

Cooperating Parties Group

**LOWER PASSAIC RIVER RI/FS
NEWARK, NEW JERSEY**

APPENDIX N

**ORGANIC CARBON MODEL OF THE
LOWER PASSAIC RIVER**

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1.0 INTRODUCTION

The Modeling Work Plan (MWP) developed by Region 2 for the RI/FS of the Lower Passaic River (LPR; HydroQual, 2006a) and Newark Bay (NB; HydroQual, 2006b), calls for a suite of models to calculate the fate and transport of contaminants in the LPR and NB. The model framework consists of a hydrodynamic sub-model (ECOM), a sediment transport sub-model (ECOM-SEDZLJS), a eutrophication sub-model (ST-SWEM), and a contaminant fate and transport sub-model (RCATOX). Region 2 and the CPG subsequently discussed a number of proposals for streamlining/optimization of the LPR/NB modeling program with the objective of reducing the LPR/NB RI/FS schedule. These discussions were also supported by analyses and information that supported a proposal for eliminating the eutrophication sub-model from the MWP.

The MWP concluded that the overall model framework should be able to address a number of specific ‘what if’ questions and was not aimed at scientific analysis nor designed to be used on a day-to-day basis for general management purposes of the LPR. Furthermore, none of the specific questions (identified in the MWP) to be addressed by the model framework are anticipated to include a change in the state of eutrophication within the LPR and NB. Therefore, it was concluded that the eutrophication sub-model most likely would not be part of the sequence of cause and effect on contaminant fate and transport that needs to be addressed with the overall model framework. The current state of eutrophication as known from available measurements could be taken as given for future conditions. Analyses using recent data were also performed to assess the state of eutrophication in the LPR and NB. The concluding proposal from this analysis was to use a judicious compilation of forcing functions for organic carbon (OC) in the water column as well as the bed sediment based on site-specific measurements.

The proposal for eliminating the eutrophication sub-model was reviewed by Region 2. Subsequent discussions between Region 2 and CPG consultants have led to a consensus on the simplification approach for the organic carbon (OC) modeling component of the LPR/NB RI/FS Modeling Program. This simplification is furthermore called the Alternative Organic Carbon Approach (AOC) and is formulated in detail in Section 2. The CPG has implemented the AOC approach and has conducted test simulations with the OC model as part of the AOC approach and with the ST-SWEM eutrophication sub-model and have analyzed the differences. These test simulations and subsequent analyses are reported in Section 3. Section 4 describes the subsequent refinement of the OC model with regard to various site-specific inputs such as initial conditions, boundary conditions, and parameterization. The linkage between the hydrodynamic, sediment transport, OC, and contaminant fate and transport models is also described in this section. Section 5 includes the results of a long-term validation of the OC model performance relative to various metrics in the sediment bed and water column. Finally, Section 6 presents a summary of the OC model development and application.

2.0 ALTERNATIVE ORGANIC CARBON APPROACH

2.1 Background

OC in the LPR and NB may originate from a number of sources, including, but not restricted to, flow coming over Dundee Dam; inflow from tributaries, combined sewer overflows, storm sewer outfalls, and sewage treatment plant outfalls; tidal exchange with NY harbor; and primary production within the water column. Based on data and experience from previous modeling studies of the LPR, NB, and the NY/NJ harbor, the MWP suggested that primary production may be important to OC dynamics in the LPR and NB. Therefore, the MWP originally proposed a complex eutrophication model to provide a mechanistic representation of primary production, die-off, and diagenesis within the water column and sediment of the LPR and NB. The proposed model relied on the regional-scale OC model developed for the NY/NJ harbor under the Contaminant Assessment and Reduction Project (CARP; HydroQual, 2007).

As part of the remedial investigation of the LPR, an analysis was conducted to understand OC dynamics within the LPR and NB, leading to a proposal to simplify the OC model proposed in the MWP (Moffatt & Nichol, 2010a). Subsequent discussions between Region 2 and the CPG (Moffatt & Nichol, 2010b; DiToro, 2010) led to a consensus on a simplified approach for representing OC dynamics within the LPR and NB study areas (de maximis, 2011). Briefly, the simplification involves the elimination of the eutrophication and sediment diagenesis elements of OC kinetics in ST-SWEM. This allows for a substantial simplification of the formulations to represent OC dynamics as well as input and calibration requirements for the model application to the LPR and NB. Accordingly, the AOC model approach has three main aspects. The first aspect concerns the reduction of the number of organic carbon fractions from the ST-SWEM representation of algal, labile, inert, and refractory (the latter three representing various forms of detrital carbon) to only algal and detrital carbon. The second aspect deals with the simplification of the organic carbon kinetics that will be used instead of the ST-SWEM eutrophication model. The final aspect involves the modeling procedure for the OC model including the development of model inputs and model application (including calibration). These aspects of the OC model are described in the following sections.

