



**U.S. Army
Corps of Engineers**

New England District
Concord, Massachusetts



**U.S. Environmental
Protection Agency**

Region I
Boston, Massachusetts

QUALITY ASSURANCE PROJECT PLAN

Modeling Study of PCB Contamination in the Housatonic River

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**Environmental Remediation Contract
General Electric (GE)/Housatonic River Project
Pittsfield, Massachusetts**

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QUALITY ASSURANCE PROJECT PLAN

Modeling Study of PCB Contamination in the Housatonic River

October 2000

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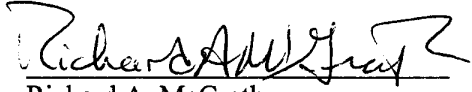
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TABLE OF CONTENTS

1		
2	INTRODUCTION.....	1
3	PROJECT MANAGEMENT	
4	1. PROJECT ORGANIZATION.....	1-1
5	2. PROBLEM DEFINITION/BACKGROUND.....	2-1
6	3. PROJECT/TASK DESCRIPTION	3-1
7	3.1 DESCRIPTION OF PROJECT TASKS	3-1
8	3.2 OVERVIEW OF MODELING FRAMEWORK AND APPROACH.....	3-1
9	4. DATA QUALITY OBJECTIVES AND CRITERIA FOR MEASUREMENT	
10	DATA AND MODEL RESULTS	4-1
11	4.1 PROJECT DATA QUALITY OBJECTIVES	4-1
12	4.2 DATA SOURCES AND AVAILABILITY	4-2
13	4.3 MEASUREMENT AND MODEL PERFORMANCE CRITERIA	4-4
14	4.3.1 Historical Model Accuracy and Performance Expectations	4-10
15	4.3.2 Proposed Model Calibration and Validation Targets.....	4-12
16	4.4 OVERVIEW OF MODEL CALIBRATION AND VALIDATION	
17	PROCEDURES	4-13
18	4.5 HSPF CALIBRATION AND VALIDATION PROCEDURES	4-15
19	4.5.1 Hydrologic Calibration and Key Calibration Parameters	4-17
20	4.5.2 Hydraulic Calibration.....	4-20
21	4.5.3 Snow Calibration and Key Calibration Parameters	4-21
22	4.5.4 Specific Comparisons To Be Performed - Hydrology.....	4-23
23	4.5.5 Sediment Erosion Calibration and Key Calibration Parameters	4-24
24	4.5.6 Specific Comparisons To Be Performed - Sediment Loadings	4-26
25	4.5.7 Nonpoint Source Calibration and Key Calibration Parameters	4-26
26	4.5.8 Specific Comparisons to be Performed - Nonpoint Loadings	4-28
27	4.5.9 Instream Sediment and Water Quality Calibration.....	4-28
28	4.6 EFDC CALIBRATION AND VALIDATION PROCEDURES.....	4-28
29	4.6.1 Specific Comparisons To Be Performed.....	4-29
30	4.6.1.1 Hydrodynamics	4-29
31	4.6.1.2 Sediment Transport.....	4-31
32	4.6.1.3 Abiotic PCBs	4-34
33	4.6.2 Key Model Calibration Parameters.....	4-36
34	4.6.2.1 Hydrodynamics	4-37
35	4.6.2.2 Sediment Transport.....	4-37
36	4.6.2.3 Abiotic PCBs	4-40

TABLE OF CONTENTS
(Continued)

1			
2			
3	4.7	AQUATOX CALIBRATION/VALIDATION PROCEDURES	4-41
4	4.7.1	Specific Comparisons To Be Performed.....	4-43
5	4.7.2	Key Model Calibration Parameters.....	4-48
6	4.8	SUMMARY OF MODEL CALIBRATION AND VALIDATION	
7		PERIODS	4-50
8	4.9	QUALITY ASSURANCE OF MODEL LINKAGE PROCEDURES	4-51
9	4.9.1	Framework for Model Linkage	4-51
10	4.9.2	Relationship of QAPP and MFD	4-52
11	4.9.3	Overview of Model Linkage	4-53
12	4.9.3.1	Physical Domain, Spatial and Temporal Scales	4-53
13	4.9.3.2	Spatial Linkage: HSPF-AQUATOX.....	4-54
14	4.9.3.3	Spatial Linkage: EFDC-AQUATOX.....	4-54
15	4.9.3.4	Temporal Linkage: HSPF-AQUATOX and EFDC-	
16		AQUATOX.....	4-55
17	4.9.3.5	Data Linkages from HSPF to EFDC	4-55
18	4.9.3.6	Data Linkages from EFDC to AQUATOX	4-55
19	4.9.3.7	Data Linkages from HSPF to AQUATOX.....	4-57
20	4.9.4	QA/QC Tests, Sensitivity Analyses, Consistency Checks.....	4-59
21	4.9.4.1	QA/QC Tests for HSPF-EFDC	4-59
22	4.9.4.2	QA/QC Tests for HSPF-AQUATOX	4-61
23	4.9.4.3	QA/QC Tests for EFDC-AQUATOX.....	4-62
24	4.10	QUALITY ASSURANCE FOR MODEL ENHANCEMENTS AND	
25		CODE DEVELOPMENT	4-65
26	4.10.1	EFDC Model Enhancements and Code Development	4-66
27	4.10.2	AQUATOX Model Enhancements and Code Development	4-66
28	5.	SPECIAL TRAINING REQUIREMENTS/CERTIFICATION	5-1
29	6.	DOCUMENTATION AND RECORDS	6-1
30		DATA ACQUISITION	
31	7.	DATA ACQUISITION REQUIREMENTS	7-1
32	8.	DATA MANAGEMENT	8-1
33		ASSESSMENT/OVERSIGHT	
34	9.	ASSESSMENT AND RESPONSE ACTIONS	9-1
35	10.	REPORTS TO MANAGEMENT.....	10-1
36			

1
2
3
4
5
6
7
8
9
10

TABLE OF CONTENTS
(Continued)

DATA VALIDATION AND USABILITY

11. DATA REVIEW, VALIDATION, AND VERIFICATION REQUIREMENTS 11-1

12. VALIDATION AND VERIFICATION METHODS 12-1

13. RECONCILIATION WITH DATA QUALITY OBJECTIVES 13-1

14. REFERENCES 14-1

LIST OF FIGURES

1		
2	Figure 1-1	Modeling Project Organization..... 1-2
3	Figure 2-1	Housatonic River Watershed 2-3
4	Figure 3-1	Housatonic River PCB Modeling Framework 3-4
5	Figure 4-1	Multi-Year Simulation of East Fork Poplar Creek, TN, Showing Seasonal
6		Fluctuations in Biomass, Especially Macrophytes, Amphipods, and
7		Minnows..... 4-45
8	Figure 4-2	Comparison of Predicted and Observed BAFs for Lake Trout in Lake
9		Ontario 4-46
10	Figure 4-3	Regression of Observed and Predicted PCB Congener BAFs 4-46
11	Figure 4-4	Cumulative Distributions of Predicted and Observed Chlorophyll in Lake
12		Onondaga Epilimnion in 1989 and 1990 4-47
13	Figure 4-5	Model Linkage Within the Modeling Framework 4-52
14	Figure 4-6	Solids Interactions Within an AQUATOX Reach..... 4-65

LIST OF TABLES

16		
17	Table 3-1	Housatonic River PCB Modeling System Components 3-5
18	Table 4-1	Data Types, Descriptions, and Sources for the Housatonic River Modeling
19		Study 4-3
20	Table 4-2	Timeline Summary of Housatonic River Data Collection above Great
21		Barrington, MA, 1979-1999 4-5
22	Table 4-3	General Calibration/Validation Targets or Tolerances for HSPF
23		Applications 4-11
24	Table 4-4	Proposed Model Calibration and Validation Target Tolerances..... 4-14
25	Table 4-5	Summary Statistics for Chlorophyll in Lake Onondaga Epilimnion..... 4-48
26	Table 4-6	Calibration and Validation Periods 4-50

1 INTRODUCTION

2 The U.S. Environmental Protection Agency (EPA) has developed the Quality Assurance Project
3 Plan (QAPP) as a tool for project managers and planners to document the type and quantity of
4 data needed for environmental decisions and to describe the methods for collecting and assessing
5 those data. The development, review, approval, and implementation of a QAPP is part of EPA's
6 mandatory Quality System. EPA requires that all environmental data used in decisionmaking be
7 supported by an approved QAPP; this requirement is defined in EPA Order 5360.1 CHG 1,
8 *Policy and Program Requirements for the Mandatory Agency-Wide Quality System*, (EPA,
9 1998a) for EPA organizations, and in 48CFR 46 for contractors. The QAPP is designed to
10 integrate all technical and quality aspects of a project, document planning results for
11 environmental data operations, and provide a project-specific "blueprint" for obtaining the type
12 and quality of environmental data needed for a specific purpose or use (EPA, 1999).

13 Considering the wide range and geographic diversity of potential environmental projects for
14 which a QAPP is required, EPA has allowed considerable flexibility in adapting the QAPP
15 requirements to fit the needs of specific projects. Accordingly, this QAPP is specifically focused
16 on the quality assurance (QA) aspects of the modeling components of the Housatonic River
17 Supplemental Investigation, as described in *Modeling Framework Design—Modeling Study of*
18 *PCB Contamination in the Housatonic River* (Beach et al., 2000), (referred to in this document
19 as the MFD). This QAPP is a companion document to the MFD, and describes the quality
20 assurance activities associated with the modeling data review and analysis, application,
21 calibration, and validation tasks. Roy F. Weston, Inc., under contract to EPA and to the U.S.
22 Army Corps of Engineers, prepared the QAPP (WESTON, 2000), which covers all quality
23 assurance issues associated with data collection being performed to support the modeling study.

24 Because no additional data collection activities are included in the modeling study covered by
25 this QAPP, all information on sampling design, sample handling/custody, analytical methods,
26 and instrumentation are provided in the WESTON QAPP.

27 Data used in the modeling study obtained from other sources (e.g., General Electric, U.S.
28 Geological Survey, National Weather Service, and National Resource and Conservation Service)

1 will be reviewed for quality issues, consistency with other relevant data, and potential errors
2 prior to use in this effort. However, it will be assumed that these data have been subject to the
3 formal QA/QC procedures and protocols of the source agency.

4 This QAPP has been prepared according to the general guidance provided in EPA Requirements
5 for Quality Assurance Project Plans (EPA, 1999). The project described in this QAPP will be
6 conducted by Roy F. Weston, Inc., and its subcontractors and consultants under USACE
7 Contract DACW33-00-D-0006. This document was prepared jointly by Roy F. Weston, Inc.,
8 and AQUA TERRA Consultants, and its subcontractors and consultants, in conformance with the
9 procedures described herein and the quality assurance program described in the quality assurance
10 program plan for AQUA TERRA's Contract 68-C-98-010 with EPA's Office of Water, Office of
11 Science and Technology, Standards and Applied Science Division, "Technical Support for
12 Environmental Assessments, Benefits Analysis and Information Systems and Multimedia
13 Environmental Fate and Transport Models."

14

1 PROJECT MANAGEMENT

2 1. PROJECT ORGANIZATION

3 The purpose of this section is to explain the organization and lines of communication for the
4 project. The project includes participants from the following organizations:

- 5 ▪ EPA Region 1
- 6 ▪ U.S. Army Corps of Engineers
- 7 ▪ Roy F. Weston, Inc.
- 8 ▪ ZZ Consulting L.L.C.
- 9 ▪ AQUA TERRA Consultants
- 10 ▪ Eco Modeling
- 11 ▪ Andrew Stoddard & Associates

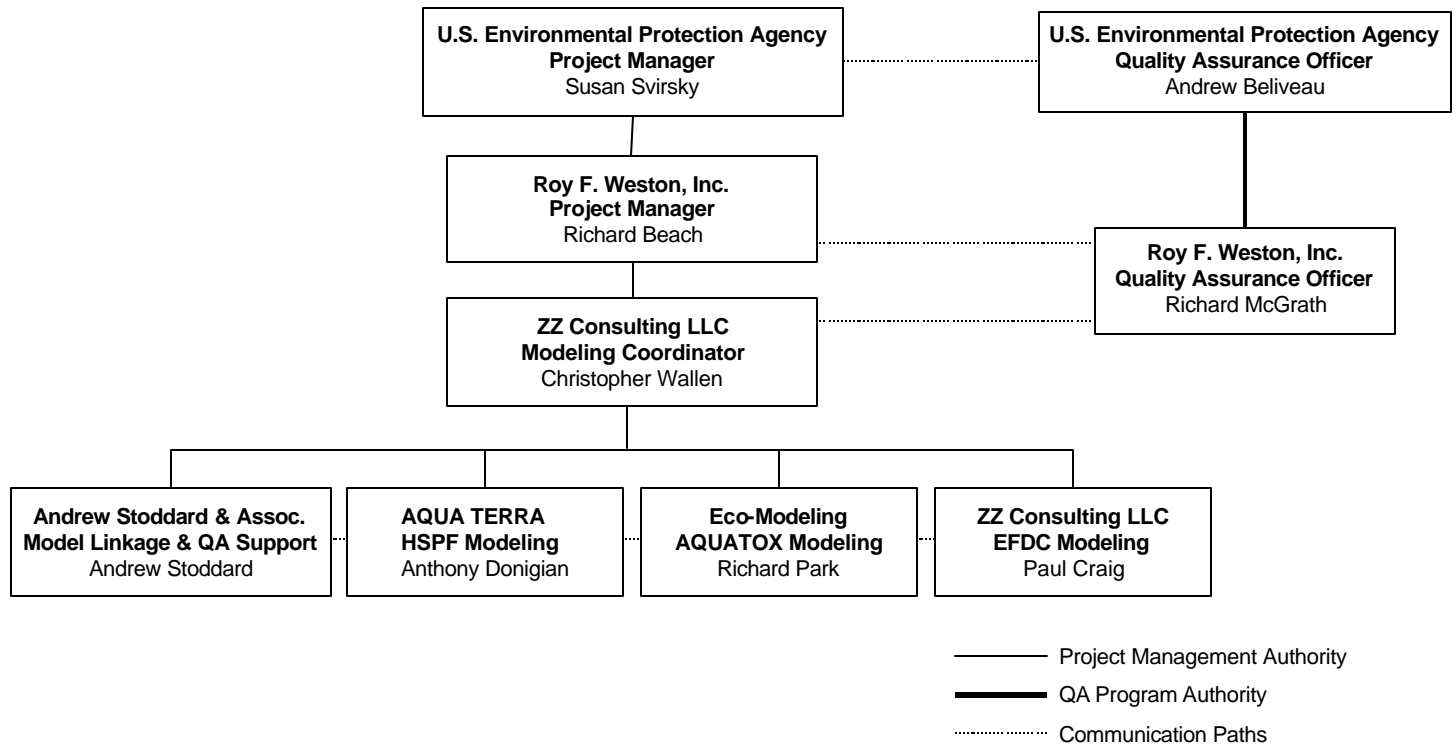
12 The project organization is displayed in Figure 1-1; the technical and quality assurance aspects of
13 the project are presented, both for the client (EPA) and the contractors.

14 Susan Svirsky is the Remedial Project Manager and Work Assignment Manager responsible for
15 the overall management of the Housatonic River Supplemental Investigation (Operable Unit 2),
16 and the EPA Work Assignment Manager for AQUA TERRA Consultants. Ms. Svirsky has
17 direct contractual/management responsibility for Roy F. Weston, Inc., and AQUA TERRA
18 Consultants. Andy Beliveau is the U.S. EPA Quality Assurance Officer for the project.

19 The Quality Assurance (QA) Officer, Richard A. McGrath for Roy F. Weston, Inc.,
20 communicates with Richard Beach, Project Manager, and Christopher Wallen, Modeling
21 Coordinator, and is independent of the modeling, data analysis, and reporting staff. Major
22 responsibilities include monitoring quality control (QC) activities to determine conformance,
23 distributing quality-related information, overseeing training of personnel on QC requirements
24 and procedures, and completing required documentation.

25 Additional projectwide oversight will be provided by the QC Officers who will not have
26 performed the original work. The QC Officers are responsible for performing evaluations to
27 ensure that QC is maintained throughout the data evaluation and modeling study. QC

Figure 1-1 Modeling Project Organization



- 1 evaluations will include reviewing work as it is completed and documenting these reviews to
- 2 ensure the standards set forth in the QAPP are met.

1 **2. PROBLEM DEFINITION/BACKGROUND**

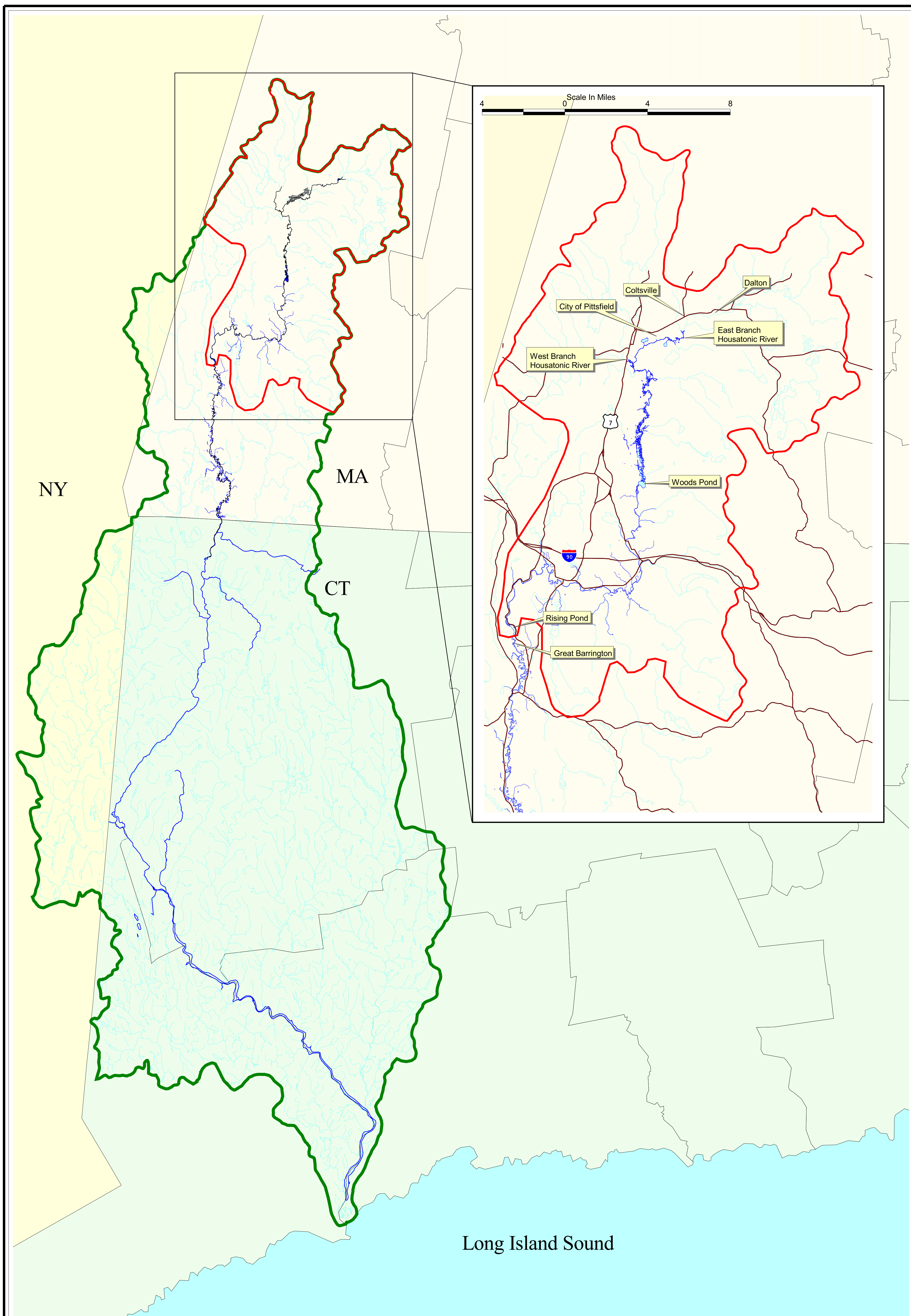
2 Historical releases of certain classes of organic and inorganic chemicals into waterbodies have
3 left a legacy of aquatic sediment enriched with these contaminants. In some sediments these
4 contaminants have accumulated to levels that may pose an unacceptable human health and
5 ecological risk. Of particular concern is the historical release to waterbodies of compounds
6 known as polychlorinated biphenyls (PCBs), given that they are toxic, persistent, and
7 bioaccumulate in the food chain.

8 PCBs historically were released to the Housatonic River (see Figure 2-1) from the General
9 Electric (GE) facility in Pittsfield, MA. Over a period of decades, these compounds have
10 accumulated in the river's bed sediment and impoundments in Massachusetts and Connecticut.
11 High-flow events have transported PCB-laden sediment onto the adjacent floodplain. Data
12 collected from 1982 to the present have documented the magnitude and extent of the PCB
13 contamination of the sediments and floodplain soils adjacent to the Housatonic River
14 downstream of the GE facility. The extent of the PCB contamination was estimated in previous
15 investigations to fall within the 10-year floodplain of the Housatonic River.




16 In addition, PCBs in fish tissue have accumulated to levels that pose a risk to human health
17 (EPA, 1998a). A recent U.S. Geological Survey (USGS) report (Garabedian et al., 1998) notes
18 that PCB concentrations in streambed sediments and fish tissue in the Housatonic River are some
19 of the highest of all their National Water-Quality Assessment Program (NAWQA) study sites
20 across the country. In 1982, the Massachusetts Department of Environmental Protection
21 (MADEP) issued a consumption advisory for fish in the Housatonic River from Dalton, MA, to
22 the Connecticut border. Previously Connecticut had issued a fish consumption advisory for
23 sections of the Housatonic River in Connecticut as a result of PCB contamination. In 1999,
24 MADEP issued a consumption advisory for ducks collected from the river from Pittsfield to
25 Rising Pond in Great Barrington, MA. Concerns expressed by local residents regarding possible
26 health effects resulting from exposure to PCB contamination are being investigated by the
27 Massachusetts Department of Public Health.

1 In September 1998, after years of scientific investigations and regulatory actions, a
2 comprehensive agreement was reached between GE and various governmental entities, including
3 EPA, MADEP, the U.S. Department of Justice (DOJ), Connecticut Department of Environmental
4 Protection, and the City of Pittsfield. The agreement provides for the investigation and cleanup
5 of the Housatonic River and associated areas. The agreement has been documented in a Consent
6 Decree between all parties that was lodged with the Federal Court in October 1999. Under the
7 terms of the Consent Decree, EPA is conducting the human health and ecological risk
8 assessments, as well as the detailed modeling study of PCB transport, fate, and bioaccumulation
9 for the Lower Housatonic River and surrounding watershed.

10 The current modeling effort will include the river reaches downstream to Woods Pond because
11 of the higher concentration of PCBs in the sediments in the main channel and PCBs accumulated
12 in this first large depositional area. Below Woods Pond, Reaches 7, 8, and 9 include the river
13 sections from Woods Pond to Rising Pond, and downstream of Rising Pond, respectively (see
14 Figure 2-1). These reaches include five dams below the Woods Pond Dam and five dams in
15 Connecticut. Although the modeling activity does not incorporate these reaches, they are
16 included in the “Rest of River” defined in the Consent Decree (October 1999) and extend
17 through Connecticut. These lower reaches may be the focus of later modeling studies.



LEGEND:

-  Surface Hydrology
-  Housatonic Watershed Boundary
-  Watershed Area Above Great Barrington

N

Scale in Miles

6 0 6 12

**Housatonic River Project
Pittsfield, Massachusetts**

**FIGURE 2-1
HOUSATONIC RIVER
WATERSHED**

1 3. PROJECT/TASK DESCRIPTION

2 3.1 DESCRIPTION OF PROJECT TASKS

3 The Housatonic River PCB modeling study is composed of four major tasks:

- 4 ▪ **Modeling Framework Development**—This task entails establishing the objective
5 and scope of the modeling study; assessing data availability; recommending data
6 collection needs; developing the conceptual model of the system; evaluating and
7 selecting the models to use; formulating and discussing the modeling approach; and
8 describing model calibration and validation procedures. The MFD (Beach et al.,
9 2000) is the product of this task.
- 10 ▪ **Quality Assurance Project Plan (QAPP) Development**—The QAPP describes in
11 detail the technical activities and quality assurance (QA) and quality control (QC)
12 procedures that will be implemented to ensure that the results of the work performed
13 for the Housatonic River PCB study satisfy the stated performance criteria and are of
14 the type, quantity, and quality needed and expected.
- 15 ▪ **Performance of the Modeling Studies**—This effort will entail development and
16 application of the Housatonic River PCB model in a phased approach consistent with
17 the modeling study’s design objectives. Required efforts will include data
18 development, model setup, model calibration and validation for the watershed, and
19 hydrodynamic, water quality, and bioaccumulation submodels.
- 20 ▪ **Evaluation of Remedial Alternatives**—After the Housatonic River PCB model has
21 been validated, the model will be used to establish baseline conditions and to explore
22 the impacts that various remedial alternatives, including no action, would have on
23 PCB concentrations. Required efforts include remedial alternative formulation,
24 modeling, and evaluation and reporting of results.

