United States Environmental Protection Agency
Office of Environmental Information Washington, DC 20460
EPA/240/R-02/007
December 2002

Guidance for Quality Assurance Project Plans for Modeling

EPA QA/G-5M

Quality

FOREWORD

The U.S. Environmental Protection (EPA) Agency has developed the Quality Assurance (QA) Project Plan as a tool for project managers and planners to document the type and quality of data and information needed for making environmental decisions. This document, *Guidance for Quality Assurance Project Plans for Modeling (EPA QA/G-5M)*, contains advice and recommendations on how to develop a QA Project Plan for projects involving the model development or application using data acquired from other sources.

EPA works every day to produce quality information products. The information used in these products are based on Agency processes to produce quality data, such as the quality system described in this document. Therefore, implementation of the activities described in this document is consistent with EPA's Information Quality Guidelines and promotes the dissemination of quality technical, scientific, and policy information and decisions.

This document was designed for internal use and provides guidance to EPA program managers and planning teams. It does not impose legally binding requirements and may not apply to a particular situation based on the circumstances. EPA retains the discretion to adopt approaches on a case-by-case basis that differ from this guidance where appropriate. EPA may periodically revise this guidance without public notice.

This document is one of the U.S. EPA Quality System Series documents. These documents describe the EPA policies and procedures for planning, implementing, and assessing the effectiveness of the Quality System. As described in EPA Manual 5360 A1 (EPA, 2000a), this document is valid for a period of up to five years from the official date of publication. After five years, this document will be reissued without change, revised, or withdrawn from the U.S. EPA Quality System Series documents. Questions regarding this document or other Quality System Series documents should be directed to the Quality Staff at:

U.S. EPA
Quality Staff (2811R)
1200 Pennsylvania Ave., NW
Washington, DC 20460
Phone: (202) 564-6830
Fax: (202) 565-2441
E-mail: quality@epa.gov

Copies of EPA Quality System Series documents may be obtained from the Quality Staff directly or by downloading them from its Home Page:

www.epa.gov/quality

ACKNOWLEDGMENTS

This guidance document benefitted greatly from comments from many reviewers with experience in environmental modeling and in quality assurance in both early internal reviews and review by the Council on Regulatory Environmental Modeling. The Models 2000 Quality Assurance and Peer Review Action Team at EPA was especially instrumental in developing the first working draft of this guidance.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

INTRODUCTION

1.1 WHAT ARE EPA'S QUALITY RELATED POLICIES REGARDING ENVIRONMENTAL MODELING?

The EPA Quality System defined in EPA Order 5360.1 A2 (EPA, 2000d), *Policy and Program Requirements for the Mandatory Agency-wide Quality System*, includes coverage of environmental data produced from models. Environmental data includes any measurement or information that describe environmental processes, location, or conditions; ecological or health effects and consequences; or the performance of environmental technology. For EPA, environmental data includes information collected directly from measurements, produced from models, and compiled from other sources such as databases or literature. The EPA Quality System is based on an American National Standard, ANSI/ASQC E4-1994.

Consistent with the National Standard, E4-1994, Section §6.a.(7) of EPA Order 5360.1 A2 states that EPA organizations will develop a Quality System that includes "approved Quality Assurance (QA) Project Plans, or equivalent documents defined by the Quality Management Plan, for all applicable projects and tasks involving environmental data with review and approval having been made by the EPA QA Manager (or authorized representative defined in the Quality Management Plan). More information on EPA's policies for QA Project Plans is provided in Chapter 5 of the *EPA Manual 5360 A1* (EPA, 2000a), *EPA Quality Manual for Environmental Programs* and *Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA, 2001). This guidance helps to implement the policies for models defined in Order 5360.1 A2.

1.2 WHAT INFORMATION DOES THIS GUIDANCE PROVIDE?

This guidance provides information about how to document quality assurance planning for modeling (e.g., model development, model application, as well as large projects with a modeling component). A "model," for the purpose of this guidance, is something that creates a prediction. The elements of QA Project Plans for data collection are described in *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA, 2001) and *EPA Manual 5360 A1* (EPA, 2000a). Further details on developing these QA Project Plans are described in *EPA Guidance for Quality Assurance Project Plans (QA/G-5)* (EPA, 1998a).

This guidance is based on the recommendations and policies from the above EPA documents, but is written especially for modeling projects, which have different quality assurance concerns than traditional environmental monitoring data collection projects. If you are familiar with the QA Project Plan structure described in these documents, you will find that the structure for the QA Project Plan for modeling is consistent with those in *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA, 2001) and *EPA Guidance for Quality Assurance Project Plans (QA/G-5)* (EPA, 1998a), though for modeling not all elements are included because not all are relevant.

1.3 WHY IS PLANNING FOR MODEL DEVELOPMENT AND APPLICATION IMPORTANT?

Planning for modeling projects is just as important as planning traditional environmental measurements for data collection projects. In order to be able to use model output for anything from regulatory purposes to research, you should be sure that the model is scientifically sound, robust, and defensible. The way to ensure this is by following a thorough planning process that incorporates the following elements:

- a systematic planning process including identification of assessments and related performance criteria;
- peer reviewed theory and equations;
- a carefully designed life-cycle development process that minimizes errors;
- documentation of any changes from the original plan;
- clear documentation of assumptions, theory, and parameterization that is detailed enough so others can fully understand the model output;
- input data and parameters that are accurate and appropriate for the problem;
- output data that can be used to help inform decision making.

These features lead to confidence in results. The steps for documenting these processes will be described in an EPA QA Project Plan for modeling efforts.

A QA Project Plan and good project management in modeling projects are closely tied together. A good QA Project Plan is valuable to a modeling project in the following ways:

- A QA Project Plan documents all the criteria and assumptions in one place for easy review and referral by anyone interested in the model.

- A QA Project Plan can be used to guide project personnel through the model development or application process and helps ensure that choices are consistent with the established objectives and project-specific requirements.

Using a consistent format makes it easy for others to review information on models and ensures that no steps are overlooked in the planning phase.

1.4 WHAT QUESTIONS DOES THIS GUIDANCE ADDRESS?

For quick reference to the information in this document, Table 1 provides a summary of the main questions addressed by this guidance and indicates the chapter and sections containing this information.

Table 1. Questions this Guidance Addresses

Questions	Chapter/Section
What are the guidelines for preparing QA Project Plans for projects that involve model development or model application?	2.1 (overview) Chapter 4 (details)
Who is responsible for developing and reviewing these QA Project Plans?	2.2
How do I document changes from the planned process described in the QA Project Plan?	2.4
How do the model development and model application processes relate to the QA Project Plan contents?	Chapter 3 (Figure 4)
How does peer review relate to quality assurance activities?	3.2.2
How are acceptance and performance criteria used in a modeling project?	3.1.3, 3.2.2, 4.1.7, 4.3.1, 4.4.1
Where are the records and documentation planned for this modeling effort described?	4.1.9
Where are the model calibration plans described?	4.2.1
What information on non-direct measurements (i.e., secondary use of existing data) should be included in a QA Project Plan for model development or application?	4.2.2
Where are the model evaluation plans described?	4.3
Where are the assessment plans for acceptance of final model results described?	4.4
Where are assessment activities documented in a QA Project Plan?	4.3, 4.4

1.5 WHO CAN BENEFIT FROM THIS DOCUMENT?

This guidance has many potential users, including all those involved in planning and implementing modeling projects or in reviewing modeling projects. Specifically,

- *Modelers* can use this guidance to see how the modeling development and application processes are linked to the various elements that are documented in the QA Project Plan. This guidance will help them to prepare and review a QA Project Plan.

- *Managers* of model development and application projects will find this guidance useful for understanding how planning is related to developing good models, and how the EPA policies defined in EPA Order 5360.1 A2 can be met.

- *QA reviewers and QA officers* will find this guidance useful for understanding the steps and details behind the planning—especially those who might not be familiar with the model development process. This guidance will help these users clearly understand how the quality system is applied to model development.

1.6 WHAT IS THE GRADED APPROACH TO QA PROJECT PLANS, AND HOW DO I DETERMINE WHAT QUALITY ASSURANCE AND QUALITY CONTROL ACTIVITIES ARE NEEDED FOR A SPECIFIC PROJECT?

EPA defines the graded approach as "the process of basing the level of application of managerial controls applied to an item or work according to the intended use of the results and degree of confidence needed in the quality of the results" (EPA, 1998a). This is an important element of the Quality System because it allows the application of quality assurance and quality control activities to be adapted to meet the rigor needed by the project at hand. Models that provide an initial "ballpark" estimate or non-regulatory priorities, for example, would not require the same level of quality assurance and planning as models that will be used to set regulatory requirements. There are no explicit categorizations or other specific guidelines for applying the graded approach, but the information in this section and in the examples (Chapter 5) should provide some insight into how to do so.

In applying the graded approach, two aspects are important for defining the level of QA effort that a modeling project needs: <u>intended use</u> of the model and the <u>project scope and magnitude</u>.

- The <u>intended use</u> of the model is a determining factor in the level of QA needed because it is an indication of the seriousness of the potential consequences or impacts that might occur due to quality problems. For example, Table 2 shows that higher standards would be set for projects that involve potentially large consequences, such as Congressional testimony, development of new laws and regulations, or the support of litigation. More modest levels of defensibility and rigor would be acceptable for data used for technology assessment or "proof of principle," where no litigation or regulatory action are expected. Still lower levels of defensibility apply to basic exploratory research requiring extremely fast turn-around, or high flexibility and adaptability. In such cases, the work may have to be replicated under tighter controls or the results carefully reviewed prior to publication. By analyzing the end-use needs, appropriate QA criteria can be established to guide the program or project. These examples are presented for illustration only, and the degree of rigor needed for any particular project should be determined based on an evaluation of the project needs and resources.

Table 2. Examples of Modeling Projects with Differing Intended Uses

Purpose for Obtaining Model-Generated Information (Intended Use)	**Typical Quality Assurance Issues**	**Level of QA**
• Regulatory compliance • Litigation • Congressional testimony	• Legal defensibility of data sources • Compliance with laws and regulatory mandates applicable to data gathering	
*		
• Regulatory development • State Implementation Plan (SIP) attainment • Verification of Model	• Compliance with regulatory guidelines • Existing data obtained under suitable QA program • Audits and data reviews	
*		
• Trends monitoring (non-regulatory) • Technology development • "Proof of principle"	• Use of accepted data-gathering methods • Use of widely accepted models • Audits and data reviews	
*		
• Basic research • Bench-scale testing	• QA planning and documentation at the facility level • Peer review of novel theories and methodology	

- Other aspects of the QA effort can be established by considering the scope and magnitude of the project. The scope of the model development and application determines the complexity of the project; more complex models need more QA effort. The magnitude of the project defines the resources at risk if quality problems lead to re-work and delays.

The scope and magnitude of the project should be considered when defining:

- type and extent of programmer's and end user's documentation,
- testing effort and documentation of test results,
- rigor of quality objectives and criteria,
- cost and schedule control.

Specific examples of how the considerations described above may be used to define a project's QA effort are provided in Chapter 5.

1.7 HOW DOES THIS GUIDANCE FIT IN THE EPA QUALITY SYSTEM?

The EPA Quality System structure was designed for data collection activities. However, because modeling can also produce data that will be used in decision making, quality issues are also relevant for these data. The paradigm needs to be modified, as indicated in Figure 1, for application to data produced by models rather than data produced by sampling and analytical measurement of environmental media. Figure 1 portrays the project portion of EPA's Quality System. Systematic planning, an important first step, calls for stated and clarified objectives. In this step, objectives are clarified. Quality control will include peer review of theory and approach, code evaluation, and/or procedures for model calibration. Quality assurance of input data and parameter values are important to model quality. Because the input data will most likely be obtained from other

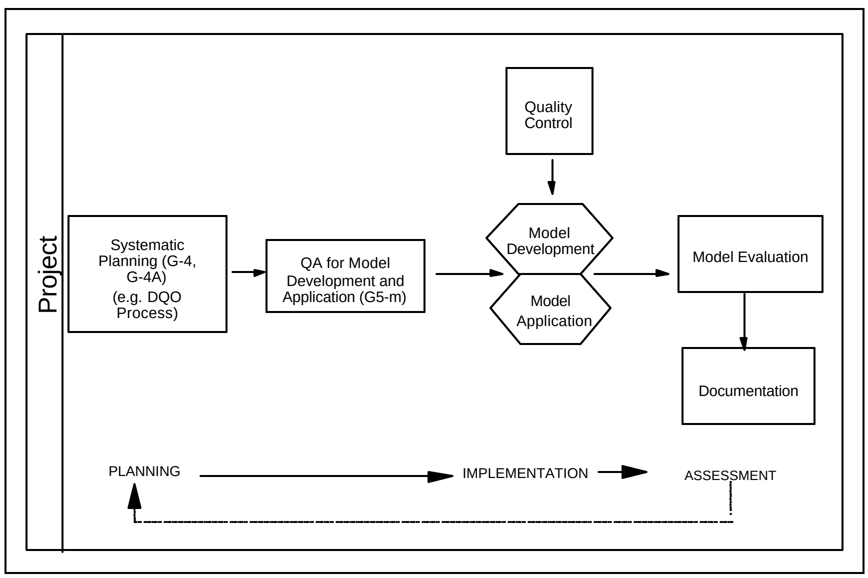

Figure 1. EPA Quality System Approach to Addressing Environmental Data Generated from Model Application

sources, data quality procedures for secondary data use should be followed. After the process of model development or application is complete, evaluation of the model output is completed. Documentation is completed or updated at the end of the model development or application process.

1.8 HOW IS THIS DOCUMENT ORGANIZED?

This document will best be used as a reference document rather than a "how-to" guide to be read front-to-back. To that end, Chapter 2 contains relevant information about EPA policies regarding QA Project Plans. Chapter 3 describes the typical planning processes a modeler would use to develop or apply a model and provides linkages to the elements in a QA Project Plan for modeling. Chapter 4 contains a description of the QA Project Plan elements, interpreted for a modeling project. Finally, Chapter 5 contains examples of the content of a QA Project Plan that illustrate the planning process for model development and model application. Three types of projects are described to give an indication of the graded approach and how different problems might be addressed with different levels of detail and description. These are not full QA Project Plans, but are meant to give an idea of the information that would be included in such a plan.

A checklist is provided in Appendix C that can be used when writing a QA Project Plan for modeling. This checklist indicates the basic pieces of information that may be relevant for each element. A glossary and a list of references are also included in the appendices.

CHAPTER 2

QA PROJECT PLAN PROCEDURES

This chapter provides a summary of guidelines for preparing QA Project Plans in projects that involve model development, modification, or application.

2.1 GENERAL EPA POLICY ON QA PROJECT PLANS

The QA Project Plan is a key component of the EPA Quality System and is the "blueprint" by which individual projects are implemented and assessed. EPA Order 5360.1 A2 (EPA, 2000d) establishes a mandatory, Agency-wide Quality System that applies to EPA and all organizations performing work for EPA. These organizations need to ensure that data collected and used for the characterization of environmental processes and conditions are of the appropriate type and quality for their intended use. The applicability of this policy to modeling is based on the "use" of environmental data (as stated in the policy).

A QA Project Plan is necessary in modeling projects even when no monitoring or other environmental data measurements are performed because modeling results frequently serve as a surrogate for these data, or are used for their interpretation. EPA allows flexibility in the organization and content of a QA Project Plan to meet the unique needs of each project or program. Note that while most QA Project Plans will describe project- or task-specific activities, there may be occasions when a *generic* QA Project Plan may be more appropriate. A generic QA Project Plan describes, in a single document, the information that is not site-, process-, or time-specific but applies throughout the program (e.g., of a specific model for a defined use). Application-specific information is then added to the approved QA Project Plan as that information becomes known or completely defined. A generic QA Project Plan is reviewed periodically to ensure that its content continues to be valid and applicable to the program over time.

2.2 QA PROJECT PLAN RESPONSIBILITIES

The QA Project Plan for a program or project may be prepared by an EPA organization, a contractor, an assistance agreement holder, or another Federal agency under an interagency agreement. Except where specifically delegated, all QA Project Plans prepared by non-EPA organizations need to be approved by EPA before implementation. However, EPA may grant conditional approval to a QA Project Plan to permit some work to begin while non-critical deficiencies in the QA Project Plan are being resolved. EPA Order 5360.1 A2 also states that all QA Project Plans shall be implemented as approved for the intended work. All personnel should understand the project-specific requirements prior to the start of data generation activities (including generation or interpretation of environmental data using modeling techniques).

For model development projects, one or more staff members who are intimately familiar with the scientific and technical details of the modeling (scientist, meteorologist, programmer, etc.) are usually designated as lead modeler of the QA Project Plan. Input from the modeling staff is critical in preparing sections of the QA Project Plan that list the critical model structure and parameters to be tested, the criteria that the tests need to meet, and the methods to evaluate the test results. In larger projects involving a staff of model developers, it is appropriate to include one or more individuals with software development, testing, and QA expertise to contribute to the QA Project Plan in areas of documentation, configuration control, test plan development, coding standards, etc. The project manager is ultimately responsible for assessing whether the performance and acceptance criteria for the intended modeling use were met and works iteratively with the intended users of the results.

In projects involving routine use of well-accepted environmental models, the project staff may lack personnel who are familiar with the software's internal operations. In this situation, a senior scientist who understands the quality objectives and performance criteria and who can assess the model's performance in the context of the project is a good candidate for preparing or reviewing the QA Project Plan and deciding if model documentation is sufficient (e.g., proprietary software). The project manager is ultimately responsible for assessing the appropriateness of the chosen model(s) for the particular application and assessing whether the performance and acceptance criteria were met and works iteratively with the intended users of the results.

2.3 QA PROJECT PLAN ELEMENTS FOR ENVIRONMENTAL MODELING

This section lists the elements of a QA Project Plan defined in *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA, 2001). Subsequent chapters of this document will provide detailed information about these elements with the emphasis on modeling projects. However, some titles of the QA Project Plan elements listed below are slightly different in subsequent chapters to emphasize the application to modeling.

Elements of a QA Project Plan Defined in the *EPA Requirements for Quality Assurance Project Plans* (EPA, 2001)			
A. Project Management			
A1	Title and Approval Sheet	A6	Project/Task Description
A2	Table of Contents	A7	Quality Objectives and Criteria
A3	Distribution List	A8	Special Training/Certification
A4	Project/Task Organization	A9	Documents and Records
A5	Problem Definition/Background		

B. Measurement/Data Acquisition			
B1	Sampling Process Design	B6	Instrument/Equipment Testing, Inspection, and Maintenance
B2	Sampling Methods	B7	Instrument/Equipment Calibration and Frequency
B3	Sample Handling and Custody	B8	Inspection/Acceptance Requirements for Supplies and Consumables
B4	Analytical Methods	B9	Non-direct Measurements
B5	Quality Control	B10	Data Management
C. Assessment and Oversight			
C1	Assessment and Response Actions	C2	Reports to Management
D. Data Validation and Usability			
D1	Data Review, Verification, and Validation	D3	Reconciliation with User Requirements
D2	Verification and Validation Methods		

2.4 REVISIONS AND RELATED GUIDANCE

2.4.1 Revisions and Review

Because of the complex and diverse nature of environmental data operations, changes to QA Project Plans, methods, and objectives are sometimes needed. When a substantive change is warranted, the QA Project Plan needs to be modified to reflect the change and those changes needs to be submitted for approval. According to EPA policy, a revised QA Project Plan needs to be reviewed and approved by the same authorities that performed the original review.

Changed procedures may be implemented only after the revision has been approved. Changes to the technical procedures should be evaluated by the EPA QA Manager and Project Officer to determine if they significantly affect the technical and quality objectives of the modeling project. If the procedural changes are determined to have significant quality impacts, the QA Project Plan should be revised and re-approved, and a revised copy should be sent to all persons on the distribution list. Only after the revision has been received and approved (at least verbally with written follow-up) by project personnel, can the change be implemented.

For programs or projects of long duration, QA Project Plans should be reviewed at least annually by the EPA Project Manager. *Guidance for Quality Assurance Project Plans (QA/G-5)* (EPA, 1998a) and *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA, 2001) contain additional information applicable to QA Project Plan revisions.

2.4.2 Related Guidance

EPA QA policy and guidelines are based on the National Consensus Standard, ANSI/ASQC E4-1994, *Specifications and Guidelines for Environmental Data Collection and Environmental Technology Programs* (ANSI/ASQC, 1995). This standard describes the quality management elements that are generally common to environmental problems, regardless of their technical scope. It also discusses the specifications and guidelines that apply to project-specific environmental activities involving the generation, collection, analysis, evaluation, and reporting of environmental data.

EPA Requirements for Quality Assurance Project Plans (EPA, 2001) and *Guidance for Quality Assurance Project Plans* (EPA, 1998a) have been developed consistent with ANSI/ASQC E4-1994. These documents are the primary references for preparing, approving, and revising QA Project Plans for EPA projects and programs. Other guidance documents are available that provide background information and techniques that may be helpful for preparing QA Project Plans for modeling projects, including: *Quality Assurance of Multi-media Model for Predictive Screening Tasks* (EPA, 1999c) and *Systems Development Life Cycle Methodology (SDLCM) Statement of Policy, Standards and Guidelines* (EPA, 2000f).

CHAPTER 3

THE MODEL DEVELOPMENT AND APPLICATION PROCESS: RELATIONSHIP TO QA PROJECT PLAN ELEMENTS

What is the purpose of this chapter? This chapter shows the modeler which elements of a QA Project Plan are linked to specific quality aspects or features of a typical model development or application project. In this chapter, the general process for conducting a model development or application project is presented. The process is divided into three basic *steps*, which are further subdivided into *tasks*. These tasks are then mapped to one or more elements of the QA Project Plan according to the types of procedures conducted and the data quality issues that need to be addressed within each task. Thus, this chapter introduces the modeler to the relevant elements of a QA Project Plan for a modeling project, within the context of a general modeling process with which the modeler is familiar.

What is the general process for conducting a model development or application project? While each modeling project is unique, most projects that involve model development and application typically follow a process similar to the one illustrated in Figure 2. The three steps in this process are the following:

1. *Modeling Needs and Requirements Analysis*: Use a systematic planning process to determine modeling needs and project-specific requirements and to decide whether or not a model currently exists that can be used to achieve these needs and requirements.

2. *Model Development*: Develop a new model in situations where no existing model can be used to address the particular study objective.

3. *Model Application*: Apply an existing model (identified from a model selection procedure when more than one model is relevant) or a newly developed model.

For projects in which modeling is only a part of the total effort, the modeling process may be preceded by a systematic planning process as indicated in Figure 2, in which quality objectives for the entire project are established. The process in Figure 2 is iterative in nature, as reviews and checks occur within the process to ensure that the model outputs will address all necessary project objectives and meet necessary performance criteria. The iterative aspect also provides flexibility to accommodate the exploratory and evolutionary nature of many model development projects.

The individual tasks performed within each step in Figure 2 are linked to one or more elements of the QA Project Plan. The QA Project Plan elements associated with a given task specify the type and quality of information that is needed to execute that task. This linkage (or "cross-walk") between

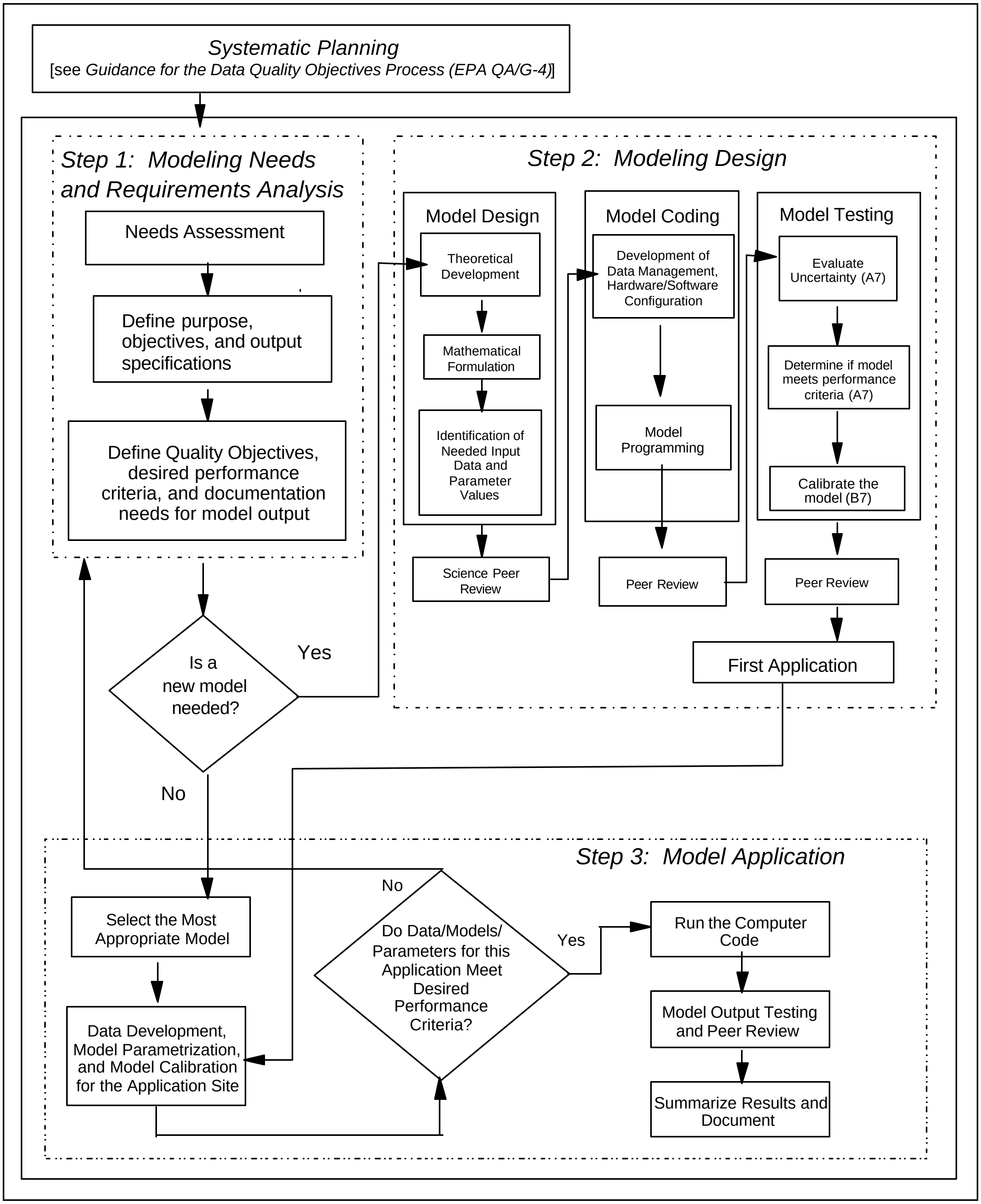

Figure 2. Typical Life-Cycle of a Three Step Modeling Project

the modeling tasks and the elements of the QA Project Plan is described in Sections 3.1 through 3.3 of this chapter.

