information is provided in the GoldSim documentation (GTG 2009a; GTG 2009b; GTG 2009c; GTG 2009d; GTG 2009e) that describes the verification and/or validation of the Spreadsheet element.

#### **11.2.13 Summary of Model Limitations**

The Spreadsheet element provides functionality that is restricted to that available in the current version of a Microsoft Excel spreadsheet.

### **11.3 External (Dynamic Link Library) Element**

There are situations in which complex functionality is needed that cannot be readily implemented using the built-in features supplied by GoldSim. GoldSim was designed to directly couple separate program modules (written in C, C++, Pascal, FORTRAN, etc.) with GoldSim algorithms. These user-defined external modules are referred to as external functions and the elements through which they interact with GoldSim are denoted External (DLL) elements.

#### **11.3.1 Identification**

This element is uniquely identified as an External element, which can be considered a Class from which specific instances are created in the GoldSim model. Instances can be created locally in Containers or globally. Global instances or local instances within the same Container must be uniquely identified.

Clones of an element can also be created. All clones are "equal" in that the original element (which also becomes a clone) is no different than the clone which was created from it. Both are clones and a change to an input to one automatically changes the corresponding input to other clones. If clones are created at the same scope, GoldSim ensures that the names of the clones are unique. If the clone is created at a different scope, then the cloned elements will have the same names.

#### **11.3.2 Type**

The External element is a GoldSim element (which can be considered a Class).

### 11.3.3 Purpose

External elements allow separate program modules to be directly coupled with GoldSim algorithms.

### 11.3.4 Function and Processing

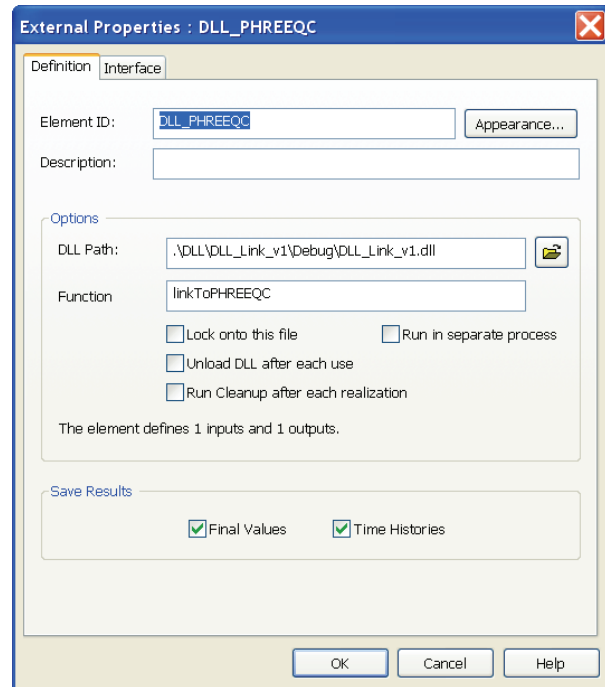
An instance of the External element provides GoldSim algorithms the ability to directly interact with separate program modules (written in C, C++, Pascal, FORTRAN, etc.). The modules are linked into GoldSim as DLLs (Dynamic Link Libraries) at run time. Integrating these external modules into GoldSim requires developing a "wrapper" (or "shell") around the existing function and compiling it into a DLL. Typically this requires a limited number of programming modifications. GoldSim supports both 32-bit and 64-bit DLLs.

An instance of the External element is created using the GoldSim dialog shown in Figure 14. The following steps are required to define an External element:

1. The external function to be used by the External element is coded.
2. The external function is compiled into a DLL (where multiple functions can be included in one DLL).
3. An External element is created within the GoldSim model where the DLL and specific function within the DLL are specified.
4. The input and output arguments that are to be sent to and received from the function are identified.

### 11.3.5 Subordinates

The required subordinate for the External element is the separate program module (compiled as a DLL) that is linked to via the element.



