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SCALE Procedure for Verified, Archived Library of Inputs and Data (VALID)

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Revision	Revision Description	Effective
	•	Date
1	Added Revision History Log Sheet	9/15/2010
1	Throughout: The name of the process/library is changed from "Models and Derived Data (MADD) to "Verified, Archived Library of Inputs and Data" (VALID). Minor editorial or other non-intent changes were made.	9/15/2010
1	Sect. 3.1: Definition of "Model" clarified to include non- critical or hypothetical systems.	9/15/2010
1	Sect. 5.1.2: Examples of reasons for rejecting a request for a VALID form were added.	9/15/2010
1	Sect. 5.1: Renumbered all steps following the new step 5.1.11	9/15/2010
1	Sect. 5.1.13: Added an explicit note that the final, reviewed files for an addition to the library by the SQA Coordinator are identified by the QA Coordinator in Section V of the VALID forms. This change is to match a current practice that minimizes the potential for an inadvertent change to a reviewed file, prior to that file being added to the library.	9/15/2010
1	Sect. 5.1.14: Added a note that the SQA coordinator provides backup copies of VALID forms and attachments on the ORNL Electronic Records System (ERS). This change matches current practice; the ERS is the only location where NSTD/NMDS staff can readily access these records.	9/15/2010
1	Sect. 5.1.15: Formerly stated that the SQA Coordinator notify "all users" of the library for each change to library. This is neither practical nor necessary. A specific list of individuals or positions to be notified is now identified.	9/15/2010
2	Formatting updated for consistency with other SCALE procedures.	
2	Introduction provided section number (Section 1) and all other sections subsequently incremented.	
2	The purpose for this revision has been added to Section 2.	
2	The applicability of this revision to work started under previous revisions has been added to Section 3.	
2	The definition of Model has been updated in Section 4.1 and the definition of VALID Case has been added as Section 4.4.	
2	A new Section 6 has been added providing general guidance on minimum standards for qualification and addressing expiration of qualifications.	
2	The Procedure as defined in what is now Section 7 has been significantly modified to support migration of the VALID procedure from a form based system to the FogBugz tracking system.	

SCALE Procedure for Verified, Archived Library of Inputs and Data (VALID)

1.0 INTRODUCTION

This procedure provides a framework for preparing, reviewing, and storing model inputs and derived data so that staff members with authorized access to the VALID library can use the inputs and data with confidence in their analyses. The procedure uses documented checks and reviews to ensure that the inputs and data were correctly generated using appropriate references. Configuration management is implemented to prevent inadvertent modification of the inputs and data or inclusion of models that have not been reviewed. The procedure also provides guidance to be followed if errors are identified or if input and/or data revisions are needed.

Although this procedure addresses quality assurance for nuclear models inputs and derived data, it remains the responsibility of each user of the inputs and data to verify that the usage complies with any specific quality assurance requirements of individual sites or projects.

2.0 PURPOSE

The purpose of this procedure is to prescribe the process used to create and maintain a collection of model inputs and associated derived data for use in nuclear analyses and validation of computational methods.

The primary purpose for this revision is to migrate the procedure from the use of electronic forms to a VALID Project within the FogBugz tracking system. The use of FogBugz automates backups, simplifies status reporting through the use of a Kanban process, and allows tracking of more information during the execution of the procedure than was available with the form based system. Future expansion of the FogBugz implementation at ORNL may also facilitate external users having direct access to the system, thus simplifying the use of external performers within this procedure.

A secondary purpose of this revision is to simplify the procedure by the elimination of some redundant steps currently in the process. The migration to FogBugz is a key enabler for some of these procedural simplifications. Experience with the procedure over the past several years has also provided insight on the value of each step. The core function of two qualified, independent individuals generating and reviewing the technical content of each VALID Case remains intact as the basis for quality in these models.

3.0 SCOPE

This procedure provides guidance for preparing, reviewing and documenting the quality of model inputs and data derived from model inputs.

Applicability of this procedure to all work in-progress under previous revisions of this procedure will be determined on a case-by-case basis by the VALID Quality Assurance Coordinator.