3.1 MODELING NEEDS AND REQUIREMENTS ANALYSIS

The first step of the modeling process consists of the following three tasks:

- assess the need(s) of the modeling project;
- define the purpose and objectives of the model and the model output specifications;
- define the quality objectives to be associated with the model outputs as described in Section 4.1.7, and the examples in Chapter 5.

The modeling planning team uses the outcomes of these three tasks to determine whether an existing model can be used or a new model needs to be developed. Figure 3 indicates how information generated in these tasks is documented in the specific QA Project Plan elements.

3.1.1 Needs Assessment

The regulatory or scientific need for using a model (versus, for example, using existing data or collecting new measurements) and the necessary features of the model should be specified within Element A5 (Problem Definition/Background) of the QA Project Plan. The individuals or organizations that would address these needs (e.g., members of the planning team, decision makers, statisticians, principal data providers and users, computer hardware and software development personnel, statistical expertise, QA Manager), along with their specific roles and responsibilities and their relationships and organizational structure within the project, should be documented in Element A4 (Project/Task Organization).

Expertise or certification requirements within the study team should be documented in Element A8 (Special Training Requirements/Certification) of the QA Project Plan. Examples are specialized computer hardware/software programmers and analysts, certified quality assurance managers, project managers, and statisticians experienced in performing goodness-of-fit tests, characterizing uncertainty, and conducting sensitivity analyses.

3.1.2 Define Purpose, Objectives, and Output Specifications

Element A6 (Project/Task Description and Schedule) of the QA Project Plan describes the approach that will be used to meet the needs identified in the needs assessment. This element also is used to provide an overall understanding of the modeling project, the work to be performed, the model outputs to be obtained, and the project implementation schedule.

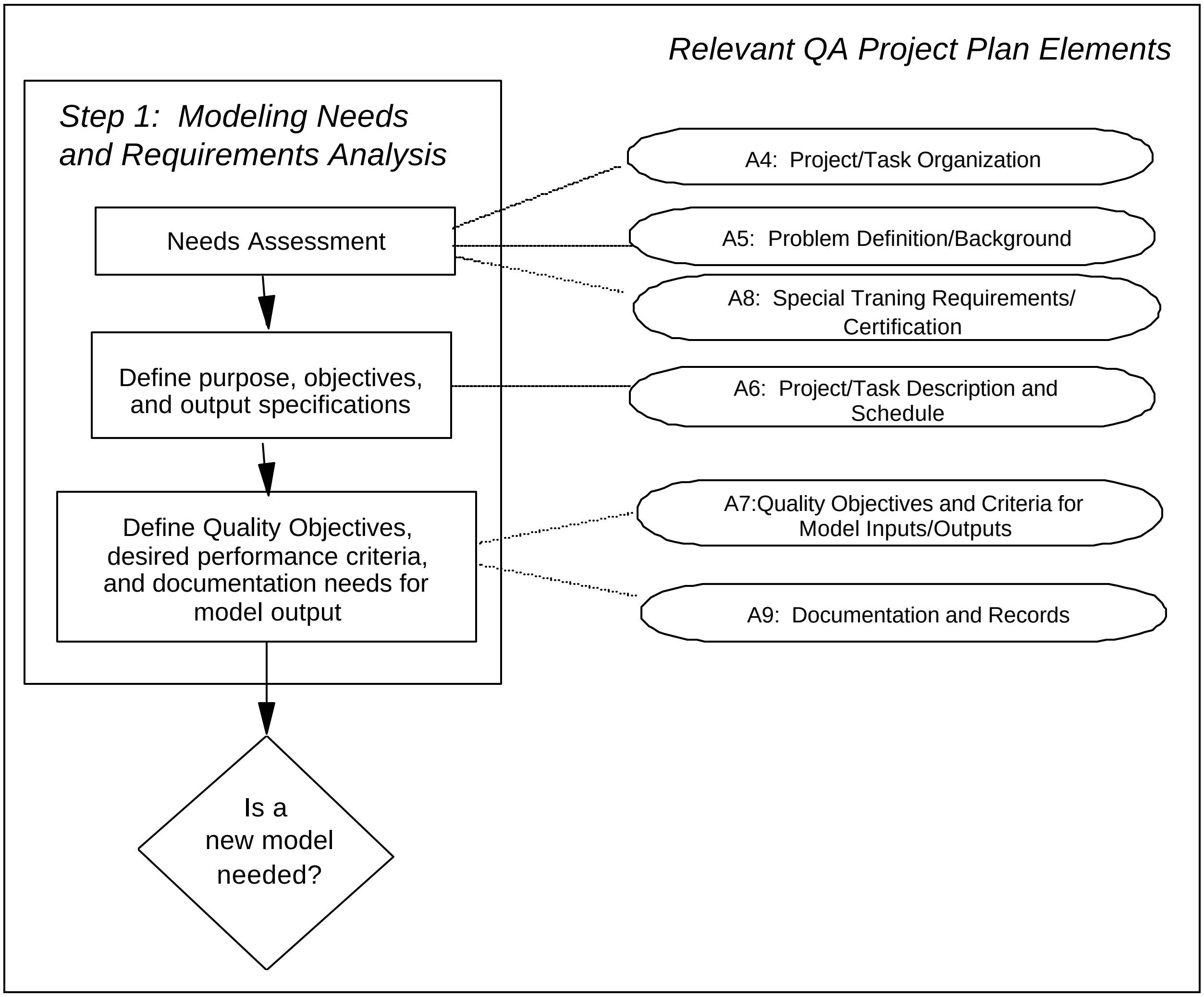

Figure 3. Map of QA Project Plan Elements to Modeling Tasks. *Information for the QA Project Plan Elements is generated in the indicated modeling task in the Modeling Needs and Requirements phase of the modeling process.*

3.1.3 Define Quality Objectives, Desired Performance Criteria, and Documentation Needs for Model Output

On a model development or application project, quality objectives and the qualitative and quantitative model performance criteria to be associated with the model output are determined by implementing a *systematic planning process*. This process addresses questions such as the following:

- How accurately and precisely does the model need to predict a given quantity at the application site or in the process step of interest in order to satisfy regulatory or scientific objectives?

- What are appropriate criteria for making a determination of whether the model estimate is accurate and precise enough (e.g., based on past general expertise combined with site or process specific knowledge)?

- How would these criteria be used to determine whether model outputs achieve the needed quality? For example, what goodness-of-fit test [e.g., chi-square test on predicted and observed frequency distributions (Snedecor & Cochran, 1989); t-test on predicted and observed Robust Highest Concentrations (Cox and Tikvart, 1990); t-test of differences in normalized means squared errors of regime averages from two models (ASTM D6589)] would be performed (e.g., to compare predicted and observed frequency distributions) and what significance level and power does this test need to achieve and what other program specific criteria will be considered (e.g., Guideline on Air Quality Models 40 CFR Part 51 Appendix W)?

The quality objectives and performance criteria that are established from implementing the systematic planning process are to be documented in QA Project Plan Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs). The possible negative consequences of making inappropriate decisions due to poor model prediction ability are a key concern.

Element A9 (Documentation and Records) of the QA Project Plan will specify those project records to be included in reports and other documents, the model testing or data assessment reporting formats, document control procedures, documentation of response actions during the project to correct model development or implementation problems, and procedures for the final disposition of records and documents, etc.

3.1.4 Is a New Model Needed?

In general, a new model is developed for a given application when an existing model cannot meet the needs and requirements for the new application without major adjustments. The process of identifying and assessing existing models for a new application begins with the analysis of modeling needs and requirements and makes use of the information documented in Elements A5 (Problem Definition/Background), A6 (Project/Task Description and Schedule), and A7 (Quality Objectives and Criteria for Model Inputs/Outputs) of the QA Project Plan, as discussed in the previous sections, along with information from Element B9 (Non-direct Measurements). Given this information, the types of questions that are generally asked when assessing the need for a new model include:

- For what specific tasks will the model be used in the given application?

- What data will be collected or obtained to characterize the application site and to develop a site conceptual model that will be compared with existing models? What is the needed spatial and temporal scale of the model inputs?

- What model outputs are needed? What is the spatial and temporal scale needed for the outputs?

- What levels of uncertainty are acceptable in model outputs?

- What are the strengths and weaknesses of existing models?

- If an existing model is available, are its parameter default values, input data, boundary conditions, and underlying assumptions acceptable?

- Is the existing model software compatible with the modeler's hardware/software configuration requirements for the new application?

- Are any improvements in the existing model's computer code operating characteristics (e.g., run time) needed?

- Do the quality and documentation associated with the existing model meet the project-specific requirements?

In addition, if multiple options for a model are being evaluated, model selection may involve evaluating the needed complexity of the model relative to the given project. Using a complex model over a simpler model may have certain drawbacks if the project does not need such complexity, while using a simpler model to address a more complex problem may result in an inability to meet certain performance criteria.

3.2 MODEL DEVELOPMENT

If the modeling needs and requirements specify that a new model is needed, then the model development process (Step 2) in Figure 2 is executed. There are four phases to Model Development: Model Design, Modeling Coding, Model Testing, and First Application, which are shown in Figure 4 and described in the sections below.

Peer review can be incorporated in many different parts of the model development, as appropriate for the level of complexity of the model and the degree of confidence needed in the model output. There are different types of peer review, from a simple review by a few easily accessible internal experts, to an elaborate peer review panel of independent experts who provide detailed written evaluations. The places in the process in which peer review can typically take place are described in subsequent sections, and is indicated by an underlining of the phrase "peer review" so that these steps can be easily found in the descriptions of the model development processes.

3.2.1 Model Design

As shown in Figure 4, the model design process consists of three phases: theoretical development, mathematical formulation, and identification of input data. As the first step in theoretical development, in order to develop a model which accurately reflects the process that takes place, a *conceptual model* of this process may be developed (e.g., identifying what is known or hypothesized to be the source, environmental transport, and fate of a contaminant) or assemble information on a toxicological pathway. This conceptual model or information should be described in Elements A5 (Problem Definition/Background) and A6 (Project/Task Description and Schedule) of the QA Project Plan. The conceptual model is then used as a starting place for the construction of explanations behind the process to be modeled. The theoretical formulation of the model would include any formulation known about the processes being modeled that will link it to the desired output.

Next, the model theory is transformed into mathematical algorithms and equations, including sub-models (modules) and model parameters, so that appropriate model outputs (predictions) can be computed. This *mathematical formulation of the theory* involves identifying algorithms and equations that have been developed to support this model theory or, if such equations are not already available, developing these equations. The sources of these algorithms, including assumptions and limitations, should be documented according to project-specific requirements contained in Element A9 (Documentation and Records) of the QA Project Plan.

Once the algorithms are developed, the *identification of needed input data and parameter values* is undertaken. The data sets that are identified as possible sources should be evaluated for quality, including relevance and appropriateness for the scenario this model is being developed to address. If non-direct measurements (i.e, existing data from computer databases, programs, literature files, or other historical sources) may be used as input to the model or as values for model parameters, the methods to be used to evaluate these data for quality should be described in Element B9 (Non-direct Measurements) of the QA Project Plan.

The scientific concepts supporting model design can be assessed in a science <u>peer review</u> during this phase. A science peer review would evaluate the soundness of the theoretical approach, the relevance of the theory to the problem at hand, and the appropriateness of the translation of the theory into mathematical formulation. The necessary documentation from this peer review process should be described in Element A9 (Documentation and Records), and might also be subject to project-specific

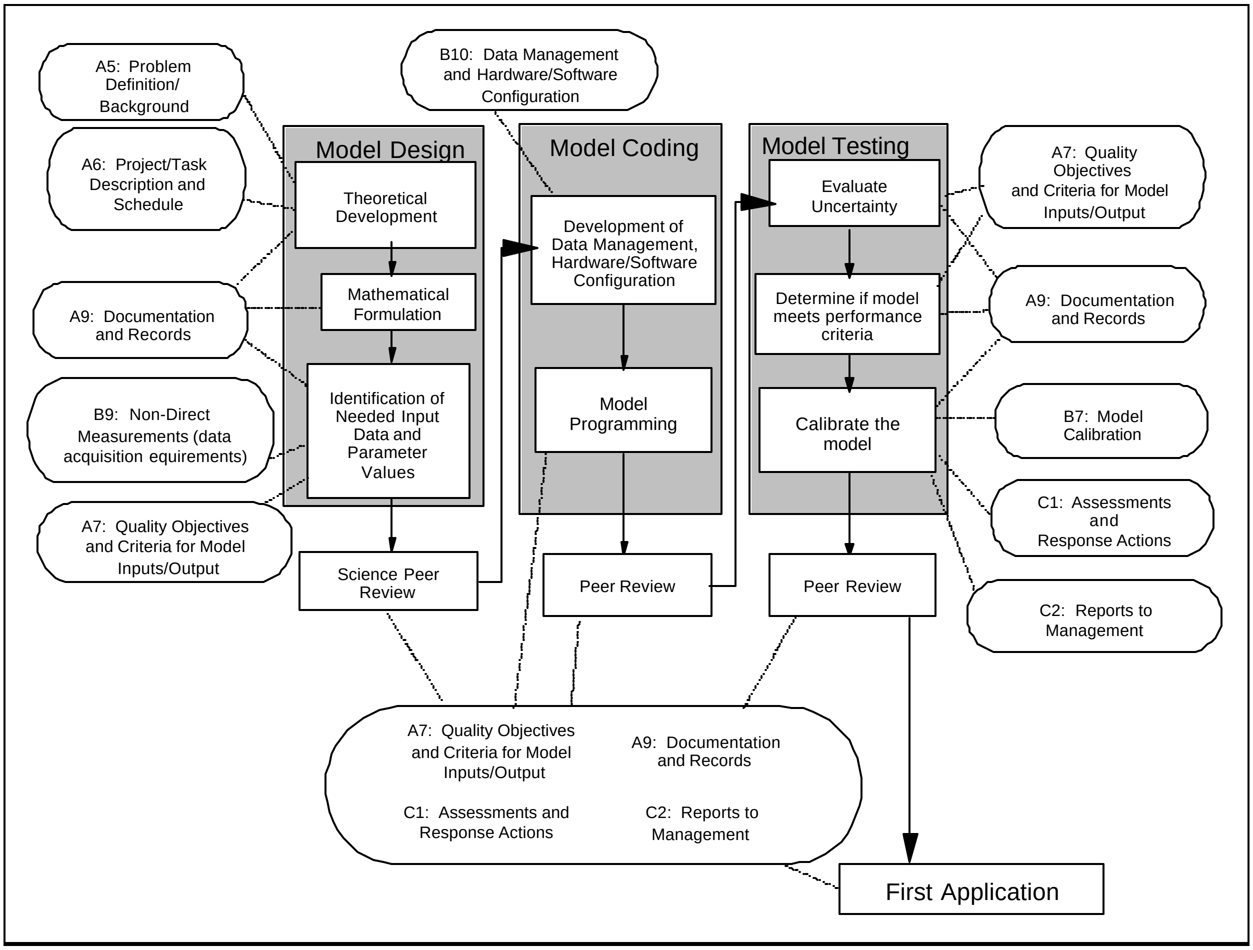

Figure 4. Map of the QA Elements to Step 2 Model Design Tasks. *Information from the QA Project Plan Elements is relevant for the indicated modeling tasks in the Model Development phase of the modeling process.*

requirements specified in Element C1 (Assessment and Response Actions) of the project's QA Project Plan.

3.2.2 Model Coding

The process of converting the science formulations to model code is usually begun after any science peer review has been completed and any necessary changes (corrective actions) have been completed. The process begins by developing the data management process and the computer hardware and software configuration requirements. The data management process consists of tracing the path, mathematical and computational operations, and quality control of "as-acquired" model input data and model predictions from their generation to their final use, storage, and documentation. Computer hardware and software configuration involves devising the data handling equipment and procedures, including required computer hardware/software and related code performance requirements (e.g., run time) needed to compile, process, manipulate, evaluate, and assess the input data and model predictions. It also involves establishing coding and configuration control requirements to ensure consistency. Modules should be compartmentalized so that they can be tested independently, and should be tested in sequence to verify consistency and compatibility between the modules. Section 3.2.3 provides more details on model testing. These requirements and criteria should be listed in QA Project Plan Element B10 (Data Management and Hardware/Software Configuration). During this phase, the results of the assessments of these requirements should be documented according to the project-specific requirements specified Element A9 (Documentation and Records) of the project's QA Project Plan.

Then, *model coding*, or the transformation of the model equations and related algorithms into an integrated and efficient computer code, is undertaken. This process involves the work of computer programmers working closely with the scientists to ensure that the theory is accurately represented in the code. Decisions might have to be made in cases where the theory cannot exactly be replicated in the code for technical reasons, and these compromises should be reached by the scientists and programmers working together.

The next part of model coding involves *calibration*. Calibration is the process of refining the model to achieve a desired degree of correspondence between the model output and actual observations of the environmental system or process the model is intended to represent. The focus is usually on the estimation and characterization of empirical parameters and parameterizations of the modeled processes. Element B7 (Calibration) specifies the procedures to be implemented to ensure that the mathematical representations and parameters used in models are reasonable to achieve the accuracy requirements specified in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs) of the project's QA Project Plan.

The final task in code development is to test the computer code and have it reviewed by external *peer reviewers* (if required) to ensure that the code is error free and achieves all requirements specified in Elements A7 (Quality Objectives and Criteria for Model Inputs/Outputs) and B10 (Data Management and Hardware/Software Configuration) of the QA Project Plan. The code assessment process (i.e., when they are to occur and the possible corrective actions to be taken) is described in Element C1 (Assessment and Response Actions). Such assessments may result in revisions to the model code, which may need additional follow-up assessments.

3.2.3 Model Testing

Before formal model testing, uncertainty (i.e., lack of knowledge) should be characterized for all stages of model design, namely: the conceptual model, the theoretical basis of the model, the mathematical formulation of the theory, the parameters and parameter values used, and the input data and assumptions. The natural variability of the relevant population(s) should also be characterized (note natural variability often limits certainty attainable, better data only provides better definition of those limits). As seen in Figure 5, these sources of variability and uncertainty affect how the model outputs are distributed and, as a result, the level of uncertainty in the output values (see EPA 1996 and 1997 for more detail). Requirements for the acceptable degree of uncertainty should have been specified in Element A7 (Quality Objective an Criteria for Model Inputs/Outputs) in the QA Project Plan during the planning stage. Element B9 (Non-direct Measurements) defines acceptable uncertainty associated with the existing data used in the modeling process. Finally, the documentation and records of assessments of uncertainty and software performance requirements are specified in Element A9 (Documentation and Records).

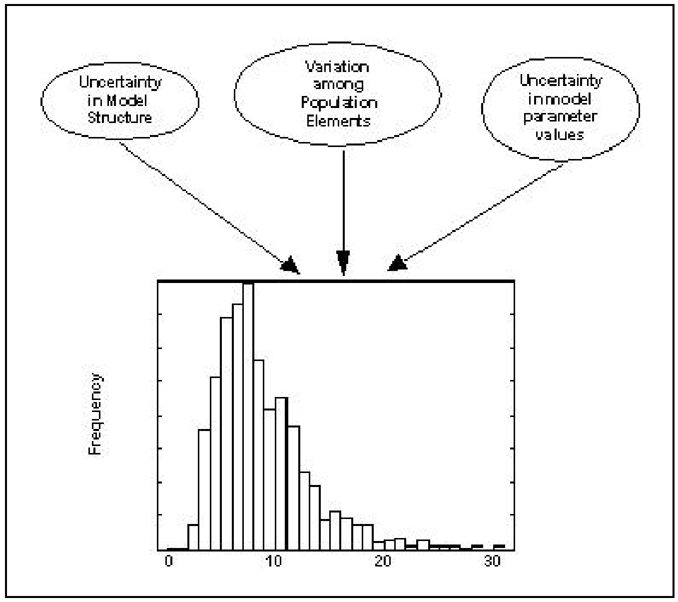

Figure 5. Propagation of Uncertainty and Variability

The model design team then *evaluates the uncertainty* in the modeling output by comparing the output with available field or lab data. If inadequacies are found [that is, if the uncertainty and variability exceed the limits specified in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs)], part of the model design process may be revisited and changes made; this assessment and review phase of model development is frequently iterative in nature. Next, the model design team assesses whether the final form of the model *can achieve the remaining performance criteria* specified in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs) of the QA Project Plan. This assessment may be done using statistical model fitting and evaluation methods (e.g., Draper & Smith, 1981) if appropriate data exist and can be obtained for comparison to model predictions. Other model-specific statistical evaluations (e.g., American Society for Testing and Materials, 2000) may also be undertaken. If appropriate data are not available, model outputs can be compared with those of an accepted model (also known as “benchmarking”) or other methods can be used (see Chen & Beck, 2000 for some examples). The method and results of these assessments are documented according to specifications given in Element A9 (Documentation and Records). If the model design team cannot be assured that the performance criteria will be met by the given model, then either the model’s needs and performance criteria need to be reassessed or revisions made to the model such that the criteria are met.

Once the model design team determines that the model will be able to achieve the overall performance criteria listed Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs), a <u>*peer review*</u> phase is recommended to assess how well the model design specifications were actually implemented. Although a formal peer review process is preferred, this may not always be possible due to project constraints. Scheduling of peer reviews, the peer review mechanism to be used, and documentation of the responses to peer review comments throughout model development is documented in Element C1 (Assessment and Response Actions). Reports to management resulting from peer reviews are described in Element C2 (Reports to Management) with management of peer review records in Element A9 (Documentation and Records).

The quality assurance assessment of the model is documented within the Group D QA Project Plan elements. Element D1 (Departures from Validation Criteria) details the criteria used to decide if the model outputs meet the requirements specified in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs) of the project's QA Project Plan. Element D2 (Validation Methods) describes the process for determining whether errors exist in the model output or if model outputs achieve required project quality levels. Element D3 (Reconciliation with User Requirements) describes the methods to be used to analyze the model outputs (as well as other site-related information and data) to determine whether anomalies exist or if assumptions established in the planning phase are not being met.

3.2.4 First Application

The first application of the model is considered to be a part of model development, because the model cannot be deemed complete until it has been shown that it can be successfully applied in a given situation. Ideally, the developers will be able to *apply the model* to a particular scenario during model testing using data from field and/or lab studies to compare the output. The *assessment of quality* for the output is assessed in the same manner that subsequent applications will be. Section 3.3 will describe the objectives and processes for these steps in more detail.

Elements C1 (Assessment and Response Actions) and C2 (Reports to Management) would apply to assessments of input data and model parameters as shown in Figure 6 and described in Sections 3.3.2 to 3.3.5. During the first application, calibrations may be employed to set parameter values with site-specific data using procedures described in Element B7 (Calibration). The records of calibration results are identified and their management defined in Element A9 (Documentation and Records). Element C1 (Assessment and Response Actions) should describe when to assess the performance of the model through comparisons with field or lab data, and also describes any corrective actions to be taken. Reports documenting the assessment methods and the results obtained are defined in Element A9 (Documentation and Records).

3.3 MODEL APPLICATION

Once models have been identified (or developed) for the project or routine application, the model application process (Step 3) in Figure 2 is executed. Figure 6 shows how the various tasks in the model application process are linked to specific QA Project Plan elements.

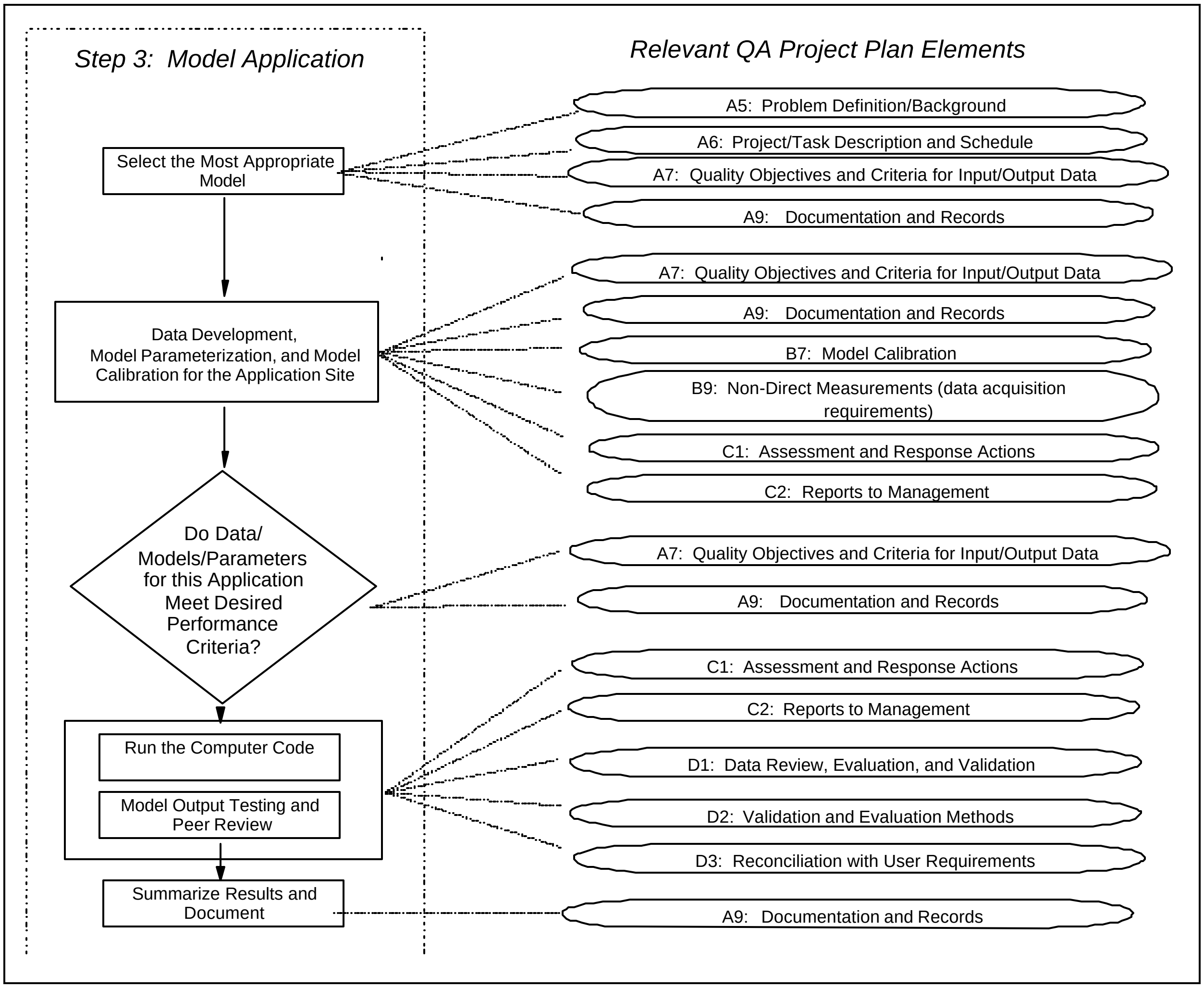

Figure 6. Map of QA Project Plan Elements to Modeling Tasks. *Information for the QA Project Plan Elements is relevant for the indicated modeling task in the* <u>*Model Application*</u> *phase of the modeling process.*

3.3.1 Select the Most Appropriate Model

When multiple models are relevant to a particular model application (see www.epa.gov/epahome/models.htm), the most appropriate model is determined by considering the particular problem that the project is addressing, any important background material that may impact the type of model used, the project's scope and available resources, the underlying objectives, and any results of statistical modeling procedures [e.g., as discussed in Draper and Smith (1981) and Berthouex and Brown (1994)]. The criteria established for selecting an appropriate model are presented in Elements A5 (Problem Definition/Background), A6 (Project/Task Description and Schedule), and A7 (Qaulity Objectives and Criteria for Model Inputs/Outputs) of the QA Project Plan. The results of the model selection procedure, in addition to the information going into the selection process, are reported according to the procedures specified in Element A9 (Documentation and Records).