25 3.2 OVERVIEW OF MODELING FRAMEWORK AND APPROACH

26 A comprehensive and integrated assessment of the watershed and a detailed analysis of the
27 hydrodynamics, sediment transport, and PCB environmental fate, transport, and bioaccumulation
28 in the most highly contaminated reaches of the Housatonic River are necessary to adequately
29 address the complex issues associated with PCB contamination. These study objectives will be
30 accomplished through the performance of an integrated watershed/hydrodynamic sediment
31 transport/water quality/bioaccumulation modeling study of PCB contamination in the Housatonic
32 River. Because no single model adequately represents these watershed and aquatic system

1 processes, a modeling framework was developed to include the component models integrated
2 within a strategy of model linkage and application.

3 The proposed modeling framework is composed of the following three component models:

- 4 ▪ U.S. EPA Hydrological Simulation Program-FORTRAN (HSPF)—Watershed Model.
- 5 ▪ Environmental Fluid Dynamics Code (EFDC)—Hydrodynamics/Sediment Transport.
- 6 ▪ AQUATOX—A Modular Toxic Effects Model for Aquatic Ecosystems.

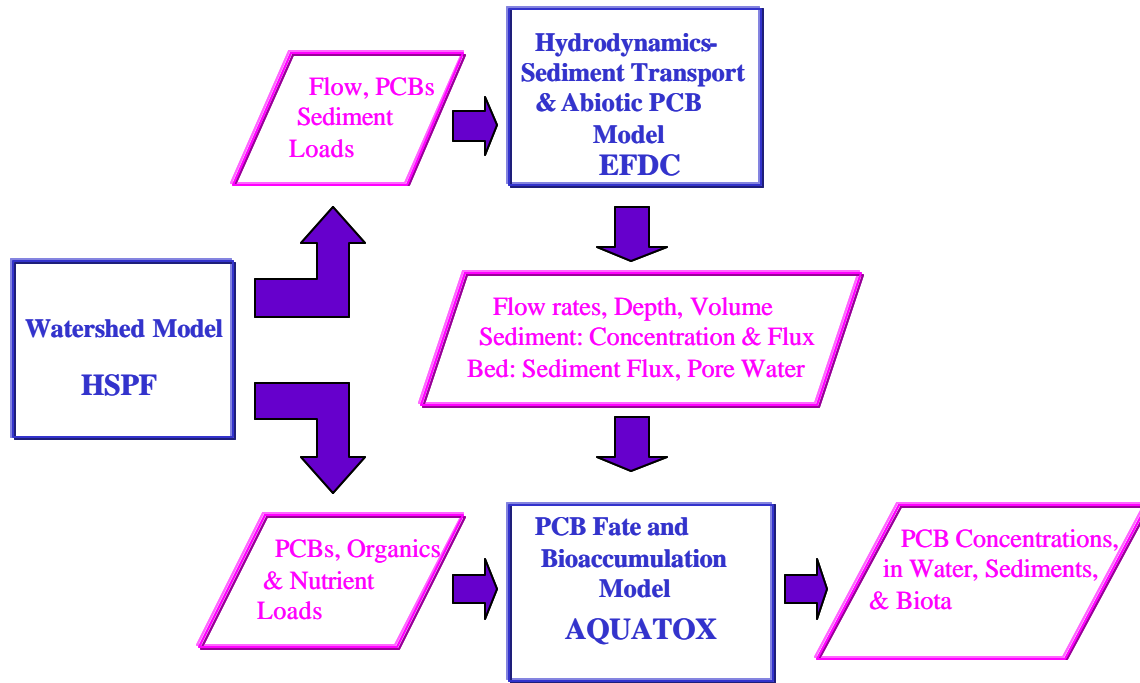
7 HSPF (Bicknell et al., 2000) is a watershed-scale hydrologic and water quality model that allows
8 simulation of both water quantity and quality in simple to complex watersheds. It provides the
9 capability to handle a diversity of water quality constituents, represent complex multi-land use
10 watersheds, include hydraulic structures and complex operational scenarios, and to represent
11 impacts of point and nonpoint sources, diversions, and various land management (urban,
12 agricultural, forest) practices. HSPF will be used to perform the hydrologic, sediment, nutrient,
13 and PCB nonpoint source loading assessment of the contributing watershed to the river
14 segments. Continuous simulation of these inputs from the contributing watershed area is
15 required to adequately establish the boundary conditions (i.e., upstream and tributary inputs to
16 network) for the hydrodynamic/water quality/bioaccumulation modeling components.

17 EFDC (Hamrick, 1996) is a sophisticated multidimensional hydrodynamic/water quality
18 numerical model that incorporates submodels for hydrodynamics (Hamrick, 1992a, 1992b),
19 sediment transport (Tetra Tech, 2000), and toxic contaminants (Tetra Tech, 1999) within a single
20 source code. It is capable of operating in 1-, 2-, or 3-dimensional modes, and can be used in a
21 wide variety of environmental settings, including rivers, lakes, reservoirs, and estuaries. EFDC
22 includes a robust numerical solution scheme to predict the system's hydrodynamic behavior, it
23 simulates both cohesive and noncohesive sediment transport, and has the ability to simulate bed
24 sediment dynamics. EFDC is capable of operating over an indefinite time period and has been
25 extensively tested and applied for numerous modeling studies of hydrodynamics, sediment
26 transport, toxic contaminants, and eutrophication in complex natural waterbodies. EFDC was
27 selected as a component of the framework because of the capability to incorporate spatial detail
28 and comprehensive, state-of-the-art process representation for hydrodynamics, sediment
29 transport, and sediment-contaminant fate and transport capabilities.

1 The AQUATOX model (Park, 1990, 1999c; EPA, 2000a, 2000b, 2000c) is a general ecosystem
2 model that represents the combined environmental fate of nutrients, sediments, and toxic
3 chemicals in aquatic ecosystems. AQUATOX has been used to model a variety of aquatic
4 systems including streams, ponds, lakes, and reservoirs. The model incorporates several trophic
5 levels, including attached and planktonic algae and submerged aquatic vegetation, invertebrates,
6 and forage, bottom-feeding, and game fish, and simultaneously represents associated organic
7 contaminants. AQUATOX simulates the fate and transfer of pollutants to the water, sediment,
8 and biotic compartments and their accumulation through the food web. The current version has
9 the potential for simulating many biotic groups and species representing a complex food web;
10 two size classes can be simulated for each fish species, and up to 15 age classes can be simulated
11 for one key species (largemouth bass in the Housatonic). As many as 20 chemicals, including
12 PCB homologs and selected congeners, can be represented simultaneously. The model
13 represents segments, such as subreaches, backwater areas, and the epilimnion and hypolimnion
14 in Woods Pond that will be linked by advection, diffusion, and migration. Up to 10 sediment
15 layers and associated pore water can be simulated. AQUATOX will be used in this modeling
16 framework to simulate the dominant PCB fate and bioaccumulation pathways, along with the
17 impacts on aquatic biota. Time-variable inputs will be provided by both HSPF and EFDC.

18 The overall modeling framework is shown graphically in Figure 3-1 and selected characteristics
19 of each model component are listed in Table 3-1. The “spatial domain” column in Table 3-1
20 defines the physical portion of the watershed/river system represented by each model, and the
21 “time step” column shows the time step of the internal model process calculations. The
22 “constituents” column identifies the key output variables calculated by each model, which are
23 either inputs to the other models, outputs that are compared with field observations as part of the
24 calibration effort, and/or the critical model predictions (e.g., PCB concentrations).

25 In essence, the framework reflects a hierarchical modeling approach. The watershed model,
26 HSPF, represents the largest spatial component of the system; it provides the boundary



1

2

Figure 3-1 Housatonic River PCB Modeling Framework

3

4 conditions for the detailed study area of the Housatonic River mainstem modeled by the
 5 hydrodynamic/sediment transport and abiotic PCB model, EFDC, and the PCB
 6 fate/bioaccumulation model, AQUATOX. Thus, the EFDC and AQUATOX models are
 7 effectively nested within the larger spatial domain of the HSPF model of the Housatonic River
 8 watershed.

9 The transport and fate of contaminants, particularly hydrophobic compounds such as PCBs, is
 10 the result of complex interacting physical, chemical, and biogeochemical processes. For
 11 example, physical transport in the water column is driven by advection and turbulent mixing of
 12 the ambient flow regime. Particulate materials are transported by gravitational settling and
 13 exchange between the water column and sediment bed by deposition, and resuspension or
 14 erosion. Contaminants adsorbed to particulates are exchanged between the water column and the
 15 sediment bed during deposition and erosion of suspended material from and to the bed.
 16 Physical/chemical processes influencing the transport and fate of sorptive contaminants include
 17 adsorption of dissolved material onto suspended particulate solids and desorption of sorbed
 18 material back into the dissolved phase. Biogeochemical processes that influence the fate of

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Table 3-1
Housatonic River PCB Modeling System Components

Model	System Component	Spatial Domain	Time Step	Constituents
HSPF	Watershed Hydrology and NPS Loads	Watershed area headwaters to Great Barrington, 282 square miles	Hourly	Flow, solids, PCBs, and nutrient loads
EFDC	Hydrodynamics, Sediment, and Abiotic PCB Transport	Confluence of East and West Branches to Woods Pond Dam	Variable, minutes	Flow, stage, abiotic PCBs and solids (cohesive and noncohesive)
AQUATOX	PCB Fate and Bioaccumulation	Confluence of East and West Branches to Woods Pond Dam	Variable; daily output	PCBs, DO, organic matter, nutrients, solids, detritus, aquatic biota

5

1 contaminants in natural waters include volatilization, biodegradation, and biological uptake or
2 bioconcentration.

3 Because of the intricate coupling between the transport and fate of particulate matter and the
4 transport and fate of contaminants, an accurate representation of the transport and fate of
5 suspended sediment is critical in developing an understanding of the transport and fate of PCBs
6 in the Housatonic River. The reliability of the sediment transport component of the model, in
7 turn, is strongly dependent on the ability of the hydrodynamic model to accurately reproduce the
8 processes of physical transport and mixing. This allows the modeler to create the appropriate
9 “physical forcing” input to dynamically simulate settling, deposition, and resuspension of
10 suspended material and of contaminants sorbed to the solids.

11 The model outputs will incorporate the effects of all critical physical, chemical, and biological
12 processes of specific importance in the evaluation of PCBs in the Housatonic River ecosystem.
13 Once calibrated and validated, these models will provide the capability for long-term predictions
14 of flows, sediment concentrations (including both fine- and coarse-grain components), nutrient
15 (nitrogen and phosphorus) concentrations, PCB concentrations (homologs, selected congeners,
16 Aroclors and total PCBs), periphyton and phytoplankton populations (estimated from
17 chlorophyll-a concentrations), and PCB biota tissue concentrations.

18 The modeling framework will allow for a detailed analysis of the effects of alternative future
19 conditions, including proposed management, cleanup, and remediation scenarios. These
20 scenarios may evaluate a broad range of options, including natural attenuation, remediation of
21 bed sediments, removal of deposited enriched sediment in the floodplain, and various
22 combinations of these alternatives.

1 **4. DATA QUALITY OBJECTIVES AND CRITERIA FOR MEASUREMENT** 2 **DATA AND MODEL RESULTS**

3 **4.1 PROJECT DATA QUALITY OBJECTIVES**

4 Data Quality Objectives (DQOs) are qualitative and quantitative statements that clarify the
5 intended use of data, define the types of data needed to support a decision, identify the conditions
6 under which the data should be collected, and specify tolerable limits on the probability of
7 making a decision error because of uncertainty in the data.

8 Data of known and documented quality are essential to the success of any water quality
9 modeling study, which in turn generates information for use in decisionmaking. Field
10 investigations that support the modeling study were conducted using QA/QC procedures
11 (WESTON, 2000b) as part of the site investigation. Model calibration will be accomplished
12 using data available from other studies in addition to these companion investigations. All data
13 used in this modeling effort will be reviewed for quality and consistency with other relevant data
14 and for reasonableness in representing known conditions of the study area.

15 The modeling study will predict concentrations of PCBs in various environmental media. The
16 quality assurance process for this type of study consists of using appropriate data, data analysis
17 procedures, modeling methodology and technology, administrative procedures, and auditing. To
18 a large extent, the quality of the modeling study is determined by the expertise of the modeling
19 and quality assessment teams, in addition to the available data. The ultimate test of quality for
20 this study, however, is that the model output is a sufficiently accurate representation of the
21 natural system to address the site-specific study objectives/data quality objectives listed below.

22 The proposed modeling study design was developed to (1) represent the full range of physical,
23 chemical, and biological processes of concern for PCB fate, transport, and bioaccumulation in
24 the Housatonic River watershed, and (2) address each of the following site-specific study
25 objectives, which also serve as the DQOs for the model output:

- 26 ▪ Quantify future spatial and temporal distribution of PCBs (both dissolved and
27 particulate forms) within the water column and bed sediment.

- 1 ▪ Quantify the historical and relative contributions of various sources of PCBs on
2 ambient water quality and bed sediment.
- 3 ▪ Quantify the historical and relevant contribution of various PCB sources to
4 bioaccumulation in targeted species.
- 5 ▪ Estimate the time required for PCB-laden sediment to be effectively sequestered by
6 the deposition of “clean” sediment (i.e., natural recovery).
- 7 ▪ Estimate the time required for PCB concentrations in fish tissue to be reduced to
8 levels that no longer pose either a human health or ecological risk based on various
9 remediation and restoration scenarios, including allowing for natural recovery.
- 10 ▪ Quantify the relative risk(s) of extreme storm event(s) contributing to the
11 resuspension of sequestered sediment and the redistribution of PCB-laden sediment
12 within the area of study.

13 The determination of whether the DQOs have been achieved is less straightforward for a
14 modeling study than for the more typical sampling and analysis type of study. The usual data
15 quality indicators (e.g., completeness, accuracy, precision) are difficult to apply and in many
16 cases do not adequately characterize model output. Nonetheless, there are objective techniques
17 that can be used to evaluate the quality of the model performance and output. These methods and
18 the proposed performance expectations are discussed below.

19 **4.2 DATA SOURCES AND AVAILABILITY**

20 The Housatonic River modeling study will use an extensive database, comprising many different
21 types of data. Application of each of the three modeling components (HSPF, EFDC, and
22 AQUATOX) will require considerable environmental data. Time series of weather data are
23 required to drive the watershed model. Additional data are required to characterize the
24 watershed terrain in terms of topography, soils, and land use/land cover. Time series data for
25 channel streamflow and stage are critical for calibrating the hydrodynamic model. Similarly,
26 data characterizing suspended and bed sediment and dissolved and sorbed chemical (PCB, TOC)
27 concentrations are required for calibration of the water quality components of EFDC and
28 AQUATOX. AQUATOX requires a subset of the data types described above and adds an
29 additional data requirement for observed PCB concentrations in biota. Table 4-1 summarizes the

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Table 4-1

Data Types, Descriptions, and Sources for the Housatonic River Modeling Study

Data Type	Data Description	Data Source
Meteorological observations	Precipitation Transpiration Evaporation Maximum/minimum air temperature Dewpoint temperature Windspeed Solar radiation Cloud cover	NOAA National Climatic Data Center (NCDC), EarthInfo, General Electric
Topography	Digital elevation model (DEM) 1:24000 scale digital terrain maps	U.S. EPA BASINS CD U.S. Geological Survey
Soil delineation and hydrological/erosion properties	Distribution of soil types and their underlying properties, e.g., permeability, soil layer depths, bulk density and soil erodibility characteristics	U.S. EPA BASINS CD U.S. Department of Agriculture STATSGO database
Land use/cover data	Classification of vegetation, water, natural surface, and man-induced features on the land surface	U.S. EPA BASINS CD U.S. Geological Survey GIRAS database
Channel characteristics	Channel lengths and slopes Channel cross-sectional geometry Bed substrate composition Hydraulic structures	General Electric/Blasland, Bouck, & Lee (BBL) U.S. EPA Reach File (RF1 & RF3) U.S. Army Corps of Engineers U.S. EPA/WESTON
Point sources	Point source flow/quality	U.S. EPA Permit Compliance/PCS City of Pittsfield
Streamflow	Base flow Storm event flows	U.S. Geological Survey U.S. EPA/WESTON
Stage/temperature	Stage and temperature data for river and Woods Pond	General Electric/QEA U.S. EPA/WESTON
Biota	Individual samples Composite samples	U.S. EPA/WESTON U.S. Geological Survey General Electric/BBL
Sediment, water quality, PCBs	Particle size distribution Total suspended solids Water column samples Grab samples Sediment cores	USGS/CAES General Electric/BBL U.S. EPA/WESTON General Electric/LMS CT DEP General Electric/Stewart

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1 data types that are required for the Housatonic River PCB modeling study. As the table
2 indicates, the data will originate from a wide variety of government and private sources.

3 The process of developing a conceptual model for the study requires an evaluation of what field
4 data are available and a determination as to what additional data collection is needed to fully
5 support the investigation. Table 4-2 (excerpted from the MFD) provides a summary of the types
6 of data that will be used as part of this investigation and the time periods over which they are
7 available. These timelines are not intended to be all-inclusive but rather to provide an overall
8 picture of available historical and current data. The MFD includes a complete list of available
9 data for stations above Canaan, CT, including meteorologic data stations, for use in the modeling
10 efforts. The references and sources used to develop the information in Table 4-2 and in the MFD
11 include published reports by GE and its consultants, USGS data, NOAA/NCDC data, the EPA
12 Housatonic River Project Database (WESTON, 2000a), and other reports. Limitations of the
13 data will be assessed, potential limitations in the data will be identified, and the data will be
14 further evaluated for usability prior to use in the modeling activities.

15 **4.3 MEASUREMENT AND MODEL PERFORMANCE CRITERIA**

16 Measurement criteria, as defined in the EPA QAPP guidance, are not directly relevant to this
17 modeling effort; criteria for current data collection efforts are addressed in the QAPP
18 (WESTON, 2000b) for the Supplemental Investigation. Issues related to measurement criteria for
19 existing data sources and data collected in the companion investigations are also addressed in
20 Sections 11 and 13.

21 This section focuses on the model performance criteria, which are the basis by which judgments
22 will be made on whether the model results are adequate to support the decisions required to
23 address the study objectives. In essence, the model performance criteria provide the numerical
24 basis for answering the question, “Are the model results, as reflected in the calibration and
25 validation comparison, of sufficient quality to be used in decisionmaking for this study?”

26 Model performance criteria, sometimes referred to as calibration or validation criteria, have been
27 contentious topics for more than 20 years (see Thomann, 1980; Thomann, 1982; James and
28 Burges, 1982; Donigian, 1982; ASTM, 1984). These issues have been recently thrust to the

Table 4-2 Timeline Summary of Housatonic River Data Studies above Great Barrington, MA, 1979-99

	General Location	Sample Type	REF / SOURCE	1979		1980		1981		1982		1983		1984		1985		1986		1987		1988		1989		1990		1991		1992		1993		1994		1995		1996		1997		1998		1999		2000					
				Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec				
Flow	Great Barrington, MA	Flow	USGS ¹	[Blue bar spanning all months from 1979 to 2000]																																															
	Coltsville, MA	Flow	USGS ²	[Blue bar spanning all months from 1979 to 2000]																																															
Stage/Temp	Woods Pond Dam	St-30min T-30min	GE/QEA GE/QEA	[Blue bars in 1997, 1998, 1999]																																															
	Woods Pond Headwaters	St-30min T-30min	GE/QEA GE/QEA	[Blue bars in 1997, 1998, 1999]																																															
	Rising Pond Dam	St-30min T-30min	GE/QEA GE/QEA	[Blue bars in 1997, 1998, 1999]																																															
	PSA Stations	SW/Events	Weston/USEPA	[Blue bar in 1999]																																															
Biota	GE - MA/CT border	Comp.	Stewart	[Blue bars in 1980, 1982]																																															
	Burlington Hatchery	Indiv.	ANS	[Blue bars in 1987, 1989]																																															
	Woods Pond Dam	Indiv.	BBL ¹	[Blue bars in 1990, 1994]																																															
	Rising Pond Dam	Indiv. F,WB,Comp. F,WB,Comp.	BBL ¹ USEPA GE	[Blue bars in 1990, 1998, 1999]																																															
	GE Plant Site	Comp.	BBL ¹	[Blue bars in 1997, 1998, 1999]																																															
	Upper E. Br. - Dalton	F,WB,Comp.	USEPA	[Blue bars in 1998, 1999]																																															
	Three Mile Pond	F,WB,Comp.	USEPA	[Blue bars in 1998, 1999]																																															
	Goodrich Pond	F,WB,Comp. F,WB	USEPA GE	[Blue bars in 1998, 1999]																																															
	W. Br. Confluence - WWTP	F,WB,Comp. F,WB,Comp.	USEPA GE	[Blue bars in 1998, 1999]																																															
	WWTP - Woods Pond Headwaters	F,WB,Comp. F,WB,Comp.	USEPA GE	[Blue bars in 1998, 1999]																																															
	Woods Pond and Backwaters	F,WB,Comp. F,WB,Comp.	USEPA GE	[Blue bars in 1998, 1999]																																															
	Sed.	Coltsville, MA	PSD TSS TSS	USGS/CAES GE,BBL ² USEPA	[Blue bars in 1979, 1990, 1994, 1998, 1999]																																														
Pittsfield, MA (PSA Stations)		PSD PSD,TSS PSD,TSS	USGS/CAES GE/BBL ² Weston/USEPA	[Blue bars in 1979, 1990, 1994, 1998, 1999]																																															
Great Barrington, MA		PSD,BD TSS PSD,TSS TSS TSS PSD,TSS	LMS LMS Stewart GE/BBL ² USGS/CTDEP USGS ¹	[Blue bars in 1979, 1982, 1990, 1992, 1994, 1998, 1999]																																															

Explanation of Sample Types			
Flow - Discharge measurement	WB - Whole Body sample of biota	GSvsC - Grain Size vs PCB Concentration	T&UNH ₃ - Total and Un-ionized Ammonia concentrations
St-30min - Stage taken at 30-minute increments	TSS - Total Suspended Solids concentration	BOD ₅ - Biological Oxygen Demand 5 day	NO ₃ - Nitrate concentration in water-column sample
T-30min - Temperature taken at 30-minute increments	PSD - Particle Size Distribution of sediment sample	WC - Water Column sample	Oil&Grease - Oil and Grease concentration
Comp. - Composite sample of biota	BD - Bulk Density (net weight) of sediment samples	Hazardous - Various Hazardous Constituents other than PCBs	Temp - Temperature measurement taken at daily increments
Indiv. - Individual sample of biota	CS - Core Sediment sample	DO - Dissolved Oxygen concentration	Nutr - Nutrients
F - Fillet sample of biota	SS - Surficial Sediment sample	GrbS - Grab Sample	

Table 4-2 Timeline Summary of Housatonic River Data Studies above Great Barrington, MA, 1979-99 (Continued)

			1979		1980		1981		1982		1983		1984		1985		1986		1987		1988		1989		1990		1991		1992		1993		1994		1995		1996		1997		1998		1999		2000							
			Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec	Jan	May	Aug	Dec						
PCBs	Coltsville, MA	CS CS,GrbS WC WC	Stewart USGS/CAES GE/BBL ² USEPA			■		■		■																																										
	Pittsfield, MA	CS CS,GrbS CS,GrbS WC WC	Stewart USGS/CAES GE/BBL ² GE/BBL ² Weston/USEPA			■		■		■					■				■											■																						
	Great Barrington, MA	CS,WC CS,GrbS WC CS,GrbS WC CS WC	Stewart USGS/CAES LMS LMS USGS/CTDEP GE/BBL ² GE/BBL ²			■		■		■					■				■																																	
TOC	Coltsville, MA	CS,GrbS CS,GrbS	USGS/CAES USEPA			■		■																																												
	Pittsfield, MA	CS,GrbS WC,CS CS,GrbS	GE/BBL ² Weston/USEPA USGS/CAES			■		■																																												
	Great Barrington, MA	CS,GrbS SS,CS	LMS USGS/CAES			■		■																																												
Other	Pittsfield, MA	Hazardous DO, pH T&UNH ₃ ,NO ₃ Oil&Grease Nutr,BOD ₅	GE/BBL ² BBL ² BBL ² BBL ² Weston/USEPA																																																	
	(PSA Stations)																																																			
	Great Barrington, MA	Tmp,DO Hazardous	USGS ¹ GE/BBL ²			■																																														

Notes:

- USGS¹ - U.S. Geological Survey: Surface-water station on the Housatonic River near Great Barrington, MA (01197500).
- USGS² - U.S. Geological Survey: Surface-water station on the Housatonic River at Coltsville, MA (01197000).
- BBL¹ - Blasland, Bouck and Lee: General Electric Company 1999. Preliminary Draft of Biota Database Summary. Prepared for discussion purposes only.
- BBL² - Blasland, Bouck and Lee: General Electric Company 1996. Supplemental Phase II/RCRA Facility Investigation Report for Housatonic River and Silver Lake. Vol. II.: with Figures and Tables. Prepared by Blasland, Bouck and Lee.
- QEA - Quantitative Environmental Analysis: Quantitative Environmental Analysis. 1998. Technical Memorandum - Spring 1997 High Flow Monitoring & Summer 1997 Bathymetric Sediment Bed Mapping Survey. Prepared to present data collected by BB&L and HydroQual.
- Stewart - Stewart Laboratories, Inc. 1982. Housatonic River Study 1980 and 1982 Investigations. Prepared for General Electric Company.
- ANS - Academy of Natural Sciences: General Electric Company 1999. Preliminary Draft of Biota Database Summary. Prepared for discussion purposes only.
- USEPA - U.S. Environmental Protection Agency: General Electric Company 1999. Preliminary Draft of 1998 Biota Database Summary. Prepared for discussion purposes only.
- GE - General Electric Company: General Electric Company 1999. Preliminary Draft of 1998 Biota Database Summary. Prepared for discussion purposes only.
- LMS - Lawler, Matusky and Skelly Engineers: General Electric Company. 1994. Housatonic River Connecticut Cooperative Agreement B Task IV.B: PCB Fate and Transport Model: Additional Monitoring and Model Verification. Prepared by Lawler, Matusky and Skelly Engineers.
- Weston - Roy F. Weston, Inc.: Roy F. Weston, Inc. 1999. Microsoft Access Database Data Mart. Preliminary summary of available data.
- USGS/CAES - CAES, CDEP, and USGS: Frink, C.R., K.P. Kulp, C.G. Fredette. 1981. PCBs in Housatonic River Sediments: Determination, Distribution and Transport. Draft. Prepared by CAES, CDEP, and USGS.
- USGS/CTDEP - USGS and CT Department of Environmental Protection: Kulp, K.P. 1991. Concentration and Transport of Polychlorinated Biphenyls in the Housatonic River Between Great Barrington, Massachusetts, and Kent, Connecticut, 1984-1988, 1991. Prepared by USGS and CT Department of Environmental Protection.
- USGS - U.S. Geological Survey: General Electric Company 1999. Preliminary Draft of 1998 Sediment Database Summary. Prepared for discussion purposes only.