**Figure 14. The GoldSim Dialog for creating an External element (Early 2007c)**

### 11.3.6 Dependencies

The External element is called at the following times:

- At the beginning of the simulation,
- At every timestep (if one of the inputs to the element has changed), and
- At any internal step in which an Event is triggered (if one of the inputs to the element has changed).

Each of these calls may be treated in a different way. For example, it may be desired that the external function ignore the call at the beginning of the simulation or carry out special initialization routines at that time. Also a call in the middle of a timestep



(i.e., due to an Event) may be treated differently from a call at the end of a timestep. To communicate this kind of information to the external function, the current elapsed time and perhaps the length of the timestep can be provided to the external function as optional input arguments.

### 11.3.7 Interface

Outputs from External elements are referenced in the same manner that outputs of other elements are referenced. This is typically done by right-clicking in the area that the output is needed and selecting **Insert Link....** A list is provided of the available outputs that can be selected from the elements in the GoldSim model.

### 11.3.8 Resources

The separate external program module with the desired functionality and a Dynamic Link Library (DLL), which is essentially a wrapper for the external module allowing interaction, are required for operation of the External element.

### 11.3.9 Data

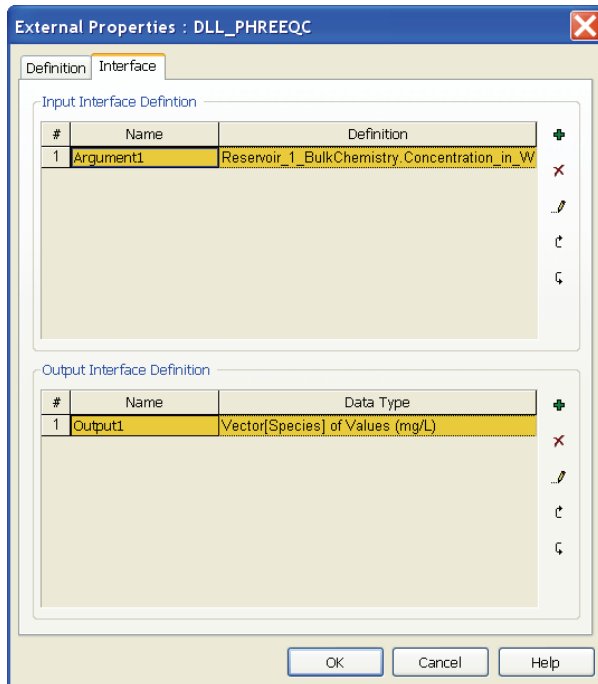
An External element is defined using the Definition Tab in the dialog shown in Figure 14. The inputs used to define an instance of the element include:

- **Element ID:** This is a text field describing the name of the instance, which may or may not be unique based on the scope. The default is the name of the element (in this case, External) with an integer suffix to create a unique name depending on scope.
- **Description:** This is an optional text field describing the instance. This field is empty by default.
- Options:
  - **DLL Path:** This is a text field defining the path to the DLL file that contains the external function, which can be selected using the Browse button.
  - **Function Name:** This is a text field identifying the (unique) name of the function in the DLL because multiple functions can be included in a single DLL. The name is case-sensitive and must match exactly the name of the external function in the object code.
  - **Lock onto this file:** If this option is selected, the following information regarding the referenced file is saved with the element: 1) file and path name, 2) date file was created, 3) date file was last modified, 4) file size, and 5) CRC signature. The CRC signature is a code that can be used to uniquely identify whether file contents have changed. When a model runs, GoldSim compares the CRC signature of the file with the original signature. If these are not identical, GoldSim displays an error message and stops. A file can be unlocked by clearing the **Lock onto selected file** item. If versioning is enabled, this information is logged with the version.
  - **Unload DLL after each use:** If this option is checked, GoldSim will unload the DLL (and continue the simulation), which is useful when running very large model files where the DLL is called infrequently. If the DLL is subsequently called again, GoldSim reloads it.
  - **Run Cleanup after each realization:** If this option is selected, then GoldSim will call the DLL with a cleanup instruction at the end of each realization.
  - **Run in separate process:** If this option is selected, GoldSim does not load the DLL into its process space, but instead launches a separate DLL server with its own private process space. Each DLL running in a separate process has its own DLL server and thus has access to a private 2 GB process space. By default, GoldSim loads DLLs used by External elements into the GoldSim

process space; thus GoldSim and external DLLs share the same address space, which is usually limited to 2 GB.