4.0 **DEFINITIONS**

- 4.1 **Model** As used in this procedure, a model is the set of computational input data that is used to describe a system of interest. For example, models of critical experiments are frequently used to validate criticality safety analyses. Models may be developed for hypothetical or representative systems (e.g., the "GBC-32" cask), or for actual process facility applications. A model is the complete set of input, (e.g., geometry, materials, cross section library, cross section processing treatments, etc.) that represents the benchmark, system, or process application.
- 4.2 **Derived Data** Derived data are data produced from computer calculations using a model. Nuclide-, reaction-, and energy-dependent *keff* sensitivity data files are examples of data derived from criticality safety analysis models.
- 4.3 **Library** The library ("VALID library") is the collection of verified models and derived data that is available for use.
- 4.4 **Case** A VALID Case is the set of experiments and/or data for which models and derived data are being generated for addition to the library. A VALID Case can contain one or more benchmark evaluations, radiochemical assay sample calculations, application models, etc. Each VALID Case moves through the procedure as a single unit. Thus multiple models can be entered into the library within the origination and review of a single case. Each VALID Case is documented in a single FogBugz case.

5.0 **RESPONSIBILITIES**

- 5.1 **Originator** The Originator is responsible for:
 - Identifying models and data that could be added to the library.
 - Identifying acceptable references describing models.
 - Documenting methods and data used to prepare the models and derived data.
 - Documenting any approximations or assumptions used in the development of models, including potential inconsistencies or

inadequacies inherent to the source references.

- Checking the models and derived data to ensure the model inputs are correct and the derived data are correctly calculated.
- Submission of models and/or data for addition to the library.
- Resolving review comments.
- Notifying the VALID Quality Assurance Coordinator if errors or problems are identified in models or data in the library.
- 5.2 **Reviewer** The Reviewer is responsible for:
 - Ensuring documentation prepared by Originator is complete and accurate.
 - Ensuring model reference is appropriate.
 - Reviewing models and derived data.
 - Working with Originator to resolve review comments.
 - Documenting review.
- 5.3 **VALID Quality Assurance Coordinator** ("QA Coordinator") The QA Coordinator is responsible for:
 - Assigning an Originator and a Reviewer to prepare and review models for the library.
 - Ensuring individuals assigned as Originator and Reviewer have background and experience levels appropriate for their responsibilities under this procedure.
 - Considering the expected use of the models and data and determining whether the references are complete, accurate, credible, and appropriate.
 - Assisting with resolution of any unresolved review comments.
 - Ensuring documentation is complete.
 - Acceptance or rejection of proposed models and/or derived data.
 - Reviewing problems reported with models and/or data in the library.
 - Ensuring users are aware of responsibilities.

5.4 **VALID Software Quality Assurance Coordinator** ("SQA Coordinator") – The SQA Coordinator is responsible for:

- Adding models and/or derived data to the library.
- Maintaining configuration control of the library.
- Maintaining documentation files.
- Maintaining a searchable data base of library contents.
- Maintaining an email notification list of staff to be informed of any changes to the VALID library.
- Notifying staff identified in the notification list regarding any changes to the VALID library.

- Maintaining a restricted-access archive of all files permanently deleted from the VALID library.
- Maintaining qualification lists for both Originators and Reviewers and documentation justifying their qualification.

NOTE: Within the VALID library, certain directories may contain proprietary data, requiring that access permissions for those directories be limited to a specific staff group. For VALID data that is proprietary, the SQA Coordinator applies directory access permissions as directed by the responsible ORNL Project Manager, and email notifications are limited to staff of the access group.

5.5 **SCALE Project Leader** – The SCALE Project Leader is responsible for:

- Ensuring this procedure is maintained and followed.
- Assigning a qualified staff member as the QA Coordinator.
- Assigning a qualified staff member as the SQA Coordinator.
- Providing interpretations of this procedure.
- Providing management direction in response to disagreements concerning the provisions of this procedure (e.g., required level of checking and reviewing or reference acceptability).
- 5.6 **Users** Users of approved models and derived data from the library are responsible for:
 - Notifying the QA Coordinator if problems are identified with models or derived data already in the library.
 - Ensuring that their use of the models and/or derived data obtained from the library meets the quality assurance requirements for their work.
 - Requesting that their name be included in the email notification list maintained by the SQA Coordinator.