Explanation of Sample Types			
Flow - Discharge measurement	WB - Whole Body sample of biota	GSvsC - Grain Size vs PCB Concentration	T&UNH ₃ - Total and Un-ionized Ammonia concentrations
St-30min - Stage taken at 30 minute increments	TSS - Total Suspended Solids concentration	BOD ₅ - Biological Oxygen Demand 5 day	NO ₃ - Nitrate concentration in water-column sample
T-30min - Temperature taken at 30 minute increments	PSD - Particle Size Distribution of sediment sample	WC - Water Column sample	Oil&Grease - Oil and Grease concentration
Comp. - Composite sample of biota	BD - Bulk Density (net weight) of sediment samples	Hazardous - Various Hazardous Constituents other than PCBs	Tmp - Temperature measurement taken at daily increments
Indiv. - Individual sample of biota	CS - Core Sediment sample	DO - Dissolved Oxygen concentration	Nutr - Nutrients
F - Fillet sample of biota	SS - Surficial Sediment sample	GrbS - Grab Sample	

1 forefront in the environmental arena as a result of the need for and use of modeling for
2 exposure/risk assessments, Total Maximum Daily Load (TMDL) determinations, and
3 environmental assessments.

4 Recently (September 1999), an EPA-sponsored workshop entitled “Quality Assurance of
5 Environmental Models” convened in Seattle, WA, to address issues related to the problems of
6 model assessment and quality assurance, development of methods and techniques, assurance of
7 models used in regulation, and research and practice on model assurance (see the following Web
8 site for details: <http://www.nrcse.washington.edu/events/qaem/qaem.asp>). This workshop
9 resulted in a flurry of web-based activity among a group of more than 50 recognized modeling
10 professionals (both model developers and users) in various federal and state agencies,
11 universities, and consulting firms that clearly confirms the current lack of consensus on this
12 topic.

13 Although no consensus on model performance criteria is apparent from the past and recent
14 model-related literature, a number of “basic truths” are evident and are likely to be accepted by
15 most modelers in modeling natural systems:

- 16 ▪ Models are approximations of reality; they cannot precisely represent natural systems.
- 17 ▪ There is no single, accepted statistic or test that determines whether or not a model is
18 validated.
- 19 ▪ Both graphical comparisons and statistical tests are required in model calibration and
20 validation.
- 21 ▪ Models cannot be expected to be more accurate than the sampling and statistical error
22 (e.g., confidence intervals) in the input and observed data.

23 All of these “basic truths” must be considered in the development of appropriate procedures for
24 quality assurance of the models to be used in this assessment of PCB contamination in the
25 Housatonic River. Despite a lack of consensus on how they should be evaluated, in practice,
26 environmental models are being applied, and their results are being used, for assessment and
27 regulatory purposes. A “weight of evidence” approach is most widely used and accepted when
28 models are examined and judged for acceptance for these purposes. Consequently, an approach

1 based on the weight-of-evidence concept, derived from the above truths, and that embodies the
2 following principles, is proposed for this study:

- 3 a. Because models are approximations of natural systems, exact duplication of observed
4 data is not a performance criterion. The model validation process will measure,
5 through comparability goals, the ability of the model to simulate measured values.
- 6 b. No single procedure or statistic is widely accepted as measuring, nor capable of
7 establishing, acceptable model performance; thus numerous graphical comparisons
8 and statistical tests are proposed to provide sufficient evidence upon which to base a
9 decision of model acceptance or rejection.
- 10 c. All model and observed data comparisons must recognize, either qualitatively or
11 quantitatively, the inherent error and uncertainty in both the model and the
12 observations. This error and uncertainty will be documented, where possible, as part
13 of this modeling study.

14 Although each of the models included in the Housatonic River PCB modeling framework will
15 use different types of graphical and statistical procedures, they will generally include some of the
16 following:

17 Graphical Comparisons:

- 18 1. Time series plots of observed and simulated values for fluxes (e.g., flow) or state
19 variables (e.g., stage, sediment concentration, and biomass concentration).
- 20 2. Observed versus simulated scatter plots, with a best-fit linear regression line
21 displayed, for fluxes or state variables.
- 22 3. Cumulative frequency distributions of observed and simulated fluxes or state variable
23 (e.g., flow duration curves).

24
25 Statistical Tests:

- 26 1. Error statistics (e.g., mean error, absolute mean error, relative error, relative bias, and
27 standard error of estimate).
- 28 2. Correlation tests (e.g., linear correlation coefficient, coefficient of model-fit
29 efficiency).
- 30 3. Cumulative Distribution tests (e.g., Kolmogorov-Smirnov [KS] test).

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1 These comparisons and statistical tests are fully documented in a number of comprehensive
2 references on applications of statistical procedures for biological assessment (Zar, 1999),
3 hydrologic modeling (McCuen and Snyder, 1986), and environmental engineering (Berthouex
4 and Brown, 1994).

5 Time series plots are generally evaluated visually as to the agreement, or lack thereof, between
6 the simulated and observed values. Scatter plots usually include calculation of a correlation
7 coefficient, along with the slope and intercept of the linear regression line; thus the graphical and
8 statistical assessments are combined. When observed data are adequate and/or uncertainty
9 estimates are available, confidence intervals for the observed data will be calculated so they can
10 be considered in the model performance evaluation.

11 For comparing observed and simulated cumulative frequency distributions, the KS test is used to
12 assess whether the two distributions are different at a selected significance level. The reliability
13 of the KS test is a direct function of the population of data values that defines the observed
14 cumulative distribution. Except for flow comparisons at the major USGS gage sites, there is
15 unlikely to be sufficient observed data (i.e., more than 50 data values per location and
16 constituent) to perform this test reliably for most water quality and biotic constituents. However,
17 we will consider this test for all appropriate model results when justified by the observed data
18 population.

19 In recognition of the inherent variability in natural systems and unavoidable errors in field
20 observations, the USGS provides the following characterization of the accuracy of its streamflow
21 records in all its surface water data reports (e.g., Socolow et al., 1997):

22	Excellent Rating	95 % of daily discharges are within 5 % of the true value
23	Good Rating	95 % of daily discharges are within 10 % of the true value
24	Fair Rating	95 % of daily discharges are within 15 % of the true value

25
26 Records that do not meet these criteria are rated as “poor.” Clearly, calibrated and validated
27 model results that are within the accuracy tolerances for a fair to excellent rating (noted above)
28 must be considered acceptable; these levels of uncertainty are inherent in the observed data. It
29 does not necessarily follow, however, that model results not meeting the threshold for “fair”
30 using this rating system are unacceptable, because they may still be of value for making

1 management decisions. For example, a result indicating that a particular regulatory criterion
2 would be exceeded by a factor of 10 would still be usable for reaching some management
3 decisions even if the model were known to produce results no closer than within 50% of the
4 “real” value.

5 **4.3.1 Historical Model Accuracy and Performance Expectations**

6 Very few QAPPs have been developed specifically for modeling assessments, and none for a
7 study that approaches the level of physical complexity of the Housatonic River. The QA Plan
8 developed for the Lake Michigan Mass Balance Project indicated a modeling quality objective
9 “... to develop a model capable of calculating pollutant concentrations in Lake Michigan to
10 within a factor of two of observed concentrations in the water column and target fish species”
11 (EPA, 1997; EPA, 2000d). PCBs are included in the Lake Michigan modeling effort as they are
12 one of the contaminants of concern.

13 A QAPP developed for an EIS for the proposed Nicollet Mine in northern Wisconsin also used
14 HSPF and specified the following acceptability criteria:

15 “The targets for acceptable calibration and verification of monthly flows are
16 a correlation coefficient greater than 0.85 and the coefficient of model-fit efficiency
17 greater than 0.8.” (EPA, 1998b)

18 Table 4-3 lists general calibration/validation tolerances or targets that have been provided to
19 model users as part of HSPF training workshops over the past 10 years (e.g., Donigian et al.,
20 2000). The values in the table attempt to provide some general guidance, in terms of the % mean
21 errors or differences between simulated and observed values, so that users can gage what level of
22 agreement or accuracy (i.e., very good, good, fair) may be expected from the model application.
23 Again, these targets should be considered as general guidance only and are not intended to be
24 “pass/fail” criteria.

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Table 4-3

General Calibration/Validation Targets or Tolerances for HSPF Applications

	% Difference Between Simulated and Recorded Values		
	Very Good	Good	Fair
Hydrology/Flow	<10	10 – 15	15 – 25
Sediment	<20	20 – 30	30 – 45
Water Temperature	<7	8 – 12	13 – 18
Water Quality/Nutrients	<15	15 – 25	25 – 35
Pesticides/Toxics	<20	20 – 30	30 – 40

Caveats: Relevant to monthly and annual values; storm peaks may differ more.
Quality and detail of input and calibration data.
Purpose of model application.
Availability of alternative assessment procedures.
Resource availability (i.e., time, money, personnel).

Source: Donigian, et al., 2000.

The caveats at the bottom of the table indicate that the tolerance ranges should be applied to mean values, and that individual events or observations may show larger differences, and still be acceptable. In addition, the level of agreement to be expected depends on many site and application-specific conditions, including the data quality, purpose of the study, available resources, and available alternative assessment procedures that could meet the study objectives.

Although not prepared as a QAPP document, model evaluation metrics prepared for the Lower Fox River sediment transport and PCB fate models (LTI & WDNR, 1998) defined quantitative model quality criteria to represent the target threshold of accuracy for the comparison of observed data with model results. Model performance criteria for the Lower Fox River models were defined on the basis of goals established for the Green Bay Mass Balance Study and the previous performance of existing models determined in a post-audit evaluation of short-term simulations of the Lower Fox River. To evaluate the models, the following model performance criteria were proposed as tolerance ranges for the mean predicted concentrations for TSS and PCBs:

1. Within $\pm 30\%$ of the observed data for the water column and sediment bed for the short-term simulation (1989-1995).

1 2. Within $\pm 50\%$ for the long-term simulation (1957-1995).

2
3 Prevailing tolerances for fate and bioaccumulation models are larger than those of hydrologic
4 and hydrodynamic models because of the inherent uncertainties in degradation, time-varying
5 bioenergetics, and alternate pathways of uptake. Based on the same Fox River study noted
6 above, while tolerances of $\pm 30\%$ and $\pm 50\%$ were proposed for PCBs in water and sediment,
7 factors of 3 and 5 for short- and long-term concentrations in fish were considered acceptable.
8 Gobas et al. (1995) found that in simulating PCBs in Lake Ontario most predictions were within
9 1 standard deviation of the observed data and all were within 2 standard deviations;
10 phytoplankton and zooplankton were within a factor of 3. Burkhard (1998), in an evaluation of
11 the Gobas and Thomann models with PCB congener data, presented results showing that the
12 predicted ratios (i.e., predicted/observed) of bioaccumulation factors (BAFs) for phytoplankton
13 were 0.17 (a factor of 5.9) for both models. For zooplankton, the ratios were 0.35 and 0.51
14 (factors of 2.9 and 1.96) in the respective models. The ratios of BAFs for amphipods were 1.82
15 and 1.86, and the mean ratios for fish were 1.28 and 2.97, respectively.

16 Standards for evaluating temporal and spatial trends and patterns have not been well quantified
17 for bioaccumulation models. Gobas et al. (1995) presented graphs showing good agreement
18 between predicted and observed trends for total PCBs in lake trout and herring gull eggs, but
19 little agreement between model results and time-varying patterns of total PCBs in amphipods,
20 zooplankton, smelt, and sculpin. With small sample size, visual inspection of patterns may have
21 to suffice; other tests are discussed in Section 4.7.1.

22 **4.3.2 Proposed Model Calibration and Validation Targets**

23 Because of the uncertain state-of-the-art in model performance criteria, the inherent error in input
24 and observed data, and the approximate nature of model formulations, absolute criteria for model
25 acceptance or rejection are not appropriate for this effort. Consequently, the tolerance ranges
26 shown in Table 4-4 are proposed as general targets or goals for model calibration and validation
27 for the corresponding modeled quantities. These tolerances will be applied to comparisons of
28 simulated and observed mean flows, stage, concentrations, and other state variables (listed
29 below), with larger deviations expected for individual sample points in both space and time.

1 There are a variety of ways to compare simulated and observed mean values. The sporadic
2 observed data can be aggregated over annual, seasonal, or monthly timeframes and compared to
3 the full range of simulated values. Alternatively, the simulated time series can be sampled to
4 include only the time periods when samples were gathered, and then limiting the model-data
5 comparisons to those sampled time periods. Clearly, both approaches have advantages and
6 disadvantages. Both of these approaches and others will be explored as part of the model
7 performance evaluation.

8 The values shown in Table 4-4 are derived from extensive past experience with the individual
9 models and the selected past efforts on model performance criteria discussed above. If
10 preliminary model results do not satisfy the target tolerances listed in Table 4-4, additional
11 efforts will be required to investigate all possible errors in, and the accuracy of, input data, model
12 formulations, and field observations. If adjustments in these tolerances are needed, they will be
13 fully investigated and documented, and revisions to this QAPP will be issued through the formal
14 QA process.

15 **4.4 OVERVIEW OF MODEL CALIBRATION AND VALIDATION PROCEDURES**

16 The application procedures for each model differ because of the variations of the specific
17 physical, chemical, and biological systems they each are designed to represent. All model
18 applications typically include three primary phases or steps: database development, system
19 characterization, and calibration and validation. QA issues are involved in all aspects of model
20 application, but they are especially critical for the calibration and validation phase since the
21 outcome establishes how well the model represents the watershed. An accurate numerical
22 representation of the study area is the primary goal of the model application effort because it
23 determines whether the model results can be relied upon and used effectively for decision-
24 making.

25 Calibration and validation have been defined by the American Society of Testing and Materials,
26 as follows (ASTM, 1984):

- 27 ▪ Calibration—A test of the model with known input and output information that is
28 used to adjust or estimate factors for which data are not available.

1
2
3

Table 4-4

Proposed Model Calibration and Validation Target Tolerances

Model/Modeled Quantity	Calibration/Validation Target Tolerances
Watershed Model	
Hydrology/Flow	± 15 %
Sediment Loadings/Concentrations	± 30 %
Water Temperature	± 10 %
Nutrient Loadings/Concentrations	± 25 %
PCB Loadings/Concentrations	± 50 %
Hydrodynamic/Sediment/Abiotic PCB Model	
Stage Height (as water column depth)	± 10 %
Solids (TSS-water column)	± 30 %
Total PCBs (water column and bed)	± 30 %
Net Sediment Accumulation Rates in Woods Pond	± 30 %
Net Solids Mass Balance/Flux	± 30 %
PCB Fate/Effects/Bioaccumulation Model	
Total PCB concentrations, short-term simulations water column, dissolved suspended and sedimented detritus Ratio of bioaccumulation factors: algae invertebrates fish	± 30 % ± 30 % ± factor of 3 ± factor of 2 ± factor of 1.5
Total PCB concentrations, long-term simulations water column, dissolved suspended and sedimented detritus Ratio of bioaccumulation factors: algae invertebrates fish	± 50 % ± 50 % ± factor of 5 ± factor of 3 ± factor of 2
Homolog profile in fish, short-term r^2 Relative bias, distributions are the same	> 0.80 p > 0.85

4
5

- 1 ▪ Validation—Comparison of model results with numerical data independently derived
2 from experiments or observations of the environment.

3 Model validation is in reality an extension of the calibration process. Its purpose is to assure that
4 the calibrated model properly assesses all the variables and conditions that can affect model
5 results. Although there are several approaches to validating a model, perhaps the most effective
6 procedure is to use only a portion of the available record of observed values for calibration; once
7 the final parameter values are developed through calibration, simulation is performed for the
8 remaining period of observed values and goodness-of-fit between recorded and simulated values
9 is reassessed. This type of split-sample calibration/validation procedure will be followed for the
10 model validation efforts on the Housatonic River, with selected adaptations required for each
11 model and available data. Model credibility is based on the ability of a single set of parameters
12 to represent the entire range of observed data; in effect, this is a form of validation.

13 As noted in Section 4.3, model performance and calibration/validation will be evaluated through
14 qualitative and quantitative measures, involving both graphical comparisons and statistical tests.
15 For flow simulations where continuous records are available, all these techniques will be used,
16 and the same comparisons will be performed during both the calibration and validation phases.
17 Comparisons of simulated and observed state variables will be performed for daily, monthly, and
18 annual values, in addition to flow-frequency duration assessments. Statistical procedures will
19 include those mentioned in Section 4.3, including error statistics, correlation and model-fit
20 efficiency coefficients, and goodness-of-fit tests.

21 For sediment, water quality, and biotic constituents, model performance will be based primarily
22 on visual and graphical presentations because the frequency of observed data is often inadequate
23 for accurate statistical measures. However, we will investigate alternative model performance
24 assessment techniques; e.g., error statistics and correlation measures, consistent with the
25 population of observed data available for model testing.

26 **4.5 HSPF CALIBRATION AND VALIDATION PROCEDURES**

27 The application of HSPF to the Housatonic River watershed will follow the standard model
28 application procedures as described in the HSPF Application Guide (Donigian et al., 1984), in
29 numerous watershed studies over the past 15 years (see HSPF Bibliography [Donigian, 1999]),

1 and recently in the HSPF application to the Chesapeake Bay watershed (Donigian et al., 1994).
2 Model application procedures for HSPF include database development, watershed segmentation,
3 and hydrology, sediment, and water quality calibration and validation. Each of these steps is
4 discussed in the MFD, with additional details provided in this section for the QA-related steps of
5 calibration and validation.

6 For HSPF, calibration is an iterative procedure of parameter evaluation and refinement, as a
7 result of comparing simulated and observed values of interest. This approach is required for
8 parameters that cannot be deterministically, and uniquely, evaluated from topographic, climatic,
9 edaphic, or physical/chemical characteristics of the watershed and compounds of interest.
10 Fortunately, the large majority of HSPF parameters do not fall in this category. Calibration is
11 based on several years of simulation (at least 3 to 5 years) to evaluate parameters under a variety
12 of climatic, soil moisture, and water quality conditions. Calibration should result in parameter
13 values that produce the best overall agreement between simulated and observed values
14 throughout the calibration period.

15 Calibration includes the comparison of both monthly and annual values, and individual storm
16 events, whenever sufficient data are available for these comparisons. All of these comparisons
17 should be performed for a proper calibration of hydrology and water quality parameters. In
18 addition, when a continuous observed record is available, such as for streamflow, simulated and
19 observed values should be analyzed on a frequency basis and their resulting cumulative
20 distributions (e.g., flow duration curves) compared to assess the model behavior and agreement
21 over the full range of observations.

22 Calibration is a hierarchical process beginning within hydrology calibration of both runoff and
23 streamflow, followed by sediment erosion and sediment transport calibration, and finally
24 calibration of water quality constituents. When modeling land surface processes, hydrologic
25 calibration must precede sediment and water quality calibration since runoff is the transport
26 mechanism by which nonpoint pollution occurs. Likewise, adjustments to the instream
27 hydraulics simulation must be completed before instream sediment and water quality transport
28 and processes are calibrated. Each of these steps is discussed below with the emphasis on the

1 key calibration parameters; Appendix B in the MFD provides a comprehensive list of model
2 parameters for HSPF, along with definitions, units, and data/evaluation sources.

3 Because parameter evaluation is a key precursor to the calibration effort, a valuable source of
4 initial values for many of the key calibration parameters is the recently developed parameter
5 database for HSPF, called HSPFParm (Donigian et al., 1999). HSPFParm is an interactive
6 database (based on MS-Access) that includes calibrated parameter values for up to 45 watershed
7 water quality studies across the United States. This will be supplemented with additional HSPF
8 hydrology studies and ongoing HSPF applications in Massachusetts and Connecticut.

9 **4.5.1 Hydrologic Calibration and Key Calibration Parameters**

10 Hydrologic simulation combines the physical characteristics of the watershed and the observed
11 meteorologic data series to produce the simulated hydrologic response. All watersheds have
12 similar hydrologic components, but they are generally present in different combinations; thus
13 different hydrologic responses occur on individual watersheds. HSPF simulates runoff from four
14 components: surface runoff from impervious areas directly connected to the channel network,
15 surface runoff from pervious areas, interflow from pervious areas, and groundwater flow.
16 Because the historic streamflow is not divided into these four units, the relative relationship
17 among these components must be inferred from the examination of many events over several
18 years of continuous simulation.

19 A complete hydrologic calibration involves a successive examination of the following four
20 characteristics of the watershed hydrology, in the order shown: (1) annual water balance, (2)
21 seasonal and monthly flow volumes, (3) baseflow, and (4) storm events. Simulated and observed
22 values for reach characteristic are examined and critical parameters are adjusted to attain
23 acceptable levels of agreement (discussed further below).

24 The annual water balance specifies the ultimate destination of incoming precipitation and is
25 indicated as:

$$\begin{aligned} 26 \quad & \textbf{Precipitation - Actual Evapotranspiration - Deep Percolation} \\ 27 \quad & \textbf{- DSoil Moisture = Runoff} \end{aligned}$$

1
2 HSPF requires input precipitation and potential evapotranspiration (PET), which effectively
3 “drive” the hydrology of the watershed; actual evapotranspiration is calculated by the model
4 from the input potential and ambient soil moisture conditions. Thus, both inputs must be
5 accurate and representative of the watershed conditions; it is often necessary to adjust the input
6 data derived from neighboring stations that may be some distance away in order to reflect
7 conditions on the watershed. HSPF allows the use of factors (referred to as MFACT) that
8 uniformly adjust the input data to watershed conditions, based on local isohyetal and evaporation
9 patterns. The MFD describes the numerous rainfall stations available within and surrounding the
10 Housatonic River watershed, whereas evaporation will need to be estimated from data collected
11 at Hartford and Albany. Fortunately, evaporation does not vary as greatly with distance, and use
12 of evaporation data from distant stations (e.g., 50 to 100 miles away) is common practice.

13 In addition to the input meteorologic data series, the critical parameters that govern the annual
14 water balance are as follows (see MFD Appendix B for complete list of HSPF parameters):

- 15 LZSN - lower zone soil moisture storage (inches).
- 16 LZETP - vegetation evapotranspiration index (dimensionless).
- 17 INFILT - infiltration index for division of surface and subsurface flow (inches/hour).
- 18 UZSN - upper zone soil moisture storage (inches).
- 19 DEEPFR - fraction of groundwater inflow to deep recharge (dimensionless).