As illustrated in Figure 15, the Interface Tab for the External element dialog provides descriptions for the inputs and outputs for the external function. The fields for the Input Interface Definition are:

- **Name:** This is a field identifying the name of the input, which is selected using the Add button. This provides a list of the output for all GoldSim elements (via the Input Link dialog) from which an output is selected.
- **Definition:** This field displays the output that was selected.



**Figure 15. The Interface Tab for creating an External element (Early 2007c)**

The fields for the Output Interface Definition are:

- **Name:** This field is the name by which the output variable is referenced in the model. For example, if the name of the External element is X and the name of the output is Y, then the output could be referenced as X.Y.
- **Data Type:** This field describes both the type (e.g., Value, Condition, Lookup Table, or Time Series) and the Units for the output.

There is no practical limit to the number of inputs and outputs that can be added to an External element. The input and output arguments are transferred between GoldSim and the external function in the order in which they are listed on the Interface tab.

### 11.3.10 Descriptions of Required External Databases and Programs

No databases are required for a GoldSim External element.

### 11.3.11 System-Level Uncertainty Considerations

There are no uncertainty considerations directly related to the External elements. However, it is possible that advanced uncertainty methods needed for the CBP may be called using these elements.

### 11.3.12 Verification and Validation

No information is provided in the GoldSim documentation (GTG 2009a; GTG 2009b; GTG 2009c; GTG 2009d; GTG 2009e) that describes the verification and/or validation of the External element.

### 11.3.13 Summary of Model Limitations

The External element provides GoldSim algorithms the ability to directly interact with separate program modules (written in C, C++, Pascal, FORTRAN, etc.). The modules are linked into GoldSim as DLLs (Dynamic Link Libraries) at run time. There are few

limitations on the use of External elements. For example, GoldSim supports both 32-bit and 64-bit DLLs. There is also no practical limit to the number of input and output arguments that can be used in an External element. Outputs from External elements can be a Value or a Condition (which can be used as inputs to other elements) or can be directly linked to a Lookup Table or Time Series element.

By default, GoldSim loads DLLs used by External elements into the GoldSim process space and thus GoldSim and external DLLs share the same address space, which is typically 2 GB under Windows. If the memory requirements for GoldSim and the DLLs exceed 2 GB, GoldSim will be unable to carry out the simulation. The user will be forced to preserve memory by saving fewer histories or time steps, turning off the saving of results for certain elements, running DLLs in separate processes, or increasing the address space in Windows.

## **11.4 File Element**

The File element is a support element in GoldSim used to control copies of auxiliary files needed by External and Spreadsheet elements. This element has no inputs or outputs and performs no calculations.

### **11.4.1 Identification**

This element is uniquely identified as a File Table, which can be considered a Class from which specific instances are created in the GoldSim model.

Instances can be created locally in Containers or globally. Global instances or local instances within the same Container must be uniquely identified.

Clones of an element can also be created. All clones are "equal" in that the original element (which also becomes a clone) is no different than the clone which was created from it. Both are clones and a change to an input to one automatically changes the

corresponding input to other clones. If clones are created at the same scope, GoldSim ensures that the names of the clones are unique. If the clone is created at a different scope, then the cloned elements will have the same names.

### **11.4.2 Type**

The File Element is a GoldSim support element (which can be considered a Class).

### **11.4.3 Purpose**

File elements control copies of auxiliary files needed by External and Spreadsheet elements.