6.0 QUALIFICATION

As stated above in Section 4.3, the QA Coordinator is responsible for ensuring the qualification of individuals acting as Originator or Reviewer for each VALID Case. General guidance for minimum requirements for qualification is provided in this section. The QA Coordinator approves each qualification, so deviations from these recommendations are allowed on a case-by-case basis.

All individuals qualified under previous revisions of this procedure maintain their qualifications. Before performing work on a VALID Case under this revision, however, they should review and understand the procedural changes instituted in Section 6.

6.1 **Originator** – Typically, an Originator will be an experienced user of the computer code or codes, which are to be used in the VALID Case. The individual will also have reviewed this procedure and provided documentation of review and understanding to the SQA Coordinator. This documentation will be combined with the resume required on file for all individuals under the SCALE QAP to form the basis for qualification.

An inexperienced code user can perform work for a VALID Case under the direction of a qualified Originator. The qualified Originator is responsible for the contents of the VALID Case. Successful completion of a VALID Case under supervision may also form the basis for a qualification for future Cases.

- 6.2 **Reviewer** Typically, a Reviewer will be an experienced user of the computer code or codes which are to be used in the VALID Case and will also have an understanding of the methods, strengths, and potential weaknesses of the techniques involved. The Reviewer will also have reviewed this procedure and provided documentation of review and understanding to the SQA Coordinator. In most cases, this documentation will already be on file to support Originator qualification. It is also desirable that in most cases and individual will serve as an Originator prior to being a Reviewer, though this is not a requirement.
- 6.3 **Expiration of Qualifications** The QA Coordinator should review the list of qualified performers periodically to ensure that personnel who should be removed from the qualified lists are appropriately identified and removed. There are neither specific requirements to maintain qualification, nor events (e.g., retirement, job changes) which necessitate termination of qualification. There is no set time limit for qualification expiration; the assignment of each performer is reviewed on a case by case basis by the QA coordinator.

7.0 **PROCEDURE**

7.1 **Initial Addition of Inputs and Data to the Library**

NOTE: If the models or data are already represented in the library, revisions and corrections should be handled according to Section 7.4 of this procedure.

7.1.1 The Requestor identifies models and derived data to be added to the library and notifies the QA Coordinator by opening a new Case in the VALID project within FogBugz. The QA Coordinator sets the Kanban status of the Case is set to "Proposed", and the FogBugz Case status is "Active (*Proposed*)". The Category for this Case should be set to "Feature".

7.1.2 The QA Coordinator either approves or rejects the request. If approved, the QA Coordinator identifies two individuals as the Originator and Reviewer for the work. The QA Coordinator may serve as either Originator or Reviewer. The Kanban status of the Case is changed to "Approved" by the QA Coordinator, and the status is changed to "Active".

The feature request is assigned a VALID Change Log (VCL) number and docketed by the SQA Coordinator. The docket number begins with VCL and is assigned a sequence number in the form *VCL-YYYY-NNN*. *YYYY* equals the current fiscal year and *NNN* represents a sequence of positive integers beginning with 001 and increasing by one for each VCL identifier assigned. The complete sequence of numbering restarts at the beginning of each fiscal year.

If rejected, the QA Coordinator notifies the Requestor, closes the Case in FogBugz, and sets the status to "Resolved (Won't Implement)". The QA Coordinator also notifies the SQA Coordinator for filing. Example reasons for rejection include (a) the requested models or data are not appropriate for library inclusion, (b) supporting references are not adequate, or (c) work cannot commence due to funding or work priority issues.

- 7.1.3 The QA Coordinator assigns the Case to an Originator and sets the Kanban status to "In Progress".
- 7.1.4 The Originator collects information about the calculations and prepares/checks the calculations using informal VALID instructions and guidance documentation.
- 7.1.5 The Originator completes documentation of the model(s) and attaches necessary documents to the Case in FogBugz. A summary of the model, a brief description of key parameters, and a list of keywords are included in the FogBugz Case. The Originator indicates in the Case that Origination is complete; this statement is equivalent to signing a document. The Case is assigned to the QA Coordinator by the Originator.
- 7.1.6 The QA Coordinator determines the necessary level of review using a graded approach. In determining level of review, the QA Coordinator may consider model source, quality of model reference, the rigor of other reviews already performed, and the expected use of the models and data. If the level of review is less

than full, the QA Coordinator provides specific review guidance to the Reviewer. A copy of the specific review guidance shall be attached to or included in the FogBugz Case. Rerunning inputs already in the library using a new version of SCALE or a new data library could be a scenario where less than the full level of review is justified.