20
21 Thus, from the water balance equation, if precipitation is measured on the watershed, and if deep
22 percolation to groundwater is small or negligible, actual evapotranspiration must be adjusted to
23 cause a change in the long-term runoff component of the water balance. Changes in LZSN and
24 LZETP affect the actual evapotranspiration by making more or less moisture available to
25 evaporate or transpire. Both LZSN and INFILT also have a major impact on percolation and are
26 important in obtaining an annual water balance. In addition, on extremely small watersheds (less
27 than 200 to 500 acres) that contribute runoff only during and immediately following storm
28 events, the UZSN parameter can also affect annual runoff volumes because of its impact on
29 individual storm events (described below). Whenever there are losses to deep groundwater, such
30 as recharge, or subsurface flow not measured at the flow gage, DEEPFR is used to represent this
31 loss from the annual water balance.

1 In the next step in hydrologic calibration, after an annual water balance is obtained, the seasonal
2 or monthly distribution of runoff can be adjusted with use of INFILT, the infiltration parameter
3 defined above. This seasonal distribution is accomplished by INFILT by dividing the incoming
4 moisture among surface runoff, interflow, upper zone soil moisture storage, and percolation to
5 lower zone soil moisture and groundwater storage. Increasing INFILT will reduce immediate
6 surface runoff (including interflow) and increase the groundwater component; decreasing
7 INFILT will produce the opposite result.

8 The focus of the next stage in calibration is the baseflow component. This portion of the flow is
9 often adjusted in conjunction with the seasonal/monthly flow calibration (previous step) because
10 moving runoff volume between seasons often means transferring the surface runoff from storm
11 events in wet seasons to low-flow periods during dry seasons. By increasing INFILT, runoff is
12 delayed and occurs later in the year as an increased groundwater or baseflow. The shape of the
13 groundwater recession; i.e., the change in baseflow discharge, is controlled by the following
14 parameters:

15 AGWRC - groundwater recession rate (per day).
16 KVARY - index for nonlinear groundwater recession.

17
18 AGWRC is calculated as the rate of baseflow (i.e., groundwater discharge to the stream) on one
19 day divided by the baseflow on the previous day; thus AGWRC is the parameter that controls the
20 rate of outflow from the groundwater storage. Using hydrograph separation techniques, values
21 of AGWRC are often calculated as the slope of the receding baseflow portion of the hydrograph;
22 these initial values are then adjusted as needed through calibration. The KVARY index allows
23 users to impose a nonlinear recession that so that the slope can be adjusted as a function of the
24 groundwater gradient. KVARY is usually set to zero unless the observed flow record shows a
25 definite change in the recession rate (i.e., slope) as a function of wet and dry seasons.

26 In the final stage of hydrologic calibration, after an acceptable agreement has been attained for
27 annual/monthly volumes and baseflow conditions, simulated hydrographs for selected storm
28 events can be effectively altered with UZSN and the following parameters:

29 INTFW - Interflow inflow parameter (dimensionless).
30 IRC - Interflow recession rate (per day).

1
2 Both INTFW and IRC are used to adjust the shape of the hydrograph to better agree with
3 observed values; both parameters are evaluated primarily from past experience and modeling
4 studies, and then adjusted in calibration. Also, minor adjustments to the INFILT parameter can
5 be used to improve simulated hydrographs; however, adjustments to INFILT should be minimal
6 to prevent disruption of the established annual and monthly water balance. Examination of both
7 daily and short-time interval (e.g., hourly) flows may be included, depending on the purpose of
8 the study and the available data. Because of the complex sinuosity of the mainstem of the
9 Housatonic River and the extensive floodplain, HSPF will focus on simulation of daily and
10 monthly flows, whereas the complex hydrodynamics of the mainstem will be modeled by EFDC.

11 In recent years, the hydrology calibration process has been facilitated with the aide of HSPEXP,
12 an expert system for hydrologic calibration, specifically designed for use with HSPF, developed
13 under contract for the U.S. Geological Survey (Lumb, et al., 1994). This package gives
14 calibration advice, such as which model parameters to adjust and/or input to check, based on
15 predetermined rules, and allows the user to interactively modify the HSPF Users Control Input
16 (UCI) files, make model runs, examine statistics, and generate a variety of plots.

17 **4.5.2 Hydraulic Calibration**

18 The major determinants of the routed flows simulated by section HYDR are the hydrology
19 results from PERLND and/or IMPLND and the physical data contained in the FTABLE; i.e., the
20 stage-discharge function used for hydraulic routing in each reach. The FTABLE specifies values
21 for surface area, reach volume, and discharge for a series of selected average depths of water in
22 each reach. This information is part of the required User's Control Input for section HYDR and
23 is obtained from cross-section data, channel characteristics (e.g., length, slope, roughness), and
24 flow calculations. Since the FTABLE is an approximation of the stage-discharge-volume
25 relationship for relatively long reaches, calibration of the values in the FTABLE is generally not
26 needed. Since the focus in the Housatonic will be simulation of daily and monthly flows, these
27 outputs will not be very sensitive to the FTABLE values and no calibration is expected.
28 However, if flows and storage volumes at high-flow conditions appear to be incorrect, some

1 adjustment may be needed; the hydrodynamics simulated by EFDC may be used, if needed, to
2 refine the FTABLEs (see model linkage discussion below).

3 **4.5.3 Snow Calibration and Key Calibration Parameters**

4 Since snow accumulation and melt is an important component of streamflow in the Housatonic
5 River watershed, accurate simulation of snow depths and melt processes is needed to
6 successfully model the hydrologic behavior of the watershed. Snow calibration, using module
7 section SNOW, is actually part of the hydrologic calibration. It is usually performed during the
8 initial phase of the hydrologic calibration since the snow simulation can impact not only winter
9 runoff volumes, but also spring and early summer streamflow.

10 Simulation of snow accumulation and melt processes suffers from two main sources of user-
11 controlled uncertainty: representative meteorologic input data and parameter estimation. The
12 additional meteorologic time series data required for snow simulation (i.e., air temperature, solar
13 radiation, wind, and dewpoint temperature) are not often available in the immediate vicinity of
14 the watershed, and consequently must be estimated or extrapolated from the nearest available
15 weather station. As discussed in the MFD, Hartford and Albany are the primary meteorologic
16 data stations that will be used for the Housatonic River Watershed, supplemented by recent data
17 collected by GE for the Pittsfield area. Snowmelt simulation is especially sensitive to the air
18 temperature and solar radiation time series since these are the major driving forces for the energy
19 balance melt calculations. Fortunately, additional nearby stations are available with air
20 temperature data. The MFACT parameter, noted above, is used to adjust each of the required
21 input meteorologic data to more closely represent conditions on the watershed; also, the model
22 allows an internal correction for air temperature as a function of elevation, using a “lapse” rate
23 that specifies the change in temperature for any elevation difference between the watershed and
24 the temperature gage.

25 In most applications, the primary goal of the snow simulation will be to adequately represent the
26 total volume and relative timing of snowmelt to produce reasonable soil moisture conditions in
27 the spring and early summer so that subsequent rainfall events can be accurately simulated.
28 Where observed snow depth (and water equivalent) measurements are available, comparisons
29 with simulated values are made. However, a tremendous variation in observed snow depth

1 values can occur in a watershed, as a function of elevation, exposure, topography, etc. Thus a
2 single observation point or location will not always be representative of the watershed average.
3 For the Housatonic, snow depth data from Hartford and Albany will be used, supplemented with
4 any additional local data.

5 The primary SNOW parameters adjusted in calibration are the following:

- 6 TSNOW - Temperature at which precipitation becomes snow (degrees F)
- 7 SNOWCF - Snow catch correction factor for precipitation gage (dimensionless)
- 8 CCFACT - Condensation/convection melt correction factor (dimensionless)
- 9 MGMELT - Daily melt factor for ground heat (inches/day)
- 10 MWATER - Liquid water storage capacity in snowpack (dimensionless)

11
12 TSNOW is used to ensure that the form of the precipitation, i.e., rain or snow, is correctly
13 assumed in the model for the majority of events in the simulation period. Since the form of the
14 precipitation will obviously have a controlling impact on the hydrologic response of each storm
15 event, TSNOW can be adjusted within a few degrees of freezing to improve the agreement with
16 observations.

17 SNOWCF is used to account for deficiencies in the accuracy of rain gages to accurately measure
18 snow fall. Traditional precipitation gages, even when equipped with snow windshields, can
19 underestimate snowfall amounts by 50% or more depending on wind conditions (Linsley et al.,
20 1975). This type of error can have major impacts on the simulation.

21 CCFACT is a factor that adjusts the theoretical condensation and convection melt equations in
22 the model to adjust for field conditions; it is often used to adjust the timing of melt events by
23 increasing or decreasing the rate of melt.

24 MGMELT is a daily melt factor that provides for a constant rate of melt due to sources of heat
25 other than through normal meteorologic conditions, such as ground thermal gradients buildings
26 and urban areas, geothermal sources, etc.

27 MWATER defines the liquid water storage capacity available in the snow pack, to reflect the
28 ability of the snow to store liquid water, within the crystal structure of the pack, up to a certain
29 limit before it releases the melt water to the land surface. This phenomenon contributes to

1 observed occurrences of dramatic releases of snowmelt during short melt periods in the middle
2 of winter and near the end of a winter season.

3 In many instances it is difficult to determine if problems in the snow simulation are due to the
4 nonrepresentative meteorologic data or inaccurate parameter values. Consequently the accuracy
5 expectations and general objectives of snow calibration are not as rigorous as for the overall
6 hydrologic calibration. Comparisons of simulated weekly and monthly runoff volumes with
7 observed streamflow during snowmelt periods, and observed snow depth (and water equivalent)
8 values are the primary procedures followed for snow calibration. Day-to-day variations and
9 comparisons on shorter intervals (i.e., 2-hour, 4-hour, 6-hour, etc.) are usually not as important
10 as representing the overall snowmelt volume and relative timing in the observed weekly or bi-
11 weekly period.

12 **4.5.4 Specific Comparisons To Be Performed - Hydrology**

13 As discussed in the MFD, hydrologic calibration will be performed for the time period of 1991 to
14 2000, whereas the period of 1979 to 2000 will be used for validation. The available flow data
15 include continuous flow records at the USGS gage sites at Coltsville and Great Barrington for
16 the entire time period, along with recent flow monitoring performed for 10 selected storm events
17 during 1999 at both tributary and mainstem sites. Since the 1999 period is the only tributary data
18 available, it was included in the calibration period to provide the most complete data set
19 available. In addition, since the nonpoint calibration will use this data, it is imperative to have
20 the most comprehensive data for calibration.

21 The same comparisons will be performed for both the calibration and validation periods.
22 Following the steps discussed above, the following specific comparisons of simulated and
23 observed values will be performed:

24 For the Coltsville and Great Barrington gage sites:

- 25 Annual and monthly runoff volumes (inches)
- 26 Daily time series of flow (cfs)
- 27 Flow frequency (flow duration) curves (cfs)

28
29 At tributary and mainstem monitoring sites:

1 Storm hydrographs (flow, cfs) for selected storm events in 1999

2 Additional comparisons:

3 Snow depth for selected land uses with available data at Hartford and Albany

4
5 In addition to the above comparisons, the water balance components (input and simulated) will
6 be reviewed for consistency with expected literature values for the Housatonic Region (e.g.,
7 Bent, 1999). This effort involves displaying model results for individual land uses for the
8 following water balance components:

9 Precipitation

10 Total Runoff (sum of following components)

11 Overland flow

12 Interflow

13 Baseflow

14

15 Total Actual Evapotranspiration (ET) (sum of following components)

16 Interception ET

17 Upper zone ET

18 Lower zone ET

19 Baseflow ET

20 Active groundwater ET

21

22 Deep Groundwater Recharge/Losses

23

24 Although observed values are not be available for each of the water balance components listed
25 above, the average annual values must be consistent with expected values for the region, as
26 impacted by the individual land use categories. This is a separate consistency, or reality, check
27 with data independent of the modeling (except for precipitation) to insure that land use categories
28 and overall water balance reflect local conditions in the Housatonic Basin.

29 **4.5.5 Sediment Erosion Calibration and Key Calibration Parameters**

30 Sediment calibration follows the hydrologic calibration and must precede water quality
31 calibration. Calibration of the parameters involved in simulation of watershed sediment erosion
32 is more uncertain than hydrologic calibration due to less experience with sediment simulation in

1 different regions of the country. The process is analogous; the major sediment parameters are
2 modified to increase agreement between simulated and recorded monthly sediment loss and
3 storm event sediment removal. However, observed monthly sediment loss is often not available,
4 and the sediment calibration parameters are not as distinctly separated between those that affect
5 monthly sediment and those that control storm sediment loss. In fact, annual sediment losses are
6 often the result of only a few major storms during the year.

7 Sediment loadings to the stream channel are estimated by land use category from literature data,
8 local Extension Service sources, or procedures like the Universal Soil Loss Equation (USLE)
9 (Wischmeier and Smith, 1978) and then adjusted for delivery to the stream with estimated
10 sediment delivery ratios. Model parameters are then adjusted so that model calculated loadings
11 are consistent with these estimated loading ranges. The loadings are further evaluated in
12 conjunction with instream sediment transport calibration (discussed below) that extend to a point
13 in the watershed where sediment concentration data is available. The objective is to represent
14 the overall sediment behavior of the watershed, with knowledge of the morphological
15 characteristics of the stream (i.e., aggrading or degrading behavior), using sediment loading rates
16 that are consistent with available values and providing a reasonable match with instream
17 sediment data.

18 In HSPF, the erosion process is represented as the net result of detachment of soil particles by
19 raindrop impact on the land surface, and then subsequent transport of these fine particles by
20 overland flow. The primary sediment erosion parameters are as follows:

- 21 KRER - Coefficient in soil detachment equation.
- 22 KSER - Coefficient in sediment washoff equation.

23
24 Although a number of additional parameters are involved in sediment erosion calibration, such as
25 those related to vegetal cover, agricultural practices, rainfall and overland flow intensity, etc.,
26 KRER and KSER are the primary ones controlling sediment loading rates. KRER is usually
27 estimated as equal to the erodibility factor, K, in the USLE (noted above), and then adjusted in
28 calibration, while KSER is primarily evaluated through calibration and past experience. The
29 calibrated parameter information within the HSPFParm database will provide a source of
30 information for initial parameter values.

1 **4.5.6 Specific Comparisons To Be Performed - Sediment Loadings**

2 The sediment erosion calibration period will coincide with the hydrology calibration and extend
3 from 1991 through 2000; the available historical data prior to 1991 will be reserved for
4 validation. The primary focus of the calibration will be the 1999 stormwater monitoring data
5 collected by EPA during 10 storm events. This is the most comprehensive dataset available for
6 storm runoff, including both tributary and mainstem sampling. Observed storm concentrations
7 of TSS will be compared with model results, and the sediment loading rates by land use category
8 will be compared with the expected ranges, as noted above. Over the calibration period, the
9 comparison locations will include Coltsville (Hubbard Avenue) and Great Barrington for
10 selected time periods in 1991 and 1995-2000; for 1999, the calibration sites will also include the
11 sampled tributary sites on Unkamet Brook, West Branch, Sackett Brook, and Roaring Brook,
12 along with the mainstem sites at Coltsville (Hubbard Avenue), Pomeroy Avenue, New Lenox
13 Road, and Woods Pond. These mainstem sites will serve primarily as consistency checks of the
14 overall sediment budgets and loading rates.

15 **4.5.7 Nonpoint Source Calibration and Key Calibration Parameters**

16 Calibration procedures and parameters for simulation of nonpoint source pollutants will vary
17 depending on whether constituents are modeled as sediment-associated or flow-associated. This
18 refers to whether the loads are calculated as a function of sediment loadings or as a function of
19 the overland flow rate. For linkage with both EFDC and AQUATOX, nonpoint source loads will
20 be provided for DO, BOD, NO_x, NH₄, and PO₄. Because of their affinity for sediment, PCBs and
21 PO₄ will be modeled as sediment-associated, and DO, BOD, NO_x, and NH₄ will be modeled as
22 flow-associated.

23 Calibration of sediment-associated pollutants begins after a satisfactory calibration of sediment
24 washoff has been completed. At this point, adjustments are performed in the contaminant
25 potency factors, which are user-specified parameters for each contaminant, defined as follows:

- 26 POTFW - mass of pollutant per mass of sediment washoff (lb pollutant/100 lb
27 sediment)
28 POTFS - mass of pollutant per mass of sediment scour (lb pollutant/100 lb
29 sediment)

1
2 Potency factors are used primarily for highly sorptive contaminants that can be assumed to be
3 transported with the sediment in the runoff. Generally, monthly and annual contaminant loss
4 will not be available, so the potency factors will be adjusted by comparing simulated and
5 recorded contaminant concentrations, or mass removal, for selected storm events. For nonpoint
6 pollution, mass removal in terms of contaminant mass per unit time (e.g., gm/min) is often more
7 indicative of the washoff and scour mechanisms than instantaneous observed contaminant
8 concentrations.

9 Calibration procedures for simulation of contaminants associated with overland flow are focused
10 on the adjustment of following three key parameters:

- 11 ACQOP - the daily accumulation rate (lb/acre/day).
- 12 SQOLIM - the maximum contaminant storage on the land surface (lb/acre).
- 13 WSQOP - the washoff factor parameter (in/hr) which is the runoff intensity that
14 produces 90% removal in 1 hour.

15
16 As was the case for sediment-associated constituents, calibration is performed by comparing
17 simulated and recorded contaminant concentrations, or mass removal, for selected storm events.

18 In most cases, proper adjustment of SQOLIM, WSQOP, and ACQOP can be accomplished to
19 provide a good representation of the washoff of flow-associated constituents; the HSPF
20 Application Guide (Donigian et al., 1984) includes guidelines for calibration of these parameters,
21 and the HSPFParm Database includes representative values for selected model applications for
22 most conventional constituents.

23 In areas where pollutant contributions are also associated with subsurface flows, such as BOD or
24 nitrate from agricultural croplands, contaminant concentration values are assigned for both
25 interflow and active groundwater. The key parameters are simply the user-defined
26 concentrations in interflow and groundwater/baseflow for each contaminant, as follows:

- 27 IOQC - Concentration of contaminant in interflow discharge (mg/L).
- 28 AOQC - Concentration of contaminant in groundwater discharge (mg/L).

29
30 HSPF includes the functionality to allow monthly values for all these nonpoint loading
31 parameters in order to better represent seasonal variations in the resulting loading rates.

1 **4.5.8 Specific Comparisons to be Performed - Nonpoint Loadings**

2 The nonpoint loading calibration will be performed in a manner directly analogous to the
3 sediment loading calibration. The calibration period will be 1996 through 2000, with the major
4 focus on the 1999 stormwater monitoring data collected by EPA for 10 storm events. The
5 historical data in the period from 1979 through 2000 will be used for validation. Observed
6 stormwater concentrations for each contaminant will be compared with model results, and for the
7 conventional pollutants (e.g., BOD, ammonia, nitrate, phosphate) the loading rates by land use
8 category will be compared with the expected ranges available from the literature and past
9 modeling studies, in a manner analogous to the sediment loading calibration. The same locations
10 as listed above for the sediment calibration will be used.

11 **4.5.9 Instream Sediment and Water Quality Calibration**

12 Instream HSPF water quality calibration procedures for sediment and other constituents are
13 discussed in the HSPF Application Guide and other model application references noted above;
14 these procedures are not discussed further here because in this study HSPF is being used
15 primarily as the watershed model to provide the nonpoint loadings to EFDC and AQUATOX.
16 The HSPF instream water quality simulation will be a means to confirm the calculated nonpoint
17 loadings, and serve as a consistency check with the observed water quality data.

18 **4.6 EFDC CALIBRATION AND VALIDATION PROCEDURES**

19 EFDC will be calibrated and validated using independent data sets selected to represent a range
20 of flow regimes from low-flow to high-flow conditions. EFDC will be calibrated using data sets
21 collected from 1999 to 2000. With a set of model parameter values calibrated to result in the
22 best agreement between the model and observed data, EFDC will then be validated using an
23 independent data set collected from 1979 through 2000. The validation of EFDC, based on this
24 continuous long-term simulation, will seek to replicate long-term trends in PCB levels measured
25 in the water column and sediment cores, sedimentation rates and sediment accumulation
26 observed in Woods Pond.

1 **4.6.1 Specific Comparisons To Be Performed**

2 Because a large component of annual solids loading, transport, deposition, and resuspension in
3 the river typically occurs only during a few episodic high-flow events, the emphasis in
4 calibration of EFDC will be on high-flow events. Based on 84 years (1914-97) of daily
5 historical records of streamflow measured at the USGS gage at Great Barrington, MA, the
6 median flow for the Housatonic River is 335 cfs with 90% of the daily flow records less than
7 1,160 cfs. Extreme high flows were recorded at Great Barrington in 1949 (11,101 cfs), 1938
8 (11,000 cfs) and 1984 (9,940 cfs) with the 1984 peak flow almost matching the 100-year flood
9 condition of 10,603 cfs. Calibration of EFDC will be based on data sets collected from 1999
10 through 2000. During this period, detailed data sets are available to characterize high-flow
11 events for 10 storm events from May through September 1999.

12 With only the boundary conditions changed to account for changes in external loading for flow,
13 suspended solids, PCBs, and climatological conditions, EFDC will be validated using historical
14 data sets collected from 1979 to 2000. The continuous long-term simulation from 1979 to 2000
15 will be the most technically demanding test of the model.

16 **4.6.1.1 Hydrodynamics**

17 In the Housatonic River, physical transport is controlled by the inflow of freshwater from the
18 upstream boundaries of the East and West Branches of the Housatonic River and its tributaries,
19 the cross section and channel slope of the river channel, bathymetry of the backwater areas and
20 Woods Pond, and bed-related bottom friction. Under flood conditions, the topography and
21 vegetation cover of the adjacent floodplain also control flow in the river-floodplain system.

22 Calibration and validation of the hydrodynamic model will be based on a comparison of EFDC
23 results to observed data sets averaged over the relevant time scales for the following parameters:

- 24 ▪ Stage height and velocity during storm events (hourly).
- 25 ▪ Water temperature (daily).
- 26 ▪ Overbank flow during floodplain inundation (storm event basis).

27
28 **Stage Height**—For the hydrodynamic model, observations of river stage height (as water
29 column depth) over a range of flows will be used as the key state variable to evaluate the ability

1 of the model to accurately represent transport processes in the Housatonic River and Woods
2 Pond. Acoustic Doppler Current Profiler (ADCP) observations of velocity recorded in the Test
3 Reach and manual observations of velocity recorded at the primary stations during 2000 will also
4 be used to check the ability of the model to represent velocity characteristics of the river as part
5 of model calibration. Time series measurements of stage height, collected during the high-flow
6 period of March to May 1997 and for 10 storm events during May through October 1999 and
7 other measurements during 2000, are available for a number of station locations within the PSA.
8 During the onset and cessation of streamflow during storm events, observed stage height records
9 will be compared to simulated stage height data at time intervals of 1 hour for calibration (1999
10 to 2000) and validation (March to May 1997) of the hydrodynamic model. For the decadal scale
11 long-term validation of the hydrodynamic model (1979 to 2000), stage height records are not
12 available except for the periods of March to May 1997 and May to October 1999 described
13 above for calibration and validation. For the long-term simulation, observed and simulated stage
14 height records will be averaged over a daily time scale for the limited model-data comparison
15 that will be possible only for the 1997 and 1999 to 2000 data sets.

16 **Water Temperature**—Spatial, vertical, and temporal observed distributions of water
17 temperature (as degrees Celsius), collected during the March to May 1997 high-flow period and
18 10 storm events of 1999 and other measurements during 2000 will be compared to simulated
19 water temperature in the river channel, backwater areas, and Woods Pond for model calibration
20 (1999-2000) and validation (1997). Observed and simulated water temperature data will be
21 averaged at daily time scales for model-data comparison. In Woods Pond, wind mixing, incident
22 solar radiation, and seasonal ice cover are important factors driving the heat balance simulation
23 of water temperature. Model-data comparison of measured and simulated vertical temperature
24 profiles and surface to bottom temperature gradients in the “deep hole” of Woods Pond will be
25 used to evaluate the accuracy of the model simulation of the seasonal onset and breakdown of
26 vertical stratification. For the decadal scale validation of the hydrodynamic model (1979 to
27 2000), water temperature records are not available except for the periods of March to May 1997
28 and May to October 1999 described above for calibration and validation. For the long-term
29 simulation, observed and simulated water temperature records will be averaged over a daily time
30 scale for graphical model-data comparison.