### **11.4.4 Function and Processing**

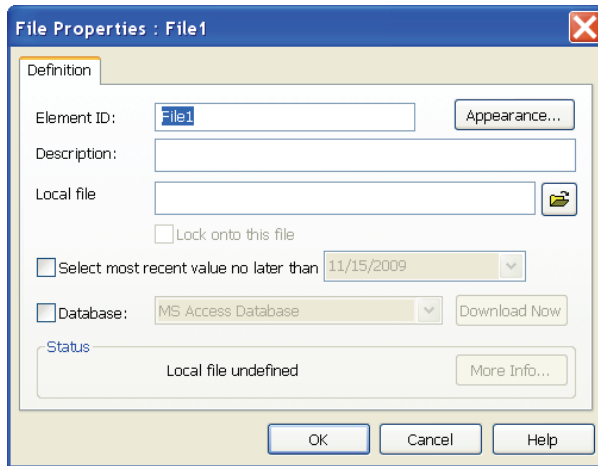
An instance of the File element is used to control copies of auxiliary files. File elements have two uses:

- To ensure that necessary support files are transferred to Slaves (clients) when using the GoldSim Distributed Processing Module (GTG 2009b), which is the most typical use; and
- To ensure that support files that are stored on a network are accessed for use in a simulation and to provide an "audit trail" for the file transfer. The element uses a database to identify a "source" file and then copy the target file to the local computer for access by GoldSim elements.

An instance of the File element is created using the GoldSim dialog shown in Figure 16.

### **11.4.5 Subordinates**

The required subordinate for the File element is the file that will be controlled by the element. If the File element is used to assure that a file stored on a network is accessed during a simulation, then the database used to control transfer of the file to the local computer for access by GoldSim elements would be an additional subordinate.



**Figure 16. The GoldSim Dialog for creating a File element**

#### **11.4.6 Dependencies and Interface and Resources and Data**

File elements are most frequently used to support distributed processing. The Distributed Processing Module allows use of multiple computers connected over a network to share the computational burden of a simulation, which is accomplished by having a Master (server) GoldSim executable connect to multiple Slave (client) GoldSim executables (GTG 2009b; GTG 2009e).

When using distributed processing, the first step is for the Master to transfer needed files to the Slaves. If External or Spreadsheet elements are used, then DLLs and spreadsheet file are transferred automatically. However, if other files are needed, then this knowledge cannot be directly captured in GoldSim. The File element can be used to overcome this issue by sending any file referenced in a File element to all Slaves in a distributed processing simulation. A File element should be created for each

file referenced by external elements. The file name is entered in the **Local file** field and the **Database** checkbox should be clear. If no path is provided, the file should be placed in the same directory as the model file. If the file cannot be found, the simulation is not allowed to proceed.

A second use of the File element is to ensure that support files that are stored on a network are accessed for use in a simulation and to provide an “audit trail” of the file transfer. When used in this manner, the **Element ID** for the File element is used as the key to access a record in a specifically formatted (Yucca Mountain) database. This record provides a network pathname for the source file and provides an integrity-checking code for the file. The **Database** box must be checked and the database name entered. Before using the GoldSim database features, all databases must be defined using the 32-bit ODBC Data Sources option in the Windows Control Panel. A name is defined for each data source and linked to a specific database file.

When the **Download Now** button is pressed or a global database download is executed, GoldSim locates the source file and copies it. The **Local file** field defines the local destination for the copy. If the local destination already exists, then it is automatically overwritten. After copying, the CRC signature<sup>13</sup> of the downloaded file is compared to that of the file represented in the database to ensure the integrity of the data transfer. If the codes are different, the download is treated as having failed.

The manner in which GoldSim interrogates the Yucca Mountain database for the most current version of the source file can be optionally set using the **Select most recent value no later than**, which provides the date for GoldSim to update. If the field

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<sup>13</sup> The CRC signature is an alphanumeric code that can be used to uniquely identify whether the file’s contents have changed.

is blank, GoldSim uses the default effective date (defined elsewhere) (GTG 2009e).

There are no inputs or outputs for the File elements.

#### **11.4.7 Descriptions of Required External Databases and Programs**

A “Yucca Mountain Database” is required for a GoldSim File element when it is used to ensure that support files that are stored on a network are accessed for use in a simulation and to provide an “audit trail” of the file transfer. A “Yucca Mountain Database” is one of several database structures supported by GoldSim, but the only one that is used by File elements.