2.2 Number of Organic Carbon Fractions

The ST-SWEM model framework includes several organic carbon fractions to represent algal carbon and detrital carbon (both, components of particulate organic carbon [POC]), and dissolved organic carbon (DOC). Detrital OC is further sub-divided to labile, refractory, and inert forms, distinguished by varying rates of diagenesis. Similarly, DOC is a sum of labile and refractory forms. In addition, since ST-SWEM is a eutrophication model, it also includes state variables representing labile and refractory forms of various nutrients such as nitrogen, phosphorus, and silica. The AOC approach, by eliminating the eutrophication and diagenesis aspects from the numerical modeling of OC dynamics, includes only two distinct OC fractions:

- The first fraction represents OC associated with algae
- The second fraction represents detrital OC that is associated with suspended sediment in the water column and sediments in the bed

Thus, the four fractions of POC inherent in the ST-SWEM model are aggregated into two fractions in the OC model – an algal fraction, and a non-algal or sediment-bound (detrital) fraction. In addition, water column DOC is treated as a model input rather than as a state variable in the OC model.

2.3 Simplified Organic Carbon Kinetics

As mentioned previously, the AOC approach does not include the eutrophication and sediment diagenesis aspects of OC dynamics included in ST-SWEM. Therefore, the process kinetics for the OC model include only the advection, dispersion, erosion, and deposition of the two carbon fractions, and the transformation of algal carbon to detrital carbon. The following text provides a description of the process kinetics for the two OC fractions in the OC model.

The following aspects are considered with respect to algal carbon:

- Algal carbon enters the LPR and NB from freshwater and marine boundaries.
- Algal carbon is subject to advection and dispersion in the water column, at rates calculated by the hydrodynamic model.
- Algal carbon is considered a conservative substance in the water column, except for settling from the water column. The settled algal carbon mass is subtracted from the water column and added to the bed, thus maintaining mass conservation.
- Following deposition to the bed, 85% of the deposited algal carbon is instantaneously lost due to diagenesis in the bed, with the remaining 15% instantaneously transformed to detrital carbon.

The following aspects are considered with respect to detrital carbon:

- Detrital carbon enters the LPR and NB from freshwater and marine boundaries and from combined sewer overflows and storm-water outfalls.
- Detrital carbon is subject to advection and dispersion in the water column, at rates calculated by the hydrodynamic model.
- Detrital carbon is considered a conservative substance in both water column and bed, except for the bed-water exchange processes of erosion and deposition.

- Detrital carbon is assumed to be inert, i.e., not subject to diagenesis in both water column and bed.
- Detrital carbon in both the water column and sediment bed is assumed to be associated only with cohesive or fine sediments (particle size <63 μm); this is an assumption in common with ST-SWEM.
- Detrital carbon settles and resuspends in accordance with settling and resuspension rates calculated for cohesive sediments by the sediment transport model. In other words, the deposition flux of carbon is determined from the sediment settling flux computed by the sediment transport model and the carbon concentration in the water column; the deposited OC mass is subtracted from the water column and added to the bed, thus maintaining mass conservation. Similarly, the erosion flux of carbon from the bed is determined from the sediment resuspension flux computed by the sediment transport model and the carbon concentration in the bed; the eroded OC mass is subtracted from the bed and added to the water column, thus maintaining mass conservation.