1 **Overbank Flow**—The ability of the hydrodynamic model to represent overbank flow during
2 inundation of the floodplain will be qualitatively checked using aerial photographs of flood
3 conditions as part of the model validation for the period 1979 to 2000. Maps delineating the
4 spatial penetration of simulated flow onto the floodplain will be compared to aerial photographs
5 that recorded overbank flow in the floodplain during flood conditions in August 1990.

6 **4.6.1.2 Sediment Transport**

7 In the Housatonic River, sediment transport is controlled by the external loading of solids from
8 the watershed, slumping and erosion of banks along the river channel, episodic flooding and
9 deposition of solids onto the floodplain, and settling and resuspension of solids within the river
10 channel, backwater areas, and Woods Pond. The external loading of solids to the river, in turn, is
11 controlled by precipitation, water runoff, soil characteristics, topography, land uses, and erosion
12 over the watershed. External loading of the cohesive (<63 microns) and noncohesive (63-250
13 microns and >250 microns) classes that will be represented in the sediment transport model will
14 be provided as total suspended solids by the calibrated watershed model (HSPF). In the
15 sediment transport model, the processes of settling, deposition, and resuspension of solids
16 control the transport and fate of solids in the river. These processes, in turn, are controlled by
17 hydrodynamics (bottom shear stress) and the physical characteristics of solids such as the
18 effective diameter, specific gravity, settling velocity, and shear strength of the sediment bed.

19 Calibration and validation of the sediment transport model will be based on comparison of EFDC
20 results averaged over the relevant time scales for the following four data sets:

- 21 ▪ Water column TSS concentrations during storm events (hourly).
- 22 ▪ Mass balance of solids within primary study area (event basis).
- 23 ▪ Areas of deposition and erosion (event basis; decadal).
- 24 ▪ Long-term sediment accumulation rates (decadal).

25
26 **Water Column TSS**—The sediment transport model will be calibrated and validated by model-
27 data comparison of observed and simulated water column concentrations of TSS as :

- 28 ▪ Time series for specific station locations and model grid cells aggregated within
29 reaches of the river.

- 1 ▪ Spatial distributions from the confluence of the East and West Branches of the
2 Housatonic River to the Woods Pond Dam time averaged by month/season and/or
3 flow regime.

4 High-resolution time series measurements of TSS, collected during the high-flow period of
5 March to May 1997 and for 10 storm events during May through October 1999 and other
6 measurements during 2000, are available for a number of station locations within the PSA.
7 During the onset and cessation of streamflow during storm events, observed and simulated TSS
8 concentrations will be compared at time intervals of 1 hour for calibration (1999 to 2000) and
9 validation (March to May 1997) of the sediment transport model. For the decadal scale
10 validation of the sediment transport model (1979 to 2000), TSS records are available for 1979-
11 80, 1991, and 1995-1999. For the long-term simulation (1979 to 2000), time series of observed
12 and simulated TSS records will be averaged over a weekly/monthly time scale for model-data
13 comparison.

14 Model-data comparisons will also be compiled to evaluate the spatial distribution of TSS along
15 the Housatonic River. To provide a consistent basis for model-data comparisons, both observed
16 TSS data and model results will be time-averaged over time scales that will be defined by flow
17 regimes (e.g., high flow; low flow). Separation of model-data comparisons by time-averaging
18 over comparable flow regime periods is essential so that data from low-flow periods do not
19 confound the evaluation of data collected during high-flow periods, for example. For the long-
20 term validation, observed and simulated TSS records will be averaged over monthly/seasonal/
21 flow regime time scales for meaningful model-data comparisons of the spatial distribution in the
22 river.

23 As noted by QEA (1998a), however, large changes in parameter values for deposition and
24 resuspension processes may result in only small changes in water column TSS concentrations if
25 external solids loading is the dominant component of the solids balance. The conventional
26 model-data comparison of TSS concentrations is not solely sufficient in itself to ensure that the
27 sediment transport model is providing the correct representation of deposition and resuspension
28 fluxes in the river.

29 **Mass Balance of Solids**—Solids loads will be integrated over an event-scale time period to
30 calculate net resuspension (or deposition) as the observed balance between inputs and output

1 over the PSA for comparison to the results of the sediment transport model. Observations of
2 flow and water column TSS concentrations will define solids inputs from the East and West
3 Branches of the Housatonic River, and tributary sources and wastewater discharges and the
4 solids outflow at Woods Pond Dam. Mass balances of inputs and the outflow from Woods Pond
5 will be computed over the (a) short-term simulation time scale (~2 to 3 months) and the (b)
6 storm event time scale (~3 to 5 days) to compare the mean and peak fluxes computed from the
7 observations and the model results. The short-term tests of the sediment transport model for
8 calibration (1999 to 2000) and validation (1997) of the model will ensure that the formulations
9 and parameter values used to represent deposition and resuspension processes are accurately
10 characterized, in an overall global sense, for the Housatonic River.

11 **Areas of Deposition and Erosion**—To assist in evaluation of the accuracy of the sediment
12 transport model simulation of spatially variable depositional or erosional areas, sediment bed
13 grain size data and geomorphology information has been collected for a number of cross sections
14 in the river for this study. This information will be used to qualitatively define areas of net
15 erosion and deposition and dynamic equilibrium in the sediment bed. Maps of depositional and
16 erosional areas simulated by EFDC will be qualitatively compared to the maps of areas of
17 deposition and erosion and equilibrium identified by the sediment bed maps and geomorphology
18 survey data. Because the inferred patterns of deposition and erosion identified by bed
19 geomorphological characteristics tend to reflect the long-term integration of sediment transport
20 processes in the river, the observed patterns of deposition and erosion will be compared to the
21 model results of the long-term validation from 1979 to 2000. Deposition and erosion fluxes
22 computed by the model will be time-averaged over annual and decadal time scales to
23 characterize the spatial distribution of these processes. Successful comparison of the model
24 results of the long-term decadal scale simulation with the inferred patterns of erosion and
25 deposition identified from the bed geomorphology survey will add considerable validity to the
26 sediment transport component of the model.

27 **Long-Term Sediment Accumulation Rates**—Sediment cores have been collected and dated
28 using Cs-137 techniques to estimate sediment accumulation rates in Woods Pond and backwater
29 areas of the river channel. In addition to the model versus data comparisons described above, net
30 deposition rates simulated with the sediment transport model for the calibration (1999 to 2000)

1 and validation (1979 to 2000) periods will be compared to sediment accumulation rates
2 estimated from sediment core measurements. For the long-term validation, the time series of
3 simulated net deposition rates in Woods Pond and the backwater areas will be averaged over a
4 relatively long time scale to reflect the slow time scale of depositional processes in the
5 Housatonic River system. The time scale will be consistent with estimates of the net sediment
6 accumulation rate in Woods Pond and the corresponding time scale required to accumulate the
7 thickness of the surface sediment layer assigned in the sediment transport model.

8 Sediment core dating methods are based on the assumption that the uniform deposition of a
9 tracer (e.g., Cs-137) onto the surface of a large body of open water controls the deposition of the
10 tracer in a sediment core. In a watershed such as the Housatonic River, uncertainty is introduced
11 into the estimation of the net sediment accumulation rate since the tracer in the sediment bed is
12 introduced directly by atmospheric deposition onto the surface of Woods Pond and indirectly via
13 deposition on the land surface of the watershed and subsequent surface runoff. This uncertainty
14 will be considered in comparing model results with observed estimates of the net sediment
15 accumulation rate for Woods Pond.

16 **4.6.1.3 Abiotic PCBs**

17 In the Housatonic River, the transport and fate of abiotic PCBs is controlled by the loading of
18 total PCBs from the source reach in Pittsfield on the East Branch (and surrounding watershed
19 area), external loading from the West Branch of the Housatonic River, resuspension and
20 deposition of PCBs sorbed onto solids, diffusive exchange across the sediment-water interface of
21 PCBs dissolved in pore water, transfer of PCBs between the solid and dissolved phases, and
22 degradation and volatilization of PCBs. In the abiotic PCB model of the Housatonic River, the
23 contributions of the source reach and watershed areas will be accounted for by the time-
24 dependent boundary conditions of total PCB loadings generated by the watershed model. PCBs
25 will be simulated in EFDC as total PCBs with the mass balance of PCBs accounted for only by
26 abiotic processes. Bioaccumulation of homologs and congeners of PCBs will be simulated in
27 AQUATOX with flow and inorganic solids loading provided by EFDC and external loading of
28 total PCBs, nutrients, and organic matter provided by HSPF.

1 Calibration and validation of the contaminant model of EFDC will be based on a comparison of
2 model results and observed total PCB concentrations averaged over the relevant time scales:

- 3 ▪ Water column concentration
 - 4 - Time series (event basis)
 - 5 - Spatial distribution (flow regime/seasonal)
- 6 ▪ Sediment bed concentration (decadal)

7
8 **Water Column PCBs**—In the water column, model-data comparisons of spatial and temporal
9 patterns of total PCB concentration will be prepared for calibration and validation of the model.

10 The abiotic PCB model will be calibrated and validated by model-data comparisons of observed
11 and simulated water column concentrations of total PCBs as:

- 12 ▪ Time series for specific station locations and grid cells aggregated within reaches of
13 the river.
- 14 ▪ Spatial distributions from the confluence of the East and West Branches of the
15 Housatonic River to the Woods Pond Dam time averaged by flow regimes.

16 Time series measurements of total PCBs, collected during 1997 and during 7 of 10 storm events
17 during May through October 1999 and other measurements collected in 2000, are available for a
18 number of station locations within the PSA. During comparable high streamflow event-scale
19 conditions, observed and simulated total PCB concentrations will be compared at time intervals
20 of 1 hour for calibration (1999 to 2000) and validation (1997) of the abiotic PCBs model. For
21 the decadal scale validation of the PCB model (1979 to 2000), total PCB records from the water
22 column are available only for 1991, and 1995 to 1999.

23 Model-data comparisons will also be compiled to evaluate the spatial distribution of total PCBs
24 in the water column. To provide a consistent basis for model-data comparisons, both observed
25 data and model results will be time-averaged over time scales defined by the flow regime and/or
26 season. The time scales used for averaging will be selected so that data from low-flow periods
27 will not be aggregated with data from high-flow periods. Under high-flow conditions (winter-
28 spring), PCBs can be introduced into the water column via scour of PCBs sorbed to particles
29 resuspended from the sediment bed. Under low-flow conditions (typically summer), scour is

1 negligible and sediment-water exchange via pore water diffusion is the primary process that
2 accounts for the mass flux of dissolved PCBs from the sediment bed to the water column. The
3 model representation of the relative significance of these processes under a range of seasonal
4 flow conditions will be tested with a range of low- to high-flow conditions recorded during the
5 calibration and validation periods of record.

6 **Sediment Bed PCBs**—In the sediment bed, spatial and temporal patterns of total PCB
7 concentration will be compared for the calibration period (1999 to 2000) and long-term
8 validation period (1979 to 2000). In the sediment bed, the spatial distribution of observed
9 surficial sediment concentrations of total PCBs will be compared to model results for the surface
10 sediment layer. Observations of vertical profiles of PCBs are available for a number of sediment
11 cores collected in depositional areas of Woods Pond and backwater regions of the river channel
12 for comparison to model results of simulated PCB sediment profiles. Particular attention will be
13 given to match the vertical resolution of the multiple sediment layers simulated in EFDC with
14 the vertical resolution of the PCB measurements reported for the sediment cores in order to allow
15 for direct comparison of the results of the long-term simulation to observed sediment core data
16 sets. Observed data and model results will be time-averaged over relatively long time scales to
17 reflect the slow time scale of net depositional processes in the river and Woods Pond. The time
18 scale assigned for averaging sediment PCB model-data comparisons will be consistent with
19 estimates of the net sediment accumulation rate in Woods Pond and the corresponding time scale
20 required to accumulate the thickness of the surface sediment layer assigned in the sediment
21 transport model.

22 **4.6.2 Key Model Calibration Parameters**

23 In developing the hydrodynamic, sediment, and contaminant transport models for the Housatonic
24 River, the input data sets used to describe the physical characteristics of the river and floodplain
25 (e.g., channel cross section, topography) and external inputs of flow, solids, and total PCB loads
26 will be compiled from site-specific data sets. Model input data are also required to describe a
27 number of physical and geochemical processes that control internal fluxes of solids (e.g.,
28 resuspension, deposition) and total PCBs (adsorption or desorption with solids) in the river. This
29 section presents the key parameters in the hydrodynamic, sediment transport, and PCB fate and

1 bioaccumulation models that will be adjusted in calibration. Appendix C in the MFD provides a
2 comprehensive list of EFDC model parameters, along with definitions, units, and data/evaluation
3 sources.

4 **4.6.2.1 Hydrodynamics**

5 The key adjustable parameter for the hydrodynamic model, the effective bottom roughness
6 coefficient, characterizes the effects of bottom friction on flow in the (a) river and (b) floodplain.
7 Parameterization of the spatially variable bottom roughness heights for the river channel will
8 take into account the dominant noncohesive and cohesive composition of the bed substrate
9 material and the channel sinuosity of the meanders. Using a method applied to the Florida
10 Everglades (Hamrick and Moustafa, 1999a, 1999b), bottom friction in the floodplain will be
11 represented by assigning spatially variable parameter values based on the relative density (i.e.,
12 sparse, moderate or thick) and the effective diameter of floodplain vegetation (e.g., grasses,
13 shrubs, and trees).

14 The key parameters that will be adjusted as spatially variable coefficients for the hydrodynamic
15 model are:

- 16 ▪ Bottom roughness coefficient in the river channel, backwater, and Woods Pond.
 - 17 ▪ Relative density of floodplain vegetation.
 - 18 ▪ Effective diameter of floodplain vegetation.
- 19

20 **4.6.2.2 Sediment Transport**

21 The hydrodynamic regime and the physical characteristics of noncohesive and cohesive solids
22 particles control settling, deposition, and resuspension processes in a river. Noncohesive solids
23 will be represented by two size classes of 63-250 microns and >250 microns. Cohesive solids
24 will be represented by a single size class <63 microns.

25 **Noncohesive Solids**—Noncohesive solids (e.g., sands) are accounted for by two classes of
26 particle sizes ranging from 63 to 250 microns and >250 microns in diameter. Using grain size
27 distribution data collected from site-specific water column and sediment bed samples in the
28 Housatonic River, effective diameters for the two classes of noncohesive solids group will be
29 assigned based on median particle diameters. Deposition of noncohesive solids is dependent on

1 the particle settling velocity and the critical Shield's stress. The critical Shield's stress, in turn, is
2 derived from the nondimensional critical Shield's parameter and particle settling velocity is
3 dependent on particle diameter. At the water column-sediment bed interface, the net
4 deposition/resuspension flux of noncohesive solids is controlled by bottom flow shear stress,
5 particle size and particle density of noncohesive solids in the surficial sediments. Three
6 empirical relationships (Smith and McLean, 1977; Van Rijn, 1984; and Garcia and Parker, 1991)
7 are available in EFDC as options to compute the near-bed equilibrium concentration and the net
8 deposition/resuspension of noncohesive solids.

9 Particle diameter, settling velocity, and the critical Shield's stress are the key parameters needed
10 for each of the three options for net deposition/resuspension in EFDC. Since functional
11 relationships have been defined to assign the settling velocity and the nondimensional critical
12 Shield's parameter based on effective particle diameter (van Rijn, 1984), particle diameter is the
13 only parameter that needs to be assigned for the two classes of the noncohesive solids model. In
14 other sediment transport models (see QEA, 1998a), the particle diameter of noncohesive solids
15 has been adjusted as a calibration parameter. Ziegler and Nisbet (1994) used the settling velocity
16 for noncohesive solids as the calibration parameter to define particle diameter.

17 The effective particle diameter, assigned as the median particle size from grain-size distribution
18 data sets, is the key parameter for noncohesive solids. Since noncohesive solids will be
19 represented as two size classes accounting for particle sizes ranging from 63 to 250 microns and
20 >250 microns, the median particle diameters determined from grain-size distributions for each
21 size class will be adjusted somewhat during model calibration to achieve the best agreement with
22 observed TSS data sets.

23 **Cohesive Solids**—Cohesive solids (silts and clays) are accounted for by particles less than 63
24 microns in diameter. The settling velocity of cohesive solids can be assigned on the basis of site-
25 specific field measurements performed in the Housatonic River. It can also be computed in
26 EFDC by selecting an empirical relationship developed for freshwater (Hwang and Mehta, 1989;
27 and Ziegler and Nisbet, 1995) that is functionally dependent on particle size, cohesive solids
28 concentration, and shear stress characteristics of the flow regime in the water column and near
29 the sediment bed. The probability of deposition of the cohesive material, used to define an

1 effective settling velocity assigned for cohesive particles, is then computed from the flow regime
2 shear stress and the critical stress for deposition (Ariathurai and Krone, 1976).

3 As a result of compaction and primary consolidation, surficial cohesive sediments typically have
4 less resistance to eroding forces than sediments deeper in the bed. For a particular flow-induced
5 bed shear stress, the mass of cohesive sediments that can be resuspended is effectively limited
6 (i.e., “armored”) by the increasing bed shear strength with depth in the bed. The time-dependent
7 nature of the bed shear strength profile of cohesive sediment beds will be accounted for in EFDC
8 by the simulation of bed formation and compaction during depositional events and the
9 subsequent primary consolidation of multiple bed layers. Using the formulations of Hwang and
10 Mehta (1989), an option can be selected in EFDC to compute the bed shear strength as a function
11 of the simulated time-dependent profile of bed bulk density.

12 The parameters needed in EFDC for the cohesive solids submodel are:

- 13 ▪ Settling velocity.
- 14 ▪ Critical shear stress for deposition.
- 15 ▪ Critical shear stress for resuspension.
- 16 ▪ Surface erosion rate.
- 17 ▪ Shear strength vertical profile of sediment bed.
- 18 ▪ Bulk density vertical profile of sediment bed.

19
20 Field data are available from Particle Entrainment Simulator (PES) (Tsai and Lick, 1986)
21 experiments in the Housatonic River (QEA, 1998b) to define the resuspension potential (or
22 surface erosion rate) of cohesive sediments under shear stresses ranging from 3 to 9 dyne cm⁻².
23 Measurements were taken in June 1997 in backwater depositional areas of Woods Pond and six
24 other dams farther downstream of Woods Pond.

25 A sediment erosion study was conducted by EPA and USACE as part of the Housatonic River
26 project during the spring of 2000, to collect both Sedflume (O’Neil et al., 1996) and PES
27 measurements. Using shear stresses ranging from ~1-100 dyne cm⁻², the Sedflume provides site-
28 specific data to define the critical erosion stress, bulk density, and shear strength as a function of
29 depth in sediment cores along the length of the river and in Woods Pond. The PES study
30 provides additional site-specific data within a smaller range of shear stress.

1 Data from the Sedflume and PES tests will be used to develop algorithms describing initiation of
2 suspension and erosion rates for Housatonic River sediments. Algorithms will relate observed
3 critical shear stresses for initiation of resuspension as a function of the measured sediment bulk
4 densities. These data will also be used to develop bulk density profiles for sediments that are
5 well consolidated and algorithms to predict bulk density profiles of consolidating sediments as a
6 function of time after deposition.

7 **4.6.2.3 Abiotic PCBs**

8 PCBs will be modeled as an abiotic constituent in EFDC. Biological processes that determine
9 the fate and bioaccumulation of PCBs will be represented in AQUATOX. Dissolved and
10 particulate phases of PCBs will be transported via advection and mixing. PCB fate in EFDC will
11 be described by partitioning for sorption and desorption between contaminants and solids, and
12 settling and resuspension of sorbed PCBs. Equilibrium partition coefficients will be assigned for
13 the water column and the sediment bed for each of the two noncohesive and the cohesive solids
14 classes. Based on a preliminary assessment of total PCBs, TSS, TOC, and grain size data in the
15 Housatonic River, a three-phase model may be required to describe the interaction of total PCBs
16 with solids.

17 In addition, EFDC contains a simple formulation that allows simulation of microbial degradation
18 and volatilization. The significance of both volatilization and degradation for assessments of the
19 fate of PCBs in the Housatonic River will be evaluated during model calibration.

20 Diffusive exchange of PCBs across the sediment-water interface, driven by the vertical gradient
21 of dissolved PCBs in the water column and pore water, can account for a significant source of
22 PCBs under low to moderate flow conditions. The depth of penetration and extent of
23 bioturbation in the sediment bed is an important sediment mixing process that can control the
24 PCB concentration in the surficial sediments. Spatially dependent vertical diffusion coefficients
25 will be derived using site-specific data and the literature and applied to define areas of (a) active
26 bioturbation and (b) negligible bioturbation.

1 Key calibration parameters for the abiotic PCB model are:

- 2 ▪ Partition coefficients for total PCBs.
- 3 ▪ Vertical diffusion coefficient in the sediment bed.

5 **4.7 AQUATOX CALIBRATION/VALIDATION PROCEDURES**

6 In keeping with established procedures (for example, Park and Collins, 1982; Connolly, 1991),
7 the calibration goal for AQUATOX is to obtain a set of parameters, consistent across model
8 segments, that are in agreement with literature and laboratory values and that reproduce the
9 observed biomass and PCB concentrations. The validation goal is to apply the model to an
10 independent set of data without changing any parameter values and reproduce the observed
11 concentrations (Collins, 1980; Park and Collins, 1982). Because it is desirable to validate over a
12 long period and the best data have been collected recently, the validation period will overlap the
13 calibration period.

14 The strategy is first to calibrate the ecosystem model and then the fate and bioaccumulation
15 model. The bioaccumulation model will then be validated with data starting 15 years earlier and
16 continuing through the calibration period (see Table 4-6 in Section 4.8 for a summary of
17 calibration/validation periods) using the same parameter values as were used in the calibration.
18 The same measures of model performance will be used for both calibration and validation.

19 Mechanistic ecosystem and bioaccumulation models are intended for application to changing
20 conditions and therefore should be general. It is important to model complex food webs because
21 of the dietary pathways of bioaccumulation, yet it is difficult to obtain site-specific data for all
22 ecosystem components. Therefore, one should look for realistic ecosystem dynamics based on
23 general principles and confirmed by those data that can be collected. It is neither reasonable nor
24 necessary to rely entirely on site-specific data; that is the advantage of using a mechanistic
25 model.

26 Proposed biotic state variables representing the complex food web of the PSA include
27 periphyton, phytoplankton, rooted macrophytes, floating filamentous algae and duckweed,
28 invertebrates (cladocerans, mayflies, snails, sphaerid clams, dragonflies, midges, oligochaetes,
29 crayfish), and fish (shiners, goldfish and carp, brown bullhead, white suckers, pumpkinseed,

1 yellow perch, and largemouth bass). Parameters are available from the literature for all these
2 variables, and AQUATOX has been used to simulate most of them in previous studies. Based on
3 initial calibration results, state variables may be added or deleted.

4 Because of its extensive application to impoundments, AQUATOX will represent the Woods
5 Pond ecosystem with little additional calibration. Application to the river ecosystem also will be
6 relatively straightforward. AQUATOX has an extensive database of parameters representing
7 many species of riverine invertebrates and fish, so that little calibration will be required. In
8 addition, the generality of the model in representing periphyton, macrophytes, various
9 invertebrates, and fish in the river will be tested using available data from other streams and
10 small rivers. In particular, published data from East Poplar Creek and Walker Branch, TN, and
11 the Little Miami River, OH, will be used to further augment the river implementation. The goal
12 is to represent the ecosystem and food web of the Housatonic River realistically so that the
13 dietary exposure and bioenergetics can be used to predict fate and bioaccumulation of PCBs.
14 Biomagnification of hydrophobic compounds such as PCBs is sensitive to the number of trophic
15 levels and to the structure of detritus-based and plant-based food webs, so it is important to
16 represent the complexity of the Housatonic biota, given the available data and general principles
17 of stream ecology.

18 The model will be calibrated to represent the PCB homologs and three or more selected
19 congeners in sufficient detail so that the selective microbial degradation and volatilization of
20 homologs and congeners can be predicted, as well as the selective bioaccumulation and
21 biotransformation by key species. The first step will be to parameterize and, as necessary,
22 modify fate and bioaccumulation formulations to best represent PCBs in the PSA. Process-level
23 equations will be tested against experimental data available in the literature. Simulations will be
24 run using newly collected PCB data, particularly congener data, from the Housatonic River.
25 Similarly, published (Hill and Napolitano, 1997) and unpublished congener data from East Fork
26 Poplar Creek, Tennessee (which is similar to the Housatonic River in several respects) will be
27 used to further refine the fate part of the model. Sensitivity analyses will be run to determine
28 which parameters have the most effect on the simulations. If a parameter is inappropriately
29 sensitive, then the formulation will be reconsidered and modified if necessary. Sensitive
30 parameters will be noted for use in uncertainty analyses in later simulations.

1 Another type of calibration will involve running the distributed version of AQUATOX in tandem
2 with the EFDC model to test and modify the hydrodynamic and sediment linkages and their
3 applicability to modeling PCB transport, sedimentation, burial, bioturbation, and resuspension.
4 This approach is discussed in Section 4.8.