#### **11.4.8 System-Level Uncertainty Considerations**

There are no uncertainty considerations directly related to File elements.

#### **11.4.9 Verification and Validation**

No information is provided in the GoldSim documentation (GTG 2009a; GTG 2009b; GTG 2009c; GTG 2009d; GTG 2009e) that describes the verification and/or validation of the File element.

#### **11.4.10 Summary of Model Limitations**

The File element is used to control copies of auxiliary files needed by External and Spreadsheet elements.

### **11.5 Contaminant/Radionuclide Transport Module**

The Contaminant Transport (CT) Module is an extension of the GoldSim simulation framework that

allows dynamic modeling of mass transport within complex engineered and/or natural environmental systems (GTG 2009a). A mass transport model is a mathematical representation of a system used to predict the release, transport, and fate of mass within the system. The “mass” that is typically simulated is that of contaminants that have been accidentally released or disposed of within the system.

There are two versions of this Module that can be added to GoldSim: the CT Module or the RT Module. The Contaminant Transport (CT) Module provides the features that most modelers will need for contaminant transport. The Radionuclide Transport (RT) Module includes all of the capabilities of the CT Module with four additional features designed to facilitate simulation of radioactive waste disposal facilities. These features give the RT Module the ability to (GTG 2009a):

- Allow decay chains including daughter product ingrowth to be simulated. The CT Module allows first-order decay, but reaction products cannot be specified.
- Provide a special element called a Source, which is used to simulate the release of contaminants from near-field engineered systems. This element is useful when simulating the behavior of waste disposal facilities, which often have as part of their design engineered packages or containers in which the waste is placed prior to disposal.
- Have a special type of element called a Network Pathway. These elements provide a computationally efficient way to simulate large, complex networks of one-dimensional conduits to describe contaminant transport through fractured systems.
- Have a special element called a CellNet Generator, which provides an easy way to rapidly create two-dimensional Cell networks.

### **11.5.1 Identification**

Either the Contaminant Transport (CT) Module or the Radionuclide Transport (RT) Module will be included in the GoldSim simulation program.

### **11.5.2 Type**

These are Modules or program extensions.

### **11.5.3 Purpose**

These program extensions allow dynamic modeling of mass transport within complex engineered and/or natural environmental systems.

### **11.5.4 Function**

The function is to predict the release, transport, and fate of contaminants and/or radionuclide within the system.

### **11.5.5 Subordinates**

Table 8 provides a summary of the elements in the Contaminant Transport (CT) and the Radionuclide Transport (RT) Modules.

### **11.5.6 Dependencies**

Either the CT or RT Module can be included in the system. The RT Module includes all the functionality in the CT Module and includes four additional features described above.

### **11.5.7 Interface**

There are no special requirements for communicating with the elements in the CT and RT modules. These elements are no different than the others in GoldSim in terms of interaction.

### **11.5.8 Resources**

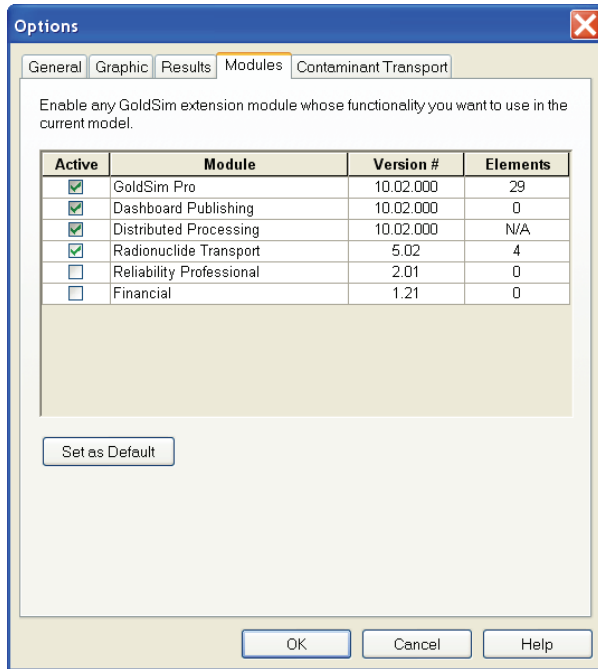
The External Pathway (Table 8) provides a mechanism to directly integrate external programs for contaminant transport into GoldSim. These elements, referred to as External Pathway functions, are linked into the model using Dynamic Link Libraries (DLLs) at runtime. These pathways are specialized extensions of the External element described in the Section entitled *External (Dynamic Link Library) Element*.