2.4 Modeling Procedure

The input and parameterization requirements for the OC model include initial conditions, boundary conditions, and the erosion/deposition kinetics for algal and detrital carbon. In addition, advection and dispersion rates calculated by the hydrodynamic model, and erosion and deposition rates calculated by the sediment transport model are also specified as inputs to the OC model. The procedure for modeling organic carbon includes:

- Measured values of chlorophyll-a (Chl-a) are used to specify the algal loadings at the model boundaries (freshwater and marine boundaries).
- A C:Chl-a ratio (based on ST-SWEM inputs) is used to convert Chl-a into algal carbon.
- As in ST-SWEM, two phytoplankton groups are modeled; these represent winter diatoms and summer flagellates, distinguished by their seasonal abundance and C:Chl-a ratios.
- Algal carbon is subject to settling from the water column at a relatively low (compared to suspended sediments) settling rate.
- Measured detrital carbon values are used to specify the detrital OC loadings at model boundaries (freshwater and marine boundaries) and at combined sewer outfalls and storm-water overflow locations.
- Detrital carbon concentration in the water column is determined using (1) detrital carbon entering from the boundaries, combined sewer outfalls, and storm-water

overflow locations, (2) detrital carbon deposition flux to the bed, and (3) detrital carbon resuspended from the bed.

- The settling and resuspension rates of detrital carbon is in accordance with the settling and resuspension rates of cohesive sediments as calculated by the sediment transport model.
- The initial condition for detrital carbon in the sediment bed is based on measured data.

2.5 ECOM-SEDZLJS to OC Linkage

Both ST-SWEM and OC models rely on information from the ECOM-SEDZLJS sediment transport model to characterize changes in bed thickness and composition. Amongst other information, the sediment transport model tabulates the time-variable erosion and deposition fluxes of cohesive and non-cohesive sediments. ST-SWEM uses this information along with an input for the initial condition of the bed composition (cohesive and non-cohesive fractions), and an input for the density of the cohesive and non-cohesive solids to calculate the time-variable composition and thickness of the various bed layers in ST-SWEM (active and archive layers, which refer to the top 15 cm in the bed and depth intervals below 15 cm in the bed, respectively). The information on bed thickness and composition is also written to a linkage file and subsequently used by the RCATOX contaminant fate and transport model. However, this means that the bed thickness and composition within ST-SWEM (and RCATOX) can differ from the sediment transport model. In order to pass consistent information and to maintain consistent layer thickness and composition between the various models, the linkage file written by ECOM-SEDZLJS, and the computations with regard to bed composition and layer thicknesses within OC were modified as described below.

The modified approach implemented in AOC seeks to maintain the same layer thickness and composition in the ECOM-SEDZLJS, OC, and RCATOX sub-models. Therefore, the linkage file written by ECOM-SEDZLJS was modified to include information on the total bed thickness, and the cohesive and non-cohesive content (in mass/unit area) of the OC active layer (the OC active layer includes the top 15cm of the sediment bed in ECOM-SEDZLJS). The modified approach also takes into consideration the fact that ECOM-SEDZLJS includes a time-variable model of bed consolidation such that a given location can experience changes in bed thickness due to consolidation, and the calculated cohesive and non-cohesive content over a fixed depth interval (eg., the top 15 cm of the bed corresponding to the active layer in the OC model). However, the OC model (nor ST-SWEM) cannot handle such transients in the bed. As mentioned previously, ST-SWEM uses an input constant dry density to calculate changes in bed thickness and cohesive and non-cohesive content in the active and archive layers. The OC model uses a somewhat similar approach, using output from ECOM-SEDZLJS on bed thickness and active layer composition calculated using the fully consolidated dry density profile for the individual layers in ECOM-SEDZLJS. This information is written to the linkage file in addition to the erosion and deposition fluxes every time-record (typically every 15 minutes). The OC

model was modified to read the additional information written to the ECOM-SEDZLJS linkage file. The formulations in OC dealing with the calculation of bed layering and composition (originally based on ST-SWEM), were modified to calculate the time-variable archive layer thickness (using the time-variable total bed thickness read from the ECOM-SEDZLJS linkage file and considering the active layer as the top 15cm of the sediment bed). The time-variable composition of the archive layer was calculated using an input initial active and archive layer composition, and the time-variable active layer composition, erosion, and deposition fluxes read from the ECOM-SEDZLJS linkage file. The active and archive layer thickness and composition in the OC model are communicated to RCATOX using the same linkage file and format as ST-SWEM. These modifications ensure the communication of consistent bed thickness and composition from the sediment transport model, to the organic carbon model, and to the contaminant fate and transport model.

The application of the OC linkage files within RCATOX simulations is further discussed in Section 3.5 of Appendix O, within the context of the contaminant sorption settings presented therein.