5 Validation will be performed using Housatonic data starting in 1979 but with the same parameter
6 values as were used for calibration. Given the limited historical data on PCBs, and especially the
7 absence of historical congener data, this process will be based on assumptions of congener
8 distributions in Aroclors most likely released to the Housatonic River, based on the site-specific
9 data. Observed data include total PCBs in sediments and in fish. Because of long half-lives of
10 the more chlorinated PCBs in adult fish, and slow degradation rates in sediments, a long
11 simulation period (e.g., 1979 to 2000), will be used for validation.

12 **4.7.1 Specific Comparisons To Be Performed**

13 The primary goal is to reproduce the long-term total PCB concentrations and mass balance and
14 the respective concentrations (or profile) of PCB homologs and selected congeners in Housatonic
15 sediments, water, and biota in river reaches, backwater areas, and Woods Pond. Because of the
16 influence of the food web and the number of trophic levels on bioaccumulation and
17 biomagnification of PCBs, a secondary goal will be to match predicted seasonal and long-term
18 dynamics of the Housatonic River ecosystem with available biomass data and known riverine
19 ecosystem dynamics.

20 There are several measures of model performance that can be used for both calibrations and
21 validations (Bartell et al., 1992; Schnoor, 1996). The difficulty is in comparing general model
22 behavior over long periods—with rapid fluctuations due to natural occurrences such as storm
23 events and algal blooms, seasonal fluctuations, and annual variability—to observed data from a
24 few points in time. Recognizing that evaluation is limited by the quantity and quality of data,
25 stringent measures of goodness of fit are inappropriate; therefore, following the proposed
26 weight-of-evidence approach discussed in Section 4.3, a sequence of increasingly rigorous tests
27 will be used to evaluate performance and build confidence in the model results:

- 1 ▪ Reasonable behavior as demonstrated by time plots of key variables—is the model
2 behavior reasonable based on general experience with aquatic ecosystems and
3 bioaccumulation? This is highly subjective, but it may provide a level of confidence
4 in less critical aspects of the modeling, such as representation of the seasonal
5 dynamics of the riverine ecosystem. An example is given for a stream in Tennessee
6 (Figure 4-1).
- 7 ▪ Visual inspection of data points compared to model plots—do the observations and
8 predictions exhibit the same general pattern with reasonable concordance of values?
9 For example, Figure 4-2 is taken from the validation of AQUATOX with data on
10 PCB congeners from Lake Ontario (Park, 1999a); note that the patterns are similar.
- 11 ▪ Do point observations fall within predicted model bounds obtained through
12 uncertainty analysis? This has the limitation of being dependent on the precision of
13 the model; the greater the model uncertainty, the greater the possibility of the data
14 being encompassed by the error bounds. Also, do model curves fall within the error
15 bands of observed data? Where data are sufficient, “box and whisker” plots showing
16 $\pm 95\%$ confidence intervals will be used.
- 17 ▪ Regression of paired data and model results—is there bias in the model results? The
18 slope, intercept, residual error, and R^2 will indicate the degree of concordance and any
19 systematic differences. Figure 4-3 is based on the data in Figure 4-2; the R^2 is
20 excellent, but the slope and intercept indicate that there is bias in the results. This
21 suggests that additional calibration is warranted.
- 22 ▪ Comparison of means—is there a statistical difference in the mean data and mean
23 model results? Student’s *t*-test pools the variance of the two distributions to compare
24 the means; however, the assumption that the variances are the same is open to
25 question, especially with sparse observed data, so we do not anticipate using this
26 metric.
- 27 ▪ Comparison of frequency distributions—how much overlap is there between data and
28 model distributions? Two procedures will be used where appropriate:
- 29 - Relative bias (Bartell et al., 1992):

$$rB = \frac{(\overline{\text{Pred}} - \overline{\text{Obs}})}{S_{\text{obs}}}$$

31 where:

- 32 rB = relative bias (standard deviation units);
33 Pred = mean predicted value;
34 Obs = mean observed value; and
35 S_{obs} = standard deviation of observations.

36

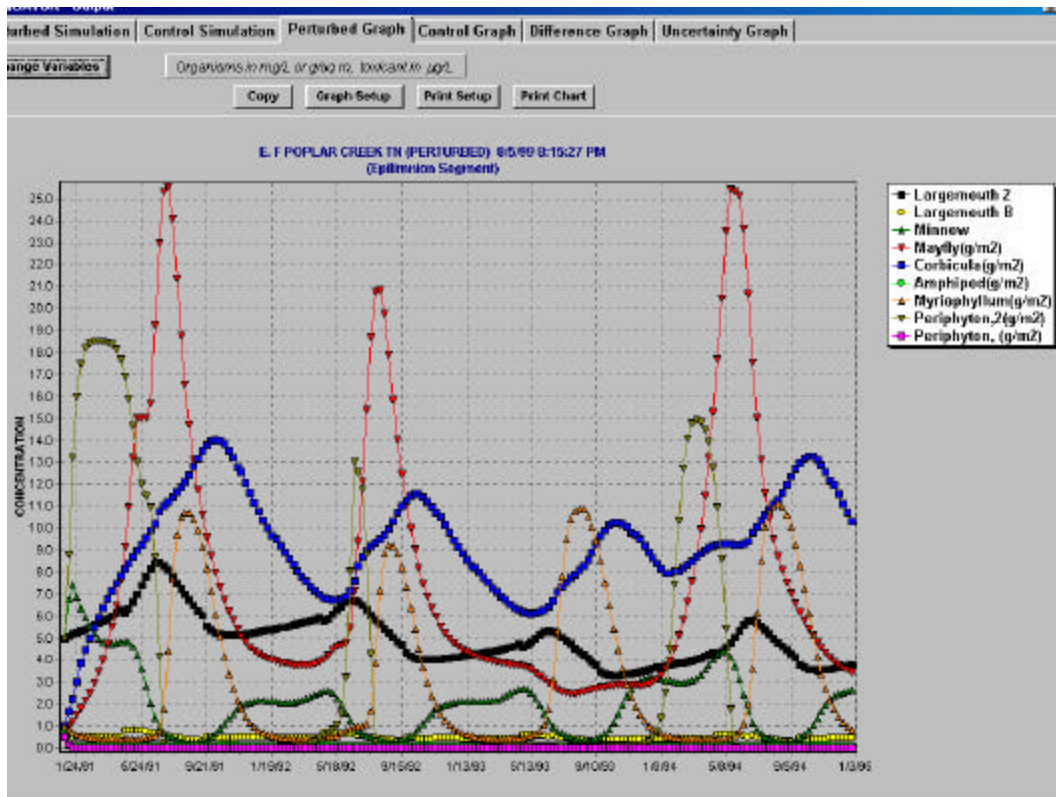


Figure 4-1 Multi-Year Simulation of East Fork Poplar Creek, TN, Showing Seasonal Fluctuations in Biomass, Especially Macrophytes, Amphipods, and Minnows

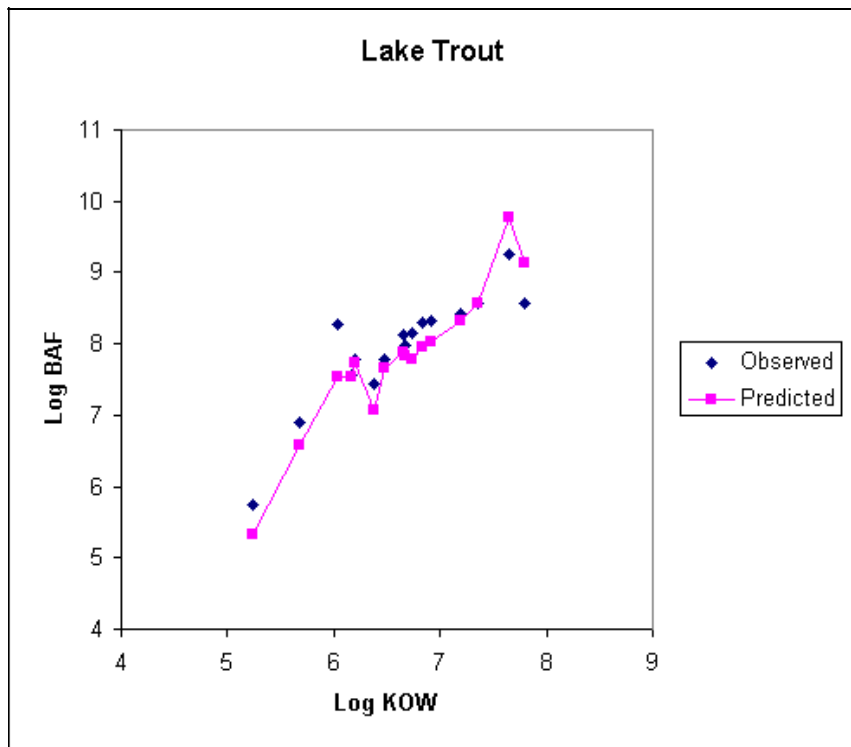


Figure 4-2 Comparison of Predicted and Observed BAFs for Lake Trout in Lake Ontario (Park, 1999a)

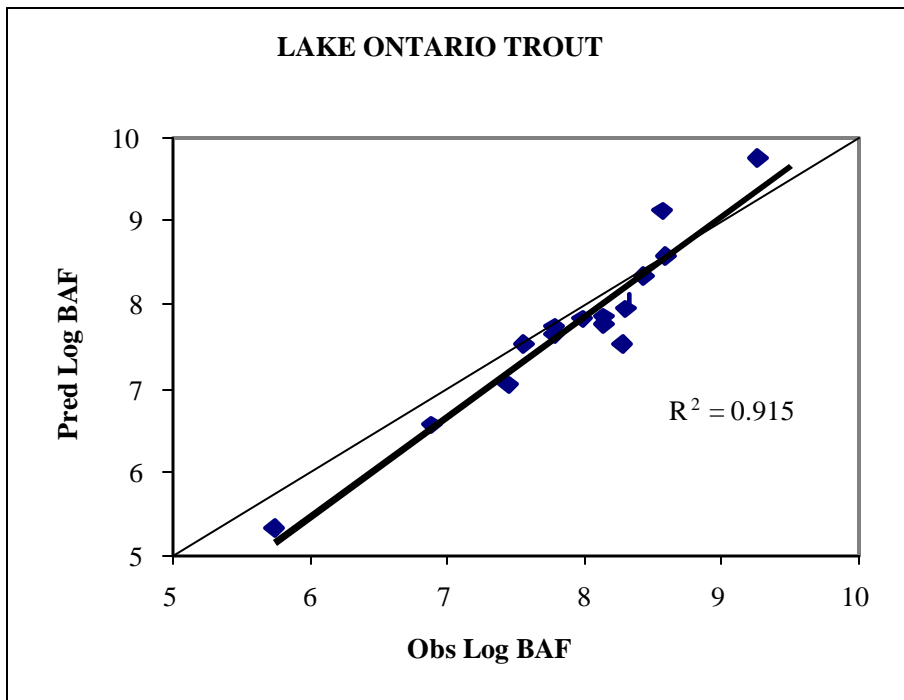


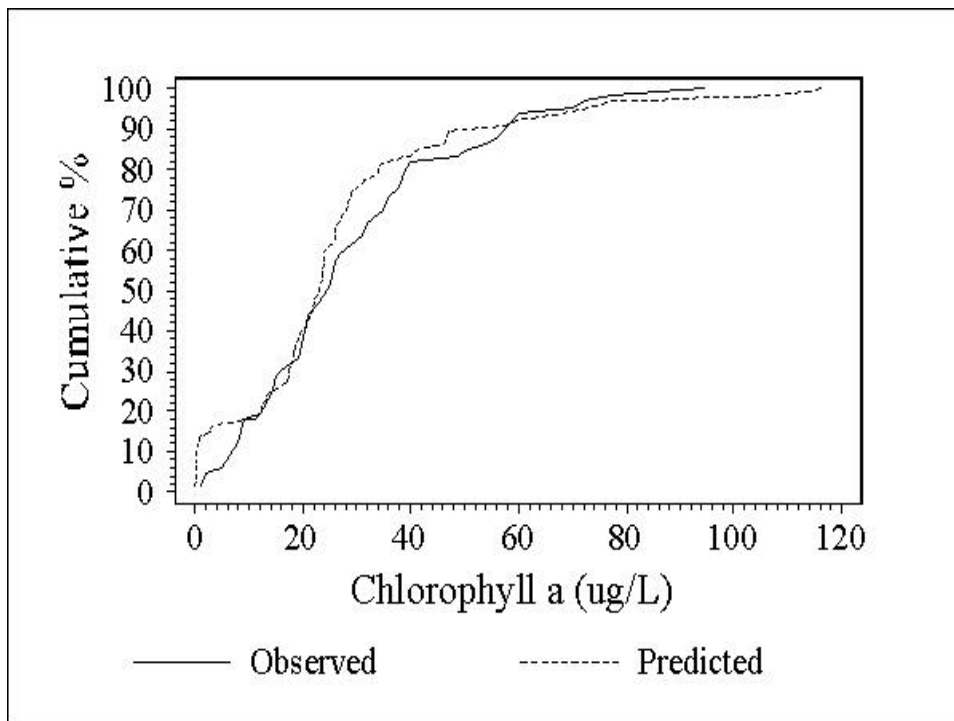
Figure 4-3 Regression of Observed and Predicted PCB Congener BAFs

1 The F test is the ratio of the variance of the model and the variance of the data.

2
$$F = \frac{S^2_{\text{pred}}}{S^2_{\text{obs}}}$$

3 Very small F values indicate that the data may be too variable to determine the goodness of fit;
4 very large F values indicate that the model is imprecise (Bartell et al., 1992). Assuming normal
5 distributions, the probability that the observed and predicted distributions are the same can be
6 evaluated. In the Lake Ontario example illustrated above, $rB = -0.195$ and $F = 2.44$, suggesting
7 that the central tendencies of the predicted and observed data are virtually identical and that the
8 probability that the two distributions are the same is rather high.

- 9
 - 10 ■ The Kolmogorov-Smirnov test can be used to determine whether or not the predicted
11 and observed cumulative distributions of time series are the same. This metric has
12 been used to compare AQUATOX model results with data from Coralville Reservoir,
13 Iowa, and Lake Onondaga, New York (Figure 4-4). Table 4-5 gives the statistics for
14 this example (Park, 1999b). Most Housatonic data are probably insufficient for
15 generating the necessary cumulative distributions, but this technique may be used for
testing some water quality variables.



16

17 **Figure 4-4 Cumulative Distributions of Predicted and Observed Chlorophyll in**
18 **Lake Onondaga Epilimnion in 1989 and 1990**

1
2
3

Table 4-5

Summary Statistics for Chlorophyll in Lake Onondaga Epilimnion

Time Period	Group	Chlorophyll (mg/L)					p-value from KS Test
		No. of Obs.	Mean	Median	Std. Dev.	Std. Err.	
1989-1990	Observed	66	28.98	25.00	19.87	2.45	0.319 ^a
	Predicted	66	26.65	23.12	23.07	2.84	

4 ^a. Not significantly different at $\alpha=0.05$.

5
6 For spatial comparisons, model results will be compared with observed data pooled by segments
7 that constitute the AQUATOX domain (respective subreaches, backwater areas, and Woods
8 Pond). Temporal comparisons will be made in several ways, depending on the metric used.
9 Visual comparisons will be based on continuous simulations with observed data plotted
10 appropriately along the date axis. Cumulative distributions, if used, will sample model results
11 from periods with available observed data. Statistical comparisons of means probably will not be
12 performed because of questions concerning applicable distributions, but if they are, model results
13 and data will be averaged over periods dictated by data availability.

14 **4.7.2 Key Model Calibration Parameters**

15 Sensitivity analyses will be run to identify the more sensitive parameters for the various
16 Housatonic River regimes. These parameters will either be set very carefully, or they may be
17 used for calibration. The goal is to calibrate with as few parameters as possible and to keep
18 those within ranges reported in the literature; Appendix D in the MFD provides a comprehensive
19 list of AQUATOX model parameters, along with definitions, units, and data/evaluation sources.
20 Key ecosystem parameters that may be candidates for calibration using biomass data collected
21 during summer 2000 include:

- 22 ▪ Half-saturation constants for nutrients; these control phytoplankton and periphyton
23 growth; these parameter values depend on trophic status and may need to be adjusted
24 for the productive, hard-water Housatonic River system.
- 25 ▪ Composite maximum photosynthetic rates; these may need to be calibrated for the
26 Housatonic algal communities.

- 1 ▪ The minimum biomass for feeding; this parameter represents both animal behavior
2 and habitat heterogeneity that can provide refuge from predation and may require site
3 calibration.
- 4 ▪ Mortality rates; these vary greatly from one site to another; intrinsic mortality is
5 usually a calibration parameter; if necessary, data may be collected to estimate
6 mortality rates for Housatonic fish.

7
8 In several bioaccumulation models prey preference is important in controlling the pathways of
9 dietary exposure; however, in AQUATOX potential preferences are balanced with prey
10 availability so that opportunistic feeding can be represented. Experience has shown that the
11 model works well with general preferences and that neither site data on gut contents—which
12 reflect short-term opportunistic feeding—nor calibration are necessary for this mechanistic
13 model. In particular, fish stomach-content and benthic invertebrate data collected on three
14 spring, summer, and fall dates from the Sudbury River, Mass., will be used (Johnson and
15 Dropkin, 1995); these will be supplemented by other pertinent literature (such as Leidy and
16 Jenkins, 1977; Thorp and Covich, 1991; Merritt and Cummins, 1996; and Exponent, 1998).

17 Key PCB parameters that may be candidates for calibration include:

- 18 ▪ Depuration—This process is difficult to measure, but it is important in controlling
19 bioaccumulation; it is likely that the size- and K_{OW} -dependent equation used in
20 AQUATOX will be adjusted for Housatonic species and to better represent PCB
21 congeners and homologs.
- 22 ▪ Biotransformation—This alters the PCB homolog profile in animals; calibration will
23 be necessary to obtain rates representing this process, if it should be modeled.

24 In addition, we will verify other key relationships including:

- 25 ▪ Microbial degradation parameters determine the persistence of PCBs in the
26 ecosystem; congener-specific values extending across all homologs are based on
27 microflora and sediments from Woods Pond (Bedard and May, 1996). Unfortunately,
28 the data are quite variable, and dechlorination is modest compared with that observed
29 in nearby Silver Lake and the Hudson River (Bedard and May, 1996) so that
30 sensitivity analysis will be used to determine if this should be included in modeling
31 homologs. However, dechlorination of congeners that are persistent in humans is
32 significant, suggesting that the straightforward assignment of degradation rates to
33 specific key congeners will be useful. Degradation rates also will be evaluated by
34 comparing spatial results to significant downstream changes that have been observed

1 (see Modeling Framework Design document) because these are presumably related to
2 time of degradation.

- 3 ■ Sorption and desorption between the freely dissolved state and algae and detritus
4 controls the bioavailability of PCBs; general estimation equations are used in
5 AQUATOX, but the results will be compared to site-specific observations to verify
6 that they are applicable to the Housatonic; parameters estimated by the model will be
7 revised as warranted; the formulation of the model has been modified to facilitate
8 direct comparison between observed data and model results.

9 **4.8 SUMMARY OF MODEL CALIBRATION AND VALIDATION PERIODS**

10 Based on the discussions for each component model, HSPF, EFDC, and AQUATOX, the
11 proposed calibration and validation periods are presented in Table 4-6.

12

13
14
15

Table 4-6
Calibration and Validation Periods

	Calibration	Validation
Streamflow	1991-2000	1979-2000
Water temperature	1991-2000	1979-2000
Sediment loads	1991-2000	1979-2000
Nonpoint loads (nutrients/BOD/organics)	1996-2000	1979-2000
Stage height	1999-2000	1979-2000
Velocity	1999-2000	suitable data not available
Suspended solids (water column)	1999-2000	1979-2000
Sediment bed solids	1999-2000	1979-2000
PCBs (water column/bed)	1999-2000	1979-2000
PCBs (fate and bioaccumulation)	1995-2000	1979-2000

16 Note: The validation period uses the longest period of time and is bounded by available data. This approach allows
17 use of the longest timeframe for which model performance can be evaluated. The resulting validated model is more
18 suitable for evaluating the model's predictive capability for simulating baseline conditions and the long-term effects
19 of potential remedial alternatives.

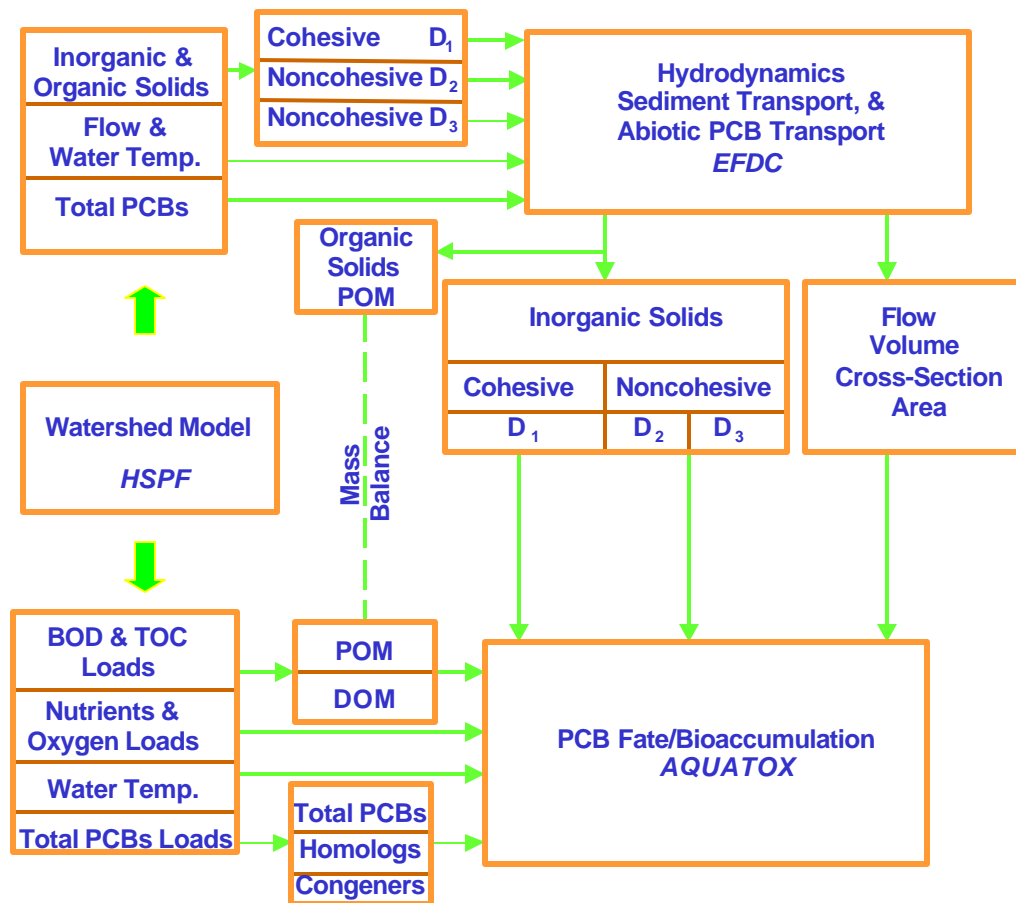
1 **4.9 QUALITY ASSURANCE OF MODEL LINKAGE PROCEDURES**

2 **4.9.1 Framework for Model Linkage**

3 The integrated modeling framework described in Section 4 of the MFD was developed because
4 no single model is capable of representing all the relevant physical, biogeochemical, and
5 biological processes that operate over a wide range of time and space scales to influence the
6 distribution of PCBs in the water column, sediments and biota of the Housatonic River, the
7 integrated modeling framework described in Section 4 of the MFD was developed. The
8 modeling framework consists of a watershed runoff model (HSPF), a hydrodynamics and
9 sediment transport model (EFDC), and a PCB bioaccumulation model (AQUATOX). The
10 design of a methodology for linkage among the three models requires consideration of both
11 spatial and temporal issues since each of the three models simulate different processes at
12 different time and space scales. The physical domains of each model and the resulting transfer
13 of information (i.e., model results) must be closely integrated to allow for the efficient operation
14 and effective representation of the Housatonic River watershed system.

15 Figure 4-5 illustrates an overview of the linkage of the outputs from the watershed model
16 (HSPF) as water inflows and constituent loads from nonpoint sources (drainage basin runoff) and
17 point sources (tributaries and wastewater dischargers), to the hydrodynamic and sediment
18 transport model (EFDC) and to the PCB fate and bioaccumulation model (AQUATOX). Figure
19 4-5 also shows an overview of the linkage of the output from EFDC as inputs of water inflows,
20 reach geometry, and solids loads to AQUATOX. HSPF will provide AQUATOX with water
21 temperature, point and nonpoint source loads for inorganic nutrients, dissolved oxygen, BOD,
22 organic matter, and PCBs. HSPF will provide EFDC with point and nonpoint source inputs for
23 streamflow, water temperature, and loads for total suspended solids and total PCBs. EFDC will
24 provide AQUATOX with streamflow, reach geometry (volume, surface area, cross-sectional
25 area), and loads of inorganic solids.