The QA Coordinator assigns the Case to the Reviewer, and sets the Kanban status to "In Testing".

- 7.1.7 The Reviewer reviews the models, derived data, and other documentation and provides comments in the FogBugz Case. The Reviewer assigns the case to the Originator.
- 7.1.8 The Originator resolves comments with the Reviewer. If there is a difficulty in comment resolution, the QA Coordinator shall be notified. If significant work is needed to resolve the comments, the Originator assigns the Case to the QA Coordinator to reset the Kanban status to "In Progress." Moderate amounts of work to address Reviewer comments can be performed without impact to the Kanban status.
- 7.1.9 After all comments are resolved and the Case is updated, the Originator assigns the Case to the Reviewer. The Reviewer indicates in the Case that Review is complete; this statement is equivalent to signing a document. The Case is assigned to the QA Coordinator by the Reviewer.
- 7.1.10 The QA Coordinator reviews the Case for completeness and accuracy. The QA Coordinator reviews and modifies the list of proposed keywords, if necessary. If needed, the Case is assigned to the Originator and/or the Reviewer to correct deficiencies identified by the QA Coordinator.
- 7.1.11 If potential discrepancies in the source reference descriptions are identified in the Case (e.g., a potential issue with Section 3 of an International Handbook of Evaluated Criticality Safety Benchmark Experiments (IHECSBE) report), the QA Coordinator determines if further notification is appropriate. The QA Coordinator notifies the SCALE Project Leader, who is responsible for further action. The QA Coordinator opens a FogBugz Case in the "Bug" category linked to the VALID Case to record the discrepancy. This subordinate case can be closed after the appropriate notifications have been sent.
- 7.1.12 If the QA Coordinator judges the Case to be complete and

accurate, the QA Coordinator indicates approval of models and derived data for inclusion in the VALID library in the FogBugz Case. This statement is equivalent to signing a document. The QA Coordinator forwards the Case and all attachments to the SQA Coordinator. The Kanban status of the Case is set to "Ready to Ship."

NOTE: The files (and file locations) to be added to the library are identified by the QA Coordinator in the Case. The SQA Coordinator should verify that the files added to the library agree with the file names, file location, and run times and dates identified in the Case documentation. Other forms of file confirmation, such as checksums, can be provided in the documentation to provide greater assurance that the files being added to the library have not been altered.

- 7.1.13 The SQA Coordinator adds the models and derived data to the VALID library.
- 7.1.14 The SQA Coordinator records in the FogBugz Case the models and data added to the library and the date on which the files were added.

NOTE: Models and/or derived data may be generated for proprietary data. Proprietary information may be archived with appropriate access restrictions but should not be included directly in the FogBugz case or the attachments. The SCALE Project Leader and responsible ORNL Project Manager will determine an appropriate storage and access strategy on a project-by-project basis.

7.1.15 The SQA Coordinator updates the configuration control list of the SCALE VALID library. The SQA Coordinator sends an email notification of the archive action to staff listed on the email notification list (or the group list for work involving proprietary data). The SQA Coordinator adds a statement to the Case that the library has been updated and that appropriate notifications have been issued; this statement is equivalent to signing a document. The SQA Coordinator assigns the Case to the QA Coordinator.

NOTE: For addition of revised models or data to the VALID library (as addressed by Section 5.4 of this procedure) the configuration control list update and the notification email will identify that the models or data are replacements for files previously removed from the library. The configuration control list will identify the revision number for the files.

7.1.16 The QA Coordinator sets the Kanban status of the Case to "Deployed". The status of the FogBugz Case can then be set to "Resolved (Implemented)".