The manner in which the External Pathway is linked to the rest of the model is by specifying the input mass flux links and the output mass flux links (GTG 2009a). GoldSim automatically calls the function representing the External Pathway at the appropriate times and passes the appropriate information between the GoldSim model and the function.

Integrating external transport pathways into GoldSim requires developing a "wrapper" around the existing function and compiling it into a DLL. In many cases, this development requires a limited number of programming modifications (GTG 2009a). GoldSim supports both 32-bit and 64-bits DLLs.

### **11.5.9 Processing**

To use the CT or RT Module, it must first be activated. GoldSim will have neither, one, or the other (but not both) Modules, depending on the license (GTG 2009a; GTG 2009d). Modules are activated by selecting **Model|Options...** from the main GoldSim menu and then selecting the **Modules** tab. All extension modules appear in the resulting dialog as shown in Figure 17.



**Figure 17. GoldSim Extensions Module Dialog (Early 2007c)**

If the GoldSim license does not allow use of either the CT or the RT module, “Contaminant Transport” will be grayed out (and the Active column will be blank) (GTG 2009a). If the license does allow use of one of these modules, either “Contaminant Transport” (for CT) or “Radionuclide Transport” (for RT) will be listed, and the Active checkbox will be available. Allowable modules can be activated and deactivated by clicking the Active checkbox. If a module (such as CT or RT) is deactivated, then any special elements associated with the module will be deleted. If a module is activated, the options associated with the module are made available.

### 11.5.10 Data

The significant conceptual models, assumptions, and parameters for the Cell and Pipe Pathway elements that are included in the CT and RT modules were

described in the Section entitled *Detailed Explanation of Computational Algorithms and Methods*.

### 11.5.11 Descriptions of Required External Databases and Programs

Although GoldSim can interact with Microsoft Excel worksheet and external databases as indicated in Table 4 and Table 8, no databases are *required* for a GoldSim model.

### 11.5.12 System-Level Uncertainty Considerations

Typically, uncertainties in predictions resulting from uncertainties in processes and parameters will likely far exceed those introduced by the numerical solution method. It is generally more worthwhile to spend time ensuring that the model captures the key aspects of the system rather than evaluating the numerical accuracy of the solution methods (GTG 2009e). However, it is important to understand the nature of inaccuracies that arise from the numerical approximations used to ensure that these remain small. The primary numerical factors affecting the accuracy of GoldSim models are (GTG 2009e):

- **Integrating Differential Equations:** GoldSim solves differential equations by numerical integration, which is the largest potential source of numerical inaccuracies in a model.
- **Solving Coupled Equations:** A model may include coupled equations or coupled differential equations that can be computationally-intensive to solve. GoldSim provides fast and accurate solution techniques for certain types of coupled systems (GTG 2009a). In other cases, coupled equations must be approximately solved using Previous Value elements, which can introduce numerical approximations on the same order as those introduced from numerical integration of ordinary differential equations.

- **Representing Discrete Events:** Discrete events may occur that impose discontinuities onto the system. Superimposing discontinuities onto a continuously-varying system that must be discretized in time can introduce inaccuracies. GoldSim provides a time-stepping algorithm for accurately representing these hybrid systems (GTG 2009a).

### **11.5.13 Verification and Validation**

No information is provided in the GoldSim documentation (GTG 2009a; GTG 2009b; GTG 2009c; GTG 2009d; GTG 2009e) that describes the verification and/or validation of the code underlying the system.