3.3.2 Consider Site- or Process (Pathway)-Specific Information

The second task is to tailor the model to the specific application by identifying the most current and appropriate data, parameter values, expert opinion, and assumptions that are consistent with model requirements. If appropriate, the model is calibrated using data and methods that apply to the site, process or pathway and application of interest following procedures and methods defined in Element B7 (Calibration), with the results managed as specified in Element A9 (Documentation and Records). Statistical methods for fitting calibration curves using appropriate data should be used whenever possible [see e.g., Berthouex and Brown (1994, pp. 213-220)]. Additional activities include implementing quality control (QC) for input data and specifying any special data management, computer hardware/software configuration, or project documentation requirements. The performance criteria for these activities are provided as appropriate in Elements A7 (Quality Objectives and Criteria for Model Inputs/Outputs), B7 (Calibration), and B9 (Non-direct Measurements), and the documentation requirements for these activities are provided as appropriate in Elements C2 (Reports to Management) and A9 (Documentation and Records) of the QA Project Plan. Element C1 (Assessment and Response Actions) describes when assessments will be conducted and the corrective actions, if any, to be taken.

3.3.3 Are Performance Criteria Met?

After the first two tasks, the model inputs and parameter estimates for the given application are evaluated based on whether they meet the performance and acceptance criteria specified in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs). If not, previous steps and tasks (e.g., overall modeling needs and requirements) need to be revisited, depending on the nature of the discrepancy. Application of the model using data from one or more field or lab studies not employed during model development allows assessments to support accepting, rejecting, or qualifying the model output for its intended use.

3.3.4 Generate and Assess Model Outputs

If model inputs and parameter estimates for the given application meet performance and acceptance criteria, the model's computer code is executed to obtain initial model outputs (predictions), and the outputs are assessed against performance criteria specified in QA Project Plan Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs). Initial assessments (i.e., site-specific code has no errors or mistakes and comparisons with field or lab data) are conducted as indicated in QA Project Plan Element C1 (Assessment and Response Actions). Assessment findings (e.g., need for corrective action) are reported as indicated in Element C2 (Reports to Management) and documented as indicated in Element A9 (Documentation and Records). The methods for final assessments [i.e., whether the final results are reasonable, address all project objectives, are technically useable, and meet performance specifications as specified in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs) are documented in QA Project Plan Elements D1 (Departures from Validation Criteria) and D2 (Validation Methods). Elements D3 (Reconciliation with User Requirements) and A9 (Documentation and Records) define the documentation needed from the assessments specified in Elements D1 (Departures from Validation Criteria) and D2 (Validation Methods). Element D2 (Validation Methods) describes the methods to be used to analyze the model outputs (as well as other site-related information and data) to determine whether anomalies exist or if assumptions established in the planning phase are not met. Once it is determined that the model provides technically useable outputs, the full suite of model runs is conducted. Each run would be subject to continued surveillance of output quality using the methods and criteria specified in the QA Project Plan [Elements A9 (Documentation and Records), C1 (Assessment and Response Actions), C2 (Reports to Management), D1 (Departures from Validation Criteria), D2 (Validation Methods), and D3 (Reconciliation and User Requirements)].

3.3.5 Summarize Results and Document

The last task in model application is to document the model outputs, the results of assessing these outputs, and the need to place caveats on the use of those outputs. The project-specific documentation and reporting requirements are described in Element D3 (Reconciliation and User Requirements) and A9 (Documentation and Records) of the QA Project Plan.

CHAPTER 4

ELEMENTS OF QUALITY ASSURANCE PROJECT PLANS FOR MODELING PROJECTS

This chapter provides details on the types of information that are included within each element of a QA Project Plan for a modeling project. This chapter differs from Chapter 3 in that Chapter 3 is focused around the general modeling process and provided an overview of how the elements of the QA Project Plan were linked to various tasks within this process. Chapter 3 follows the typical sequence of these tasks within a modeling project. In contrast, this chapter describes each QA Project Plan element in the order in which the elements appear in the QA Project Plan. As such, it is structured similarly to Chapter 3 of *EPA Requirements for Quality Assurance Project Plans (EPA QA/R-5)* (EPA, 2001) and Chapter 5 of EPA Order 5360 A1 (EPA 2000a).

As discussed in Section 1.6, EPA quality assurance guidance allows for a graded approach to preparing QA Project Plans, in which the level of detail is based on the scope and magnitude of the project and the intended use of the model. This chapter describes QA Project Plan elements for projects where a new model is developed or an existing model is revised, and this model is being applied for the first time to a given test application. Various types of modeling projects may need more or less detail (e.g., subsequent applications) than what is suggested in this chapter based on the scope, magnitude, and intended use of the model output.

Like the QA Project Plan, this chapter presents each element in a separate section, with the sections organized by the four element groupings. Each section is preceded by a text box containing a summary of the element's features as specified within *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA, 2001), with alterations occasionally made to this summary to make it more specific to a modeling project.

4.1 GROUP A: PROJECT MANAGEMENT

All nine Group A elements presented in *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA, 2001) are relevant and important to address in the QA Project Plan for a modeling project, and each is addressed in the following Sections 4.1.1 through 4.1.9.

4.1.1 Title and Approval Sheet (A1)

Include title of plan; name of the organization(s) implementing the project; effective date of the plan; and names, titles, signatures, and approval dates of appropriate approving officials.

The title and approval sheet documents the following information on the QA Project Plan:

- title, document number (if appropriate), revision number (Revision 0 corresponds to the first version), and effective date of the given revision;

- name of each organization involved in implementing the various stages of the modeling project (e.g., modeling organization, software contractor);

- names, titles, and affiliation of the officials of each organization who will approve the QA Project Plan (e.g., project managers, principal investigators, QA Managers, EPA project manager/program officer, EPA QA Officer), along with space for their dated signatures. [These officials are also represented in the project's organizational chart within Element A4 (Project/Task Organization).]

Examples of title and approval sheets can be found within QA Project Plans that are posted on EPA's Quality Staff web site (www.epa.gov/quality). The signatures of the key project officials on this page document their official awareness and approval of the QA Project Plan, and therefore, the project's goals and procedures. The specified dates of the signatures indicate when the plan was approved, which constitutes the earliest start date for the model development and/or application efforts addressed in the plan (i.e., Steps 2 and 3 of the modeling process as documented in Chapter 3.)

4.1.2 Table of Contents and Document Control Format (A2)

Provide a table of contents for the document, including sections, figures, tables, references, and appendices. Apply a document control format on each page following the Title and Approval Sheet when required by the EPA Project Manager and QA Manager.

The table of contents allows easy access to information contained in the plan. It includes the titles of all sections, subsections, tables, and figures, along with the page numbers within the document where each of these can be found. When required by the EPA Program Manager and QA Manager, a document control format such as that in Figure 7 appears in the upper right-hand corner of each page of the QA Project Plan. It includes the QA Project Plan's section number, revision number and date (as stated on the title and approval sheet), the page number, and the total number of pages either in the given section or the entire document.

Section No.________
Revision No._______
Date______________
Page_____of_______

Figure 7. Example of a Document Control Format

4.1.3 Distribution List (A3)

List the individuals and their organizations who need copies of the approved QA Project Plan and any subsequent revisions, including all persons responsible for implementation (e.g., project managers), the QA Managers, and representatives of all groups involved. Paper copies need not be provided to individuals if equivalent electronic information systems can be used.

The QA Project Plan's distribution list facilitates the control of the document by helping ensure that the most current QA Project Plan is in use by all project participants.

4.1.4 Project/Task Organization (A4)

Provide a concise organizational chart showing the relationships and the lines of authority and communication among all project participants. Include other model results users who may be outside the group that are developing and applying the model, but for whom the model outputs are intended. Identify any subcontractor relationships relevant to the modeling project.

Identify the individuals or organizations participating in the project and discuss their specific roles and responsibilities. Include the principal users of the model output, the decision makers, the project QA Manager, and all persons responsible for implementation. The project QA Manager must be independent of the unit generating the data or software. Identify the individual responsible for maintaining the official, approved QA Project Plan.

A model development or application project often consists of several different tasks that can involve different groups and organizations. It is important for the QA Project Plan to officially document the responsible organizations and key players on the project, lines of authority and reporting, and the relationships and official lines of communication between and among them.

The organizations involved and their responsibilities on the project should be identified, followed by text descriptions of key individuals participating in the project and an organizational chart such as the example in Figure 8. The key individuals on modeling projects may include the project manager, project QA Manager, managers of the software/hardware configuration, the person responsible for maintaining the QA Project Plan, principal users of the model output, decision makers (such as the person responsible for model selection, if a selection is possible), and other persons responsible for implementing the QA Project Plan and for approving deliverables. The specific roles, activities, and responsibilities of these positions on the project should be highlighted in their descriptions.

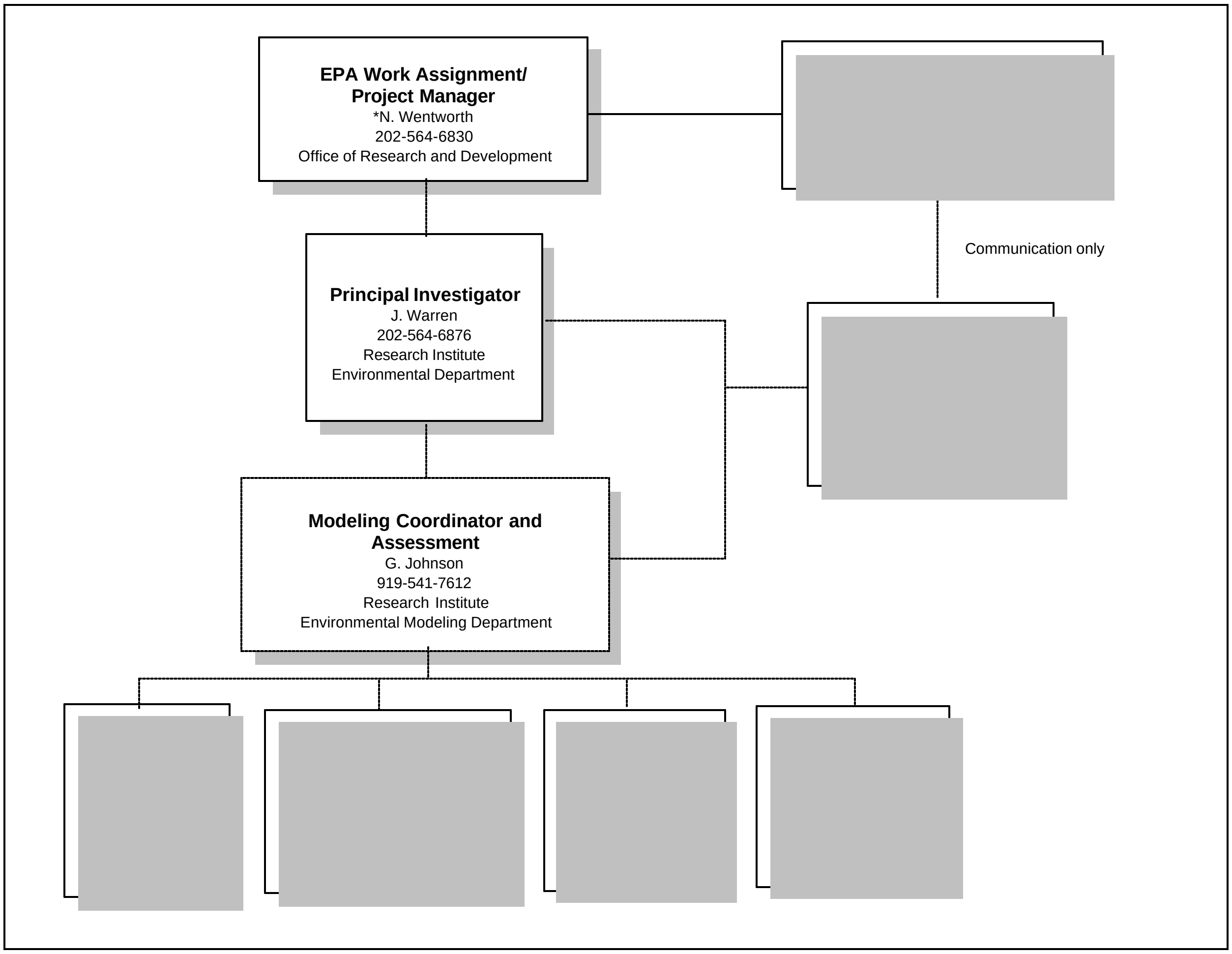

Figure 8. Example of an Organizational Chart for a Modeling Project

The project organization chart shows the lines of authority and communication among key individuals on the project. If direct contact between project managers and users of model output does not occur (e.g., between modelers and decision makers), the organization chart should show the path that the information takes from one group to the other.

4.1.5 Problem Definition/Background (A5)

State the specific problem to be solved, decision to be made, or outcome to be achieved. Include sufficient background information to provide a historical, scientific, and regulatory perspective for this particular project.

This element of the QA Project Plan states the problem to be addressed by the modeling project with detail sufficient to allow a technically-trained reader to understand both the scientific need for the project and how the project's objectives and activities will address the problem. The types of decisions to be made are also documented in this QA Project Plan element. "Stating the Problem" and "Identifying the Decision" are the first two steps of EPA's approach to systematic planning and the Data Quality Objectives Process, as documented in *Guidance for the Data Quality Objectives Process (QA/G-4)* (EPA, 2000b) and highlighted in Section 4.1.7 below. Questions that the QA Project Plan may address when defining the problem include the following:

- What is the specific problem? What are the goals and objectives of this project that will address this problem?

- What population in the environment does the problem specifically target, and what measure(s) within this population does the problem address?

- Why should a modeling approach be used to address the problem? Is there a regulatory requirement for a modeling analysis?

- What specifically will this project produce to address this problem (e.g., a new predictive tool, modeling results for a new scenario)?

- What types of decisions regarding the problem may be made as a result of this project?

- Who will be responsible for making these decisions?

- Will any aspect of the problem not be addressed in this project?

- What other types of problems may this project address?

It is important to place the problem in historical perspective to give readers and users a sense of the project's purpose and position relative to other project and program phases and initiatives. Such information also indicates the importance of generating new information and suggests tools that may be available to do this. Therefore, sufficient background information should be provided in the QA Project Plan to answer the following types of questions, when applicable:

- Why is this project important, and how may it support proposed or existing research, programs, initiatives, regulations, or other legal directives?

- How may this project "fit in" with other on-going, broader efforts?

- What types of conflicts or uncertainties currently exist that will be resolved by this project?

- What information, previous work, or previous data may currently exist that this project can use?

- Given that the problem is best solved by a modeling approach, what models currently exist (if any) that can be used to achieve this project's goals and objectives? If multiple models exist, how is one determined to be better than the others for this application?

The presentation of background information can include a discussion of initial ideas or approaches for model development or application that were considered when selecting the approach described under "Project/Task Description and Schedule" (Element A6).

4.1.6 Project/Task Description and Schedule (A6)

Provide a summary of all work to be performed, products to be produced, and the schedule for implementation. The discussion need not be lengthy or overly detailed, but should give an overall picture of how the project will resolve the problem or question described in Element A5 (Problem Definition/Background).

An overview of the various tasks to be involved in the model development and/or application effort is provided in this section of the QA Project Plan, along with the general technical approach and the quality activities and procedures associated with these tasks. The discussion should present the various tasks in relation to each other, and as a result, should allow the effort to resolve the problem specified in Element A5 (Problem Definition/Background). This discussion need not be overly lengthy or burdensome to prepare, as it is primarily meant to provide an overview. For detailed information, references can be made to other available documents, other sections of the QA Project Plan, or to a contact person who can distribute the information.

For modeling projects, examples of tasks that can be addressed in the overview (but not necessarily detailed here) include the following:

- how the conceptual model of the problem or site will be developed;

- how the structural model and data processing software will be obtained;

- how data may be acquired for model development, calibration, and testing;

- the criteria used to decide whether probabilistic model output or point estimates are needed; and

- assessments relative to associated project-specific quality requirements.

This element of the QA Project Plan also lists the products, deliverables, and milestones to be completed in the various stages of the project, along with a schedule of anticipated start and completion dates for the milestones and deliverables, and the persons responsible for them.

4.1.7 Quality Objectives and Criteria for Model Inputs/Outputs (A7)

Describe the quality objectives for the project and the performance criteria to achieve those objectives. EPA policy is to use a systematic planning process [see EPA Order 5360.1 A2 (EPA, 2000d)] to define quality objectives and performance criteria.

This element of the QA Project Plan introduces the quality criteria that the expected components and outcomes of the modeling project need to achieve in order to meet the needs of the user. These criteria are specified within *performance or acceptance criteria* that are developed in a *systematic planning process*. Systematic planning identifies the expected outcome of the modeling project, its technical goals, cost and schedule, and the criteria for determining whether the inputs and outputs of the various intermediate stages of the project, as well as the project's final product, are acceptable. This is usually an iterative process involving at least modelers and users. The goal is to ensure that the project will produce the right type, quality, and quantity of data to meet the user's needs. EPA Order 5360.1 A2 (EPA, 2000d) states that EPA environmental programs should use a systematic planning process to develop acceptance or performance criteria when collecting, evaluating, or using environmental data (e.g., information produced from models).

The systematic planning process can be applied to any type of data-generating project. The seven basic steps of the systematic planning process are illustrated in Figure 9. The first three steps can be considered preliminary aspects of scoping and defining the modeling effort, while the last four steps relate closely to the establishment of performance criteria or acceptance criteria that will help ensure the quality of the model outputs and conclusions. While both are measures of data quality, *performance criteria* are used to judge the adequacy of information that is newly-collected or generated on the project, while *acceptance criteria* are used to judge the adequacy of existing information that is drawn from sources that are outside of the current project. Generally, performance criteria are used when data quality is under the project's control, while acceptance criteria focus on whether data generated outside of the project are acceptable for their intended use on the project (e.g., as input to a model) [see *Guidance on Systematic Planning for Environmental Data Collection Using Performance and Acceptance Criteria (QA/G-4A)* (EPA, 2002)].

Systematic planning is based on a graded approach. This means that the extent of systematic planning and the approach to be taken should match the general importance of the project and the intended use of the data. For example, when modeling is to be used on a project that generates data to be used either for decision making (i.e., hypothesis testing) or to determine compliance with a standard, EPA recommends that the systematic planning process take the form of the *Data Quality Objectives (DQO) Process* that is explained in detail within *Guidance for the Data Quality Objectives Process (QA/G-4)* (EPA, 2000b).

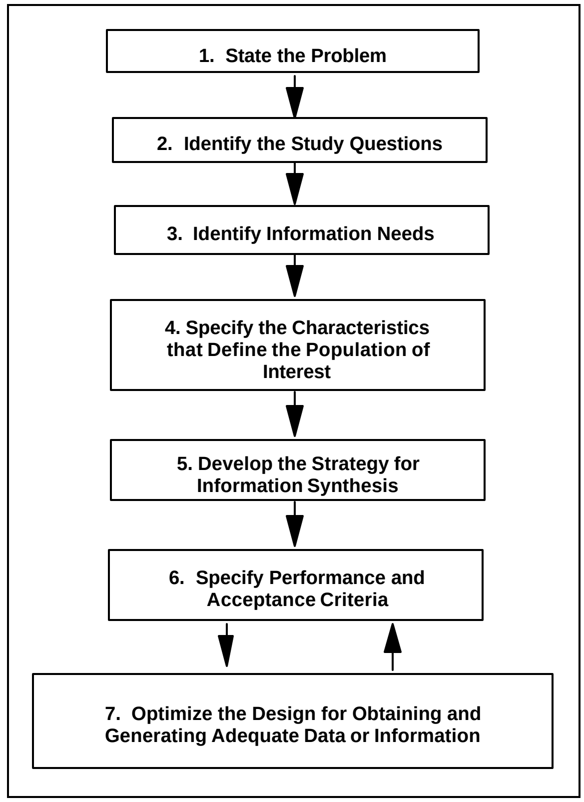

Figure 9. The Systematic Planning Process

The primary feature of this QA Project Plan element is the set of performance or acceptance criteria associated with data quality within the various stages of the modeling process, as determined from applying a systematic planning process. For decision-making programs in which the systematic planning process takes the form of the DQO Process, these criteria are represented within DQOs (EPA, 2000b) that express data quality relative to achieve tolerable levels of potential decision errors.

What types of issues do the performance or acceptance criteria that result from systematic planning address in a modeling project? The performance or acceptance criteria developed by the project planning team (see Section 3.1.1) address the following types of components for modeling projects:

- the particular type of task being addressed and the intended use of the output (e.g., predictions) of the modeling project to achieve this task;
- the type of output needed to address the specific regulatory decision (if relevant), including whether probabilistic or point estimates are needed;
- the statistical criteria (e.g., limits on decision error) to be used in the model-building process to identify those variables considered statistically important to the prediction process and included as input to the model;

- desired limits placed on the probability of making a certain type of decision error due to the uncertainty associated with the model output (if a decision is to be made) and/or criteria to demonstrate the model performs adequately (e.g., as well or better than a previously accepted model for a given situation);

- how the parameter, input, calibration, and test data necessary for this project are acquired and evaluated for use in model development and/or in producing output;

- requirements associated with the hardware/software configuration (e.g., run time or processing capabilities) for those studies involving software evaluation.

While DQOs state the user's data needs relative to a given decision, corresponding criteria need to be placed on the data to determine whether the data have satisfied these needs. For modeling projects, such quality criteria can be placed on outcomes such as software performance (e.g., run time or processing capabilities) and model prediction (e.g., acceptable level of uncertainty associated with model prediction, relative to decision error). This element of the QA Project Plan links the DQOs with appropriate *data quality indicators (DQIs)*, which measure features of data quality such as precision (i.e., variability in data under prescribed similar conditions), bias (i.e., systematic error), accuracy, representativeness, completeness, and comparability. Although the level of rigor with which this is done and documented within the QA Project Plan can vary widely depending on the particular type of modeling project, this linkage represents an important advancement in implementing quality assurance.

Evaluation of model data may also include uncertainty and variability assessment which can be introduced here, with details provided in the Group C and D elements. Requirements for a specified level of uncertainty and/or variability can also be specified under this element.

Once the performance or acceptance criteria have been established, it is possible to specify software performance and corresponding parameterization, input, and test requirements. These specifications are made within the Group B elements of the QA Project Plan.

4.1.8 Special Training Requirements/Certification (A8)

Identify and describe any specialized training or certifications needed by personnel in order to successfully complete the project or task. Discuss how such training will be provided and how the necessary skills will be assured and documented.

This element identifies and documents any specialized training requirements and technical expertise of the project team for the modeling project. Training requirements can include expertise in certain scientific disciplines (e.g., statistics), in code development or testing in a specific computer language, in data assessment, and in model development, evaluation or application. Usually the organizations participating in the project are responsible for conducting training and obtaining any required certification for their staff.

The issues outlined in this element (when relevant) include:

- the specific training, expertise, and certifications required, and the project team member(s) required to have them;
- specific dates or a time frame for training sessions or certifications;
- plans for securing the services of qualified staff with the necessary training and/or certification;
- plans for documenting the achievement of training requirements and certifications. (All certificates or documentation representing completion of specialized training should be maintained in personnel files.)

4.1.9 Documentation and Records (A9)

Describe the process and responsibilities for ensuring that appropriate project personnel have the most current approved version of the QA Project Plan, including version control, updates, distribution, and disposition. Itemize the information and records that must be included in the given data reporting format and specify the reporting format for hard copy and any electronic forms. Records can include data from other sources, model input and output files, and results of model calibration and testing. Identify any other records and documents applicable to the project that will be produced, such as test or data assessment reports, interim progress reports, and final reports. Specify or reference all applicable requirements for the final disposition of records and documents, including location and length of retention period.

Preparing appropriate documentation for quality assurance purposes is important for all environmental data operations, but especially so for modeling projects. Note that the title for this element uses the broader term documentation instead of "documents" as in *Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA, 2001) because in modeling items like internal notes in the code may need to be described. Information on how a model was selected, developed, evaluated, and applied (as relevant) on a given project needs to be documented so that sufficient information is available for model testing and assessment, peer review, and future model application.

Like the other QA Project Plan elements, the scope and magnitude of the project drives the types of records and level of detailed documentation to be kept, and consequently, specified within this element. For example, organizations conducting basic model research have different reporting requirements than organizations producing predictions for regulatory decision making, in which documentation needs to be sufficient to allow the model results to be re-created. Examples of specific types of issues related to records and documentation for a modeling project that this element may address include the following:

- formats of the different types of data reporting packages (e.g., model parameterization, model input, model calibration, model output), which need to be consistent with the requirements and procedures for data assessment described in the remainder of the QA Project Plan;

- document control and distribution procedures;

- storage requirements (may be governed by regulatory requirements, organizational policy, or contractual project requirements);

- backup plans for paper and electronic storage;

- approvals (e.g., when changes or updates to records or documents are necessary);

- retention periods; and

- persons responsible for the various facets of record keeping (e.g., storage, tracking, access, updates, obtaining approvals, distribution, final disposition).

Table 3 contains examples of records and documentation that may be relevant for some modeling projects. Note that the QA Project Plan itself is addressed here, although information on document control, distribution, updates (as necessary), and approvals for the QA Project Plan are specified in earlier elements.

Table 3. Examples of Important Reporting and Documentation on a Modeling Project

Project Phase/Document	Type of Documentation
Systematic Planning	Quality Assurance Project Plan
Implementation (Oversight)	Approach/Concept Peer Review Reports Model User's Guide (including application examples)
	Standard Operating Procedures

Table 3. Examples of Important Reporting and Documentation on a Modeling Project

Project Phase/Document	Type of Documentation
	Assessment Reports for Acquired Data Input and Test Data Sets Code Verification Report Hardware/Software Configuration Test Report Source Code Calibration Report Model Assessment Reports (i.e., sensitivity analyses, comparison of output to field or lab data or output of another model, reasonableness checks, uncertainty analyses) Configuration Management and Maintenance Manuals
Results Assessment	Assessment Reports for Output Data Output Data Set and Use Constraints Metadata Report of Peer Review Comments

When peer review is necessary during the modeling process, the materials required for peer review drive reporting and documentation needs on a modeling project. For example, peer reviewers need access to model evaluation records in order to address the following types of peer review charge questions (see EPA, 1994):

- What databases were used to provide an adequate test?
- What were key assumptions and the model's sensitivity to them?
- Is the documentation of model code and verification testing adequate?
- How well does the model report variability and uncertainty in its output?