2.6 Navigation Scour

Navigation scour has been implemented within RCATOX for model cells that were identified as being subject to significant ship traffic within the LPR and Newark Bay, as described in Appendix M. The implementation includes both the scour of sediment bed POC as well as POC loading to the water column associated with the scoured sediments. For cells within the LPR subject to navigation scour, the total bed elevation change due to the navigation scour is predicted by the sediment transport model for each discrete time period of simulation, and this change is applied at the beginning of every discrete period in the OC model. The POC mass scoured from the bed is computed from the initial profile at the start of the corresponding time period, and its release to the water column is evenly divided over the duration of the time period. For cells within NB subject to navigation scour, the bed elevation change due to the navigation scour is distributed over time and added to the erosion driven by hydrodynamic forcing. In both scenarios, the POC release is distributed uniformly over the water column. No additional parameterization of navigation scour was imposed as part of the OC model inputs, as the depth and timing of navigation scour were provided by the sediment transport model similar to flow-driven erosion.

2.7 Summary

A simplified numerical model framework, referred to as the AOC, for representing OC dynamics in the LPR and NB was developed during the remedial investigation studies of the LPR. The information required to define inputs to the OC model is based on various data surveys implemented as part of the remedial investigation of the LPR and NB, secondary data sources, and using the results of the hydrodynamic and sediment transport models. This is further described in Section 4. The following section describes a few tests of the AOC approach, and comparing AOC performance to ST-SWEM model performance

for various metrics over a one-year period. In addition, contaminant fate and transport model performance using the results of AOC and ST-SWEM models is also assessed.

3.0 TEST SIMULATIONS: AOC AND ST-SWEM

The OC model was implemented following the approach described in Section 2. Results from a one-year simulation using the OC model were compared to ST-SWEM model results to assess the performance of the OC model. A complete test simulation with hydrodynamics, sediment transport, the ST-SWEM eutrophication model and the RCATOX model for contaminants was obtained from the Region 2 modeling team in 2012. The results obtained using the OC model were compared to the results of the ST-SWEM eutrophication model for the same model inputs and parameterization. Subsequently, RCATOX model results for contaminants using the organic carbon results from both approaches were obtained and compared. The differences were identified and analyzed. It should be stressed that the ST-SWEM and RCATOX test simulation provided by Region 2 do not represent calibrated models and was only meant to represent a test case. This reporting is only meant to compare the results of both organic carbon model approaches to assess the impact of the organic carbon approach on the contaminant model results in the test simulation examined. It is aimed at identifying differences arising from the different organic carbon modeling approaches.

3.1 OC Model Implementation

The code used for the OC model derives from the ST-SWEM code received from Region 2. The code modifications to implement the AOC approach involved essentially a simplification of the ST-SWEM model formulations and parameterization following the approach described in Section 2. The implementation consisted of 7 distinct elements:

- a. Set up a AOC simulation for two OC fractions

The OC model for the test simulations used the same grid schematization and other input features such as the locations of freshwater and other point sources as the original ST-SWEM simulation from Region 2. The model was set up for 2 substances or state variables: algal POC and sediment-bound POC. The test simulation used the ECOM hydrodynamic model results in the same way as the original ST-SWEM approach.

- b. Create equivalent model boundary conditions for the two OC fractions

All boundary conditions, point sources, and non-point sources of the organic carbon fractions input to the ST-SWEM simulation were identified and assigned, as appropriate, into algal POC and sediment-bound POC and applied to the model setup mentioned under a).

- c. Develop an OC kinetics subroutine reading the ECOM-SEDZLJS results

This routine reads through the ECOM-SEDZLJS sediment transport results in the same manner as the ST-SWEM routines and obtains sedimentation and resuspension rate results for further processing and use in the OC model computations.

- d. Develop the bed sediment POC initial conditions inputs

Sediment bed POC for the test simulations was set to the same initial condition as the ST-SWEM simulation received from Region 2.

e. POC resuspension kinetics

The kinetics subroutine mentioned under c) was expanded with the input bed-sediment POC content. From the information from c) and d) the resuspension of bed POC is determined in the kinetics subroutine.

f. Settling rates

The kinetics subroutine was updated with settling rates for both POC fractions corresponding to the settling rates used in ST-SWEM for algal POC and ECOM-SEDZLJS results for sediment-bound POC.

g. Create output file for RCATOX

The kinetics subroutine was set up to produce an organic carbon linkage file that exactly matches the structure of the file that ST-SWEM produces. This linkage file is subsequently used for performing the RCATOX contaminant test simulations described below.