### **11.5.14 Summary of Model Limitations**

Although GoldSim was designed to be a flexible tool to simulate contaminant transport in environmental systems, there are limitations depending on how the program will be used. Only certain types of functionality are built into GoldSim and its extension modules, which may compel the user to create their own functionality using either built-in functions or calling external programs. For example, if external programs are used, then the ability to ensure that the material balance is maintained becomes difficult. The transport functions available in the GoldSim extension modules are one-dimensional in nature.

## **11.6 Reliability Module**

The Reliability Module is a program extension to GoldSim which allows probabilistic simulation of the reliability and performance of complex engineered systems over time (GTG 2009c). The outputs of the Reliability Module consist of predicted reliability metrics (e.g., reliability and availability) for the overall system and for individual components. The Module can also be used to compute the probability of specific consequences to

support risk analysis. GoldSim catalogs and analyzes failure scenarios, which allows key sources of unreliability and risk to be identified (GTG 2009c).

### **11.6.1 Identification**

This program extension is denoted the Reliability Module.

### **11.6.2 Type**

The Reliability Module is a program extension (or module).

### **11.6.3 Purpose**

This module allows the probabilistic simulation of the reliability and performance of complex engineered systems over time.

### **11.6.4 Function**

This module is used to predict reliability metrics (e.g., reliability and availability) for the overall system and individual components, to compute the probability of specific consequences, and to catalog and analyze failure scenarios to allow key sources of unreliability and risk to be identified.

### **11.6.5 Subordinates**

The elements included in this module are described in Table 9.

### **11.6.6 Dependencies**

The discrete event elements described in Table 5 are often used in conjunction with the Reliability elements. For example, the Triggered and Timed Events are often used to create initiating events (e.g., events external to the system being modeled, such as an earthquake) that can lead to the failure of a system component (GTG 2009c).



### **11.6.7 Interface**

There are no special requirements for communicating with the elements in the Reliability Module. These elements are compatible with other GoldSim elements in terms of interaction.

### **11.6.8 Resources**

There are no external elements specific to the Reliability Module.

### **11.6.9 Processing**

To use the Reliability Module, it must first be activated. Modules are activated by selecting **Model|Options...** from the main GoldSim menu and then selecting the **Modules** tab. All extension modules appear in the resulting dialog as shown in Figure 17.

### **11.6.10 Data**

There are no external functions that require resource allocation that are specific to the Reliability Module.

### **11.6.11 Descriptions of Required External Databases and Programs**

Although GoldSim can interact with Microsoft Excel worksheets and external databases as indicated in Table 4 and Table 8, no databases are required for a GoldSim model, including the elements in the Reliability Module.

### **11.6.12 System-Level Uncertainty Considerations**

There are no issues specifically related to the computation of reliability metrics using the elements in the Reliability Module.

### **11.6.13 Verification and Validation**

No information is provided in the GoldSim documentation (GTG 2009a; GTG 2009b; GTG 2009c; GTG 2009d; GTG 2009e) that describes the verification and/or validation of the code underlying the system.

### **11.6.14 Summary of Model Limitations**

The elements included in the Reliability Module are meant to complement and not replace existing methods (GTG 2009c).

## **12 DATA DICTIONARY**

The data dictionary is provided by Table 1 through Table 9.

## **13 SUMMARY AND CONCLUSIONS**

The goal of the Cementitious Barriers Partnership (CBP) is to develop a reasonable and credible set of tools to predict the structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over extended time frames (e.g., >100 years for operating facilities and >1000 years for waste management).

GoldSim is a graphical, object-oriented computer program for executing dynamic, probabilistic simulations. GoldSim is a "visual spreadsheet" allowing the user to visually create and manipulate data and equations including linking to external program and databases (GTG 2009d). Although GoldSim can be run deterministically, one of its key features is to manage uncertainties through the use of probability distribution functions. The features described for GoldSim make it an adequate candidate for the initial integration efforts for the CBP tools.

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