This element of the QA Project Plan should specify the types of documentation that will be necessary for peer review and how such information will be generated, maintained, and distributed.

If candidate models are assessed as part of a model selection process, certain documentation (e.g., code verification, testing results, user's guide, application examples) are needed to ensure that the model selected meets necessary acceptance criteria, such as criteria placed on hardware/software configuration. Details on documentation of the project's hardware/software configuration are provided within Section 4.2.3 of this guidance document [QA Project Plan Element B10 (Data Management and Hardware/Software Configuration)].

The final output data reporting package includes individual records that represent actions taken to achieve the objectives of the modeling project and the performance of specific QA functions. The QA Project Plan should discuss how these various components will be assembled to represent a concise and accurate record of all activities that impact data quality.

Example of EPA policy on documentation. EPA's Risk Assessment Forum (EPA, 1997) has established policy requiring sufficient documentation of the approach to a risk assessment before its conclusions can be considered acceptable (EPA, 1996). Examples of model-related features that should be documented on risk assessment projects include:

- all models used and assumptions made that can impact results,
- the rationale used to select the methods to propagate uncertainty and variability through the model and to conduct sensitivity analyses of the model,
- the statistical goodness-of-fit methods and other rationale used to decide which statistical distributions should be used to characterize the uncertainty or variability of model input parameters,
- how the number of Monte Carlo simulations necessary to achieve sufficiently stable probabilistic model results was determined,
- how the methods used to elicit expert opinion on models and model inputs were selected and implemented.

4.2 GROUP B: MEASUREMENT AND DATA ACQUISITION

The Group B elements focus on the quality procedures that are implemented when acquiring, generating, and handling data to develop or apply a predictive tool or model. Chapter 3 showed that the Group B elements are addressed when determining whether a new model needs to be developed, when performing various tasks within model design and coding, and when preparing a model for a particular application. The data acquisition methods are introduced within the project overview provided in Element A6 (Project/Task Description and Schedule), and the Group B elements provide detailed information on these methods.

Input data for model development and application efforts are typically collected outside of the modeling effort or generated by other models or processing software. These data need to be properly assessed to verify that a model characterized by these data would yield predictions with an acceptable level of uncertainty. To this end, the Group B elements address various aspects of data acquisition, the calibration of the model based on these data, management of the data, and the software/hardware configuration needed for data processing. Of the ten Group B elements presented in *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA, 2001), the following three are especially relevant for a modeling project:

- *[Model] Calibration (B7)*: Documenting the procedures for calibrating the model that will perform the designated regulatory predictive task.

- *Non-direct measurements (data acquisition requirements) (B9)*: Introducing the types and sources of existing data to be used in building and/or executing the model(s) to be considered, specifying how these data will be acquired, and documenting the quality associated with these data and their relevance in addressing project objectives.

- *Data management and hardware/software configuration (B10)*: Documenting the data management process from data acquisition through transmission and processing, and to final use; documenting the components of the process to generate model outputs; and highlighting the QA procedures associated with the configuration of the hardware and software utilized by the model.

Although other Group B elements may occasionally be relevant for certain modeling projects, they are generally geared toward projects that collect new data. These elements need to be represented within the QA Project Plan for modeling projects, but they can be labeled as "not relevant" for the given project if it is so determined. Sections 4.2.1 through 4.2.3 provide guidance on the above three QA Project Plan elements for modeling projects.

When addressing the Group B elements, detailed copies of quality assurance methods and/or standard operating procedures (SOPs) can be either included directly in the discussion, provided as attachments to the QA Project Plan, or, if easily obtained and readily available to all project participants [e.g., American Society for Testing and Materials (ASTM) methods], cited within the discussion and included in the reference list.

4.2.1 [MODEL] Calibration (B7)

Identify all tools affecting quality that must be controlled and, at specified periods, calibrated to maintain performance within specified limits. Describe or reference how calibration will be conducted. If no nationally recognized standards exist, document the basis for the calibration. Identify the certified equipment (approved model) and/or standards used for calibration. Indicate how records of calibration shall be maintained and be traceable to the instrument (model).

General QA Project Plan guidance indicates that Element B7 (Calibration) for data collection addresses calibration of the analytical instruments that will be utilized to generate analytical data. For modeling projects, by analogy the "instrument" is the predictive tool (the model) that is to be developed and/or applied. All models, by definition, are a simplification of the environmental processes they are intended to represent. When formulating the mathematical representations of these processes, there are empirical relationships and parameters that need to be defined (e.g., the rate of formation or destruction of a chemical). The estimation of parameters involved in formulating these empirical relationships is called *(model) calibration*, and it is most often performed once in the model development phase. However, some model parameters may need to be estimated for every application of the model, using site-specific field data. Similar to an analytical instrument, models are calibrated by comparing the predictions (output) for a given set of assumed conditions to observed data for the same conditions. This comparison allows the modeler to evaluate whether the model and its parameters reasonably represent the environment of interest [as determined based on accuracy requirements specified in Element A7 (Qaulity Objectives and Criteria for Model Inputs/Outputs) of the QA Project Plan]. Statistical methods typically applied when performing model calibrations include regression analyses (Draper & Smith, 1981) and goodness-of-fit methods (as discussed in EPA, 1999e; Gilbert, 1987; and D'Agostino & Stephens, 1986). In this portion of the QA Project Plan, the details of the model calibration procedure, including any statistical analyses that are involved, are documented.

On projects supporting regulatory decision making, the level of detail on model calibration in the QA Project Plan should be sufficient to allow another modeler to duplicate the calibration method, if the modeler is given access to the model and to the actual data being used in the calibration process. For other projects (e.g., some basic research projects), it may be acceptable to provide less detail on this issue for the QA Project Plan. For example, some projects may use procedures that are somewhat different from standard calibration techniques, such as "benchmarking" procedures, and although such procedures may be relevant to document in Element B7 (Calibration), the level of detail may differ from what is generally portrayed for calibration. Even though some modeling projects may use techniques other than standard calibration techniques, this section uses the term "calibration" to facilitate the discussion.

Examples of different features of the model calibration effort that the QA Project Plan may address include the following:

- objectives of model calibration activities, including acceptance criteria;
- frequency of model calibration activities;
- details on the model calibration procedure;
- method of acquiring the input data;
- types of output generated by the model calibration;
- method of assessing the goodness-of-fit of the model calibration equation to calibration data;

- method of incorporating variability and uncertainty in the model calibration results;
- corrective action to be taken if acceptance criteria are not met.

Each of these items is addressed in detail in the paragraphs that follow.

Objectives of Model Calibration Activities, Including Acceptance Criteria – Information related to objectives and acceptance criteria for calibration activities that generally appear at the beginning of this QA Project Plan element includes the following:

- *Objectives of the model calibration*, including what the calibration should accomplish and how the predictive quality of the model might be improved as a result of implementing the calibration procedures.

- *Acceptance criteria*: The specific limits, standards, goodness-of-fit, or other criteria on which a model will be judged as being properly calibrated (e.g., the percentage difference between reference data values from the field or laboratory and predicted results from the model). This includes a mention of the types of data and other information that will be necessary to acquire in order to determine that the model is properly calibrated (e.g., field data, laboratory data, predictions from other accepted models).

- *Justifying the calibration approach and acceptance criteria*: Each time a model is calibrated, it is potentially altered. Therefore, it is important that the different calibrations, the approaches taken (e.g., qualitative versus quantitative), and their acceptance criteria are properly justified. This justification can refer to the overall quality of the standards being used as a reference or of the quality of the input data (e.g., whether data are sufficient for statistical tests to achieve desired levels of accuracy).

Frequency of Model Calibration Activities – Inputs to the model calibration process can highly influence the quality of information generated by the model. Therefore, the calibration process may need to be iterative in nature, repeated whenever some key aspect of the environment changes. Each iteration would utilize data that accurately portray the changing environment and, therefore, would provide further necessary refinements to the model. This element of the QA Project Plan should contain a schedule for addressing model calibration issues, with explanation as needed for the specified frequency and timing of calibration.

Details on the Model Calibration Procedure – The QA Project Plan documents the procedures to be used when performing model calibrations during the project, providing information such as the following:

- An overview of each model or model component requiring calibration should be given, along with the various components of the calibration procedure, some of which may coincide with the model's components. This could be specified in text format and/or in a graphic, flow diagram-type figure. This presentation can incorporate how schedule and other time-dependent factors interplay with the various stages of the calibration procedure.

- Details on specific methods to be used to perform the calibration, for each portion of the model and at each stage of the procedure. SOPs detailing the methods can be appended to the QA Project Plan.

- Any need to modify the calibration method to accommodate data acquired for calibration purposes (see below).

- The resources necessary to conduct the model calibration, along with the individual responsible for directing the model calibration efforts [as specified in the organizational chart in Element A4 (Project/Task Organization)].

- The approach to maintaining calibration records and ensuring that the results can be traced to the appropriate version of the model should be specified [over and above what has already been discussed in Element A9 (Documentation and Records) on this subject].

<u>Method of Acquiring the Input Data</u> – Element B9 (Non-direct Methods) provides details on the types of existing data to be acquired and used as input to model calibration activities. This element can document some introductory information on these data, such as the following:

- The types of data necessary at each stage of the calibration procedure and for each model component (or each model), along with any need for the data to represent a specific environmental situation determined by location or some other unique characteristic;

- How the data will be acquired;

- How the quality of the data for model calibration will be determined and verified throughout the calibration procedure. If previous investigations on these data provide information on the quality of the data, references documenting the level of data quality should be included in the QA Project Plan. Otherwise, any methods used to verify data quality in the context of this project should be documented.

Types of Output Generated by the Model Calibration – The important measures and outputs that are expected to be generated upon implementing the model calibration procedure and that will be used to assess whether the model is properly calibrated should be documented. In addition, statistical QC techniques to be used to process the output data for comparison to reference values or other acceptance criteria should be described. The quality assurance aspects of these analyses should also be addressed.

Method of Assessing the Goodness-of-fit of the Model Calibration Equation to Calibration Data – Statistical procedures such as chi-square tests and various regression diagnostic reviews (e.g., residual plots, tests for lack of fit) are generally used when comparing the distribution of model output data that results from calibrating the model to the distribution of data measured within the particular environment that the model output is to simulate. If such procedures are used on the project, they should be referenced here along with the criteria to be used in judging the "goodness-of-fit" of the model-generated distribution with the reference distribution.

Method of Incorporating Variability and Uncertainty in the Model Calibration Results – For a given environmental condition, uncertainty in the representativeness of the model input data (e.g., incompleteness, variability, and unintentional bias) will affect uncertainty in the outcome of model calibration. Deviations to the input data (reflecting the data's inherent uncertainty) or to the calibration methods and acceptance criteria can yield different model calibration outcomes. The QA Project Plan addresses uncertainty in the outcome of model calibration and its potential impact on decisions being made from this outcome by documenting the following:

- The expected sources of uncertainty and variability in the model and their potential effect on the outcome of model calibration.

- The tools to be used to characterize uncertainty and variability in the outcome of model calibration (e.g., Monte Carlo techniques, sensitivity analysis).

- Acceptance criteria to be used to evaluate the level of uncertainty and variability, relative to whether the resulting uncertainty in the outcome of model calibration falls within acceptable limits.

Corrective Action to Be Taken If Acceptance Criteria Are Not Met – The QA Project Plan should document what corrective action would be taken when situations such as the following occur:

- when limits, standards, or other criteria that identify whether the model is properly calibrated are not achieved;

- when sensitivity or uncertainty analysis imply that uncertainty in the model calibration outputs exceeds pre-specified criteria.

Situations in which the model calibration process may need to be repeated after any corrective action is taken should also be specified.

4.2.2 Non-direct Measurements (Data Acquisition Requirements) (B9)

Identify any types of data needed for project implementation or decision making that are obtained from non-measurement sources such as computer data bases, programs, literature files, and historical databases. Describe the intended use of the data. Define the acceptance criteria for the use of such data in the project and specify any limitations on the use of the data.

"Non-direct" measurements refer to data and other information that have been previously collected or generated under some effort outside the specific project being addressed by the QA Project Plan. Examples include computer databases, literature files, and software processing. Frequently, using existing data rather than generating new data is sufficient to meet the needs of some phases of a modeling project. Because the data have already been collected and therefore, the needs of the project cannot influence how the measurements were generated, these data need special consideration. Issues regarding how relevant non-direct measurements are identified, acquired, and used on the project are addressed within this QA Project Plan element. Additional guidance on the secondary use of data may also be found in other EPA documents currently under development.

Consider an example where the sources of certain model input data are historical databases or nationally-representative surveys. This element of the QA Project Plan would document how the approach to collecting these data (as determined from the data's sources) could impact the ability to meet the modeling project's quality objectives [detailed in Element A7 (Qaulity Objectives and Criteria for Model Inputs/Outputs)]. The issue is not one of the credibility of the organization which generated the data, but rather whether this particular data set is relevant for the problem at hand. When used uncritically, data with characteristics that do not meet the quality objectives of the project may lead to a higher chance of making decision errors. Therefore, it is important to scrutinize the applicability of any non-direct measurements to a project, regardless of their sources.

The QA Project Plan should address the following four issues regarding information on how non-direct measurements are acquired and used on the project:

- the need and intended use of each type of data or information to be acquired;
- how the data will be identified or acquired, and expected sources of these data;

- the method of determining the underlying quality of the data; and
- the criteria established for determining whether the level of quality for a given set of data is acceptable for use on the project.

Each of these items is addressed in detail below.

The Need and Intended Use of Each Type of Data or Information to Be Acquired – This QA Project Plan element can begin by introducing those components of the modeling process [introduced in Element A6 (Project/Task Description and Schedule)] in which non-direct measurements are expected to be utilized as input. For each of these components, the following items should be addressed:

- the particular need for non-direct measurements, relative to how the need will allow the objectives in Element A6 (Project/Task Description and Schedule) to be achieved;

- justification for using non-direct measurements, rather than generating new data;

- details on the intended use of the data to satisfy the given need.

How the Data Will Be Identified or Acquired, and Expected Sources of These Data – Once the need for and the intended use of non-direct measurements have been introduced, the approach to obtaining data to meet these needs can be specified. Sources of non-direct measurements identified for possible use on the project would be documented here. In addition, the procedure for selecting data sources would be detailed here, along with the types of information that these sources would be anticipated to provide. This discussion would also mention the criteria and critical judgment that would be used to determine whether certain data sources are relevant and how certain data sources would be selected if competing sources were available. If sources of potentially acceptable data are available but would likely not be considered for the project, then reasons for not considering these sources should be given to address the potential for selection bias that this may introduce.

The QA Project Plan should also indicate the extent to which project objectives (or other criteria, such as limits on decision errors) can be achieved by using specific sources and types of data and parameters that have been identified through the data acquisition process. One example of how this may be done is to rank the different data sources relative to how critical their data are to the modeling process and its output and the extent to which the data have been collected according to specifications of the modeling project. Data receiving high rankings would have a high likelihood of being selected (if multiple sources exist or if budgeted resources are limited) and would be placed under greater scrutiny during data assessment and software testing processes [Elements B10 (Data Management and Hardware/Software Configuration) and C1 (Assessment and Response Actions)].

The Method of Determining the Underlying Quality of the Data – Once specific types of data and information and the sources of these data have been identified, it is necessary to express the *acceptance criteria* introduced in Element A7 (Qaulity Objectives and Criteria for Model Inputs/Outputs) relative to each anticipated data source and how these criteria will determine whether the given data source is an acceptable input to the modeling project. Because these acceptance criteria are directly tied to the underlying quality of the data, this QA Project Plan element should precede this discussion by specifying what is known about the quality of the non-direct measurements to be used in the modeling project.

A first step in gathering information on acceptance criteria for a given source of non-direct measurement data is to determine whether a QA Project Plan or a sampling and analysis plan exists and is available for that source. Complete SOPs, other standard procedures, and laboratory-specific deviations and specifications associated with these procedures may also be important to review and reference in the QA Project Plan. When analytical data are being considered, it may be sufficient for the QA Project Plan to simply cite the analytical method if it is a complete SOP. If other analytical methods were used, a reference to a procedure (e.g., from *Test Methods for Evaluating Solid Waste,* SW-846) should be identified, along with other relevant information (e.g., options and variations used by the lab, detection limits actually achieved, calibration standards, and concentrations used). If the analytical procedure is unique or an adaption of a "standard" method, the QA Project Plan should describe or cite the complete analytical and sample preparation procedures.

From these references, the results of data assessment and the quality guidelines associated with the given type of measurement may be cited in the QA Project Plan for the modeling project, as well as the extent to which the data abide by these guidelines. In particular, any limitations on the use of the data that may result from any uncertainty that may exist in the data's quality should be noted.

One approach to determining whether non-direct measurements satisfy acceptance criteria involves referring to references obtained from the data sources to identify information on *data quality indicators (DQIs)* associated with the measurements (Section 4.1.7). The QA Project Plan should document the relevant findings for the non-direct measurements.

Other information about the projects and procedures that generated the non-direct measurements may also be important to cite in the QA Project Plan. For example, the extent to which the measurements reflect the modeling project's target population, the sampling and analytical methods used, and the parameters of interest to the modeling project would be important to document. The sampling method can materially affect the representativeness, comparability, bias, and precision of the final analytical result. Similarly, the analytical methods influence the outcome of the measurements and, as a result, their ability to achieve decision performance criteria for the model's intended predictive task. These types of information serve as examples; the information relevant to a given project will depend on the project's overall scope and objectives.

The Criteria Established for Determining Whether the Level of Quality for a Given Set of Data is Acceptable for Use on the Project – Documenting how the non-direct measurements achieve pre-established acceptance criteria is one step toward satisfying the quality objectives for the modeling project that were specified within Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs) of the QA Project Plan. Thus, as a first step in determining acceptance criteria, the project's objectives for the quality of the intended output [as determined through the systematic planning process documented in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs)] are reviewed. During this first step, the quality objectives can be translated into a statement about the likelihood of making certain decision errors as a result of using the model output in statistical analysis. This first step corresponds to the first stage of the Data Quality Assessment process that EPA has established to evaluate data based on scientific and statistical criteria in order to determine whether the data are of the right type, quality, and quantity to support their intended use. The first stage of the Data Quality Assessment process is documented in Chapter 1 of *Guidance for Data Quality Assessment (QA/G-9)* (EPA, 2000c).

Note that information on project objectives and/or limits placed on decision errors (as determined within systematic planning) would be used as the basis for ranking the various data types by their criticality to achieving these objectives, as discussed previously.

Acceptance criteria for individual data values generally address issues such as the following:

- *Representativeness:* Were the data collected from a population sufficiently similar to the population of interest and the model-specified population boundaries? Were the sampling and analytical methods used to generate the collected data acceptable to this project? How will potentially confounding effects in the data (e.g., season, time of day, location, and scale incompatibilities) be addressed so that these effects do not unduly impact the model output?

- *Bias:* Would any characteristics of the data set directly impact the model output (e.g., unduly high or low process rates)? For example, has bias in analysis results been documented? Is there sufficient information to estimate and correct bias? If using data to develop probabilistic distributions, are there adequate data in the upper and lower extremes of the tails to allow for unbiased probabilistic estimates?

- *Precision:* How is the spread in the results estimated? Is the estimate of variability sufficiently small to meet the uncertainty objectives of the modeling project as stated in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs) (e.g., adequate to provide a frequency of distribution)?

- *Qualifiers:* Have the data been evaluated in a manner that permits logical decisions on the data's applicability to the current project? Is the system of qualifying or flagging data adequately documented to allow data from different sources to be used on the same project (e.g., distinguish actual measurements from estimated values, note differences in detection limits)?

- *Summarization*: Is the data summarization process clear and sufficiently consistent with the goals of this project (e.g., distinguish averages or statistically transformed values from unaltered measurement values)? Ideally, processing and transformation equations will be made available so that their underlying assumptions can be evaluated against the objectives of the current project.

In addition to addressing these questions when establishing acceptance criteria, the QA Project Plan can document the likely consequences (e.g., incorrect decision-making) for selecting data that do not satisfy one or more of these areas (e.g., are non-representative, are inaccurate), as well as procedures in place to minimize the likelihood of selecting such data.

Certain types of data may be needed to meet the project's data needs [Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs)] but may not need to meet the same level of quality as other data (e.g., data meant only to provide background information). This should be noted in the QA Project Plan when relevant.

4.2.3 Data Management and Hardware/Software Configuration (B10)

Describe the procedures for assuring that applicable Agency information resource management requirements (EPA Directive 2100) are satisfied (EPA QA Project Plans only). If other Agency data management requirements are applicable, such as the data standards, discuss how these requirements are addressed.

This QA Project Plan element focuses on the procedures in place to manage (i.e., compile, handle) the data that are expected to be either acquired or generated by the modeling project. Different phases of the project may consider different types and sources of data, and the use of certain data may span across multiple project phases. Therefore, the first segment of this QA Project Plan element (Data Management, labeled "Element B10a") documents the approaches that the project will take to manage the various forms and types of data on the project from acquisition or generation - through their final use. The first subsection (Section 4.2.3.1) provides guidance on documenting the approach to data management.

Linked with data management is the hardware/software configuration required to input the acquired data in an existing model and to generate the model output necessary to meet the objectives of the prediction task. Also, as indicated in Figure 4, the hardware/software configuration will influence how a model is coded. Therefore, the second segment of this QA Project Plan element (Hardware/Software Configuration, or Element B10b) documents the software and hardware configuration needed for data processing within the modeling project. The type of information included about the hardware/software configuration should be consistent with what is specified in the Software Quality Assurance Plan addressed by American National Standards Institute/Institute of Electrical and Electronics Engineers Standard 730 (IEEE, 1999), as integrated into overall project planning. The second subsection (Section 4.2.3.2) provides guidance on specifying the requirements of and the approach to developing the hardware/software configuration.

4.2.3.1 Data Management (B10a)

In general, the QA Project Plan should provide enough documentation on the project's data management procedures (e.g., data entry, data tracking, data manipulation) to permit the data to be traced from their source and acquisition through their transmission and processing, to their final use on the project. Data management procedures are addressed for all types and sources of data, from the non-direct measurements [introduced in Element B9 (Non-direct Measurements)] used as input to the model through the model outputs.

Describing how the various data sources can be traced through the life cycle of the project, from initial source to final use, can be a difficult task. It is often better to portray this process graphically rather than textually through one or more *process flow diagrams.* An example of a process flow diagram is given in Figure 10. The process flow diagram shows the various data inputs and outputs for each procedure in the modeling process, the interaction of these procedures, and the reports that the process produces. Therefore, the diagram documents the intermediate and final stages of the data relative to the flow of the different project phases, as well as the roles that each type of data play within the modeling process and in generating the final products.

The QA Project Plan also documents the tools to be used to facilitate the data management process. Examples of such tools include forms, checklists, database documentation, on-line interactive screens, and program code. Some tools can be included as attachments to the QA Project Plan.

This element of the QA Project Plan should present an overview of the mathematical operations and data processing operations that will be performed on the data during the pre-processing, model computation, and post-processing stages of the modeling process, as described below.

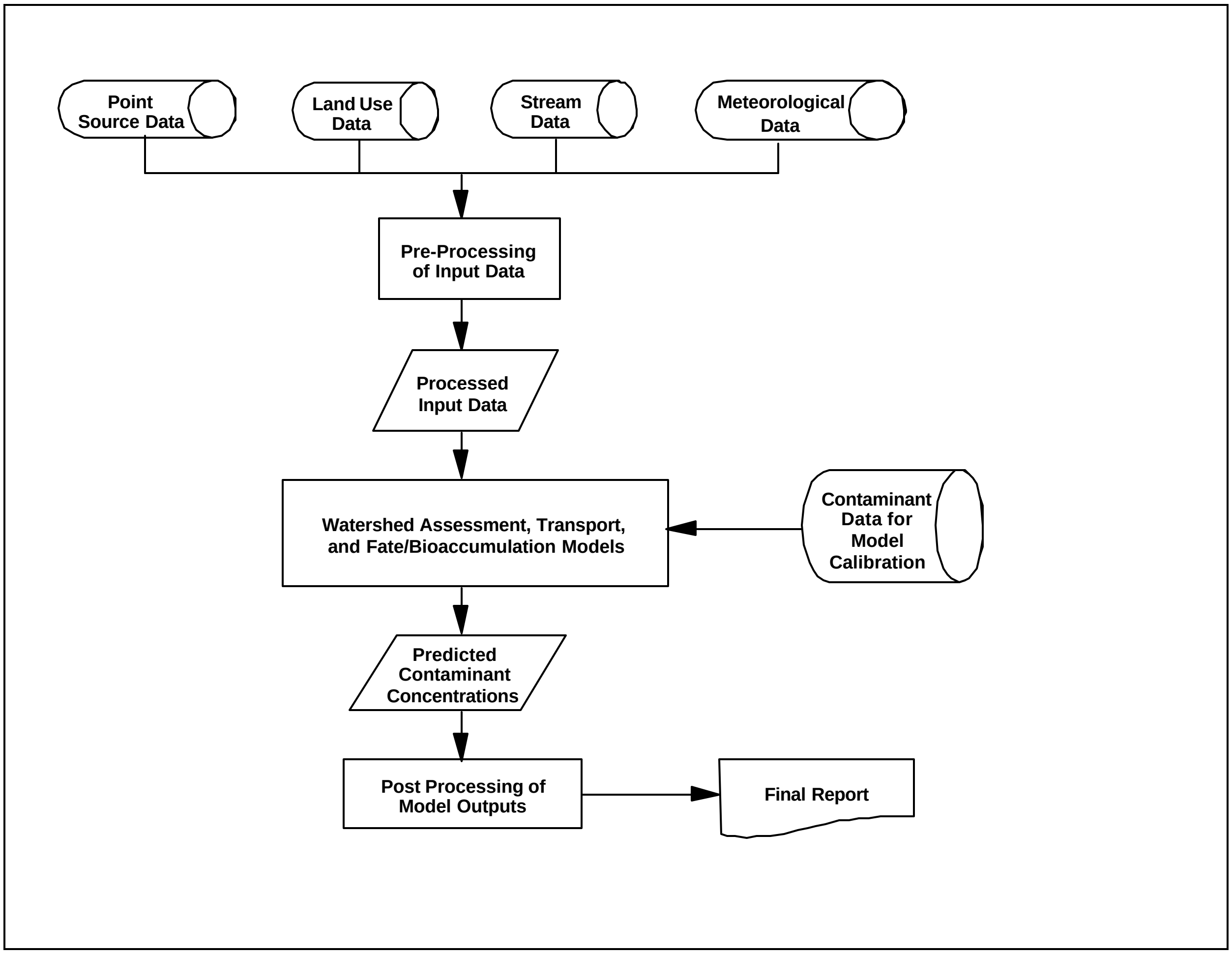

Figure 10. Example of a Process Flow Diagram for a Modeling Project

- In the pre-processing stage, the input data are prepared for use in the modeling stage by performing procedures such as data formatting, reduction, transformations, conversions, and subsetting. [Analyses used to verify whether the data satisfy pre-determined assumptions for statistical analysis are addressed in QA Project Plan Element D3 (Reconciliation and User Requirements).] As necessary, the discussion should justify why certain data procedures need to be implemented and address the impact that the data procedures may have on the ability to achieve the project's quality objectives documented in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs).