3.2 Comparison, ST-SWEM and OC models – Organic Carbon

The test simulation with ST-SWEM was repeated with the OC model and graphically compared for a grid-cell located at RM 2.0 in the LPR at grid indices (18,42) of the collapsed grid (see Figure 1).

The algal carbon concentration calculated by ST-SWEM at this location is shown in Figure 2 with the black line labeled 'ST-SWEM'. That result does not appreciably differ from the results calculated by the OC model (shown with the red line) until May 1996. From June 1996 until the end of September 1996 there are relatively large differences between the two models. The OC model results are more in line with measurements (3 mg C/l corresponds to about 40 - 100 ug/l Chl-a concentrations which is approximately the upper bound of the range of recent values measured within the LPR). The higher ST-SWEM values may be caused by continuation of algal growth and probably by a lack of additional mortality due to the higher salinity concentrations in this area of the model domain. The OC model does not simulate other algal dynamics such as growth, mortality, respiration, etc. Rather, the OC model only includes a settling process that results in a decline in OC concentrations downstream. Subsequent sections will address the importance of this on the contaminant simulation results.

Both the ST-SWEM model as well as the OC model computes the time-variable POC content in the bed. Figure 3 shows a comparison of POC concentration in the upper 15 cm of the sediment bed for the grid cell location shown in Figure 1. Although both models tend to show mostly similar temporal patterns and responses to short-term events, over the course of the year, the OC model calculates an increase of 6% whereas ST-SWEM calculates a decrease of 7% relative to the initial condition. Further analysis of the

differences showed that while the OC model uses a constant settling rate for algae related carbon, ST-SWEM uses a temperature dependent rate as shown in Figure 4.

In addition to the afore-mentioned differences, ST-SWEM models phytoplankton with temperature and nutrient depending growth rates and mortality rates. In contrast, the AOC model does not include any algal growth nor any nutrient or temperature dependencies which can cause a net increase in algal concentrations within the LPR and NB. The only fate and transport process for algae in the OC model (in addition to advection and dispersion) is settling. These differences between the algal kinetics in the OC and ST-SWEM models likely explains the difference in algal concentrations between the two approaches during the summer months when algal growth would be expected to be occurring within the LPR.

3.3 Comparison, ST-SWEM and OC models – Contaminants

The results of both ST-SWEM and OC models were used with the one-year RCATOX test simulation received from Region 2 and the impact of the varying approaches to modeling OC assessed for contaminant fate and transport. The test simulation was performed over the same one-year period simulated in the OC and ST-SWEM models. The OC linkage results from ST-SWEM and OC model runs were used to perform a fate and transport simulation for 2,3,7,8 TCDD using the RCATOX model setup received from Region 2. The results are presented in terms of the contaminant mass in the water column and various sediment layers (active layer which refers to the top 15 cm of the bed, archive layer which refers to the depth-interval between 15 cm and 107 cm, and deep bed which includes the depth-interval below 107 cm) over two reaches in the LPR – one from RM 8 to Dundee Dam and one from RM 8 down to RM 0. Figure 5 through Figure 8 show the results of this comparison. RCATOX results using the ST-SWEM model linkage results are labeled with legend ‘ST-SWEM’ and shown in green, and RCATOX simulations using the OC model linkage results are labeled with legend ‘AOC’ and shown in red.

a. Upper part of the LPR (RM 8 – 17)

Figure 5 shows model-calculated results for 2,3,7,8 TCDD mass in the water column and in the active layer between RM 8-17. Figure 6 shows similar results for mass in the archive and deep bed layers. Although both simulations start with the same initial condition, the results diverge over time. Water column and active layer mass shows differences within about a month from the start of the simulation, and the archive and deep bed layers after about 2-3 months. These non-negligible differences are further discussed in the following section.

b. Lower part of the LPR (RM 0 – 8)

Figure 7 shows model-calculated results for 2,3,7,8 TCDD mass in the water column and in the active layer between RM 0-8. Figure 8 shows similar results for mass in the archive and deep bed layers. As with the comparisons for RM 8-18, although both simulations start with the same initial condition, the results diverge over time. Water column and active

layer mass shows differences shortly after the start of the simulation, and the archive and deep bed layers after about 1-2 months. These non-negligible differences are further discussed in the following section.