26



1
2

Figure 4-5 Model Linkage Within the Modeling Framework

3 **4.9.2 Relationship of QAPP and MFD**

4 Section 4.4 of the MFD presents a detailed description of the methodology and assumptions used
 5 to construct the data linkages for the model framework consisting of HSPF, AQUATOX, and
 6 EFDC. A brief overview of the methodology described in the MFD is presented in this section
 7 of the QAPP. Since the linkage between the three models is complex, it is essential to design
 8 procedures to ensure that the linkages are coded correctly and maintain proper mass balances of
 9 constituents. The purpose of this section of the QAPP document is to provide a detailed
 10 description of the QA/QC tests proposed to ensure that the linkages between HSPF, AQUATOX,
 11 and EFDC are performed correctly. The guiding principle in designing the QA/QC tests of the
 12 model linkage is the strict requirement to maintain a mass balance of water volume, heat content,
 13 inorganic solids, organic matter, nutrients, and PCBs loads provided by HSPF and EFDC to
 14 AQUATOX.

1 **4.9.3 Overview of Model Linkage**

2 Using streamflow, water temperature, solids, and PCB loadings provided by the watershed
3 runoff model (HSPF), EFDC will simulate water temperature, streamflow, velocity, and stage
4 height in the hydrodynamic model. EFDC will simulate three size classes of solids as: (1)
5 cohesive (<63 microns); (2) noncohesive (63-250 microns); and (3) noncohesive (>250 microns)
6 in the sediment transport model. Using streamflow, reach geometry (volume, surface area,
7 cross-sectional area) and inorganic solids loadings provided by EFDC, AQUATOX will account
8 for inorganic solids in the water column and simulate evolution of the sediment bed using
9 erosion and deposition fluxes of solids provided by EFDC. Using simulated water temperature
10 and loadings provided directly by HSPF, AQUATOX will simulate organic matter, dissolved
11 oxygen, inorganic nutrients, and trophic levels of biota that include algae, macrophytes, benthic
12 invertebrates, and fish. Using the total PCB loadings provided by HSPF, AQUATOX will
13 simulate multiple homologs and selected congeners of PCBs in the water column and sediment
14 bed and bioaccumulation of PCBs in the biota.

15 **4.9.3.1 *Physical Domain, Spatial and Temporal Scales***

16 The framework for the three models represents a hierarchical modeling approach with each
17 model defined by its own physical domain and relevant spatial and temporal scales.

18 The watershed runoff model (HSPF) accounts for the largest physical domain, covering the
19 Housatonic River watershed from the headwaters to Great Barrington, MA.

20 The hydrodynamic and sediment transport model (EFDC) provides the finest spatial resolution to
21 represent the river channel, floodplain, backwater areas, and Woods Pond. The physical domain
22 for EFDC extends from the confluence of the East and West Branches of the Housatonic River
23 downstream to the outlet of Woods Pond at the Woods Pond Dam. The physical domain of
24 EFDC is represented using two coupled grid schemes as the (1) river channel and floodplain
25 (R/FP Model); and (2) backwater areas, Woods Pond (WP model), and floodplain.

26 The PCB fate and bioaccumulation model (AQUATOX) provides a coarse spatial resolution to
27 represent the river channel, backwater areas, and Woods Pond. The upstream and downstream

1 boundaries of the coarse reaches for AQUATOX are matched with the in-stream reaches of
2 HSPF. The physical domain for AQUATOX extends over the same domain as the
3 hydrodynamic model from the confluence of the East and West Branches of the Housatonic
4 River downstream to the outlet of Woods Pond at the Woods Pond Dam. Note that the physical
5 domain of AQUATOX does not include the floodplain.

6 The watershed model (HSPF) and the hydrodynamic and sediment transport model (EFDC) are
7 driven by, and generate, high-frequency time series of streamflow and solids loads at a time scale
8 of hours. Hourly streamflow and solids loadings provided by HSPF as input to EFDC are
9 linearly interpolated within EFDC to match the sub-hourly time step needed for numerical
10 integration of the hydrodynamic and sediment transport model. The PCB fate and
11 bioaccumulation model (AQUATOX) is designed to represent physical, biogeochemical, and
12 ecological processes operating on a lower frequency time scale with the input load time series
13 data specified at a daily (24-hour) time scale.

14 **4.9.3.2 Spatial Linkage: HSPF-AQUATOX**

15 The linkage of pollutant loads provided by HSPF to AQUATOX is a straightforward procedure
16 since the upstream and downstream boundaries of the AQUATOX reaches are matched to the
17 boundaries of the in-stream reaches defined for the watershed model.

18 **4.9.3.3 Spatial Linkage: EFDC-AQUATOX**

19 The procedure for the linkage of streamflow, water temperature, reach geometry, and solids
20 loads from EFDC to AQUATOX, however, is less straightforward because the mass fluxes (i.e.,
21 [flow] x [concentration]) of water and solids simulated within each EFDC grid cell of the river
22 channel and Woods Pond must be summed horizontally and vertically for the array of EFDC grid
23 cells located within the boundaries of each AQUATOX reach. The horizontal flux of water and
24 solids is summed for each grid cell across the upstream boundary to define the upstream input to
25 each AQUATOX R/FP reach and WP segment. The export (or import) of fluxes of water
26 volume, solids, and PCBs between the river channel and floodplain will be tracked by
27 summation of the fluxes over each grid cell along the floodplain/channel boundary.

1 Because the domain of AQUATOX does not include the floodplain, fluxes of water and solids
 2 to/from the floodplain must be provided by EFDC to the AQUATOX reaches and WP segments
 3 to maintain the correct mass balance of water volume and solids. In the R/FP model and in the
 4 WP model, solids deposition and resuspension fluxes between the bed and water column
 5 (vertical fluxes) are summed over the array of grid cells that match each AQUATOX reach to
 6 define total vertical fluxes for input to AQUATOX.

7 **4.9.3.4 Temporal Linkage: HSPF-AQUATOX and EFDC-AQUATOX**

8 The spatial processing of model results generated by HSPF and EFDC described above is
 9 followed by temporal processing of the spatially aggregated data sets to prepare the input time
 10 series needed for AQUATOX. To link the time series of high-frequency simulation results
 11 generated by HSPF and EFDC with AQUATOX, the high frequency time series are numerically
 12 integrated over a 24-hour period to provide daily time series for input to AQUATOX.

13 Listings of the input time series provided by HSPF to EFDC, EFDC to AQUATOX, and HSPF
 14 to AQUATOX are summarized below. Details of the methodologies used to determine the
 15 various parameters are given in the MFD.

16 **4.9.3.5 Data Linkages from HSPF to EFDC**

17 Streamflow, water temperature, solids, and total PCBs simulated in HSPF are assigned as hourly
 18 time series loads for input to EFDC grid cells as follows:

19	Boundary inflow of water volume	(m ³ sec ⁻¹)
20	Water temperature.....	(°C)
21	TSS#1 (cohesive, <63 microns)	(mg/L)
22	TSS#2 (noncohesive, 63-250 micron)	(mg/L)
23	TSS#3 (noncohesive, >250 microns)	(mg/L)
24	Total PCBs	(µg/L)

26 **4.9.3.6 Data Linkages from EFDC to AQUATOX**

27 After spatial aggregation of fine resolution EFDC grid cells over each coarse AQUATOX reach,
 28 geometry, streamflow, and dispersive mixing are assigned as daily time series for input to
 29 AQUATOX as follows:

1 Volume.....(m³)
2 Cross-sectional area at upstream-downstream interfaces(m²)
3 Surface area (horizontal).....(m²)
4 Horizontal flow at upstream boundary of reach.....(m³ day⁻¹)
5 Horizontal flow to/from channel/floodplain(m³ day⁻¹)
6 Horizontal dispersion rate for all upstream-downstream interfaces(m² day⁻¹)
7 Vertical dispersion rate for WP epilimnion-hypolimnion(m² day⁻¹)

8
9 The sediment transport model simulates three size classes of solids (TSS) that account for both
10 inorganic and organic material. Since HSPF provides particulate organic matter (POM) to
11 AQUATOX, the POM portion of TSS simulated in EFDC must be subtracted out to maintain a
12 proper mass balance of solids and organic matter in AQUATOX. Using a dry weight:carbon
13 (DW:C) ratio and spatially and temporally dependent estimates of TOC:TSS ratios defined from
14 mainstem and tributary data sets collected for the Housatonic River study, loads of particulate
15 inorganic matter (PIM) solids for each of the three size classes are computed from the following
16 relationships:

17 TSS = POM + PIM..... Eq. (4-1)
18 PIM = noncohesive (sands) + cohesive (silts & clays) Eq. (4-2)
19 POM = TSS * (TOC:TSS) * (DW:C)..... Eq. (4-3)
20 PIM = TSS - POM = TSS * [1 - (TOC:TSS) * (DW:C)]..... Eq. (4-4)

21
22 Upstream boundary loads are provided for each size class as daily time series for input to
23 AQUATOX as:

24 PIM#1 (cohesive, <63 microns)..... (g day⁻¹)
25 PIM#2 (noncohesive, 63-250 microns)..... (g day⁻¹)
26 PIM#3 (noncohesive, >250 microns)..... (g day⁻¹)

27
28 The export/import (E/I) of particulate inorganic solids (PIM) are provided by EFDC as daily time
29 series for input to AQUATOX to track the mass flux exchange of solids and sorbed PCBs
30 between the river channel and floodplain (R/FP) as:

31 PIM#1 R/FP E/I (cohesive, <63 microns)..... (g day⁻¹)
32 PIM#2 R/FP E/I (noncohesive, 63-250 microns) (g day⁻¹)
33 PIM#3 R/FP E/I (noncohesive, >250 microns)..... (g day⁻¹)

34

1 The loss of PCBs from the river channel to the floodplain during flood events is accounted for by
2 the solids flux provided by EFDC and internally generated sorbed and dissolved PCB
3 concentrations simulated in AQUATOX.

4 The deposition and resuspension fluxes of particulate inorganic solids (PIM) are provided by
5 EFDC as daily time series for input to AQUATOX as:

6	PIM#1 Deposition (cohesive, <63 microns)	(g day ⁻¹)
7	PIM#2 Deposition (noncohesive, 63-250 microns)	(g day ⁻¹)
8	PIM#3 Deposition (noncohesive, >250 microns)	(g day ⁻¹)
9	PIM#1 Resuspension (cohesive, <63 microns).....	(g day ⁻¹)
10	PIM#2 Resuspension (noncohesive, 63-250 microns).....	(g day ⁻¹)
11	PIM#3 Resuspension (noncohesive, >250 microns).....	(g day ⁻¹)

12
13 The deposition and resuspension fluxes of POM are parameterized in AQUATOX by assuming
14 that the behavior of cohesive solids subject to deposition and resuspension in EFDC can be used
15 to infer equivalent deposition and resuspension velocities for POM. This is considered a
16 reasonable assumption since POM would be subject to the same physical processes as cohesive
17 solids. Deposition and resuspension fluxes simulated in EFDC for the cohesive size class of
18 solids are aggregated over the grid cells corresponding to each AQUATOX reach to assign
19 equivalent POM deposition and resuspension velocities for input to AQUATOX. as:

20	TSS#1 (cohesive, deposition velocity)	(m day ⁻¹)
21	TSS#1 (cohesive, resuspension velocity)	(m day ⁻¹)

22

23 **4.9.3.7 Data Linkages from HSPF to AQUATOX**

24 Water temperature and the sum of point and nonpoint source loads of dissolved oxygen and
25 inorganic nutrients simulated by HSPF are assigned as daily time series for input to each
26 AQUATOX reach as follows:

27	Water temperature.....	(°C)
28	Dissolved oxygen.....	(g day ⁻¹)
29	Ammonium-N	(g day ⁻¹)
30	Nitrite-N + Nitrate-N	(g day ⁻¹)
31	Orthophosphate-P.....	(g day ⁻¹)

32

1 The watershed model (HSPF) simulates BOD and TOC to represent dissolved and particulate
 2 oxidizable organic matter. Since AQUATOX is designed to account for external loads and
 3 internal production of dissolved (DOM) and particulate (POM) organic matter, the BOD and
 4 TOC loads simulated in HSPF must be transformed to provide dissolved and particulate
 5 components of organic matter for input to AQUATOX. Using a dry weight:carbon (DW:C) ratio
 6 and spatially and temporally dependent estimates of TOC:BOD, dissolved (DOC:TOC) and
 7 particulate (POC:TOC) fractions of TOC defined from mainstem and tributary data sets collected
 8 for the Housatonic River study, dissolved (DOM) and particulate (POM) organic matter loads are
 9 computed using the following relationships:

10 BOD = dissolved BOD + particulate BOD Eq. (4-5)
 11 TOC = DOC + POC Eq. (4-6)
 12 TOC = BOD * (TOC:BOD) Eq. (4-7)
 13 DOM = TOC * (DOC:TOC) * (DW:C) Eq. (4-8)
 14 POM = TOC * (POC:TOC) * (DW:C) Eq. (4-9)

15
 16 The sum of point and nonpoint source loads of dissolved (DOM) and particulate (POM) organic
 17 matter are assigned as daily time series for input at the upstream boundary of each AQUATOX
 18 reach as:

19 DOM (g day⁻¹)
 20 POM (g day⁻¹)

21
 22 The watershed model (HSPF) simulates loading of total abiotic PCBs as dissolved and sorbed
 23 forms of PCBs. Using total PCBs and solids loads provided by HSPF, EFDC simulates the
 24 transport and fate of total abiotic PCBs, including the export, or import, of solids between the
 25 floodplain and the river channel. Because the physical domain of AQUATOX does not include
 26 the floodplain, the total PCB load provided by HSPF to AQUATOX must be adjusted internally
 27 within AQUATOX to account for the mass flux export(loss)/import(gain) of PCBs sorbed onto
 28 solids between the river channel and floodplain. The mass flux of solids exchanged between the
 29 river channel and the floodplain provided by EFDC is coupled with the internally generated
 30 concentration of sorbed and dissolved PCBs simulated in AQUATOX to specify the mass flux
 31 exchange of sorbed PCBs from the river channel to the floodplain. Floodplain resuspension of
 32 PCBs is considered to be a very rare occurrence, and thus is assumed to be negligible.

1 AQUATOX simulates the bioaccumulation of three categories of PCBs: (1) total PCBs; (2)
 2 multiple homologs of PCBs; and (3) selected congeners of PCBs. The total PCB loads provided
 3 by HSPF and adjusted internally in AQUATOX to account for the sorbed PCB exchange
 4 between the river channel and floodplain, must be transformed to provide homolog and selected
 5 congener loads of PCBs as input to AQUATOX. Using splits of total PCBs to define fractions
 6 that represent homologs and selected congeners, total PCB loads are defined for input to
 7 AQUATOX as total PCBs, multiple homologs and selected congeners of PCBs as follows:

8	Total PCBs	(g day ⁻¹)
9	Selected PCB congener(s)	(g day ⁻¹)
10	Multiple PCB homolog(s).....	(g day ⁻¹)

11

12 **4.9.4 QA/QC Tests, Sensitivity Analyses, Consistency Checks**

13 In designing procedures to link the three models, a number of data processing steps will be coded
 14 and implemented to couple the output of HSPF and EFDC in both time and space for input to
 15 AQUATOX. In order to ensure that these data processing steps provide the correct linkage of
 16 HSPF to EFDC, HSPF to AQUATOX, and EFDC to AQUATOX, QA/QC tests will be
 17 performed using time invariant (steady-state) data sets input to simplified (a) kinetic and (b)
 18 spatial model representations. All time series data input from HSPF to EFDC and HSPF to
 19 AQUATOX will be assigned time-invariant values to represent constant inflows of water, solids
 20 loads, total PCBs, nutrients, organic matter, and dissolved oxygen loads. Unit values of flow and
 21 concentration (i.e., 1, 10, 100 etc.) will be used to simplify the input data sets to allow easy
 22 checking of the results of the models.

23 **4.9.4.1 QA/QC Tests for HSPF-EFDC**

24 Using constant inputs to define the time series for external flow and solids loads from HSPF and
 25 assignment of model parameter values in EFDC to represent cohesive and noncohesive solids as
 26 conservative materials, the linkage between HSPF and EFDC will be tested by comparison of
 27 solids in the water column defined for an idealized HSPF instream reach and the corresponding
 28 group of EFDC grid cells.

1 The QA tests will include the following three cases to test the linkage of the spatial groups of
2 EFDC grid cells with a corresponding HSPF instream reach:

- 3 • 1-D river channel; depth averaged with one lateral cell.
- 4 • 2-D river channel; depth averaged with three lateral cells.
- 5 • 3-D open water (pond) with two water column layers.

6 In each of these cases, the spatial representation will be simplified by assigning uniform
7 geometry for the length, width, and depth of EFDC grid cells over an idealized physical domain.
8 Although the sediment bed will be uncoupled from the water column for the QA tests of HSPF
9 and EFDC linkage, the sediment bed will be represented with two layers as: (1) active layer of
10 surficial sediments; and (2) deep layer of buried sediments. The spatial linkage of solids will
11 be tested for a set of EFDC grid cells mapped to a corresponding HSPF instream reach. For
12 each of the 1-D, 2-D, and 3-D test cases described above, the kinetic linkage of the models will
13 be simplified by assuming that solids are a conservative material (i.e., solids always in
14 suspension with zero mass flux from deposition and resuspension). Appropriate values will be
15 assigned to the deposition and resuspension parameters for cohesive and noncohesive solids so
16 that the simulation results are driven only by steady-state forcing from hydrodynamics and
17 upstream and nonpoint source loads.

18 The time series results for flow and solids loading simulated for the HSPF instream reach will be
19 compared to the time series of flow and solids loading summed over the matching set of EFDC
20 cells. Because the conservative case is a simple test of transport routing within an idealized river
21 channel in EFDC, the output results from EFDC should be identical to the input data provided by
22 HSPF for (a) total solids; (b) cohesive solids; and (c) two size classes of noncohesive solids.
23 Recognizing that the additive effects of machine error can result in a loss of about an order of
24 magnitude precision over thousands of calculations, the input data from HSPF should match the
25 output data from EFDC within the precision of floating point arithmetic used in the computers
26 for this test. If the data sets do not match, the code used in the linkage procedures will be
27 checked and debugged for possible code errors until the HSPF input and EFDC output data sets
28 match and thus demonstrate that all linkage errors have been found and corrected.

1 **4.9.4.2 QA/QC Tests for HSPF-AQUATOX**

2 Using constant inputs to define external loads from HSPF and assignment of model parameter
3 values in AQUATOX to represent conservative materials, the linkage between the two models
4 will be tested by comparison of the total mass for each state variable calculated within each
5 AQUATOX reach and the corresponding HSPF reach.

6 **Organic Matter**—For organic matter, AQUATOX calculates the uptake of organic matter into
7 the food web as well as burial of organic matter. These effects on total organic matter are not
8 accounted for in HSPF. To perform a meaningful QA test, therefore, we will turn off (i.e., assign
9 zero values) the uptake and burial of organic matter within AQUATOX. Based on the
10 representation of organic matter as a conservative substance in AQUATOX, the mass of organic
11 matter for each AQUATOX reach should balance against the mass of organic matter in the HSPF
12 reach.

13 **Nutrients and Dissolved Oxygen**—The HSPF nutrient and dissolved oxygen loadings will be
14 input to AQUATOX through the AQUATOX loadings interface. Two tests will be performed to
15 ensure that this linkage has been correctly performed. First, following completion of the whole
16 model linkage, every category of loading that has been input into the AQUATOX model will be
17 checked against original data to ensure that the input time series are derived from the proper
18 category. This review will be logged to ensure that each category of loadings coming into
19 AQUATOX has been tested. Second, the debug mode within AQUATOX will be activated to
20 check that the loading data is being properly read from the appropriate loading input data set.

21 **PCBs**—The linkage of PCBs from HSPF to AQUATOX will be tested by comparing the total
22 PCB loads generated by HSPF to the loads received by AQUATOX. Because the total PCB
23 loads input from HSPF will be separated into homologs for the AQUATOX simulations, the
24 summed mass of PCB homolog loads within AQUATOX will be compared with the total mass
25 of PCBs calculated by HSPF. Thus, this will test both the mass balance of the model linkage,
26 and that the HSPF data has been properly divided into homologs for input to AQUATOX.

1 **4.9.4.3 QA/QC Tests for EFDC-AQUATOX**

2 Using constant inputs to define external flow and loads from HSPF and assignment of model
3 parameter values in EFDC to represent cohesive and noncohesive solids as conservative
4 substances, the linkage between EFDC and AQUATOX will be tested by comparison of the total
5 water column and sediment bed solids mass calculated within each AQUATOX reach and the
6 corresponding group of EFDC grid cells.

7 The QA tests will include the following three cases to test the linkage of the spatial groups of
8 EFDC grid cells with the corresponding AQUATOX reaches:

- 9 ▪ 1-D river channel; depth averaged with one lateral cell.
- 10 ▪ 2-D river channel; depth averaged with three lateral cells.
- 11 ▪ 3-D open water (pond) with two water column layers.

12
13 In each of these cases, the spatial representation will be simplified by assigning uniform
14 geometry for the length, width and depth of EFDC grid cells over an idealized physical domain.

15 In each case, the sediment bed will be represented with two layers as: (1) “active” layer of
16 surficial sediments; and (2) “deep” layer of buried sediments. The spatial linkage of mass will
17 first be tested with the EFDC grid cells mapped to a single AQUATOX reach. The linkage will
18 then be further tested with AQUATOX reaches mapped to the EFDC grid. In the later, the 1-D
19 and 2-D river channel cases will serve as a QA test of the “cascade” downstream advection
20 scheme developed for AQUATOX. The 3-D test case will provide a QA test of the explicit finite
21 difference scheme developed for AQUATOX to represent horizontal transfers from dispersive
22 mixing, advection and migration between adjacent reaches.

23 For each of the 1-D, 2-D, and 3-D test cases described above, the kinetic linkage of the models
24 will be tested with simplified representations of kinetic parameters for solids as (a) conservative
25 and (b) nonconservative materials. For the conservative test, values will be assigned to the
26 following parameters so that the simulation results are driven only by steady-state
27 hydrodynamics:

- 28 ▪ Noncohesive solids
 - 29 - Settling rate
 - 30 - Resuspension rate

- 1 - Critical stresses for erosion and deposition
- 2
- 3 ▪ Cohesive solids
- 4 - Settling rate
- 5 - Resuspension rate
- 6 - Critical stresses for erosion and deposition
- 7

8 For the nonconservative test, constant values will be assigned for the parameters listed above so
9 that the kinetic behavior of the model will be represented as a simple first-order gain or loss.
10 Using different channel slopes in EFDC, cases will be prepared to test losses (net deposition) and
11 gains (net erosion) in the solids model. The EFDC test simulations for the two size classes of
12 solids will be compared to steady-state analytical solutions for the 1-D river channel case.

13 For the conservative materials case, the time series results for flow and solids loading from
14 AQUATOX for each reach will be compared to the time series of flow and solids loading
15 provided by HSPF to EFDC and linked to AQUATOX. Since the conservative case is
16 essentially a test of advective routing in EFDC and AQUATOX, the output results from
17 AQUATOX should be identical to the input data provided by HSPF. Recognizing that the
18 additive effects of machine error can result in a loss of about an order of magnitude precision
19 over thousands of calculations, the input data from HSPF should match the output data from
20 AQUATOX within the precision of floating point arithmetic used in the computers for this test.
21 If the data sets do not match, the code used in the linkage procedures will be checked and
22 debugged for possible code errors until the HSPF input and AQUATOX output data sets match
23 and demonstrate that all linkage errors have been found and corrected.

24 For the conservative and nonconservative test cases, the time series results simulated by EFDC
25 and AQUATOX will be compared at the downstream outflows of the AQUATOX reaches for
26 the following model parameters:

- 27 ▪ Flow.
- 28 ▪ Volume.
- 29 ▪ Concentration of cohesive and noncohesive solids in water column.
- 30 ▪ Mass of cohesive and noncohesive solids in water column.

- 1 ▪ Mass of cohesive and noncohesive solids in sediment bed.
- 2 ▪ Gain (or loss) of mass of cohesive and noncohesive solids between water column and
- 3 sediment bed.