- In the model computational stage, the mathematical equations within the model are derived and applied to the data. [This is different from the mathematical approaches used to calibrate the model, which are addressed in Element B7 (Calibration).] While a purpose of the project may be to develop the specific mathematical procedures and equations that constitute the model computational stage, this element can still highlight the primary mathematical approaches that are expected to be applied and how these approaches will ensure that the model's underlying scientific principles will be properly incorporated.

- In the post-processing stage, statistical procedures are applied to analyze the model output, to generate data summaries and reports introduced in Element A9 (Documentation and Records), and to characterize variability and uncertainty in the model output.

This element should outline the proposed methodology for data analysis (e.g., summary statistics, frequency distributions, etc.), verifying that the methodology can be applied successfully to collected or existing data. If the final report will provide details on the methodology, this should be mentioned in the QA Project Plan. This element should also address how the final forms of the data will be processed in support of the project's requirements for the types of information generated from the outputs of the project (i.e., reporting the synthesis of results in the form of charts, tables, graphs, figures, visualizations) and how deviations from these requirements would be handled.

Examples of "control mechanisms" associated with data management that can be documented in the QA Project Plan include the following:

- the approach to detecting and correcting errors that may occur during data entry to forms, reports, or databases, and to preventing loss of data during data reduction and data reporting;

- internal checks to be implemented during data entry or data pre-processing;

- the proposed approach to generating an audit trail associated with certain data management activities such as data reduction and conversion;

- guidelines for transmitting data from one person or location to another or copying data from one form to another;

- the approach to characterizing data transmittal error rates;

- the approach to minimizing information loss during data transmittal; and

- descriptions of the established procedures for tracking the flow of data through the data processing system portrayed within the process flow diagram.

Relevant control procedures are determined based on the project's overall scope and importance of the project's objectives.

Examples of what may be addressed in the QA Project Plan regarding documentation of the data management process include standard record-keeping procedures, audit trails, a system for controlling and tracing the whereabouts of data and documents, and the approach to storing and retrieving data records for various storage media types (e.g., hardcopy, electronic).

4.2.3.2 Hardware/Software Configuration (B10b)

This section of the QA Project Plan provides information on the types of computer equipment, hardware, and software to be used on the project, including information on how they will be used (e.g., for conducting the data management procedures specified earlier in this element of the QA Project Plan). If different types of equipment, hardware, and software are available, a brief justification should be provided, as necessary, for selecting certain types over other types. Reasons should also be given if a certain type of equipment, hardware, or software is required to be used on the project. This type of information may be best presented in table format.

This element may also address performance requirements (e.g., run times) and other features that characterize and assess the hardware/software configuration. This discussion should be incorporated within a general overview of the configuration's QA program. (Assessments that target the model itself and its ability to make predictions are addressed by the Group C elements within the QA Project Plan.) The configuration's QA program is jointly planned and implemented by the project management team and the software developer's independent QA staff, generally as part of systematic planning [Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs)]. It addresses the use of standards, test planning and scheduling, level of documentation required, personnel assignments, and change control. It also ensures that timely corrective action will be taken as necessary. Items within the systems development life cycle that are relevant to the particular modeling project should also be considered when establishing the configuration's QA program. Examples of such items, taken from Chapter 4 of EPA's *Information Resources Management Policy Manual* (Directive 2100) (EPA, 1998b) and the Information Technology Architecture Roadmap[1], are provided in Table 4.

---

[1]Published by EPA's Office of Technology Operations and Planning, formerly the Office of Information Resources Management, Directive 2100 establishes a policy framework for managing information within EPA. It can be accessed online at www.epa.gov/irmpoli8/polman/index.html. The Information Technology Architecture Roadmap, which contains annual updates of this document, can be found at (Internal EPA website) http://Basin.rtpnc.epa.gov:9876/etsd/ITARoadMap.nsf.

Table 4. Typical Activities and Documentation Prepared Within the System Development Life Cycle of a Modeling Project that Should be Considered When Establishing the QA Program for the Hardware/Software Configuration

Life Cycle Stage	Typical Activities	Documentation
Needs Assessment and General Requirements	• Assessment of needs and requirements interactions in systematic planning with users and other experts	• Needs assessment documentation (e.g., QA Project Plan) • Requirements document
Detailed Requirements Analysis	• Listing of all inputs, outputs, actions, computations, etc., that the modeling framework is to perform • Listing of ancillary needs such as security and user interface requirements • Design team meetings	• Detailed requirements document, including performance, security, user interface requirements, etc. • System development standards
Framework Design	• Translation of requirements into a design to be implemented	• Design document(s) including technical framework design, software design (algorithms, etc.)
Implementation Controls	• Coding and configuration control • Design/implementation team meetings	• In-line comments • Change control documentation
Testing, Verification, and Evaluation	• Verification that the modeling code, including algorithms and supporting information system, meets requirements • Verification that the design has been correctly implemented • Beta testing (users outside team) • Acceptance testing (for final acceptance of a contracted product) • Implement necessary corrective actions	• Test plan • Test result documentation • Corrective action documentation • Beta test comments Acceptance test results
Installation and Training	• Installation of data management system and training of users	• Installation documentation • User's guide
Operations, Maintenance, and User Support	• Usage instruction and maintenance resources for model framework and data bases	• User's guide • Maintenance manual or programmer's manual

It is important that the QA Project Plan specify the particular QA procedures that will be implemented within the modeling project to ensure that the data generated by the modeling framework (i.e., the model and its supporting hardware and operating system) are defensible and appropriate for its planned final use. This section of the QA Project Plan would address QA efforts performed as the data management and processing systems are being developed. The schedule for these efforts should also be included in task scheduling [Element A6 (Project/Task Description and Schedule)]. These efforts may include:

- identifying necessary requirements for the hardware/software configuration and establishing quality criteria that address these requirements within the systematic planning and needs analysis phase of the project [Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs)];

- implementing an appropriate project management framework to ensure that the requirements and quality criteria established for the hardware/software configuration are achieved [as discussed in Elements A4 through A9 and B9 (Non-direct Measurements)]; and

- performing testing and other assessment procedures on the configuration to verify that the project-specific requirements and quality criteria are being met [details on the assessment procedures are addressed in Element C1 (Assessment and Response Actions)].

The magnitude of these QA efforts will depend on the underlying complexity of the modeling effort and the required hardware/software configuration. Therefore, EPA's graded approach (Chapter 1) will direct the overall scope on which these QA efforts need to focus.

Elaborating further on the first bullet above, the systematic planning phase of the study [Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs)] defines requirements and quality criteria for the data processing system to ensure that the project's end-use needs can be adequately met. For example, criteria on errors propagated by data processing would be established during systematic planning to ensure that uncertainty requirements for the model outputs can be met. Such requirements and criteria, therefore, impact the project's hardware/software configuration.

In systematic planning, questions such as the following may be addressed when defining these requirements and quality criteria:

- What are the required levels of accuracy and uncertainty for numerical approximations?

- Are the selected mathematical features of the model (e.g., algorithms, equations, statistical processes) appropriate for the model's end use?

- Are the correct data elements being used in the calculations performed within the model's algorithms?

- What requirements regarding documentation and traceability are necessary for the model's inputs, interim outputs, and final outputs?

Other items addressed during systematic planning that are likely to impact assessment of the hardware/software configuration include security, communication, software installation, and system performance (e.g., response time). These issues are addressed briefly below.

Security issues: Examples of QA efforts that address security issues regarding data handling and communication (e.g., viruses, hackers, e-mail interception) and system vulnerability include the following:

- ensuring that security needs are included among project requirements and can be found within the project requirements documentation;

- ensuring that security features of the configuration are adequately and thoroughly tested and the results documented;

- planning for audits addressing system vulnerability to be conducted by security personnel outside the immediate project team.

Other security issues that may be relevant to a particular project (preferably during system planning) are found in EPA's *Information Security Manual* (Directive 2195A1) (EPA, 1999a).

Communication issues: The QA program should address communication among the model developers and users regarding configuration acceptance and control of changes, such as:

- ensuring that all user communication interfaces are adequately defined, and that beta testing is performed to have users test the connections of these various interfaces;

- ensuring that proper and complete testing of the communications hardware and software is done, preferably under "worst-case" (i.e., high-load, adverse) conditions.

Software installation issues: The QA program should specify those QA techniques associated with installing or uninstalling the software configuration on users' computers. Examples of such techniques include the following:

- performing adequate beta testing to ensure that installation can be performed successfully on a wide variety of different platforms, including various combinations of processors, memory sizes, and video controllers;

- ensuring that uninstall routines are complete (e.g., removing entries in the initialization and registry files as well as deleting files);

- ensuring that any "auto-install" or "auto-uninstall" routines are thoroughly tested and debugged before release.

Response time issues: If the QA program provides explicit, testable objectives for response time performance in various phases of the modeling procedure (e.g., real-time data processing, pre-processing, post-processing, uncertainty analyses), these should be documented in the QA Project Plan for all interactive and real-time systems.

When documenting planning and performance components of the hardware/software configuration, project and QA Managers should tailor the documentation to meet the specific needs of their project. Examples of different types of documentation that can be generated for various tasks within the planning phase of the system's life cycle include the following:

- *Requirements Documentation (IEEE, 1998b):* The general requirements document gives an overview of the functions that the model framework will perform. Detailed requirements documents define all critical functions that the completed framework needs to support. Performance goals derived from analysis of the project's quality objectives [QA Project Plan Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs)] should be included among the requirements. Requirements documentation should be reviewed by the regulatory program end user, if possible, to ensure that critical functions and other requirements have not been overlooked.

- *Design Documentation:* Design documents plan and describe the structure of the computer program. These are particularly important in multi-programmer projects in which modules written by different individuals interact. Even in small or single-programmer projects, a formal design document can be useful for communication and for later reference.

- *Coding Standards or SOPs:* These may apply to a single project or a cumulative model framework and need to be consistent across the development team. Uniform standards for code formats, subroutine calling conventions, and in-line documentation can significantly improve the maintainability of models and processors.

- *Testing Plans (IEEE, 1986):* Testing needs to be planned in advance and address all requirements and performance goals. Specific procedures for corrective action and retesting process should be described in the QA Project Plan (similar to IEEE, 1999) and implemented within the assessments discussed in the QA Project Plan's Group C elements.

- *Data Dictionary:* A data dictionary can be useful to developers, users, and maintenance programmers who may need to modify the modeling framework later. The data dictionary is often developed before code is written as part of the design process. The dictionary should be updated as necessary when new elements are added to the data structure. A data dictionary need not be a separately written document. For example, the record definition files needed for many database systems can serve this purpose, provided that they are available in a form that is readily accessible to the user or maintenance programmer.

- *User's Manual:* The user's manual can often borrow heavily from the requirements document because all the software's functions should be specified there. The scope of the user's manual should take into account such issues as the level and sophistication of the intended user and the complexity of the interface. Online help can also be used to serve this function.

- *Maintenance Manual:* The maintenance manual's purpose is to explain a framework's software logic and organization for the maintenance programmer. This manual should also contain crucial references documenting algorithms, numerical methods, and assumptions. Instructions for rebuilding the system from source code are included. The maintenance manual will often borrow heavily from the design manual.

- *Source Code:* It is very important to securely store downloadable code and to archive computer-readable copies of source code according to the policies of the relevant regulatory program.

- *Configuration Management Plan (IEEE, 1998a):* The configuration management plan provides procedures to control the software/hardware configuration during development of the original model version and subsequent revisions. It ensures that only approved deletions, additions, and changes are introduced in a controlled way to maintain the integrity of the model. The configuration management process starts when the unit is successfully tested and placed under project configuration control. Upon deployment, a documented product baseline configuration enhances the reliability and maintainability of the software/hardware configuration through the remainder of its useful life.

Additional information and examples can be found in Chapter 17 of EPA's *Information Resources Management Policy Manual* (Directive 2100) (EPA, 1998b). In general, any discussion of documentation in the QA Project Plan should be coordinated with information presented in Element A9 (Documentation and Records).

The configuration should be designed to comply with applicable EPA information resource management and data standard policies, which can be found within EPA's *Information Resources Management Policy Manual* (Directive 2100) (EPA, 1998b). Other policies and standards may also be applicable and should be cited, such as the Federal Information Processing Standards, which govern the acquisition of U.S. Government information processing systems. This portion of the QA Project Plan should introduce these standards and discuss how the project will ensure that they will be addressed.

Sources for determining specific types of standards include the following:

- EPA's *Information Resources Management Policy Manual* (Directive 2100) (EPA, 1998b) includes the EPA hardware and software standards to promote consistency in use of standard support tools such as computer-aided software engineering tools and coding languages, as applicable, by contractors and EPA staff in model software development and maintenance efforts.

- Chapter 5 of EPA's *Information Resources Management Policy Manual* (Directive 2100) (EPA, 1998b) defines applicable EPA data standards.

- EPA's Environmental Data Registry (www.epa.gov/edr) promotes data standardization, which allows for greater ease of information sharing.

- The EPA Information Technology Architecture Roadmap (Internal EPA website: Basin.rtpnc.epa.gov:9876/etsd/ITARoadMap.nsf) provides guidance for the selection and deployment of computing platforms, networks, systems software, and related products that interconnect computing platforms and make them operate.

- Publications on Federal Information Processing Standards govern the acquisition of U.S. Government information processing systems.

Directives and standards such as these are frequently revised. Therefore, it is important that these directives and standards be reviewed frequently to ensure that the latest versions are being utilized. The QA Project Plan should specify how the acceptability of the configuration will be verified or demonstrated according to these and other standards.

4.3 GROUP C: ASSESSMENT AND OVERSIGHT

The purpose of the assessment and oversight section of the QA Project Plan for a modeling project (i.e., the Group C QA Project Plan elements) is to describe the internal and external checks and activities necessary to assess the effectiveness of the modeling project implementation and associated QA and QC activities. These checks and activities are needed to detect errors and to ensure that using the model being developed and applied achieves the modeling task (i.e., meets user requirements) at the prediction ability and levels of quality specified in QA Project Plan Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs) (Section 4.1.7). Furthermore, the assessment is needed to ensure that adequate coordination and documentation of all planned internal and external assessments (e.g., peer reviews) are achieved, and that any needed corrective actions are implemented and their effectiveness assessed and documented in a timely manner.

All models need to include this type of evaluation in the planning stages—even data-poor or qualitative models for which traditional model evaluations cannot be done. The QA Project Plan for these projects should contain information to address the following questions:

- Are more studies needed?
- How good does my confidence have to be to move forward?
- What do I need to know to be able to show this model is sound?

Assessment and Response Actions (Element C1) includes various model theory and algorithm evaluation assessments, assessments of the effect of variability within a population and uncertainty of model structure and parameter values on model outputs, the sensitivity of model outputs to a particular model and model inputs used, data quality assessments, model verification tests by statistical comparisons of model outputs with field or laboratory data, internal and external peer reviews, and hardware/software configuration testing. These assessments may lead to response actions to make mid-course corrections in project activities. Reports to Management (Element C2) identifies the frequency and distribution of reports issued to inform management of the project status and ensures prompt and appropriate corrective actions are taken during model development or application.

Because both Groups C and D of the QA Project Plan address assessment activities, information presented in these two groups of elements may overlap (as discussed in Section 4.4). Generally, Group C of the QA Project Plan focuses on <u>interim</u> assessments conducted iteratively throughout both the model development and application processes to ensure that pre-determined modeling criteria are being achieved as the model is being developed or implemented. In contrast, Group D focuses on <u>final</u> assessments performed in the final stages of model development and after the model has been applied in a given instance to evaluate whether the outcomes meet the project's original objectives. This distinction between the Group C and Group D elements is consistent with *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA, 2001) for environmental sampling and data analysis projects, which specifies that the assessments documented in Group C occur first, focusing on how samples are being collected and data are being generated, while assessments in Group D focus on ensuring that the newly generated data can be used to achieve the project's objectives.

4.3.1 Assessment and Response Actions (C1)

Describe each assessment to be used in the project, including the frequency and type. Discuss the information expected and the success criteria (i.e., goals, performance objectives, acceptance criteria and specifications, etc.) for each assessment proposed. List the approximate schedule of assessment activities.

For any planned self-assessments (utilizing personnel from within the project groups), identify potential participants and their exact relationship within the project organization. For independent assessments, identify the organization and person(s) that shall perform the assessments, if this information is available. Describe how and to whom the results of each assessment shall be reported. Define the scope of authority of the assessors, including a description of when assessors are authorized to act.

Discuss how response actions to assessment findings, including corrective actions for deficiencies and other non-conforming conditions, are to be addressed and by whom. Include details on how the corrective actions will be verified and documented.

This element of the QA Project Plan documents the types of assessments to be performed throughout the various stages of both model development and application, the purpose of each assessment and the specific model features that each assessment is to address, and the expected periods of time in which the assessments will take place. The specific assessments are based on a clear understanding and statement of the purpose of the model, the way the model will be used in management and/or regulatory tasks and decision making, and the accuracy of the model outputs needed (predictions).

In general, this QA Project Plan element specifies the following types of information:

- a description of the assessment/oversight strategies and schedule of assessment activities, including the order in which the assessments will be conducted and how the total set of assessments is structured to provide a complete and comprehensive assessment;

- a description of how each assessment will be planned and conducted;

- the organizations and individuals that are expected to participate in assessments, including peer reviews;

- the information expected, success criteria, and documentation for each assessment;

- a description of how and to whom the results of each assessment will be reported;

- a discussion of the limits of authority of assessors to recommend or direct changes (including corrective actions) in the development or application of models; and

- a description of how, when, and to whom response actions to assessment findings will be addressed and verified as successfully completed and documented.

When relevant, the QA Project Plan addresses the following two classes of project assessments that are typically used on a modeling project:

- *Internal assessments* are those conducted by the organizations developing or applying the model. These assessments are usually initiated or overseen by the internal QA Officer [specified within QA Project Plan Element A4 (Project/Task Organization)]. Such assessments include:

  – reviews of the model theory, mathematical structure, parameters, and data to ensure the objectives of the new model or application of an existing model are being met;
  – reviews of the model evaluation and hardware/software configuration testing conducted to assure the quality requirements for a new application of an existing model;

  – reviews to assess the appropriateness of data being used or considered for use in a new application of a model.

- *External assessments* are those conducted by organizations that are not directly involved with the development and application activities. External assessments are often peer reviews. Such assessments typically address the same issues as listed above for internal assessments, but the broader perspectives that external reviewers may provide can lead to new insights into problems not fully recognized or discussed by internal reviewers.

Since models produce estimates that are averaged in many ways (e.g., in time, over some volume or space), it is to be expected that the model output will differ from observed field data. Environmental processes are inherently stochastic, so differences (often quite large) will be seen even when conditions are apparently identical. Evaluating the effectiveness of model development or model application projects involves several types of assessments so that all significant sources of uncertainty (i.e., lack of knowledge) in model output and input parameters and variability in relevant populations and data can be evaluated. For these reasons, the assessments of model performance will involve both qualitative and quantitative assessments.

- *Quantitative Assessments:* The uncertainty in some sources—such as some model parameters and some input data—can be estimated through *quantitative assessments* involving statistical uncertainty and sensitivity analyses. In addition, comparisons can be made for the special purpose of quantitatively describing the differences to be expected between model estimates of current conditions and comparable field observations. However, model predictions are not what is directly observed, so special care needs to be taken in any exercise that attempts to make a quantitative comparisons of model predictions with field data.

- *Qualitative Assessments:* Some of the uncertainty in model predictions may arise from sources whose uncertainty cannot be quantified. Examples are uncertainties about the theory underlying the model, the manner in which that theory is mathematically expressed to represent the environmental components, and theory being modeled. The subjective evaluations of experts may be needed to determine appropriate values for model parameters and inputs that cannot be directly observed or measured (e.g., air emissions estimates). *Qualitative assessments* are needed for these sources of uncertainty.

Additional discussion of quantitative and qualitative assessments is provided in various publications such as *Standard Guide for Statistical Evaluation of Atmospheric Dispersion Model Performance* (ASTM D 6589-00)*, A Guide for Uncertainty Analysis in Dose and Risk Assessments Related to Environmental Contamination* (NCRP, 1996), *Uncertainty: A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis* (Morgan & Henrion, 1990), and *Uncertainty Analysis,* (Kirchner, 2000), and in recent EPA documents available on the web, *Report of the Workshop on Selecting Input Distributions for Probabilistic Assessments* (EPA, 1999d at www.epa.gov/NCEA/input.htm) and *Risk Assessment Guidance for Superfund: Volume 3 (Part A): Process for Conducting Probabilistic Risk Assessments* (EPA, 1999e at www.epa.gov/superfund/pubs.htm).

The following two categories of assessment activities are typically addressed when preparing the QA Project Plan for a model development or application project:

- *Surveillance Activities*: Surveillance consists of the continual or frequent monitoring of the status and progress of the modeling project and the analysis of records to ensure that management and technical aspects are being properly implemented according to the specified schedule and quality requirements developed during systematic planning. Surveillance activities are conducted to uncover any problems that may adversely impact the ability to achieve project goals. Surveillance activities include assessing how project milestones are achieved and documented, corrective actions, budgets, communications among project staff, peer reviews, data management and timely acquisition of data, computers and software, and prompt attention to problems that arise.

- *Model Performance Evaluations*: Model performance evaluations are conducted to answer the question, "Does the model perform the required task while meeting the quality objectives?" Examples of such evaluations include the following:

  - *model theory assessments*, which assess whether the theory underlying the model is appropriate and capable of explaining the processes critical to the regulatory task or scientific hypotheses being addressed by a new model or a new application of an existing model;

  - *model algorithm assessments*, which ensure that the mathematical algorithms (equations) used to obtain quantitative predictions provide an appropriate translation of the accepted underlying theory into equation form;

  - *data acquisition assessments*, which assess the quality of non-direct measurements (e.g., computer databases, programs, literature files, and historical databases) using criteria specified in the QA Project Plan [Element B9 (Non-direct Measurements)];

  - *model calibration studies*, which quantitatively assess the uncertainty and suitability of data used to develop values of model parameters and the amount of discrepancy between model predictions and appropriate, measured field or laboratory data [Element B7 (Calibration)];

  - *sensitivity analyses*, which identify key model inputs (assumptions, expert opinion, data) and model parameters whose uncertainties account for a large proportion of the uncertainty of model predictions;

  - *uncertainty analyses*, which assess the range of predicted values from the model that could occur because of the uncertainty of model components, assumptions and input data, or the uncertainty over space and time of the value of some model parameters (if necessary to meet risk assessment guidelines);

  - *hardware and software configuration testing* for programming errors (e.g., the coded model equations or modules are correctly inserted, linked, and used in the software code) and other problems with the development and implementation of hardware and software needed for obtaining model predictions (Element B10b);

– *data quality assessments*, which use statistical design and analysis tools to assess whether (1) the model input data have the precision and accuracy needed and satisfy all assumptions (e.g., lognormality) needed for use in the model, and (2) the variability and/or uncertainty of initial model outputs achieve the specified Data Quality Objectives (decision performance criteria) and model performance criteria specified in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs of the QA Project Plan;

– *model evaluations (or verification tests)*, which compare model results with laboratory tests, field data, analytical solutions, synthetic test data sets, or other well-accepted models ("benchmarking") to provide documented information about the model's strengths and weaknesses and permit programmatic evaluations to identify areas needing corrective action.

– *internal and external peer reviews*, in which individual experts or a group of experts not previously involved in the project review all aspects of the model development, code preparation and use, model application, and results.

Note: This is a list of examples of different types of model performance evaluations that may be performed on a modeling project and is not meant to imply that all would be required on each project.

For data quality assessments, *Guidance for Data Quality Assessment: Practical Methods for Data Analysis (QA/G-9)* (EPA, 2000c) provides nonmandatory statistical guidance for planning, implementing, and evaluating retrospective assessments of the quality of results from environmental data collection operations, including methods to characterize and describe data sets, test for outliers, test distribution assumptions, test for differences between two data sets, and test for deviation from a population standard. Other resources on data quality assessment include *Goodness of Fit Techniques* (D'Agostino & Stephens, 1986), *Risk Assessment Guidance for Superfund: Volume 3 (Part A): Process for Conducting Probabilistic Risk Assessment* (EPA, 1999e), and *Statistical Methods for Environmental Pollution Monitoring* (Gilbert, 1987), which provide statistical goodness-of-fit tests of data to hypothesized distribution forms.

If EPA contractual or regulatory requirements specify that peer reviews of certain aspects of the modeling process are necessary on the project (e.g., on the theoretical basis for the model, the mathematical model structure, model algorithms and methods of solution of the model code, model predictions and alternative interpretations, model calibration data, uncertainty and sensitivity analysis methods, data quality assessment methods, conclusions), the QA Project Plan should specify criteria that the peer review will meet [e.g., EPA's peer review policy (EPA 2000e) and guidance given in *Guidance for Conducting External Peer Review of Environmental Regulatory Models* (EPA, 1994)]. When peer review is to be performed on the project, the QA Project Plan implementation file should include the names, titles, and positions of the peer reviewers, their report findings, the project management's documented responses to their findings (or reference to where responses to peer review comments are located).

Among the model performance evaluations discussed above, hardware and software configuration testing is conducted to ensure that:

- programming errors are minimized;
- the coded model equations or modules are correctly inserted, linked, and used in the software code;
- the code is linked to or performs analyses that assess the uncertainty and variability of predicted results (if necessary to meet risk assessment guidelines); and
- the total completed modeling software package meets all user requirements.

While QA Project Plan Element B10b (Hardware/Software Configuration) introduces the needs and goals of the hardware/software configuration and presents the configuration's QA program, this element of the QA Project Plan should address the tests performed to assess the configuration's adherence to the requirements specified in the QA program. Examples of such tests include the following:

- *Software code development inspections:* Software requirements, software design, or code are examined by an independent person or groups other than the author(s) to detect faults, programming errors, violations of development standards, or other problems. All errors found are recorded at the time of inspection, with later verification that all errors found have been successfully corrected.

- *Software code performance testing:* Software used to compute model predictions is tested to assess its performance relative to specific response times, computer processing usage, run time, convergence to solutions, stability of the solution algorithms, the absence of terminal failures, and other quantitative aspects of computer operation.

- *Tests for individual model module:* Checks ensure that the computer code for each module is computing module outputs accurately and within any specific time constraints. (Modules are different segments or portions of the model linked together to obtain the final model prediction.)

- *Model framework testing:* The full model framework is tested as the ultimate level of integration testing to verify that all project-specific requirements have been implemented as intended.