3.4 ST-SWEM and OC Models, Differences – Contaminants

In depth analysis of the differences presented in Figure 5 through Figure 8 indicated that the differences in contaminant results are primarily related to the use of different particle mixing rates within the active layer in ST-SWEM and OC. As shown in Figure 9, ST-SWEM calculates a temperature-dependent (i.e., seasonal) particle mixing rate, whereas the RCATOX model uses a constant mixing rate to calculate mixing of particulate-phase contaminants between the individual layers (on the order of 1 cm each in thickness) within the active layer in the RCATOX model. The particle mixing rate calculated by ST-SWEM shows seasonal variations, with lower values in winter and higher values during the summer months, and varying by over an order of magnitude from low to high. In contrast, the OC model simulation used for this test simulation used a constant particle mixing rate of about $0.65 \times 10^{-4} \text{ m}^2/\text{d}$ or $237 \text{ cm}^2/\text{year}$.

In addition to affecting particulate-phase concentrations within the active layer, the seasonal variations in particle mixing rate also affect the dissolved-phase mixing within the active layer and the dissolved-phase contaminant flux between the sediment bed and the water column. However, the most crucial mixing term is the particle mixing rate because the majority of the contaminants are partitioned to sediment particles in the bed. In the contaminant model, higher particle mixing rates are expected to reduce contaminant concentration gradients across the individual layers that make up the active layer of the sediment bed.

Figure 10 (for RM 8-17) and Figure 11 (for RM 0-8) show the results of a RCATOX sensitivity run examining the impact of difference in particle mixing rates. RCATOX results using ST-SWEM model output for OC linkage are shown with a black line, and RCATOX results using OC model output for OC linkage are shown with a red line; these are also the results shown in Figure 5 and Figure 7. RCATOX results using the same particle mixing rate as the ST-SWEM model output but using the remainder of the OC model output for OC linkage are shown with a green line. In both the upper LPR (RM 8-17) as well as the lower miles of the LPR (RM 0-8), RCATOX results driven using ST-SWEM are practically identical to that using OC with ST-SWEM mixing rates. The only differences occur during the summer months (June – September). As seen in the comparisons presented in Figure 2, there is a significant difference in the algal carbon results between ST-SWEM and OC models during the summer months. The higher algal carbon calculated by ST-SWEM during the summer months results in a higher proportion of contaminants to be partitioned to the slower settling algae in the RCATOX simulation using ST-SWEM as compared to the RCATOX simulation using OC. This causes a higher contaminant mass in the water column and thus a higher net export of contaminants in the case of the RCATOX simulation driven by ST-SWEM linkage output.

In addition to the particle mixing rate, another source of the difference between the RCATOX results driven by ST-SWEM and OC models, primarily in contaminant mass in the archive and deep bed layers, originates from differences in the thickness of the archive layer and the changes calculated therein. ST-SWEM uses the sedimentation and resuspension information from ECOM-SEDZLJS along with a spatially and vertically constant dry density to calculate changes in bed and archive layer thickness. However, the OC model uses the ECOM-SEDZLJS outputs of bed thickness to calculate archive layer thickness.

In order to examine the impact of the difference in bed layer thicknesses between ST-SWEM and OC, a RCATOX sensitivity simulation was performed using the same particle mixing rate and active/archive/deep bed layer thicknesses as the ST-SWEM model output but using the remainder of the OC model output for OC linkage. Figure 12 through Figure 15 show the results of this sensitivity run (shown with green line) in comparison to RCATOX results using ST-SWEM model outputs (shown with black cross-marks), and RCATOX results using OC model outputs (shown with red line). The results show that by eliminating the two important physical differences in model inputs, the OC model and the ST-SWEM driven results are almost identical. Only Figure 14 shows a minor difference for the months of June – September due to differences in Chl-a concentrations between ST-SWEM and OC models.

3.5 Summary

The OC model was implemented following the simplified approach for representing OC dynamics within the LPR and NB study areas as agreed upon in discussions between the EPA and the CPG. The OC model performance was compared against ST-SWEM model performance for OC. A few differences related to primary production and algal dynamics were identified and attributable to the lack of eutrophication dynamics in the AOC model. A similar comparison was also performed for contaminants in the bed and water column using RCATOX simulations driven by ST-SWEM and OC models. Differences in contaminant results were identified as primarily driven by differences in particle mixing rates and bed layer thicknesses between ST-SWEM and OC models. Differences in contaminant results driven by primary production were relatively minor and primarily limited to the summer months and between RM 0-8.