7.2 Use of Input and Data

- 7.2.1 Users of inputs and derived data obtained from the VALID library shall ensure that the quality assurance requirements are satisfied for the particular analyses where they use the data.
- 7.2.2 Users shall report any errors or deficiencies in the data to the QA Coordinator.

7.3 **Configuration Management of Input and Data**

- 7.3.1 File access permissions are set so that only the SQA Coordinator may modify or delete folders and files in the library.
- 7.3.2 The SQA Coordinator shall ensure that the VALID library, the configuration control list and all supporting documentation is backed up on a schedule consistent with the configuration of the hardware where the archive is maintained.

7.4 **Revisions or Corrections of Library Content**

Revision of inputs and data in the VALID library may be necessary when references are revised, model improvements are identified, modeling approximations are determined to be inappropriate, modeling errors are discovered, methodology errors are discovered, or nuclear data errors are identified. Such revisions shall be conducted in accordance with this procedure.

- 7.4.1 Upon identification of potential errors in inputs or derived data in the VALID library, the QA Coordinator instructs the SQA Coordinator to relocate the identified inputs and/or data from the library to a quarantined storage area (or to install file access restrictions) so that users cannot access the potentially flawed models and/or data.
- 7.4.2 The QA Coordinator opens a FogBugz Case in the "Bug" category, and links it to the original Case from which the files were added to the library. If the files were added under a previous revision of this procedure, this Case will not link to an older Case, but will reference the previous documentation using the VALID Form number.

- 7.4.3 The SQA Coordinator relocates the identified files or otherwise restricts general access to the files, updates the configuration control list for the VALID library, and sends an email notification of file restriction to staff listed on the email notification list (or to staff in the appropriate access group, for proprietary data).
- 7.4.4 The QA Coordinator identifies a staff member to evaluate the need for a revision and, if a revision is needed and appropriate, act as the revision Originator. The QA Coordinator assigns the Bug Case to this staff member.
- 7.4.5 The Originator reviews the potential error or proposed revision and recommends either "no revision needed," "revision recommended," or "removal of inputs and/or data from library recommended" and assigns the Case to the QA Coordinator.
- 7.4.6 If the QA Coordinator disagrees with a recommendation, the issue is forwarded to the SCALE Project Leader for resolution.
- 7.4.7 If the QA Coordinator concurs with a recommendation of no changes needed, the QA Coordinator notifies the person who originally identified the problem. He/she instructs the SQA Coordinator to (a) return the models and/or derived data to the library (or remove access restrictions) and update the configuration control list and (b) send an email notification of file reinstatement to appropriate staff. The QA Coordinator assigns the Bug Case a status of "Resolved (By Design)".
- 7.4.8 If the QA Coordinator concurs with a recommendation that the models and/or data should be revised, the QA Coordinator notifies the revision Originator to proceed with the revision. The revision is processed as described in Section 6.1. The QA Coordinator opens a new Feature Case, linked to the Bug Case, for use in the revision process described in Section 6.1. Both the Bug and Feature cases are closed when the replacement files have been added to the library.

NOTE: All replacement files shall contain, as the first characters of the title card, identification of the revision number and associated VALID Case or form number. For replacement files, example formats are "REVISION N (VALID Case XXXX)" or "REVISION N (VALID FORM XX-XXX)" followed by the case title, where "N" is the revision number (e.g., 1, 2, ...). This information must be present in the title card for all replacement files (e.g., input, output, sensitivity data files). Original files are

considered to be "Revision 0" and do not require this labeling. Revision information is <u>not</u> allowed within VALID library file names or directory names as that may interfere with the functionality of software used to perform library searches.

7.4.9 If the QA Coordinator concurs with a recommendation that the models and/or data should be permanently removed from the library, the QA Coordinator notifies the person who originally identified the problem. He/she instructs the SQA Coordinator to archive the removed files with restricted access, and to update the configuration control list to reflect that the models and/or data have been permanently removed from the library. The QA Coordinator assigns the Bug Case a status of "Resolved (Won't Fix)". The SQA Coordinator notifies the VALID user list that the files have been removed and will not be replaced, and the QA Coordinator provides the SCALE project leader with justification for the permanent removal of the files.