- *Integration tests:* The computational and transfer interfaces between modules need to allow an accurate transfer of information from one module to the next, and ensure that uncertainties in one module are not lost or changed when that information is transferred to the next module. These tests detect unanticipated interactions between modules and track down cause(s) of those interactions. (Integration tests should be designed and applied in a hierarchical way by increasing, as testing proceeds, the number of modules tested and the subsystem complexity.)

- *Regression tests:* All testing performed on the original version of the module or linked modules is repeated to detect new "bugs" introduced by changes made in the code to correct a model.

- *Stress testing (of complex models):* This ensures that the maximum load (e.g., real-time data acquisition and control systems) does not exceed limits. The stress test should attempt to simulate the maximum input, output, and computational load expected during peak usage. The load can be defined quantitatively using criteria such as the frequency of inputs and outputs or the number of computations or disk accesses per unit of time.

- *Acceptance testing:* Certain contractually-required testing may be needed before the new model or model application is accepted by the client. Specific procedures and the criteria for passing the acceptance test are listed before the testing is conducted. A stress test and a thorough evaluation of the user interface is a recommended part of the acceptance test.

- *Beta testing of the pre-release hardware/software:* Persons outside the project group use the software as they would in normal operation and record any anomalies encountered or answer questions provided in a testing protocol by the regulatory program. The users report these observations to the regulatory program or specified developers, who address the problems before release of the final version.

- *Reasonableness checks:* These checks involve items like order-of-magnitude, unit, and other checks to ensure that the numbers are in the range of what is expected.

Again, it should be noted <u>that the actual types of tests performed depend on the level of assessment needed for the program, and not all of these tests would be performed on each project</u>.

Types of information that can be specified in the QA Project Plan for hardware and software configuration tests include the following:

- a list of user needs and code requirements based on the end use of the model;

- a description of the types, number, and frequency of configuration tests that will be conducted;

- a structured, orderly, and documented test schedule for testing and audits;

- a specification of "correct" or "acceptable" outputs for each configuration test to compare with test results;

- a list of necessary documentation for the planned configuration testing;

- a discussion of potential corrective actions that could result from uncovered problems; and

- a description of the internal and external peer reviews that are planned to assess the hardware/software configuration testing effort and results.

When executed, the assessments discussed above may reveal that the quality measures associated with the outcomes of the model development or application project do not conform to the quality specifications defined in the QA Project Plan. The QA Project Plan may specify certain types of documentation or assessment procedures, such as:

- occurrences of specific unsatisfactory conditions upon which the assessors are authorized to act;
- specific response actions needed;
- protocol for managing, conducting, evaluating, reporting, and documenting the response actions and rationale for such actions;
- person(s) responsible for seeing that response actions are successfully completed [see Element C2 (Reports to Management)];
- person(s) responsible for overseeing response actions and person(s) to whom the results of the response action will be reported; and
- decision-making hierarchy and the schedule and format for oral and written reports.

4.3.2 Reports to Management (C2)

Identify the frequency and distribution of reports issued to inform management (EPA or otherwise) of the project status; results of software tests, model performance evaluations, and other assessments such as output data quality assessments; and significant quality assurance problems and recommended solutions. Identify the preparer and the recipients of the reports, and any specific action recipients are expected to take as a result of the reports.

Reports to management are a critical part of the communication process among all participants in a model development or application project. Planned reports provide a structure for notifying management of the following:

- adherence to project schedule and budget;
- deviations from approved QA Project Plans, as determined from project assessment and oversight activities (discussed in the previous subsection);
- the impact of these deviations on model prediction, application quality, and uncertainty;
- the need for and results of response actions to correct the deviations;
- potential uncertainties in decisions based on model predictions and data; and
- Data Quality Assessment findings regarding model input data and model outputs (predictions).

Reports to management should provide an understanding of the potential effect that changes made in one segment of the model input data, the algorithms, or the development and application process may have on segments of the model algorithms, process, or predictions.

Certain management reports and deliverables mandated by contractual or project requirements should be specified in the QA Project Plan, along with the necessary routing procedures, due dates, and distribution lists [if they differ from the distribution list specified in Element A3 (Distribution List)]. Other reports that are less formal in nature (e.g., a report on the outcome of the model selection process) can be handled less formally in the QA Project Plan. The QA Project Plan specifies the personnel responsible for preparing reports, evaluating their impact, and implementing response actions. It also specifies the planned frequency, content, and distribution of relevant reports to ensure that management may be alerted to data quality problems, necessary changes to the data, viable response actions, and proposed solutions. The frequency of reports should allow management to properly anticipate certain events and take corrective actions (e.g., propose viable solutions, procure additional resources).

Examples of certain types of reports to management that may be relevant to mention for a modeling project (depending on the scope of the project) include the following:

- final version of the QA Project Plan,
- monthly progress reports detailing the status of each phase of the project from both a technical and cost standpoint,
- needs assessment report,
- modeling framework report,
- model documentation,
- model calibration report,
- model evaluation report,
- model outputs uncertainty report,
- disposition of peer review comments (for the various stages of peer review on the project),
- summary report of the model application, and
- final report of the model application.

4.4 GROUP D: DATA VALIDATION AND USABILITY

The primary purpose of this group of elements is to describe the process to assess the usability of the model results (whether from the first application of a new or revised model or from application of an accepted model). Therefore, these elements refer to quality procedures that occur near or at the end of the modeling project. The QA Project Plan contains the criteria and methods for deciding the degree to which each component of the modeling process has met its quality specifications as described in the Group B elements as well as the requirements for the final output [Elements A5 (Problem Definition/Background) and A7(Quality Objectives and Criteria for Model Inputs/Outputs)].

As mentioned at the beginning of Section 4.3, both Groups C and D of the QA Project Plan address assessment-type activities regarding the model output (i.e., predictions) generated in a given application. Therefore, information in these elements may overlap. Generally, Group D elements focus on final assessments performed in the final stages of model development for a first application or in subsequent applications to evaluate whether the outcomes meet the project's original objectives.

Group D of the QA Project Plan describes data review, verification, and validation processes (EPA, 2001). For modeling projects, this is analogous to confirming that the steps of the modeling process were followed correctly to produce the model outputs and that the results meet project objectives.

Data (or information) validation and usability activities for modeling projects are represented within the following three QA Project Plan elements:

- *Departures from Validation Criteria (D1):* This first element documents the criteria used to evaluate how deviating from the specifications given in the QA Project Plan may impact the quality and usability of final results and decisions that are made based on these results.

- *Validation Methods (D2):* This second element describes the process and methods for determining whether deviations have occurred within the model components.

- *Reconciliation with User Requirements (D3):* This element combines the information from the previous two elements to make a final assessment of the usability of the model results.

Each element is addressed in the following subsections.

4.4.1 Departures from Validation Criteria (D1)

State the criteria used to review and validate—that is, accept, reject, or qualify—the model results, in an objective and consistent manner.

Along with Element D2 (Validation Methods), this element of the QA Project Plan elaborates on the acceptance criteria mentioned in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs), which evaluate the model and its components based on its ability to produce results that can be used to achieve project objectives. For example, this element would state acceptance criteria associated with the degree to which each model output item has met its quality specifications. The possible types of discrepancies that may arise when the acceptance criteria and other QA Project Plan specifications are not met in their entirety are also addressed, along with the effects that such discrepancies are likely to have on the outcome of the model development and application processes.

Examples of such acceptance criteria and details about how such criteria may be evaluated in the various stages of the modeling process are as follows, presented in the context of specific model applications:

- *Mathematical basis for the model:* Criteria to be used to determine how well the mathematical theory behind the model represents the processes being modeled are addressed, in addition to how the criteria were established. In all cases, the possible ways in which the criteria may not be met are specified, and the effects these conditions may have on the model output are discussed.

- *Numerical models:* The criteria confirming that the numerical (coded) model accurately estimates the mathematical theory behind the model are discussed, along with how the modeling outcome is affected if these criteria are not met. The criteria for assessing the numerical model (e.g., convergence criteria) and reasons for their appropriateness are discussed. Also, the expected level of uncertainty from model structure and parameterization and its effects on the model output are addressed.

- *Code verification:* The final set of computer code is scrutinized to assure that the equations are programmed correctly and that sources of error, such as rounding, are minimal. This process is likely to be more extensive for new computer code. For existing code, the criteria used for previous verification, if known, can be described or cited. Any additional criteria specific to the modeling project can be specified, along with how the criteria were established. Possible departures from the criteria are discussed, along with how the departures can affect the modeling process.

- *Model evaluations:* A model can be evaluated by comparing model predictions of current conditions with similar field or laboratory data not used in the model calibration process, or with comparable predictions from accepted models or by other methods (uncertainty and sensitivity analyses).

- *Validation of input data:* For a first application of the model, where parameter values are specified and site-specific data are input into the model or subsequent applications, the input data may need to be validated for their requirements planned in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs). In addition how the criteria were established and the possible ways in which the criteria may not be met are specified, and the effects these conditions may have on the model output are discussed.

- *Model output:* The criteria used to assess the usability of the model output include its regulatory task requirements, as specified in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs) of the QA Project Plan. For model applications in production mode, model outputs are similarly assessed against program uncertainty and variability requirements. Comments on the process of choosing these criteria and objectives should refer to Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs). If the model output fails to meet these criteria, the resulting course of action is detailed.

Note that many of the assessment approaches used to evaluate these acceptance criteria may have already been provided in Element C1 (Assessment and Response Actions), and references back to this section are acceptable.

4.4.2 Validation Methods (D2)

Describe the process to be used for validating the model results, including (if appropriate) procedures that maintain the integrity of data throughout the life of the project or task. Discuss how issues shall be resolved and the authorities for resolving such issues. Describe how the results are conveyed to users. Provide examples of any forms or checklists to be used. Identify any project-specific calculations required.

The purpose of this element is to describe, in detail, the process for making a final assessment of whether model components and their outputs satisfy the user requirements specified throughout the QA Project Plan. The appropriate methods of evaluation are determined by the quality objectives developed for the project and detailed in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs). The individuals responsible for the evaluation of the various components of the model together with the lines of authority should be shown on the organizational chart presented in Element A4 (Project/Task Organization). The chart should indicate who is responsible for each activity within the process.

The review process should be described for each component of the model and its results discussed in Element D1 (Departures from Validation Criteria). Discussion should address the difference between processes for newly-developed versus established models and between existing versus new software code. The review procedure for all model output results should be documented in the SOPs (e.g., graphical displays or videos).

Examples of issues to be addressed include the following:

- *Mathematical basis for the models:* The process should be described that will be used to assure that the mathematical basis for the model accurately reflects the process it represents. For example, the mathematical model can be assessed through peer review. The method of model evaluation, including responsibilities and schedules for peer review or other methods of assessment, should be described.

- *Numerical models:* For new or existing models, the process of measuring characteristics of the numerical model against the set criteria should be addressed, along with the procedure for confirming that the numerical model is accurately estimating the mathematical model.

- *Code verification:* The process of specifying how and when code will be checked to ensure that the program correctly solves the equations representing the mathematical model should be discussed. The new software code is examined and existing code is evaluated with respect to the current modeling process. If possible, the verification status of existing code should be addressed.

- *Model evaluation:* The process of specifying how and when model output will be compared with independent data to ensure that the modeling results meet project objectives.

- *Validation of input data:* The process of specifying how and when parameter values and site-specific data that are input into the model will be validated for their requirements planned in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs) [or B9 (Non-direct Measurements)].

- *Model output:* The usability of the model output is assessed by comparing it against its regulatory task requirements and other criteria specified in QA Project Plan Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs). The procedure that will be used to assess the model output should be documented.

4.4.3 Reconciliation with User Requirements (D3)

Describe how the results obtained from the project or task will be reconciled with the requirements defined by the data user or decision maker. Outline the proposed methods to analyze the output data and determine possible anomalies or departures from assumptions established in the planning phase of the modeling process. Describe how reconciliation with user requirements will be documented, how issues will be resolved, and how limitations on the use of the output data will be reported to decision makers.

The purpose of Element D3 (Reconciliation with User Requirements) is to outline and specify, if possible, methods for evaluating (relative to user requirements) the model outputs that the project generates. These methods include scientific evaluations of the model predictions to determine if they are of the right type, quantity, and quality to support their intended use.

This element discusses the procedures in place to determine whether the final set of model results meets the requirements for the data quality assessment. This element should also discuss how departures from the underlying assumptions or output criteria associated with statistical procedures applied in the data quality assessment will be addressed, the possible effects of departures from assumptions or specified output criteria on the model results, and what potential modifications will need to be made to adjust for these departures. Finally, the discussion should specify model limitations that may impact the usability of the results.

Data quality assessment (DQA) follows the procedures that are documented within the Group DQA Project Plan elements. Discussed in detail within*, Guidance for Data Quality Assessment: Practical Methods for Data Analysis (QA/G-9*) (EPA, 2000c), DQA determines how well the validated output can support their intended use. In cases where formal DQOs have been established [Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs)], DQA is a key part of the assessment phase of the data life cycle. It focuses on evaluating the ability of information to be used for decision making and provides graphical and statistical tools. If a probabilistic model has been developed, then the distribution of the model outputs, which is a measure of the uncertainty of the model predictions, should be compared with the allowable model output uncertainties specified in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs Data). The uncertainties of the various inputs and assumptions used in the model should be examined if that has not been done under Element C1 (Assessment and Response Actions). Also, sensitivity analyses may be used to gain information on the particular model inputs that contribute the most uncertainty to model outputs. This information can be used to provide clues to how reductions in model output uncertainties can be most cost-effectively reduced to acceptable levels.

Risk Assessment Guidance for Superfund: Volume 3 (Part A): Process for Conducting Probabilistic Risk Assessment (EPA, 1999e) provides uncertainty and sensitivity analysis methods. *Uncertainty Analysis in Ecological Risk Assessment* (Warren-Hicks & Moore, 1998) and *Uncertainty Analysis* (Kirchner, 2000) also provide case studies describing current state-of-the-practice ecological uncertainty analyses. Statistical methods should be used to assess the uncertainty (e.g., variability and unintended bias) and any abnormalities in the differences (residuals) between model outputs and comparable data. Graphical and statistical methods as discussed in *Applied Regression Analysis* (Draper & Smith, 1981 and in ASTM D6589) are useful for this purpose.

For modeling projects that are data poor (i.e., that have high uncertainty in model inputs and consequently in model outputs), it is particularly important that procedures are in place to address whether the high levels of uncertainty that are likely can allow user requirements to be met, and if not, the actions needed to address that issue

CHAPTER 5

EXAMPLES

This chapter is designed to provide an illustration of the information that could be included in a QA Project Plan for modeling. The previous chapters discuss the type of content that could be included, and this chapter is meant to provide examples of this content. This chapter is important for two reasons: (1) implementation of a new process is always more understandable with examples and, (2) these examples will provide the reader with some insight into the implementation of the "EPA graded approach."

In this chapter, three levels of projects are described to illustrate the varying level of detail and emphasis that may be needed for a QA Project Plan based on the nature of the modeling project and the intended use of the output data. The first example describes the development of an entire model made up of many different modules. The second example describes application of a less complex model. The third describes the planning information needed to test a single module in development as part of building a larger model system.

In each example, the information provided under each relevant QA Project Plan element is described to illustrate the application of the QA Project Plan elements to that example. These examples also discuss the documentation appropriate for each project.

5.1 COMPLEX MODELS – LAKE MICHIGAN MASS BALANCE PROJECT

A QA Project Plan for this complex project describes how planning, implementation, and assessment activities are coordinated across the extensive model framework (see www.epa.gov/glnpo/lmmb/planning.htm). Although this would be an overview document, an adequate level of detail is needed to clearly communicate agreed-upon development, assessment, and reporting activities and evaluation criteria from project management to the model developers. Referral to accompanying project documents would be used where possible to keep this QA Project Plan for the entire framework at a reasonable size.

5.1.1 Part A: Project Management

Section A3: Distribution List. Due to the large scope of this modeling project, this section contains an extensive list of individuals who will be involved in the review and approval of the QA Project Plan. This list can include but is not limited to module project managers, QA Managers, data suppliers, individual module developers, funding managers, and data users.

Section A4: Project/Task Organization. Because coordination among modeling teams and communication of progress will be a critical part of this QA Project Plan, the management plan for the project is described. Because this is such a long-term project, management will take a phased approach to development in order to accommodate the increasing complexity of the system and changes in resources over time. The stages would be clearly defined, with reviews, evaluations, and interim decision making clearly identified and described. The planned stages for this project include using historical data to refine modeling theory and sampling designs, working with data suppliers on data quality assessment, developing and testing the final models, and documenting the models and quality assurance results.

Section A5: Problem Definition/Background. The purpose of this model is to develop a tool to improve the understanding of the sources, transport, fate, and bioaccumulation of toxic chemicals in Lake Michigan. The information needs driving the model development are twofold: (1) to determine sources of chemicals in tributary, atmosphere, and sediment categories and, (2) to predict future in-lake chemical concentrations [e.g., polychlorinated biphenyls (PCBs) in lake trout] under alternative management scenarios. The target fish species are lake trout and coho salmon.

Section A6: Project/Task Description and Schedule. It is important to have an overall schedule so that individual module developers take into account testing and evaluating of other modules. This section lists all the modules being developed, the schedule for testing and evaluation, and the schedule for testing interfaces between/among modules.

The modeling framework is shown in Figure 11. The relationships between the modules are clearly specified in the planning documents, including input, output, any processing needed, and the measurement unit to be used at each transition. The method for moving the data from one module to another is specified under Element B10 (Data Management and Hardware/Software Configuration).

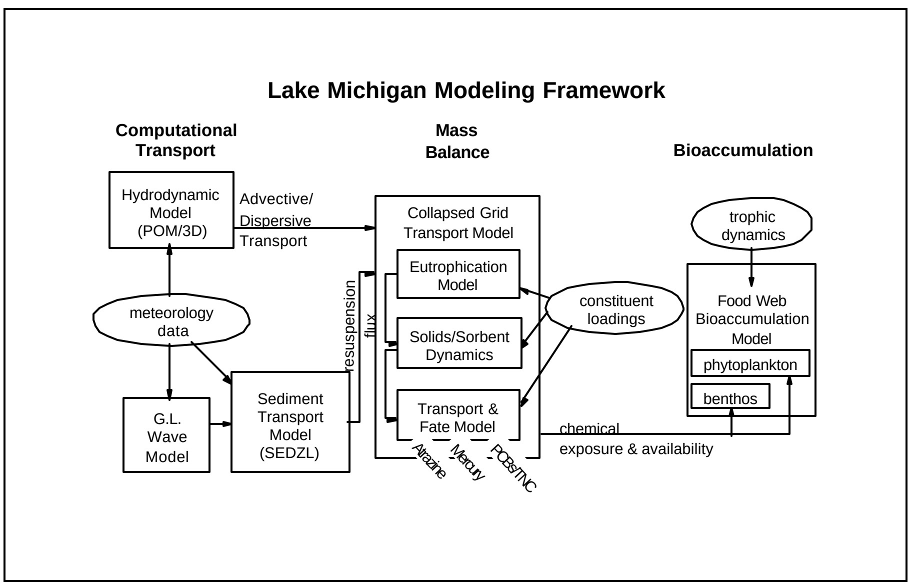

Figure 11. Modeling Framework for Lake Michigan Mass Balance Project

The model framework QA Project Plan would include QA information on the individual modules within the framework. Each model team would develop its own individual quality assurance plan to be included in the QA Project Plan for the framework. These QA plans would include:

- background and main features of the model;
- source(s) and quality of the data (e.g., used in calibration or testing of the model);
- plans for model software code development and maintenance;
- information on model parameters (source of the data, other values considered and reasons for rejection, information supporting the use of these data for this model);
- plans for model documentation (e.g., equations, underlying assumptions, boundary conditions, and numerical methods);
- plans for code verification;
- plans for code documentation (e.g., code, internal documentation, documentation of adaptations for the Great Lakes, user's guide);
- plans for model calibration, evaluation, and uncertainty;
- references, especially to any earlier documentation of the model if it was previously developed.

Section A7: Quality Objectives and Criteria for Model Inputs/Outputs. This section will describe several different levels of quality objectives. The Technical Coordinating Committees for this modeling project developed modeling quality objectives (EPA, 1999b) that were translated into quality objectives for the individual modules to be used to evaluate the model. The data quality objectives for the entire framework specified that the model should be capable of calculating pollutant concentrations in Lake Michigan to within a factor of 2 of observed concentrations in the water column and target fish species. Furthermore, study managers agreed to accept an uncertainty level for each input to the model within 20-30% of the mean at the 95% confidence level. The modeling objective was to simulate the average water quality within ± 2 standard errors of the observed mean (by cruise/segment average) or to provide 95% confidence that the actual mean falls within this specified range.

Section A9: Documentation and Records. This section includes the plan for long-term documentation, which is especially important in a multi-year and multi-stage project like this one. The type of information that will be part of the record is itemized so that modelers are informed beforehand of the records they should keep. All records, including modeler's notebooks and electronic files, would be maintained by the laboratory QA officer in a central project archive upon completion of the project.

These records would include documentation of model testing, calibration, and evaluation. Records would be kept of written rationale for selection of models, record of code verification (hand-calc checks, comparison to other models), source of historical data, source of new theory, and documentation of adjustments to parameter values due to calibration. These records will be maintained by each modeler and transferred to a central project archive. Agency standards and ANSI/IEEE standards for software QA plans need to be followed.

5.1.2 Part B: Data Acquisition and Management

Section B7: Calibration. In this section, outputs of interest are clearly identified, with special attention to issues that will need to be coordinated for consistency between different modules. The analysis procedures and acceptance criteria would be specified in the QA Project Plan for each module (this might be done under the QA Project Plan for each module under Section A6). If field or other data will be used for calibration, the QA Project Plan would describe why those data were chosen, how those data will be acquired, and how the quality of those data will be assessed.

Adjustments due to calibration need to agree with scientific knowledge and with the process rates within a reasonable range of values found in literature. A list of internal variables used to calibrate the model outputs would be included in this section.

For this model, simulations will be used to attempt to reproduce the statistical distribution properties of the data. Parameter optimization will be used to minimize residuals. Model simulation results will be compared to measurements obtained from the project data collection program.

Section B9: Non-direct Measurements (Data Acquisition Requirements). For this project, the preference is to use published data that have been through a peer review process overseen by an editorial board. Unpublished data can be used, and will be reviewed using data quality assessment (DQA) tools. Instructions for performing DQA are presented in this section. This section also includes a table listing major data needs and potential and confirmed sources for these data. A list of the available QA information is included along with identification of the QA information that will be sought for data sources that are utilized.

For this QA Project Plan, historical data from a variety of sources and data collected for this modeling project need to be assessed to determine if they meet the objectives of the modeling project. Information on acquired data would be obtained from the relevant data collection QA Project Plans or related materials. This information would be used to evaluate indicators such as the comparability of the data for aggregation and time analyses, its representativeness of lake conditions, bias, and precision.

Assessment of the data by both the Great Lakes National Program Office and the modelers would be preferred.

Section B10: Data Management and Hardware/Software Configuration. For this model, the Revision Control System will be used to coordinate version input and output files. The compatibility of the input database formats and modeling framework will be worked out along with hardware/software requirements. Hardware/software configuration would be described in some depth in accordance with document planning requirements for developers of the individual models, and pre- and post-processors.

Test planning and results reporting need to be specified and implemented to assure compatibility of parts of the model framework and final usability. Plans would be needed for configuration management of revised code throughout the phased development.

5.1.3 Part C: Assessments and Response Actions

Uncertainty will be estimated in a two-step process. The parameter variance-covariance matrix resulting from calibration will be estimated and applied to generate exceedence levels for model predictions using Monte Carlo methods. The goal of this process is 95% exceedence limits within a factor of 2 of the predicted toxic chemical concentrations in water and top predator fish over the duration of the calibration period (1994-1995).

The ability of the code to correctly represent model theory will be assessed. In addition, specific tests are planned to ensure operations are verified. Continuity checks, mass conservation checks, and testing of numerical stability and convergence properties will be conducted.

5.1.4 Part D: Output Assessment and Model Usability

Plans for testing need to be worked into the phases of the project. Model simulations will be planned to reproduce the statistical distribution properties of the field and laboratory data. Evaluation will be done by comparing cumulative frequency distribution plots of data to frequency distributions plots from comparable model predictions. This quantitative evaluation will be integrated with qualitative assessment. A science review panel independent of the model development process will provide reviews on a regular basis.

As the individual modules evolve through different scales and levels of uncertainty with development (e.g., screening models, a medium-resolution segment scheme, and a high level resolution phase), assessments will be planned to determine if they are acceptable to pass on to the next phase. Ultimately, the whole framework needs to be assessed, and these individual assessment results will provide background for planning such an assessment.

5.2 INTERMEDIATE MODELS – PORT RIVER NITROGEN AND PHOSPHATE TOTAL MAXIMUM DAILY LOAD (TMDL) PROJECT

In this example, a state's Department of the Environment (DOE) wishes to estimate a Total Maximum Daily Load (TMDL) for selected nutrients (nitrogen and phosphorus) that have impaired the ability of a given waterway to achieve water quality standards, and estimate how the TMDL is allocated among different sources of these nutrients. A TMDL is an estimate of the maximum amount of a pollutant that a waterway can receive and still remain within water quality standards established by the Section 303 of the Clean Water Act (CWA). The state DOE plans to use EPA's existing Water Quality Analysis Simulation Program (WASP5), and in particular, its EUTRO5 component on water quality/eutrophication, as a modeling tool for obtaining the necessary information for establishing the TMDL estimates. For this project, a QA Project Plan is prepared to describe how planning, implementation, and assessment activities would be accomplished to achieve defensible outputs from this modeling process. The following discussion indicates the type of information that would be included in the QA Project Plan.

5.2.1 Part A: Project Management

Section A4: Project/Task Organization. Because this is largely the effort of a single state's DOE, this section of the QA Project Plan would focus on roles and responsibilities of internal departments and managers who will contribute to the modeling effort. For example, each department that is to provide necessary model input data would be specified here, along with appropriate contact people. Departments that will contribute to TMDL development but may not be directly involved in the modeling effort may also be specified here. Individuals will be noted according to their responsibilities in overseeing various stages of the project. Examples of these project stages include the following:

- refining the problem using historical data
- working with data suppliers on data quality assessment
- reviewing the model for this specific application
- calibrating and testing the selected model
- performing model fits and identifying appropriate model inputs for each fit
- conducting sensitivity analyses
- documenting the model application and quality assurance results.

Section A5: Problem Definition/Background. The Port River, a 8.5 mile-long tributary of the Large River, was included on the CWA Section 303(d) list of impaired waters due to demonstrated eutrophication and low dissolved oxygen levels that violated water quality standards. Elevated nitrogen and phosphorus levels in the river have contributed to excessive algae blooms and wide diurnal fluctuations in dissolved oxygen content which have the potential to cause fish kills. Estimated TMDLs for total nitrogen and total phosphorus are needed because technology-based controls and other types of controls did not allow water quality standards to be attained for water contact recreation, aquatic life protection, and shellfish harvesting. The goals are to keep the concentration of chlorophyll-*a* (a surrogate indicator of algae blooms) to below 52 :g/L and dissolved oxygen to no lower than 5mg/L. Thus, the purpose of this model application is to provide predictions (or projections) on total nitrogen and total phosphorus to be used in developing TMDLs that will be protective of the river's designated uses. Information would be generated for both low (base) flow and annual average conditions.