4.0 AOC IMPLEMENTATION IN RI/FS SIMULATIONS

This section documents the OC setup and implementation for the remedial investigation of the LPR. The OC setup consists of the model grid, initial conditions, boundary conditions, and various parameter settings.

4.1 Computational Grid and Domain

The computational grid and domain used for the OC model application to the LPR and NB is the same as that used for the hydrodynamic and sediment transport model applications described in Appendix L and Appendix M, respectively. The model domain and the model grid are shown in Figure 16.

The model domain includes the 17.4-mile tidal stretch of the LPR extending from Dundee Dam to the mouth at Newark Bay, the Hackensack River (including the Meadowlands wetlands) from Oradell Dam to its mouth at Newark Bay, Newark Bay, and the tidal entrances to Newark Bay, namely the Arthur Kill extending to Raritan Bay and the Kill van Kull extending to upper New York bay. In addition to the algal and detrital OC entering from the freshwater and open boundaries listed above, several minor tributaries (Hackensack River, Second River, Third River, Saddle River), combined sewer outfalls, and storm-water outfalls also discharge OC into the LPR and NB. The model grid consists of 1942 horizontal elements, with an average grid size within the LPR of 40 m wide and 180 m long. The LPR is represented with 4 cells across (decreasing to 3 cells above RM 4.4, and 2 cells above RM 15.7).

4.2 Initial Conditions

The initial conditions for the OC model consists of inputs for detrital carbon in the active and archive layers of each grid cell, and for algal carbon and detrital carbon in the water column. Due to the relatively short residence time in the water column, the initial conditions for algal and detrital carbon are not relevant over the long-term simulations used in the calibration of the OC model. Initial conditions in the water column were therefore set using the ST-SWEM inputs developed by Region 2 as part of the Focused Feasibility Study (FFS; USEPA 2016).

Initial conditions for detrital carbon in the sediment bed were defined based on an analysis of data from the LPR and NB. Data from several historical and recent surveys were examined as part of this analysis. Figure 17 shows the locations in LPR and NB with measurements of detrital carbon in surficial sediments (top 15 cm of bed) and in the sub-surface (depth intervals below 15 cm in the bed). In NB, the data sources primarily include the 2005 Newark Bay Phase I and the 2007 Newark Bay Phase II survey data. In the LPR, due to the presence of several unrealistically and unexplainably high measurements of sediment total organic carbon (TOC) in some of the historical data, only data collected after 2004 were included for purposes of developing initial conditions. Accordingly, these data surveys correspond to:

- 2005 High Res Core Sampling
- 2007 EPA EMBM
- 2007-2008 Sediment Sampling Program
- 2008 CPG Low-resolution Coring Program
- 2009-2010 FSP2 Benthic Sediment Sampling
- 2012 CPG Benthic Sediment Sampling
- 2012 River Mile 10.9 Addendum A
- 2013 CPG Second Supplemental Sampling Program

Figure 18 and Figure 19 show spatial plots (along the longitudinal axis) of the LPR and NB for data collected in the top 15 cm of the bed (corresponding to the active layer in the OC model) and below the top 15 cm (corresponding to the archive layer in the OC model) for various survey programs following 2004. The data from the various surveys include measurements of sediment TOC (in units of mass of OC per unit mass of dry sediment), the fines content (fraction of sediment less than 63 μm), and the dry density of the sediments. These have been used to calculate the fraction organic carbon (f_{OC}) which is the OC content expressed in percentage terms relative to mass of dry sediments and shown on the upper panels in Figure 18 and Figure 19. The middle panels in Figure 18 and Figure 19 show the apparent f_{OC} on fine sediments (fraction of sediment less than 63 μm), a quantity calculated using the measured f_{OC} and measured fines content. The calculation of apparent f_{OC} on fine sediments follows the assumption implicit in the ST-SWEM and OC models, that all the detrital carbon in the bed and water column is associated only with fine sediments. The bottom panels in Figure 18 and Figure 19 show the POC in the sediments, a quantity calculated using the measured TOC and measured dry density.