4

5 **Streamflow and Reach Geometry**—All the physical geometry and water flow data coming into

6 AQUATOX from EFDC will be treated as time series of external input data by AQUATOX. As

7 such, these data will be input through the AQUATOX loadings interface. Two tests will be

8 performed to ensure that the EFDC to AQUATOX linkage is acceptable. First, each category of

9 loading that has been input into the AQUATOX model will be checked against original data and

10 logged. Secondly, the debug mode will be used within an AQUATOX run to ensure that each

11 category of data is being properly used.

12 One additional test will be performed with the water flow data. Because AQUATOX is

13 receiving daily flow rates from EFDC, the AQUATOX model can calculate its own daily volume

14 data for each reach. This can then be compared to the daily EFDC volume data for each reach to

15 ensure that the water volume linkage has been correctly set up. The volume that AQUATOX

16 calculates must equal the EFDC incoming volume data for the linkage to be verified.

17 **Solids Linkage**—The EFDC-AQUATOX solids linkage will be tested by comparing the mass of

18 solids within each AQUATOX reach with the integrated solids mass calculated by EFDC for the

19 matching grid cells. Figure 4-6 shows the solids interactions within an AQUATOX reach

20 (export/import between the river channel and floodplain not shown) to illustrate the linkage test.

21	<i>Wup</i>	=	upstream boundary inflow of suspended and bedload solids.....	(g day ⁻¹)
22	<i>Wps</i>	=	point source input of solids	(g day ⁻¹)
23	<i>Wnps</i>	=	nonpoint source input of solids	(g day ⁻¹)
24	<i>Wres</i>	=	resuspension of solids	(g day ⁻¹)
25	<i>Wdep</i>	=	deposition of solids	(g day ⁻¹)
26	<i>Wout_{susp}</i>	=	outflow of suspended solids	(g day ⁻¹)
27	<i>Wout_{bed}</i>	=	outflow of bedload solids	(g day ⁻¹)

28

29

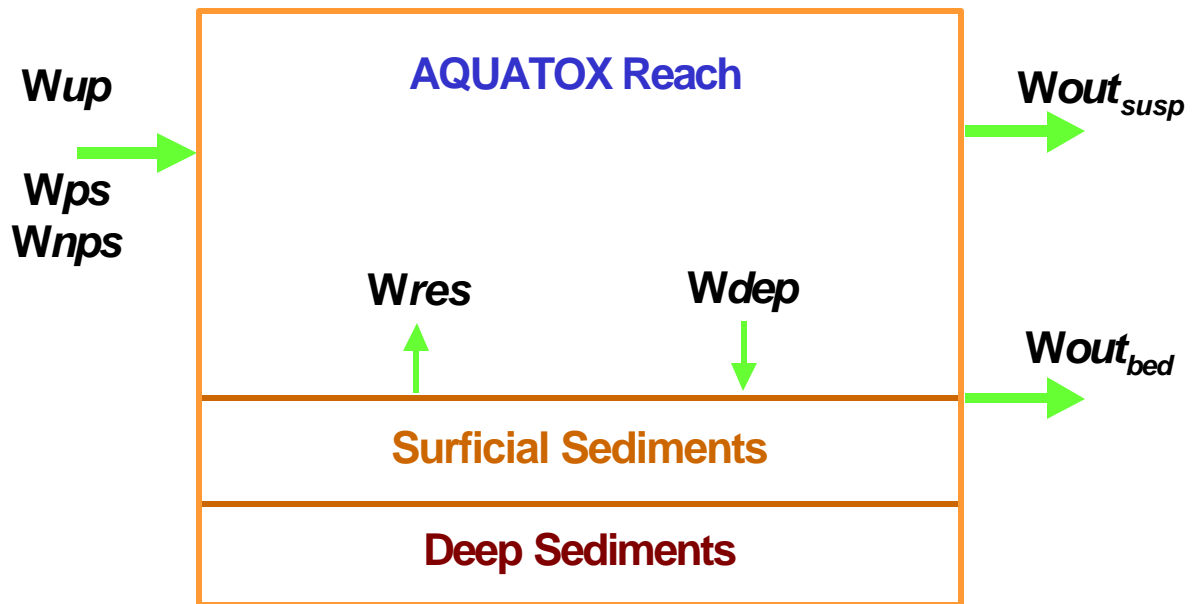


Figure 4-6 Solids Interactions Within an AQUATOX Reach

AQUATOX will calculate the mass of solids within the reach using the sum of the external input loads for that day and the rates of resuspension and deposition. This mass of suspended solids within the reach will then be compared to the EFDC calculation mass. If the mass of the suspended solids is found to be the same, the solids linkage is working properly.

AQUATOX also will calculate a value for the outflow of solids to the adjacent downstream reach ($W_{out_{susp}}$). The $W_{out_{susp}}$ value calculated by AQUATOX will use the calculated solids concentrations in water and the water flow rates for that segment. Because the EFDC calculation of $W_{out_{susp}}$ will not include bedload, the $W_{out_{susp}}$ value passed by EFDC will be tested against the AQUATOX calculation. When these $W_{out_{susp}}$ values are equivalent, this will confirm that the aggregation of solids mass flux is working properly within EFDC and that AQUATOX is correctly using the solids flux rates from EFDC.

4.10 QUALITY ASSURANCE FOR MODEL ENHANCEMENTS AND CODE DEVELOPMENT

As part of the Housatonic River model framework, model enhancements and associated code changes are anticipated for AQUATOX and EFDC.

1 Any changes to the AQUATOX and EFDC codes will undergo thorough review and testing and
2 be documented in the model calibration report. QA procedures for these enhancements are
3 discussed in the sections below.

4 **4.10.1 EFDC Model Enhancements and Code Development**

5 As documented in Section 4.2.2 of the MFD, the version of EFDC being used for the Housatonic
6 River study has been developed and used for numerous applications to rivers, lakes, reservoirs,
7 estuaries, and coastal waters. The computational burden for the application of EFDC in the
8 Housatonic River is anticipated to be quite large. Work is being conducted to investigate
9 enhancements and model constructs to improve the EFDC model's computational efficiency.
10 Areas being investigated include parallel processing, coding optimizations/streamlining, variable
11 time step schemes, and stepped hydrodynamics.

12 If code modifications (FORTRAN 90) are made to EFDC and used in the Housatonic River
13 study, rigorous QA/QC tests will be implemented to ensure the correctness and accuracy of the
14 code changes. Simplified test problems will be designed to provide benchmark comparisons of
15 model results generated with the existing version of EFDC code and the modified version of the
16 code. Using constant parameter values for flow, loads, external forcing functions and physical
17 characteristics, simple uniform grid schemes will be specified to test 1-D, 2-D, and 3-D idealized
18 physical domains. Benchmark test cases will be developed to enable comparison of existing vs.
19 modified numerical model results with analytical solutions for hydrodynamics and transport and
20 fate of conservative and nonconservative constituents.

21 **4.10.2 AQUATOX Model Enhancements and Code Development**

22 AQUATOX Version 2.00 has been developed for the Housatonic River project. It has several
23 enhancements over previous versions that are intended to optimize its application to this specific
24 project. It is a linked-segment model that can represent Housatonic tributaries, sequential
25 reaches, and backwater areas, and stratified and unstratified segments of Woods Pond. Upstream
26 reaches can be run separately with a downstream "cascade" link, and more intimately connected
27 segments can be run simultaneously with bidirectional links that allow the modeling of such
28 processes as advection, diffusion, and migration. The model is capable of simulating up to 20

1 chemicals, including PCB homologs or congeners, simultaneously. It can represent two size
2 classes of all modeled fish species and up to 15 age classes for one species.

3 AQUATOX is written in modular, object-oriented Pascal using the Delphi programming system,
4 and individual units can be recompiled and tested quickly. Self-documenting long variable
5 names and commented structure facilitate evaluation. All code is written by a single experienced
6 programmer and reviewed and verified by the scientist responsible for the formulations.
7 Furthermore, descriptions of any algorithmic solutions are incorporated into the written
8 documentation. All changes are logged and sequential version numbers are assigned; these same
9 version numbers are used for automatic updating of data structures.

10 When making changes, the model is run in Delphi debug mode so that intermediate values can
11 be inspected during a test simulation. The model also can save time-varying rates for all
12 processes represented by the differential equations and those rates can be imported into a
13 spreadsheet program for tabulation and plotting. Thus, both changes in state variable values and
14 the rates contributing to those changes can be evaluated. After modification, the model is tested
15 by running a test suite based on analytical solutions with known results from several published
16 sources.

17 AQUATOX calculates the transfer of contaminants through the food web and within the
18 sediments. These movements require that various differential equations are properly linked for
19 mass balance to be maintained. To test this linkage, all contaminant loss processes (such as
20 microbial degradation) can be turned off within the model to ensure that mass balance is
21 perfectly maintained as the contaminant is distributed throughout the system. This is also a
22 robust test of the segment linkages. Contaminant loss can be temporarily turned off for an entire
23 linked system. The contaminant then moves up the food-web in each segment and is distributed
24 throughout the system (through drift, migration, and diffusion) while the total contaminant mass
25 within the system stays constant. These tests ensure that mass balance is being maintained
26 throughout the linked system as well as within each individual segment.

27 AQUATOX is designed to facilitate documentation of assumptions and data sources for specific
28 applications and to archive results. Note fields are provided for the study and for each of the
29 state-variable loading screens. These provide the user with a way to record an overview of the

1 study and to describe sources and salient features of the loading data. Furthermore, almost every
2 parameter has an associated comment field to document the source of the value used.

3 Both input and output are designed for efficient use. Input files can be imported in a variety of
4 formats, expediting linkage with the HSPF and EFDC companion models. Output is in the form
5 of tables, graphs, and exported files of mass, concentrations, and rates of biotic and chemical
6 constituents; and graphs and exported files of statistical distributions of concentrations based on
7 sensitivity and uncertainty analyses.

8 Simulations, with all associated data and output, are archived in study files. The version of
9 AQUATOX used for the application also is saved to facilitate later auditing and, if necessary,
10 additional application. Versions are upward compatible; therefore, if an old study is opened with
11 a newer version of the model, the data structure will be updated automatically and the user will
12 be advised of any necessary manual additions.

1 **5. SPECIAL TRAINING REQUIREMENTS/CERTIFICATION**

2 No special training requirements or certifications are needed by modeling study personnel with
3 regard to field monitoring techniques or laboratory analysis procedures. The development and
4 application of each of the three models (HSPF, EFDC, AQUATOX) to be used in the Housatonic
5 River study will be guided by individuals with highly specialized expertise in their respective
6 model. The staff who are involved in the development of model input data sets and model
7 application for this project have gained experience in numerical modeling through their work on
8 numerous model application projects over the past 20 to 30 years. Any staff training, if needed,
9 and oversight will be provided by one or more of the senior modelers.

1 **6. DOCUMENTATION AND RECORDS**

2 All data and assumptions used in the modeling study of the Housatonic River will be recorded
3 and documented in a series of reports as described in Section 10, Reports to Management. As
4 directed by the EPA Project Manager (EPA PM) and/or the USACE PM, the modeling team will
5 prepare additional interim progress reports, technical memoranda, and other deliverables, which
6 will be distributed to project participants as directed by the EPA PM. The originals of all records
7 and documents, including soft copy versions of the data and model input data sets, will be
8 maintained at the Roy F. Weston, Inc., West Chester, PA, office for a period of at least 3 years
9 after final payment (unless otherwise directed).

10 The modeling team will develop a central file as a repository for information and data used in the
11 preparation of any reports and documents during the project and will supervise the use of
12 materials in the file. The following information will be included:

- 13 ▪ Any reports and documents prepared.
- 14 ▪ Contract and work assignment information.
- 15 ▪ Copies of e-mail correspondence that contain critical instructions or document
16 important decisions.
- 17 ▪ Project QAPP.
- 18 ▪ Results of technical reviews, data quality assessments, and audits.
- 19 ▪ Communications (memoranda; internal notes; telephone conversation records; letters;
20 meeting minutes; and all written correspondence between AQUA TERRA and other
21 members of the modeling team, EPA, and other project team personnel,
22 subcontractors, suppliers, or others).
- 23 ▪ Maps, photographs, and drawings.
- 24 ▪ Studies, reports, documents, and newspaper articles pertaining to the project.
- 25 ▪ Special data compilations.

26
27 Photographs taken of the watershed area and locations along the river will be kept with the
28 project file records. Records of receipt with information on source and description of

1 documentation shall be filed along with the original data sheets and files to ensure traceability.
2 Records of such actions and subsequent findings need to be kept during additional data
3 processing. Examples include unit conversions, contouring, data gap interpolation, and data
4 extrapolation. Recordkeeping shall also include example calculations and conversions, and
5 software references for data processing (e.g., name of software, provider, version, etc.).

6 The model application will include complete recordkeeping of each step of the modeling process.

7 The documentation will consist of reports and files addressing the following items:

- 8 ▪ Assumptions.
- 9 ▪ Parameter values and sources.
- 10 ▪ Nature of grid and grid design justification.
- 11 ▪ Changes and verification of changes made in code.
- 12 ▪ Actual input used.
- 13 ▪ Output of model runs and interpretation.
- 14 ▪ Calibration and validation procedures and results from the model.
- 15 ▪ Intermediate results from iterative calibration runs.

16
17 All data files, source codes, and executable versions of the computer software used in the
18 modeling study will be retained for auditing or post-project reuse, including:

- 19 ▪ Version of the source and executable image of the code used.
- 20 ▪ Calibration input and output.
- 21 ▪ Validation input and output.
- 22 ▪ Application input and output (i.e., for each scenario studied).

23
24 If any modifications are made to the source code used in the modeling study, the code will be
25 tested again according to a standard testing protocol. All new input and output files must be
26 saved for inspection and possible reuse together with existing files, records, codes, and data sets.

27 The main objective of most model applications is a scenario analysis and screening of the
28 proposed alternative scenarios. The scenario analysis steps for the Housatonic River PCB Study
29 will be carefully executed and extensively documented. Important elements of this
30 documentation include code execution options used, a complete set of input data, output model
31 result files, and an overview of the results of the simulations.

1 The project reporting will also include descriptions of calibration targets, measures of
2 calibration, calibrated variables, calibration assessment, and model validation results, as
3 described in Section 4.3.

4 If any change(s) in this QAPP are required during the study, a memo will be sent to each person
5 on the distribution list describing the change(s), following approval by the appropriate persons.
6 Each individual will be responsible for attaching a copy of each memo to his/her copy of the
7 QAPP.

1 DATA ACQUISITION

2 7. DATA ACQUISITION REQUIREMENTS

3 As discussed in Section 4, data of known quality will be used to the extent possible, which
4 means that QC data accompanying the measurement data must be available. If such QC data are
5 unavailable, this will be noted. Data obtained from government databases and peer-reviewed
6 publications will be assumed to be accurate. However, all data will be reviewed for usability,
7 general quality, and consistency with other data sources, prior to use in the modeling activities
8 (see Section 11). A complete description of the procedures and criteria to be used in reviewing
9 data for usability is provided in the Project QAPP (WESTON, 2000b). Limitations in the data
10 sets will be acknowledged and included in discussions of their use. All data entered manually or
11 electronically will be confirmed by checking the source data. Computer-generated metric
12 calculations will be confirmed by manually calculating a subset of the values to the extent
13 possible.

1 **8. DATA MANAGEMENT**

2 All data directly or indirectly collected as part of this project will be managed (maintained) as
3 hard copy only, both hard copy and electronic, or electronic only, depending on the ir nature.

4 Guidelines for data formatting, including data element type, format, allowable values and ranges,
5 and other parameters, will be developed before creating the final version of the project database.

6 All data used to populate the modeling database will be screened before upload and model
7 application for adherence to those rules as well as completeness, timeliness, and consistency. All
8 manually entered parameter values from paper sources will be screened by reviewing printouts
9 of summaries of randomly selected portions of the model application. This review will include
10 comparison to the original data sources (e.g., USGS, NWS) and comparison to the paper
11 documentation. Any record identified as having problems will be reviewed to determine whether
12 corrected data can be acquired or the record omitted. Appropriate policies, standards, and
13 guidelines will be followed.

14 All data collection efforts planned to support the modeling study, as described in the MFD, are
15 being performed by Roy F. Weston, Inc.; the QAPP prepared for that comprehensive data
16 collection effort (WESTON, 2000b) covers all quality assurance issues associated with data
17 collection. The project database for the overall Housatonic River PCB contamination
18 investigation is called the DataMart, and its maintenance, update, and distribution are performed
19 by Roy F. Weston, Inc. Any data used for the modeling study that are obtained from the
20 DataMart will undergo scrutiny similar to that described above. The watershed model database
21 will be maintained by AQUA TERRA for the duration of the project. This database will use a
22 Watershed Data Management (WDM) file (Lumb and Kittle, 1986) as the central repository of
23 both the model input data files and output files.

24 Modifications to this section of the QAPP to address changes in database security and storage
25 may be required later in the project since the needs of the project may vary as it proceeds. All
26 files pertaining to the data, calculations, figures, and text for data reporting will be stored by
27 AQUA TERRA, Roy F. Weston, Inc., or EPA, as appropriate. The final version will be provided
28 to the EPA PM or USACE PM for archiving when analyses are complete. Electronic copies of

- 1 databases will be supplied to EPA with the final report, and copies will be maintained by Roy F.
- 2 Weston, Inc., for a period of at least 3 years after final payment, unless otherwise directed.

1 **ASSESSMENT/OVERSIGHT**

2 **9. ASSESSMENT AND RESPONSE ACTIONS**

3 Because this is a modeling project and not an environmental sampling and analysis project,
4 traditional performance and system audits are not appropriate, nor will traditional corrective
5 actions be needed. Data generated as modeling results will be evaluated during the validation
6 process.

7 Model performance assessments as described in Section 4.3 will be made continually by the
8 modeling group. Performance audits will consist of comparison of model results with observed
9 historical data, and general evaluation to ensure reasonable model behavior for state variables
10 and other output lacking historical data. Performing control calculations and post-simulation
11 validation of predictions are major issues in the quality assurance framework. As data entries,
12 calculations, or other activities are checked, the QC Officer will document these activities, as
13 appropriate, and provide this documentation to the Modeling Team and Modeling Coordinator
14 for inclusion in the project file.

1 **10. REPORTS TO MANAGEMENT**

2 Given that the focus of this study is on modeling rather than data collection, there will be no
3 formal QA reports generated or submitted to management. However, appropriate and timely
4 technical reports are required as a component of project performance.

5 Once a month, as part of the normal reporting requirements, the modeling team members will
6 provide the Roy F. Weston Project Manager with a brief technical status and cost report
7 describing the status of the project, accomplishments during the reporting period, planned
8 activities for the next period, any special problems or events, planned/completed travel, and the
9 budget status of the effort.

10 The project requirements call for submittal of the following four key reports to management:

- 11 ▪ Final Modeling Framework Document
- 12 ▪ Final Quality Assurance Project Plan
- 13 ▪ Final Model Calibration Report
- 14 ▪ Final Model Validation Report

15
16 The final draft Modeling Framework Document (MFD) has been completed (Beach et al., 2000).
17 The MFD will be peer reviewed in conjunction with the final draft of this Quality Assurance
18 Project Plan. Upon completion, the final drafts of the Model Calibration and Model Validation
19 Reports will also be peer reviewed. In addition, reports on baseline conditions and scenario
20 simulations and results may be required.

1 DATA VALIDATION AND USABILITY

2 11. DATA REVIEW, VALIDATION, AND VERIFICATION 3 REQUIREMENTS

4 This section discusses the criteria for determining whether to accept, reject, or qualify the data
5 collected for a project. *Validation* criteria are those that are used to determine whether the data
6 satisfy user requirements, whereas *verification* criteria determine whether the data are sufficient
7 for drawing conclusions related to the data quality objectives (DQOs).

8 The focus of this project is using environmental data to calibrate and validate models, rather than
9 collecting new environmental field data. Consequently, it would not be meaningful to establish
10 traditional data validation and verification criteria in this QAPP, because the modeling
11 component of the project does not include collection of additional data. Input data and model
12 results will, however, undergo extensive review, with established review procedures and
13 assessment criteria as described below.

14 A number of historical studies and data sets exist for the Housatonic River. These data sets will
15 be evaluated to determine if and how the data may be used in the modeling effort. The process
16 to be followed for evaluating the data sets will be similar to that developed for determining the
17 usability of historical data for the Ecological Risk Assessment being conducted concurrently
18 with the modeling. The evaluation process is based on procedures for assessing data usability
19 detailed in *Guidance for Data Usability in Risk Assessment* (EPA, 1992). In outline, this
20 evaluation process will score each data set using six data quality criteria including, for example,
21 such categories as level of documentation and validity of analytical methods. The combined
22 score for each data set will be used to assign it to one of the following categories:

- 23 ▪ Level A: Acceptable, unrestricted use
- 24 ▪ Level B: Acceptable, use with caution, some use restrictions may apply
- 25 ▪ Level C: Conditionally acceptable for limited uses
- 26 ▪ Level D: Not acceptable

27
28 The criteria necessary to achieve the Level A designation are strict, and it is anticipated that few
29 of the historical studies will fall into this unrestricted use category. The majority of the studies

1 are expected to be either Level B or Level C and may therefore be used for limited purposes. No
2 studies assigned to Level D will be used in the calibration or validation of the model.

3 Experienced professionals will perform the data review, compilation, and evaluation phases of
4 the study. The modeling team members will be responsible for reviewing data entries,
5 transmittals, and analyses for completeness and adherence to QA requirements. The data shall
6 be organized into a standard database on a microcomputer. A screening process will be used that
7 scans the database and flags data that are outside of typical ranges for a given parameter. The
8 database will be scanned to ensure data for all parameters are within typical ranges. Values
9 outside of typical ranges will not be used to develop model calibration data sets or model kinetic
10 parameters.

11 Raw data received in hard copy format will be entered into the standard database. All entries
12 will be compared to the original hard copy data sheets by the team personnel. Data manipulation
13 will also be accomplished using specialized programs and/or commercial spreadsheet programs.
14 A selected fraction of the calculations will be recalculated by hand to ensure correct formula
15 commands were entered into the program. If 5% of the data calculations are incorrect, all
16 calculations will be rechecked after the correction is made to the database. Data quality will be
17 assessed by comparing entered data to original data or by comparing model results with the
18 measurement performance criteria summarized in Section 4 to determine whether to accept,
19 reject, or qualify the data.

1 **12. VALIDATION AND VERIFICATION METHODS**

2 This section refers to data validation and verification methods, not modeling issues; model
3 validation is discussed in Section 4. *Data validation* is the process of determining whether the
4 data satisfy user requirements, whereas *data verification* is the process of ensuring that the data
5 are sufficient for drawing conclusions related to the DQOs.

6 Given that the focus of this modeling effort is using environmental data to calibrate and validate
7 models, rather than collecting environmental field data, traditional data validation and
8 verification procedures are not applicable. For the overall Housatonic River Supplemental
9 Investigation, these issues are addressed in the QAPP for the accompanying data collection effort
10 (WESTON, 2000b). Input data and model results will, however, undergo extensive review, as
11 described in Sections 8 and 11.

12 The WESTON QA Officer is responsible for establishing and maintaining a QA program that
13 includes QA and QC processes to ensure the quality of the project data. The Modeling
14 Coordinator and WESTON Project Manager (see Figure 1-1) will make all data available to the
15 QA Officer within 2 weeks of receipt of data. The QA Officer will identify any issues of
16 concern to the Modeling Coordinator and Project Manager, who will then will resolve these
17 issues with the modeling team.

1 **13. RECONCILIATION WITH DATA QUALITY OBJECTIVES**

2 For most QAPPs that include field sampling activities, this section addresses the issue of whether
3 the collected data meet the DQOs, based on selected data quality indicators. Each data type is
4 evaluated for adequacy in terms of the common data quality indicators, such as precision,
5 accuracy, representativeness, comparability, and/or completeness.

6 The Housatonic River PCB Modeling Study focuses on using environmental data to calibrate and
7 validate the components of a modeling system that will predict PCB environmental fate and
8 transport. Section 4.1 describes the six DQOs of the project. All DQOs relate to
9 quantifying/estimating current and future environmental conditions. In this context
10 *reconciliation* with DQOs connotes establishing how model results will be tested and evaluated
11 in order to ensure that the models are producing results of sufficient quality. This topic is
12 addressed in detail in Section 4.3.

13 Since the focus of the project is not on collecting or generating new field data, the evaluation of
14 certain data quality indicators such as precision, accuracy, and completeness is not warranted.
15 However, an evaluation of the comparability and representativeness of available data is
16 appropriate, and will be performed as part of the model calibration and validation process.
17 Assessment of data set comparability will determine when there is confidence that (1) two sets of
18 data can be considered equivalent with respect to the measurement of a specific variable or group
19 of variables, or (2) a set of data collected at one site may be reasonably used to represent
20 conditions at another site. Evaluation of data *representativeness* will determine the degree to
21 which data accurately and precisely represent characteristic conditions (e.g., chemical
22 concentrations) and, therefore, address the natural variability or the spatial and temporal
23 heterogeneity of a site.

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