Section A6: Project/Task Description and Schedule. It is important to establish a schedule that will allow time requirements on approving TMDLs to be met with a defensible product. This section of the QA Project Plan lists all critical activities for planning criteria; acquiring and assessing existing data; model evaluation for selection, calibration, and application; and reporting. A process for tracking this schedule to complete these activities is also needed to assure that deadlines in the overall TMDL process are met.

Section A7: Quality Objectives and Criteria for Model Inputs/Outputs. This section will describe the several different levels of quality objectives for the various stages of this modeling project, as determined from a systematic planning process. The following types of quality objectives are among those relevant for this effort:

- Acceptance criteria for intended use of existing data: Existing data will be used as input to the modeling effort. This data will be judged acceptable for their intended use if they meet acceptance criteria that are determined from a systematic planning process and documented here. The sources of existing data to be used in this effort and their intended uses are documented in Element B9 (Non-direct Measurements). Examples of acceptance criteria and the types of data issues addressed by these criteria are as follows:

  – Data reasonableness: Loading data from surveys conducted in 1984 and 1985 will be used as input to the models when predicting baseline conditions. The reasonableness of these dates needs to be documented here. For example, these dates occur prior to the implementation of non-point source nutrient reduction controls placed on this waterway.

  – Data completeness: Data from at least four surveys need to be available for all available sampling stations within the tidal portion of the Port River from its confluence with the Large River to the upper free flowing areas of an unnamed tributary located above the Orange Sewage Treatment Plant. This criterion reflects the agreed-upon spatial domain of the model. Overall, the data need to achieve a 95% minimum criterion on completeness.

– Data representativeness: Certain criteria on data representativeness will need to be achieved, such as time and location for sample collection and comparability in sampling and sample analysis methods for input data from the DOE's water quality monitoring and point source databases (e.g., point source loading data from the most recent year for the four point sources). Other methods for assessing data representativeness relative to current conditions (e.g., photograph verification, visual assessment, considering data from bathymetric and ground truth land use surveys) can be detailed in Element C1 (Assessment and Response Actions).

- Acceptability of model calibration and testing inputs and outputs: Element B7 (Calibration) discusses the approach to be taken to determine whether the EUTRO5 model is properly calibrated. Project managers are defining model calibration in this setting as how well the model is able to reproduce current observed flow rates and concentrations of nutrient, dissolved oxygen, and chlorophyll-*a* (e.g., trends and peak values), as measured from multiple field surveys and stored in a state-maintained monitoring database. Because water quality data for multiple surveys exist for each sampling station in the waterway, each station has multiple measurements for the water quality parameters that are used as input to the models. Thus, the calibration procedure is able to divide the total variability of the model predictions into two sources: within-station variability in the input measurements, and variability and uncertainty associated with how well the model fits the data (i.e., lack-of-fit). The following criteria, as determined from stakeholders consulting with study statisticians, have been established for acceptable model calibration inputs and outputs, respectively:

  – At least 90% of the input nutrient concentration measurements at a given sampling station should be within two standard errors of the mean measurement at that station.

  – The percentage of total variability and uncertainty that is attributable to lack-of-fit of the model should not exceed 25% in any of the calibration model fits.

  Other goodness-of-fit evaluations may also be considered (EPA, 2000c; Gilbert, 1987) when determining corrective action associated with these criteria. For example, data may need to be transformed (e.g., logarithmic) to better achieve these criteria and other model assumptions, or further investigations into specific data values may be necessary. Such corrective actions are addressed in Element C1 (Assessment and Response Actions).

- Acceptability of model outputs: Any limitations on uncertainty associated with model outputs are specified here. For example, managers within the state's Wastewater Management Program may specify a goal that the uncertainty associated with the predicted value at a given location will need to be within 25% of the predicted value with 95% confidence.

- Acceptability of flow rate estimates: As discussed in Element B9 (Non-direct Measurements), multiple regression techniques will be used to predict low and average flows within various segments of the watershed as a function of land use data. The regression equations will need to achieve certain criteria on their goodness-of-fit (e.g., R^2 of at least 0.90).

The above types of data quality criteria tend to be quantitative in nature. However, certain stages of the model application process may benefit from assessments that are more general and qualitative. For example, when evaluating the outcome of model calibration, qualitative assessments may be done by evaluating how well the outputs of the fitted model are able to match the overall trend in prediction over time or over the entire watershed area. This evaluation would be documented in a final report by using graphs — the axes of these graphs and the data to be used should be documented in the QA Project Plan. An evaluation of how well these model outputs reflect peaks and valleys in the predicted water quality values at specified time points or at certain points in the watershed can also be compared to what has been observed and collected in surveys. Again, these can be documented in the final report by graphs that should be described in this element.

Section A9: Documentation and Records. This section includes the plan for documentation which will be important for defending the model predictions used in supporting the TMDLs. The type of information that will be part of the record would be itemized here so that modelers are aware before the project begins of the records that should be kept. Examples of appropriate documentation in this study include: calibration and sensitivity analyses results, records of written rationale for selection of models or modules, record of code verification (e.g., hand-calculated checks, comparison to other models), sources of existing data used, and any adjustments to model parameter values that result from model calibration. All records, including modeler's notebooks and electronic files, should be maintained by the project manager in a central project archive upon completion of the project.

5.2.2 Part B: Data Acquisition and Management

Section B7: Calibration. Water quality data on such measures as chlorophyll-*a*, phosphorus, nitrate, and dissolved oxygen that were collected from earlier surveys on the waterway, in addition to flow measurements obtained from the United States Geological Survey, will be used in calibrating the EUTRO5 model to this particular application. Element B9 (Non-direct Measurements) will document the sources of these data, and Element A7 (Quality Objectives and Criteria for Model

Inputs/Outputs) will specify the criteria for which these data will be judged acceptable for use in model calibration.

The calibration will judge the extent to which the model is able to predict current water quality measures that agree with what was actually observed in the surveys. For instance, the extent to which the model accurately captures observed trends in the water quality data at the various sampling points in the river and its tributaries, after taking into account the underlying variability in these monitored data, will be determined and appropriately documented. The discussion should note that in this particular application, model testing is also occurring during the model calibration process, as the inputs to the model calibration and the model's corresponding outputs represent a given water quality scenario that will be used as part of the TMDL development process. The performance criteria upon which the calibration will be deemed acceptable will be noted in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs).

Within the model calibration exercise, model rate coefficients will be adjusted as necessary to meet the calibration criteria and to reflect current scientific knowledge and various process rates that fall within a reasonable range of values found in the scientific literature. A list of internal variables used to calibrate the model outputs should be included in this section, along with any adjustments made to the model. The rationale for any needed model adjustments based on the results of the calibration process would be documented according to the procedures specified in Element A9 (Documentation and Records).

Section B9: Non-direct Measurements (Data Acquisition Requirements). As indicated previously, different types of data already existing within the state's databases will be used for model calibration and as input to the model. This section of the QA Project Plan discusses the different sources of these data, the intended uses of these data on the project, the specific criteria for accepting an existing data source for use on the project, and any limitations that the use of these data may have on this project.

The primary types of existing data to be used in the modeling effort are nutrient point source loads and non-point source loads for the watershed. Loads for the contributing point sources are taken from discharge monitoring reports that exist in the state's point source database. When average flow conditions are assumed, non-point source loadings are calculated as a sum (across the different types of land uses) of land use areas multiplied by their respective land use loading coefficients. Land use areas originate from the State's Office of Planning. Land use loading coefficients are previously-published outputs that resulted from fitting a continuous simulation model representing the bay in which the river deposits. Non-point sources represent such contributors as atmospheric deposition, as well as loads from septic tanks, urban development, agriculture, and forest land.

The modeling effort will consider four different scenarios that represent either baseline or future conditions and low versus average flow characteristics. These scenarios simulate seasonality effects. Therefore, different sets of existing data (i.e., point source loads and non-point source loads) will be needed as model inputs for each scenario. These data sources should be listed here for each scenario, along with any limitations that these data may have in terms of predicting the scenarios.

For this project, the water quality and physical field data were collected by the state's field operations program in earlier surveys according to documented field and laboratory protocols and at documented monitoring stations. In order to ensure this data is appropriate for use in this model, survey records will be checked to assure conformance with procedures established for their initial collection and to assure that the resulting data meet the requirements established in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs). Data will be reviewed to be sure that their values fall within previously-observed and reasonable ranges (e.g., base flow nutrients and groundwater).

As part of the modeling procedure, the watershed will be subdivided into subwatersheds, and low and average flows will be determined at each subwatershed using multiple regression procedures that predict flow as a function of land use data (Draper & Smith, 1981). The regression equation predicting low flow was determined from flow data collected at two sampling stations. Because no average flow data were available for the basin, the regression equation for average flow was determined using long-term average daily flow data originating from survey gauges and relating these data to land use acres within the basins. The equations will need to achieve acceptance criteria specified in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs). The source and relevance of these regression equations will be documented in this element of the QA Project Plan.

In determining whether existing data sources meet acceptance criteria for the project [as defined in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs)], information on acquired field data to be used for assessing acceptance criteria would be obtained from the QA Project Plans of the operations collecting these data or from related materials from the state's field operations branch. Any limitations on the existing data that may impact a model's predictive ability for this project should be discussed here. For example, water quality surveys for which data were used in model calibration were collected over 15 years ago, and therefore, any changes to the waterway and its environment since then needs to be taken into consideration.

Section B10: Data Management and Hardware/Software Configuration. EPA's model WASP 5 and its sub-model EUTRO5 are being used to estimate the fate and transport of nutrients because they are capable of studying time-variable or steady state (up to three dimensional), linear or non-linear, kinetic water quality problems. This element of the QA Project Plan discusses the resource needs for the modeling system. A process flow diagram would be included to illustrate how various types of data are input to the system and the different types of model outputs. Details would be provided on how the model input and output data will be manipulated, managed, and maintained as part of this project (e.g., all data to be input to the model need to be stored in metric units), along with how the overall integrity of the data will be ensured through the various stages of the project. For example, information on how the water quality survey data used in model calibration are averaged across the different surveys would be discussed here.

The future form of the model needs to be compatible with the input database formats and with the hardware/software capabilities of the department (e.g., Department PC-compatible, pre- and post-processors available from distributor). Thus, these types of resource requirements are mentioned in this element of the QA Project Plan. If available, case histories on prior use of this model will be reviewed with the test results generated in the model development phase to assure that the model is adequate to meet the goals of this project.

5.2.3 Part C: Assessments and Response Actions

The different types of assessments and model performance evaluations to be performed in this project are documented in Element C1 (Assessment and Response Actions) of the QA Project Plan. Examples are the following:

- *Testing the Model* - The ability of the selected model and modules to correctly represent modeled conditions will be assessed focusing on changes in eutrophication due to increases in stream flow. A sensitivity analysis will be performed to determine the effect of flow in the Port River system focusing on non-point flows and corresponding loads. The goal of this analysis is to test the sensitivity of the model during high flows to assure its responses are reasonable. If needed, further verification will be done by comparing model prediction results with survey data for base conditions.

- *Performing Multiple Runs of the Model to Simulate Seasonality Effects* - To assess the extent to which seasonality impacts the model outputs and, ultimately, to incorporate seasonality into the TMDL development process, the model will be fitted under different scenarios for nutrient loading and stream flow conditions. Some assessment is necessary to verify that the different scenarios that are selected represent the critical conditions for which the TMDL needs to satisfy water quality standards. Results of all runs will be used in the TMDL development process.

- *Evaluating Existing Data* - As described in Element B9 (Non-direct Measurements), modeling staff will evaluate data to be used in calibration and as model input according to criteria discussed in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs Data) and will follow-up with the various data sources on any concerns that may arise.

- *Calibrating the Model* - The model calibration procedure is discussed in Element B7 (Calibration), and criteria for acceptable outcomes are provided in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs).

- *Sensitivity Analyses* - The different considerations that are to be addressed in sensitivity analyses will be documented here. One example is fitting the model after increasing the assumed non-point source flows and the corresponding loads, in order to test the sensitivity of the model under high flow situations.

5.2.4 Part D: Output Assessment and Model Usability

This section will describe how the modeling staff will complete and document the following tasks:

- review the set of future model predictions for reasonableness and relevance based upon observed field data and the literature,

- determine the consistency with the requirements documented in Element A7 (Quality Objectives and Criteria for Model Inputs/Outputs) on acceptable uncertainty,

- verify the model predictions relative to the requirements of the TMDL development process, and

- confirm that all steps of the modeling process were followed correctly.

Any problems will be reported to the project manager and corrective actions discussed with the Wastewater Management Program. The findings, including any limitations associated with their use in developing TMDLs, will be discussed in the project report.

Note from Element B9 (Non-direct Measurements) above that estimated non-point source load data for future conditions, representing future conditions after treatment improvement and used as input to the model, includes a margin of safety factor to account for uncertainty in future projections that are based on existing data. This margin of safety is generally specified in percentage terms within the QA Project Plan and is based on previous knowledge of uncertainty in forecasting nutrient levels. It generally accounts for uncertainty in a manner that is conservative from the standpoint of environmental protection. For example, it improves the likelihood that the allowable nutrient loads the system can incorporate without incurring an impairment is not underestimated. In determining whether this margin of safety was selected appropriately and meets user requirements, some evaluation should be conducted to assess where the magnitude of this margin of safety is adequate relative to the level of uncertainty associated with these model inputs. In addition, this margin of safety may be included in the evaluation of uncertainty in model outputs that is performed within the data quality assessments documented within Group D of the QA Project Plan.

5.3 SINGLE MODULE – LAND APPLICATION MODULE

This is an example of critical QA Project Plan elements for a single module that is part of a larger existing model. This QA Project Plan covers the assessment phase of the model development task. At the beginning of this project, the model has already been developed and will be tested with this project.

5.3.1 Background

The Land Application Unit (LAU) module is one of five source emission models that are components of EPA's Multimedia, Multipathway, Multi-receptor Risk Analysis (3MRA) software system. In a LAU, waste is applied to the land at regular intervals and is tilled into the soil. The LAU module simulates this process and estimates how much of each waste constituent volatilizes into the air, leaches into the groundwater, runs off into the stream, or remains bound to the soil. All of these output concentrations (air emissions, leachate concentration, runoff concentration, and amount bound to the soil) are used as input to other modules in 3MRA. The LAU module is described in detail in a technical background document (EPA, 1999c).

The 3MRA model was developed for use in implementing the Hazardous Waste Identification Rule (HWIR). The 3MRA model establishes risk-based concentration limits that, if exceeded for a constituent in a waste stream, will identify that waste stream as hazardous, necessitating management of the waste in a regulated waste management unit designed for hazardous waste. The 3MRA system schematic diagram is presented in Figure 12. As a 3MRA source module, the LAU Module is the first module fired by the 3MRA's Multi-Media Simulation Processor.

5.3.2 Part A: Project Management

Section A4: Project Organization. The team will include the following members: client (Hazardous Waste Program Project Manager), program QA Manager, contractor (Project Manager), modelers, scientists, information management personnel, and QA personnel. Some of the scientists, information management personnel, and modelers assigned to the QA project are not assigned to the LAU model development project and, therefore, are independent in their assessments.

Section A5: Problem Definition/Background. The objective for this project is identified as follows: to evaluate whether the outputs of the LAU module are acceptable and correspond to the expectations that the total model places on the LAU module; and to summarize and report to the project manager and client the results of those assessment tests. Because 3MRA is a probabilistic risk

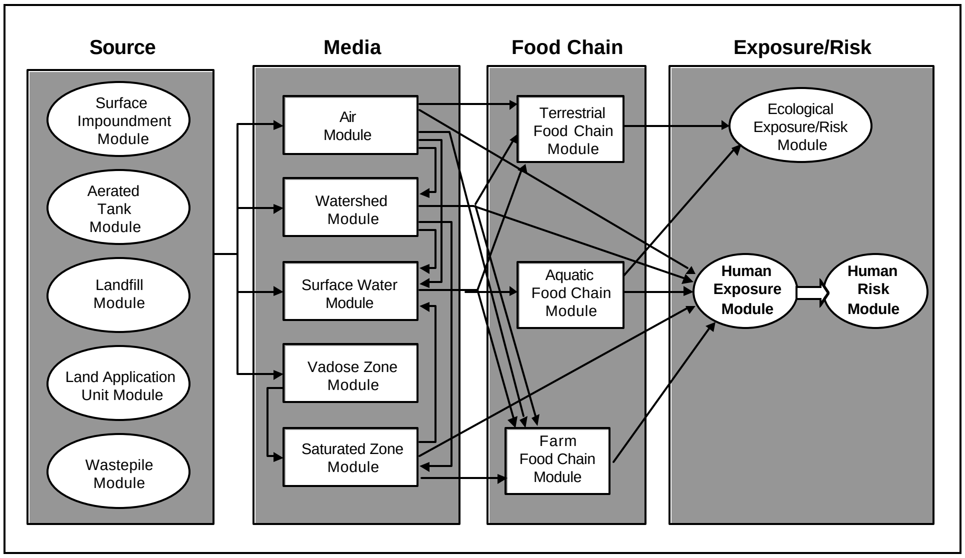

Figure 12. Module Components of 3MRA.

assessment model, reporting of uncertainty and variability associated with the output of the LAU module is specified in EPA policy.

Section A6: Project/Task Description and Schedule. It is important to document the overall schedule because some assessments must be performed sequentially while others may be conducted independently. This task lists all of the assessments and the time frame in which the tests should be performed. The schedule for assessment of this module is constrained by the schedule for the testing of the larger model. Thus, because this module is the first module run for the entire model, it needs to be assessed first. However, if unforseen problems with the output of this module are discovered during the assessment of other modules receiving these data outputs, the LAU module must be revised and re-assessed. This overall project schedule is also constrained by regulatory deadlines.

Section A7: Data Quality Objectives and Criteria for Model Inputs/Outputs. Because this project involves the assessment of module development, performance and acceptance criteria are more appropriate than DQOs. Model performance criteria include: (1) evaluation of pre-simulation calculations and accuracy of calculated input data, (2) evaluation of algorithms for subarea coupling and water balance, (3) performance of the Generalized Soil Column model for benzene diffusion and convection and the subarea coupling process, and (4) overall performance of the LAU module by benchmarking of the LAU module with the widely accepted HELP model. The criteria for acceptance are specified for each test requirement in Table 5.

The module assessment requirements for the LAU module include testing of algorithms using hand calculations to ensure that the model calculates as intended, writing another program to ensure that the results of certain calculations within this model agree within ± 0.1%, or benchmarking the model using data from an external source for comparison.

Table 5. Description of Modeling Project Tasks

Project Tasks	Technical Approach	Quality Requirements and Procedures	Personnel Requirements	Types of Reports/Records
Read input data	Echo inputs to outputs, 10% check of data points	100% agreement	Information specialists	Input and output records
Pre-simulation calculations	Hand Calculations	100% agreement check. Complete agreement with modeled values	Scientists	Algorithm spreadsheet and program documentation
Benzene diffusion	Independent computer program to check vertical transport calculations	Agreement between output within 0.1%	Computer modeler	Output of model and independent comparison model
Subarea coupling process	Set runoff parameters to nonzero and zero values	Check of output is a nonzero value and zero as expected	Scientists	Inputs and outputs of models, checking nonzero and zero values where appropriate
HELP benchmarking	Compare 10% of modeled values to external benchmarks from HELP model	100% agreement	Scientists familiar with external benchmark data	Model outputs and corresponding external benchmark data
Logical flags	Output logical flags to external file and check for agreement	Compare to see that 100% of logical flags were carried forward in the analysis	Information specialist	Output of logical flags from multiple portions of the model to assure correspondence

All data used in the model will be subjected to quality control procedures. All data that are acquired through electronic transfer from quality-controlled sources will be subjected to 10% check to assure a valid data transfer has occurred. Any data that are hand entered specifically for this module will be subjected to a 100% check against primary or secondary data sources.

Section A8: Special Requirements/Certification. This section states that experience with hazardous waste modeling and information management is needed for this project.

Section A9: Documentation and Records. The documentation of the assessments from Sections B7 and B9, and Groups C and D will include model input and output files used in the assessment process, inputs and outputs and model code from any external computer programs developed to validate the model, and any external data sources used to benchmark the modeled outputs. In addition, each module assessment step will include a signed QA documentation form for the model. Any changes made to the model code as a result of QA checks will be documented using the appropriate change control process.

5.3.3 Part B: Data Generation and Acquisition

Section B7: Calibration. Calibration will not be used for this model due to lack of data [see Section C1 (Assessment and Response Actions) for benchmark testing].

Section B9: Non-direct Measurements (Data Acquisition Requirements). This section documents the data used to generate the input data files (site layout data, LAU Module-specific parameters, chemical properties parameters, and four types of meteorological data—daily, monthly, annual, and long-term average). This documentation will include the sources of these data, quality assurance information about these data sources, and an indication of how the data were assessed to determine if they were appropriate for this model.

They will be assessed based on project requirements (e.g., acceptable uncertainty and variability). All data used in model testing are provided by EPA and will be evaluated for data quality for use in the LAU source model (e.g., representativeness, bias, completeness, and comparability to expected input data). In addition, the data will be checked (100% for data that are hand-entered and 10% for data that are entered by direct electronic transfer) to assure that the correct values have been recorded in the data files. The sources of data used in the LAU model will be numerous because many types of data are necessary for this module. For example, meteorologic and climate data are acquired from the National Climate Center electronically, soil texture data are available from an online database, and chemical and physical data are available from literature sources (such as hard copies of handbooks).

Section B10: Data Management and Hardware/Software Configuration. In this section, a flow diagram (like Figure 13) would be used to show the relationship between the parts of the module and describe how data flows through these parts. The QA Project Plan would contain details about how the data were pre-processed (in this case, unit conversions were needed) and how this pre-processing was done. Also in this section, details would be included about how the data were entered into the Generalized Soil Column Model—whether it was hand-entered, read from a database or other file, generated internally, or otherwise entered into the model.

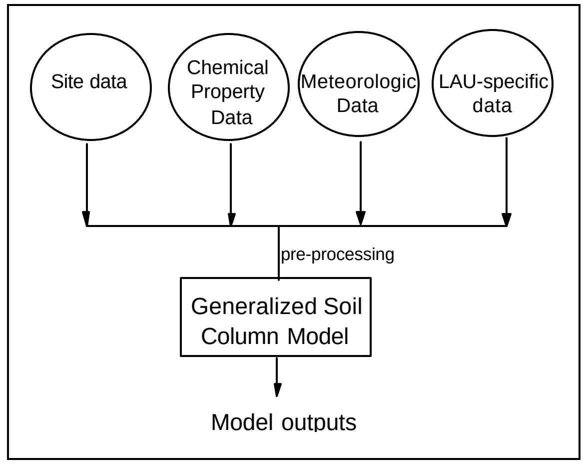

Figure 13. Data Flow Diagram for the LAU Module

The hardware and operating system for running this module would be described with enough detail to determine if they meet the requirements specified for the model (e.g., operating system compatibility, run time, memory).

5.3.4 Part C: Assessment and Response Actions

These assessments are representative examples of what was planned to be done, and are not a complete list of model assessments.

Correctly Read Input Data. The LAU Module reads input data from several files, which are either preexisting (meteorological data) or are generated. Input data will be verified for: (1) site layout data, (2) LAU Module-specific parameters, (3) chemical properties parameters, and (4) four types of meteorological data—daily, monthly, annual, and long-term average—by running the simulation in a mode that documents as output all of the input parameter values to an external file. Ten percent of the parameter values documented in the output file will be randomly selected and compared with the corresponding values from the input files.

Results will be reported to the project QA officer in the format provided in Section A9. If exact agreement is not achieved between the input values and the output values, corrective action will be taken by the modeling coordinator to assure that the correct files are read appropriately and the test is repeated to document compliance.

Evaluation of Pre-simulation Calculations. Prior to executing the algorithms in the LAU Module, each calculation in the spreadsheet will be evaluated for mathematical correctness (checked against the parent equation in the documentation, if applicable), reviewed for correct coding [e.g., ensuring that parentheses were correctly placed in the assignment statement or that the internal calculation order is correct, (e.g., multiplication before addition)], and reviewed for consistency among units.

In addition, a number of parameters that are internally generated as a function of the input data will be assessed to see if they are correct. Single representative calculations of each type will be selected for testing by the QA officer. A spreadsheet will be created to independently perform the calculations that generate the parameters of the selected representative LAU Module code for comparison. To be correct, values can differ by no more than a rounding error (usually less than ±0.1%).

Results will be reported to the project QA officer and the modeling coordinator in the format provided in Section A9. If incorrect algorithms or deviations from the independent spreadsheet calculation values are found, corrective action will be taken by the modeling coordinator to assure that the algorithms are corrected and this test is repeated.

Assessment of Correct Operation of the Generalized Soil Column Model. The Generalized Soil Column Model is the fundamental chemical fate and transport algorithm driving the LAU simulation. It simulates the time-variable, vertical distribution of chemical mass in a one-dimensional soil column as well as losses due to internal sinks, emissions to the atmosphere of volatile and sorbed chemical, losses from the surficial soil layer due to storm water runoff and erosion, and losses to the vadose zone from leaching. Computationally, it is a semi-analytical solution to the one-dimensional, time-variable advective/diffusive differential equation including first-order losses.

The assessment of correct operation of the Generalized Soil Column Model will be conducted by several test cases, including benzene diffusion and convection, to check the model's response to several individual key parameters. The planned test cases are described in this section.

<u>Benzene Diffusion</u>. This test case will assess the most computationally intensive aspect of the LAU Module, the diffusive mass transfer algorithm, which simulates the diffusive mass flux emanating from N individual computational elements constituting the "soil column," combines the effects of each element on all the other elements, and performs the same operations in a "reflected" soil column to achieve a zero concentration gradient boundary condition at the soil column's lower boundary.

The diffusion algorithm is impractical to check in a spreadsheet environment because of its computational complexity. Therefore, an independent computer program will be developed in BASIC and used to check these calculations. This will be a "clean-room" exercise in which only the documentation and previous knowledge of the algorithm's theoretical basis will be used to develop it, rather than by "reverse-engineering" the LAU Module code. The compiled program will be documented and reported according to requirements specified in Section A9.

An output file of the vertical concentration profile will be produced by running the simulation in a mode that will also document all of the corresponding input parameter values to an external file. The simulation will represent the times after the waste application and again after the diffusion algorithm are applied. Separately, the post-diffusion vertical concentration profile will be simulated by the module and documented. The results will be reported to the project QA officer and the modeling coordinator in the format provided in Section A9. If deviations from the independent values are found, corrective action will be taken by the modeling coordinator to assure that the algorithms are corrected, and this testing process will be repeated to document compliance.

Benzene Convection. This test case for benzene will be used to check the convective transfer algorithm of the Generalized Soil Column Model that shifts the vertical concentration gradient downward by one computational cell when a convection event occurs (i.e., when the chemical mass, moving at the effective convection velocity, has completely traversed the cell's depth). This test will be conducted by producing before- and after-convection vertical profiles from a convection event in an external file mode and comparing them to ensure that the profile has been translated downward by one cell.

A spreadsheet presenting excerpts from the external file on the convection event will document the results of the Generalized Soil Column Model convection algorithm assessment, and will be reported to the project QA officer and the modeling coordinator in the format provided in Section A9. If the results do not show the downward translation in the profile, corrective action will be taken by the modeling coordinator to assure that the algorithms are corrected, and this testing process will be repeated to document compliance.

Assessment of the Correct Operation of the Subarea Coupling Processes. A local watershed is a land area containing the LAU and over which surface runoff is assumed to occur as sheet flow (overland flow). It contains up to three subareas: the LAU, a downslope buffer between the LAU and the water body, and possibly an up-slope subarea lying between the LAU and the local watershed drainage divide. The local watershed subarea coupling algorithm serves to take chemical (and solids) mass being transported off the LAU during a runoff event as overland flow and contaminating the downslope buffer via settling and diffusion. The Generalized Soil Column Model is essentially a one-dimensional model (vertical), simulating the fate and transport of chemicals in a single subarea. These subareas are coupled for purposes of simulating fate and transport across the local watershed by code external to the Generalized Soil Column Model, which is the code of interest for assessing Requirement 4 in Section A7 (Quality Objectives and Criteria for Model Inputs/Outputs).

Subarea Coupling Algorithm Decoupling Test. As noted above, the mechanisms by which a buffer area downslope of the LAU is contaminated are: (1) settling of eroded solids onto the buffer and, (2) diffusive exchange of dissolved chemicals between the storm water runoff and the underlying pore space of the buffer's surficial soil layer. These mechanisms are controlled by the solids' settling rate in storm water runoff and the diffusion coefficient. A test case will be assessed as a two-run sensitivity analysis to ensure that cancellation of these two coupling parameters would result in no contamination of the downslope buffer subarea. Run 1 will use the default values (nonzero) for storm water runoff and the diffusion coefficient to establish that contamination of the downslope buffer occurs when these values are nonzero. Run 2 will change these two parameter values to zero to assess whether contamination will occur.

The buffer concentrations will be reported to the output file, and if the results of Run 1 were not positive and the results of Run 2 were not zero, corrective action will be taken. The results will be reported to the project QA officer and the modeling coordinator in the format provided in Section A9. If the results are not appropriate, corrective action will be taken by the modeling coordinator to assure that the algorithms are corrected, and this testing process will be repeated.

Benchmark Testing. Benchmark testing will be performed on portions of the module, and additional model assessment will be performed to test model performance. Benchmark testing is used in this case because there are no existing data to use in model calibration. This assessment will compare hydrology outputs of the LAU's water balance algorithm to a widely accepted EPA hydrology model, the HELP model, which is more complex than the LAU module's water balance algorithm but uses a similar underlying mathematical construct. Approximate comparability of long-term average results is expected with the benchmarks. General agreement of the various water balance outputs with the outputs generated by the HELP model will be acceptable.

This test case will benchmark the water balance algorithm against results of the HELP model for six sites (e.g., Miami, Dallas, San Diego, Madison, Denver, and Seattle) over five years. Meteorological files generated for these benchmark sites will be used with edited daily meteorological files to replace daily precipitation and daily temperature with the precipitation and temperature time series for the benchmark site being run. The monthly meteorological file will also be edited to replace the monthly maximum and minimum average temperature time series values with those from the benchmark site. Each file will end the time series at five years. The appropriate data file will also be edited to replace the site latitude with the latitude of the benchmark site. In addition, the appropriate data file will be edited to make any non-LAU sub-areas have an area of 1.0 m^2 to minimize water balance effects of those subareas. Identical values of the following water balance parameters will be used for the HELP and HWIR water balance algorithm runs.

Results of comparisons of HWIR and HELP will be presented in spreadsheets for infiltration rates and average run-off. In addition, this assessment will also include average annual runoff rates for the regions of the country pertaining to each of the six sites as taken from the *Water Atlas* (Geraghty et al., 1973). The five-year average runoff values will be compared to those of the *Water Atlas* for each of the six sites as well as the predictions of the HELP model as a check of reasonableness of the HELP output. This approach assumes that these empirical *Water Atlas* data are indeed an appropriate basis of comparison[2]. The results will be reported to the project QA officer and the modeling coordinator in the format provided in Section A9. If the results do not show the appropriate correspondence with the benchmarks, corrective action will be taken by the modeling coordinator to assure that the algorithms are corrected, and this testing process will be repeated to document compliance.

5.3.5 Part D: Output Assessment and Model Usability

If the model outputs meet the internal criteria of the module as described in this test plan, they should meet the requirements for the overall model. Total model planning, development, and testing are intended to assure that if each module meets its own internal quality standards, the module output will meet the requirements for the entire model.

Assessment of Correct Operation of System Requirements. Because the LAU is a source module and is the first module fired by the overall modeling system, system-level interactions with other modules are relatively minor. However, some system-level functionality is needed—for example, outputting warning/error messages, output of logical flags, and time series management.

Logical Flags. A set of seven logical outputs will be generated by the LAU Module to check that the outputs are properly generated. That is, the LAU need only have the *potential* to output that variable for the flag to be set at "true." It need not actually have a non-zero output during the run. The criteria for properly generated flags will be checked via hand calculations.

The data file results with the logical flags will be checked for agreement with the module documentation, and the agreement will be reported to the project QA officer and the modeling coordinator in the format provided in Section A9. If the logic flags are incorrectly set, corrective action will be taken by the modeling coordinator to assure that the logic flags are corrected, and this testing process will be repeated to confirm compliance.

---

[2]More benchmark testing would be required for more definitive statements regarding relative accuracy. For example, only a single curve number was used in the comparisons, and it is unknown to what extent that curve number might represent average conditions as reflected by the *Water Atlas* data.

APPENDIX A

BIBLIOGRAPHY

40 CFR 51, Code of Federal Regulations, *Guideline on Air Quality Models*, Appendix W.

American National Standards Institute/American Society for Quality Control (ANSI/ASQC). (1995). *Specifications and Guidelines for Quality Systems for Environmental Data Collection and Environmental Technology Programs (E4-1994)*. American National Standard.

American Society for Testing and Materials. 2000. Standard Guide for Statistical evaluation of Atmospheric Dispersion Model Performance. Standard D6589–00. West Conshohocken, Pennsylvania.

Berthouex, P.M. and Brown, L.C. (1994). *Statistics for Environmental Engineers*. Boca Raton, FL: Lewis Publishers

Chen, J. and Beck, M.B. (2000). *Quality Assurance of Multi-media Model for Predictive Screening Tasks (EPA/600/R-98/106)*. U.S. EPA.

Cox, W. M. and Tikvart, J.A., (1990). A Statistical Procedure for Determining the Best Performing Air Quality Simulation Model. *Atmospheric Environment*. Vol. 24A: pp. 2387-2395.

D'Agostino, R.B. and Stephens, M.A. (1986). *Goodness-of-fit Techniques.* New York: Marcel Dekker.

Draper, N.R. and Smith, Jr., H. (1981). *Applied Regression Analysis* (2nd ed.). New York: Wiley.

Geraghty, J. A., D. W .Miller, F. van der Leeden, and F. L. Troise. (1973). *Water Atlas of the United States*. 3rd edition. Water Information Center, Incorporated, Port Washington, NY.

Gilbert, R.O. (1987). *Statistical Methods for Environmental Pollution Monitoring*. New York: Wiley.

Institute of Electrical and Electronics Engineers (IEEE). (1986). Standard 1012: IEEE standard for software verification and validation plans. *IEEE Standards Collection: Software Engineering* (Volume 2: Process Standards). Piscataway, NJ.

Institute of Electrical and Electronics Engineers (IEEE). (1998a). Standard 828: IEEE standard for software configuration management plans. *IEEE Standards Collection: Software Engineering* (Volume 2: Process Standards). Piscataway, NJ.

Institute of Electrical and Electronics Engineers (IEEE). (1998b). Standard 830: IEEE recommended practice for software requirements specifications. *IEEE Standards Collection: Software Engineering* (Volume 4: Resource and Technique Standards). Piscataway, NJ.

Institute of Electrical and Electronics Engineers (IEEE). (1999). Standard 730: IEEE standard for software quality assurance plans. *IEEE Standards Collection: Software Engineering* (Volume 2: Process Standards). Piscataway, NJ.

Kirchner, T.B. (2000). Uncertainty analysis. In T.B. Borak (Ed.), *Applications of Probability and Statistics in Health Physics*. (pp. 115-161). Madison, WI: Medical Physics Publishing.

Morgan, M.G. and Henrion, M. (1990). *Uncertainty: a Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis*. New York: Cambridge University.

National Council on Radiation Protection and Measurements (NCRP). (1996). *A Guide for Uncertainty Analysis in Dose and Risk Assessments Related to Environmental Contamination.* (NCRP Commentary No. 14). Bethesda, MD.

National Institute of Standards and Technology (NIST). (1996). *NIST Special Publication 500-234: Reference Information for the Software Verification and Validation Process* [On-line]. Available: http:\\hissa.ncsl.nist.gov\HHRFdata\Artifacts\ITLdoc\234\val-proc.html

Snedecor, G.W. and Cochran, W.G. (1989). *Statistical Methods* (8th ed.). Ames, IA: Iowa State University Press.

U.S. Environmental Protection Agency. (1994). *Guidance for Conducting External Peer Review of Environmental Regulatory Models* (EPA 100-B-94-001). Washington, DC: Office of the Administrator.

U.S. Environmental Protection Agency. (1996). *Summary Report of Workshop on Monte Carlo Analysis* (EPA/630/R-96/010). Washington, DC: Office of Research and Development.

U.S. Environmental Protection Agency. (1997). *Guiding Principles for Monte Carlo Analysis* (EPA/630/R-97/001). Washington, DC: Office of Research and Development

U.S. Environmental Protection Agency. (1998a). *Guidance for Quality Assurance Project Plans (QA/G-5)* (EPA/600/R-98/018). Washington, DC: Office of Research and Development.

U.S. Environmental Protection Agency. (1998b). *Information Resources Management Policy Manual* (Directive 2100). Washington, DC.

U.S. Environmental Protection Agency. (1999a). *Information Security Manual* (Directive 2195A1). Washington, DC.

U. S. Environmental Protection Agency. (1999b). *Quality Assurance Plan for Mathematical Modeling.* Washington, DC: Office of Research and Development.

U.S. Environmental Protection Agency. (1999c). *Quality Assurance of Multi-media Model for Predictive Screening Tasks* (EPA/600/R98/106). Washington, DC: Office of Research and Development.

U.S. Environmental Protection Agency. (1999d). *Report of the Workshop on Selecting Input Distributions for Probabilistic Assessments* (EPA/630/R-98/004) [On-line]. Available: www.epa.gov/ncea/input.htm

U.S. Environmental Protection Agency. (1999e). *Risk Assessment Guidance for Superfund: Volume 3 (Part A): Process for Conducting Probabilistic Risk Assessments* (EPA 000-0-99-000) (Draft) [On-line]. Available: www.epa.gov/superfund/pubs.htm

U.S. Environmental Protection Agency. (1999f). *Source Modules for Nonwastewater Waste Management Units (Land Application Units, Wastepiles, and Landfills): Background and Implementation for the Multimedia, Multipathway, and Multireceptor Risk Assessment (3MRA) for HWIR99*. Washington, DC: Office of Solid Waste.

U.S. Environmental Protection Agency. (2000a). *EPA Quality Manual for Environmental Programs* (Order 5360 A1). Washington, DC.

U.S. Environmental Protection Agency. (2000b). *Guidance for the Data Quality Objectives Process (QA/G-4)* (EPA/600/R-96/055). Washington, DC: Office of Environmental Information.

U.S. Environmental Protection Agency. (2000c). *Guidance for Data Quality Assessment: Practical Methods for Data Analysis (QA/G-9)* (EPA/600/R-96/084, QA00 Update). Washington, DC: Office of Environmental Information.

U.S. Environmental Protection Agency. (2000d). *Policy and Program Requirements for the Mandatory Agency-wide Quality System* (EPA Order 5360.1 A2). Washington, DC.

U.S. Environmental Protection Agency. (2000e). *Science Policy Council Handbook: Peer review* (EPA 100-B-00-001). Washington, DC: Office of Research and Development, Office of Science Policy.

U.S. Environmental Protection Agency. (2000f). *Systems Development Life Cycle Methodology (Sdlcm) Statement of Policy, Standards and Guidelines*. Washington, DC: Office of Research and Development, Center for Exposure Assessment Modeling.

U.S. Environmental Protection Agency. (2001). *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA/240/B-01/003). Washington, DC: Office of Environmental Information.

U.S. Environmental Protection Agency. (2002). *Guidance on Systematic Planning for Environmental Data collection Using Performance and Acceptance Criteria (QA/G-4A).* Peer Review Draft.

U.S. General Accounting Office. (1997). *Report to the Chairman, Subcommittee on Oversight and Investigations, Committee on Commerce, House of Representatives: Air Pollution Limitations of EPA's Motor Vehicle Emissions Model and Plans to Address Them* (GAO/RCED-97-21).

Warren-Hicks, W. J. and Moore, D.R.J. (1998). *Uncertainty Analysis in Ecological Risk Assessment (*SETAC Special Publications Series). Pensacola, FL: Society of Environmental Toxicology and Chemistry.

APPENDIX B

TERMS AND DEFINITIONS

assessment - the evaluation process used to measure the performance or effectiveness of a system and its elements.

audit (quality) - a systematic and independent examination to determine whether quality activities and related results comply with planned arrangements and whether these arrangements are implemented effectively and are suitable to achieve objectives.

boundary condition - mathematical expression of a state of the environmental system that constrains the equations of the mathematical model.

conceptual model - an interpretation or working description of the characteristics of the physical system.

contractor - any organization or individual that contracts to furnish services or items or perform work; a supplier in a contractual situation.

data quality assessment - a statistical and scientific evaluation of the data set to determine the validity and performance of the data collection design and statistical test, and to determine the adequacy of the data set for its intended use.

design - specifications, drawings, design criteria, and performance requirements. Also the result of deliberate planning, analysis, mathematical manipulations, and design processes.

environmental data - any measurements or information that describe environmental processes, location, or conditions; ecological or health effects and consequences; or the performance of environmental technology. For EPA, environmental data include information collected directly from measurements, produced from models, and compiled from other sources such as data bases or the literature.

environmental data operations - work performed to obtain, use, or report information pertaining to environmental processes and conditions.

environmental processes - manufactured or natural processes that produce discharges to or that impact the ambient environment.

environmental programs - work or activities involving the environment, including but not limited to characterization of environmental processes and conditions; environmental monitoring; environmental research and development; the design, construction, and operation of environmental technologies; and laboratory operations on environmental samples.

evaluation - a test of the model with known input and output information that is used to assess that the calibration parameters are accurate without further change and to demonstrate model performance.

graded approach - the process of basing the level of application of managerial controls applied to an item or work according to the intended use of the results and the degree of confidence needed in the quality of the results.

inspection - an activity such as measuring, examining, testing, or gauging one or more characteristics of an entity and comparing the results with specified requirements in order to establish whether conformance is achieved for each characteristic.

management system - a structured, non-technical system describing the policies, objectives, principles, organizational authority, responsibilities, accountability, and implementation plan of an organization for conducting work and producing items and services.

method - a body of procedures and techniques for performing an activity (e.g., sampling, modeling, chemical analysis, quantification) systematically presented in the order in which they are to be executed.

model calibration - the process of refining the model representation of the environmental framework, properties, and boundary conditions to achieve a desired degree of correspondence between the model simulations and observations of the environmental system and processes. The focus is usually on the estimation and characterization of empirical constants used in parameterizations and mathematical representations of environmental processes.

participant - when used in the context of environmental programs, an organization, group, or individual that takes part in the planning and design process and provides special knowledge or skills to enable the planning and design process to meet its objective.

performance evaluation - a type of audit in which the quantitative data generated in a measurement system are obtained independently and compared with routinely obtained data to evaluate the proficiency of an analyst or laboratory.

quality - the totality of features and characteristics of a product or service that bear on its ability to meet the stated or implied needs and expectations of the user.

quality assurance - an integrated system of management activities involving planning, implementation, documentation, assessment, reporting, and quality improvement to ensure that a process, item, or service is of the type and quality needed and expected by the client.

quality assurance manager - the individual designated as the principal manager within the organization having management oversight and responsibilities for planning, documenting, coordinating, and assessing the effectiveness of the quality system for the organization.

quality assurance project plan - a document describing in comprehensive detail the necessary QA, QC, and other technical activities that must be implemented to ensure that the results of the work performed will satisfy the stated performance criteria.

quality control - the overall system of technical activities that measures the attributes and performance of a process, item, or service against defined standards to verify that they meet the stated requirements established by the customer; operational techniques and activities that are used to fulfill requirements for quality.

quality system - a structured and documented management system describing the policies, objectives, principles, organizational authority, responsibilities, accountability, and implementation plan of an organization for ensuring quality in its work processes, products (items), and services. The quality system provides the framework for planning, implementing, documenting, and assessing work performed by the organization and for carrying out required QA and QC activities.

record - a completed document that provides objective evidence of an item or process. Records may include photographs, drawings, magnetic tape, and other data recording media.

sensitivity - the variation in the value of one or more output variables or quantities calculated from the output variables due to variability or uncertainty in one or more inputs to a model.

sensitivity analysis - a quantitative evaluation of the impact of variability or uncertainty in model inputs on the degree of calibration of a model and on its results or conclusions.

simulation - one complete execution of the computer program, including input and output.

source code - the program instructions written in a programming language [FIPS PUB 106 (NIST) definition].

specification - a document stating requirements and which refers to or includes drawings or other relevant documents. Specifications should indicate the means and the criteria for determining conformance.

supplier - any individual or organization furnishing items or services or performing work according to a procurement document or financial assistance agreement. This is an all-inclusive term used in place of any of the following: vendor, seller, contractor, subcontractor, fabricator, or consultant.

surveillance (quality) - continual or frequent monitoring and verification of the status of an entity and the analysis of records to ensure that specified requirements are being fulfilled.

uncertainty – lack of knowledge about specific factors, parameters, or models.

variability - observed differences attributable to true heterogeneity or diversity in a population or exposure parameter (variability can be better characterized but not reduced by further measurement or study).

verification - confirmation by examination and provision of objective evidence that specified requirements have been fulfilled. In design and development, verification concerns the process of examining a result of a given activity to determine conformance to the stated requirements for that activity.

APPENDIX C

CHECKLIST FOR QA PROJECT PLAN ELEMENTS FOR MODELING

Name of Project this QA Project Plan is for: ________________________________

GROUP A: PROJECT MANAGEMENT

A1. Title and Approval Sheet
Contents this element may contain:

- Title of QA Project Plan
- Revision number of QA Project Plan
- Effective date of QA Project Plan revision
- Names of all organizations involved in modeling project
- Names of all key project officials responsible for the work, with space for dated signatures

A2. Table of Contents and Document Control Format
Contents this element may contain:

- Title of all sections, including subsections, tables, figures, references, appendices
- Page numbers for each section
- Section for each QA Project Plan element
- Document control box

A3. Distribution List
Contents this element may contain:

- List of all individuals (and their role on the project) who will be provided copies of the approved QA Project Plan, including all persons responsible for implementation, including project managers, QA Managers, and representatives of all groups involved.

A4. Project/Task Organization
Contents this element may contain:

- Concise organizational chart showing the relationships and lines of communication among all project participants, other data users, and any subcontractors relevant to environmental data operations
- Project name and organizations involved, and a description of their respective responsibilities

A5. Problem Definition/Background

Contents this element may contain:

- Goals and objectives of this project that will address this problem
- Definition of the population the problem targets and what measures within this population the problem addresses
- Reason the project includes a modeling approach to address the problem (is it a new predictive tool?)
- Types of decisions that may be made as a result of this project
- Names of those responsible for making these decisions
- Any other types of problems that the project may address
- Background information on the problem
- Reasons the project is important, how it supports other existing research, programs, or regulations
- Conflicts or uncertainties that will be resolved by this project
- Reasons one model is determined to be better than another for this application

A6. Project/Task Description and Schedule

Contents this element may contain:

- Summary of all work to be performed, products to be produced, and the schedule for implementation
- List of products, deliverables, and milestones to be completed in the various stages of the project
- Schedule of anticipated start and completion dates for the milestones and deliverables, and persons responsible for each

A7. Quality Objectives and Criteria for Model Inputs/Outputs

Contents this element may contain:

- Project data quality objectives (DQOs), performance criteria, and acceptance criteria
- Description of task that needs to be addressed and the intended uses of the output of the modeling project to achieve the task
- List of requirements associated with the hardware/software configuration for those studies involving software evaluation

A8. Special Training Requirements/Certification

Contents this element may contain:

- Types of required training and certification needed by the project team
- Plan for obtaining training and/or certification
- Documentation of training and/or certification

A9. Documentation and Records
Contents this element may contain:

- Description of information to be included in reports
- Proper document control and distribution procedures
- Details on document storage
- Backup plan for records stored electronically
- Description of the change control process (who approves changes, etc.)
- Length of retention periods for each record
- Data assessment reports, interim project progress reports
- Model science formulation report, peer review reports
- Model assessment reports, interim project progress reports
- Code standards, code auditing and testing reports, interim project progress reports
- Model calibration report
- Model evaluation records (How well does the model report variability and uncertainty in its output?)
- User's manual
- Configuration management (after production version) and code maintenance (e.g., or software internal documentation of logic and structure) manuals

GROUP B: MEASUREMENT AND DATA ACQUISITION

B7. Calibration
Contents this element may contain:

- Objectives of model calibration activities, including acceptance criteria
- Frequency of model calibration activities
- Details on the model calibration procedure
- Method(s) of acquiring input data
- Types of output generated by the model calibration
- Approach to characterize uncertainty (e.g., sensitivity analysis)
- Corrective action to be taken if criteria are not met
- Resources and responsibilities for calibrating the model
- Analysis of model output relative to acceptance criteria

B9. Non-direct Measurements (Data Acquisition Requirements)
Contents this element may contain:

- Types of data needed for implementing a project that are obtained from non-measurement sources such as databases, literature files
- Need for non-direct measurements, intended use of data
- Method(s) of identifying and acquiring data
- Method of determining the underlying quality of the data
- SOPs and field or lab-specific deviations associated with these procedures
- Acceptance criteria for non-direct measurements: such as completeness, representativeness, bias, precision, qualifying data

B10. Data Management and Hardware/Software Configuration
Contents this element may contain:

- Information on the project data management process (field, office, and lab)
- Record-keeping procedures, document control system, audit trails
- Control mechanism for detecting and correcting errors, preventing loss of data
- Procedures for assuring applicable Agency resource management requirements are satisfied
- Required computer hardware/software and any specific performance requirements

Data Management

- Any data forms, checklists, on-line interactive screens used in the modeling process
- Any graphics developed to document the data management process (process flow diagrams, modeling flow charts, etc.)
- Documentation of internal checks used during data entry
- Data calculations and analyses that should to be highlighted in the QA Project Plan
- Plans for characterization of uncertainty and variability in the model results (e.g., summary statistics, frequency distributions, goodness-of-fit tests)

Hardware/Software Configuration

- List of equipment, hardware, and software that will be used on the project
- Description of performance requirements
- Decisions regarding security issues
- Decision regarding communication issues
- Decisions regarding software installation issues
- Decisions regarding response time issues
- Plans for requirements documentation

- Coding standards
- Testing plans
- Plans for data dictionary (may not need to be a separate document)
- Plans for a user's manual
- Plans for a maintenance manual (explaining software logic and organization)
- Plans for source code for the ultimate user of the model or model framework
- Configuration management plan (procedures to control software/hardware configuration during development of the original model version)

GROUP C: ASSESSMENTS AND OVERSIGHT

C1. Assessment and Response Actions

Contents this element may contain:

- Assessment/oversight strategies and schedule of assessment activities, order of events
- Organizations and individuals expected to participate in assessments, including peer reviews
- Information expected, success criteria
- Scope of authority of assessors to recommend or direct changes to the model (corrective actions)
- Qualitative and quantitative assessments
- Internal assessments (internal QA officer's review of input data, code verification, calibration, benchmarking) and external assessments (peer review of model theory or mathematical structure)
- Surveillance activities (continued monitoring of status and progress of the project, tracking project milestones and budgets)
- Plans for model performance evaluations
- Plans for sensitivity analysis
- Plans for uncertainty analysis
- Plans for data quality assessment
- Plans for code testing

Hardware/Software Assessments

- Plans for hardware and software configuration testing, if appropriate
- Plans for code verification tests
- Plans for internal and external peer reviews
- Plans for checking for programming errors
- Plans for checking for correct insertion of model equations
- Plans for checking for code's linkage to analysis of uncertainty

Hardware/Software Configuration Tests

- Plans for software code development inspections
- Plans for software code performance testing
- Plans for a test of the model framework
- Plans for integration tests (check computational and transfer interfaces between modules)
- Plans for regression tests
- Plans for stress testing of complex models (to ensure that maximum load during peak usage does not exceed limits of the system)
- Plans for acceptance testing (contractually-required testing needed before a new model or model application is accepted by the customer and final payment is made)
- Plans for beta testing of pre-release hardware/software, recording of anomalies
- Plans for checking for programming errors

Plans for science and product peer review

- Theoretical basis for the model
- Mathematical model structure
- Model algorithms
- Model predictions
- Model calibration
- Plans for data quality assessment
- Plans for peer review of final technical product

C2. Reports to Management

Contents this element may contain: plans for documentation of:

- Project reporting schedule
- Frequency, content, and distribution of reports
- Deviations from approved QA Project Plan
- Need for response actions to correct deviations
- Potential uncertainties in decisions based on input data and model limitations
- Data Quality Assessment findings

GROUP D: DATA VALIDATION AND USABILITY

D1. Departures from Validation Criteria

Contents this element may contain:

- Criteria used to review and validate (accept, reject, or qualify) model components such as theory, mathematical procedures, code, and calibration (convergence criteria, etc.)
- Criteria used to review and validate input data
- Criteria used to test model performance
- Criteria used to review or validate model outputs

D2. Validation Methods

Contents this element may contain:

- Methods for review of model components such as theory, mathematical procedures, code, and calibration (peer review, etc.)
- Methods for review of input data
- Methods for review of model performance tests
- Methods for assessment of model output and usability

D3. Reconciliation with User Requirements

Contents this element may contain:

- Discussion of project or task results
- List of departures from assumptions set in the planning phase of the model
- Report on limitations on use of output data for decision makers or users