Apparent f_{OC} on fine sediments shown in Figure 18 and Figure 19 follows a general spatial pattern, decreasing from upstream to downstream in the LPR, and is relatively constant in NB. This general pattern also correlates with fines content in the LPR which increases from upstream to downstream. The correlation of apparent f_{OC} on fine sediments with fines content was therefore evaluated as shown in Figure 20, separately for the LPR (upper panels) and NB (lower panels). The evaluation was performed separately for the active layer (left panel) and archive layer (right panel). The data exhibit a general trend of decreasing apparent f_{OC} with increasing fines content in the LPR; this trend was quantified using a power function as shown in Figure 20. The dataset also includes a few data samples with apparent $f_{\text{OC}} > 100\%$ which likely reflects an artifact of the model framework assumption that detrital OC is only associated with fine sediments; these samples were therefore not included in the regression analysis. The regression was used as the basis for defining the initial condition in the LPR for detrital OC in bed. In NB, the data do not indicate a trend with fines content. Rather, the only trend in NB is a slight spatial trend in

bulk sediment f_{OC} as seen on the top panel of Figure 18, decreasing from the mouth of the LPR to the vicinity of the intersection of the navigation channels leading to the Kill van Kull, Arthur Kill, and middle of southern NB (located at approximately RM -5), followed by a slight increase in f_{OC} . Therefore, the f_{OC} data in NB were averaged over 1-mile intervals and the averages were used to assign detrital carbon initial conditions.

The detrital carbon initial conditions in the bed were determined by first calculating the apparent f_{OC} on fines using the results of the sediment transport model for fines content in the active and archive layers at the beginning of WY1996 along with the regressions (in the LPR; Figure 20). The calculated apparent f_{OC} on fines was converted to bulk sediment f_{OC} and used to compare against measured values for an assessment of the calculated initial conditions. Figure 21 and Figure 22 shows the calculated initial conditions for apparent f_{OC} on fines and f_{OC} in the active and archive layers in relation to measured values. Since the sediment transport model incorporates spatial trends in grain size distribution, the calculated apparent f_{OC} on fines (upper panels in Figure 21 and Figure 22) follows the spatial trends noted in Figure 18 and Figure 19. The resulting f_{OC} on bulk sediments (lower panels in Figure 21 and Figure 22) is also consistent with the range of measured values. The calculated bulk sediment f_{OC} was subsequently converted to POC for model input using the dry density calculated by the sediment transport model in the active and archive layers at the beginning of WY1996. The initial conditions thus developed represent the net POC in the sediment, i.e., the sum of inert, labile, and refractory carbon.

4.3 Boundary Conditions

The boundary conditions for the OC model consist of specification of concentrations of algal and detrital OC entering the model domain from (1) various freshwater inflows such as Dundee Dam, Hackensack River, Saddle River, Second River, Third River, and MacDonald Brook, (2) combined sewer overflows and stormwater outfalls, and (3) the inflowing tide at the Arthur Kill and Kill van Kull tidal boundaries. Although these inputs were defined based on ST-SWEM model inputs derived by Region 2 for the FFS (USEPA, 2016; LBG, 2014), the approach is described here briefly.

4.3.1 Dundee Dam, Hackensack River, and Saddle River

Being the dominant source of freshwater to the LPR and NB, algal and detrital OC loadings from Dundee Dam incorporate recent measurements conducted as part of various programs. Loadings for detrital OC were derived based on measurements from various programs (2005 EPA Small Volume water column sampling study, the 2008 EPA High Flow Storm Event Sampling, and the Physical Water Column Monitoring [PWCM; AECOM 2009] and Chemical Water Column Monitoring [CWCM; AECOM 2011] sampling programs conducted between 2009 and 2013 as part of the LPR and NB remedial investigation). Briefly, the detrital OC loadings were developed as a function of river flow, and the resulting function applied to the long-term time-series of river flow to estimate detrital OC loadings from Dundee Dam.

Loadings for algal carbon were based on a simpler approach using data from the Passaic Valler Sewerage Commission (PVSC) and New Jersey Harbor Dischargers Group (NJHDG). The measured values of Chl-a after conversion to algal OC (using a C:Chl-a ratio) were specified for the day of measurements. For periods with data, the values were linearly interpolated between data points and for months without any data the long-term average of the data collected in that month across all years was used.

Algal OC loadings from the Hackensack and Saddle Rivers were based on seasonal average concentrations calculated using data collected in 1994-1995 (HydroQual, 2007). POC loadings in the Hackensack and Saddle Rivers were estimated using the rating curve approach described for Dundee Dam and using data collected in 1994-1995 (HydroQual, 2007).

4.3.2 Combined Sewer Overflows and Stormwater Outfalls

OC loadings from combined sewer overflows and stormwater outfalls are restricted to detrital carbon. These were calculated using temporally-constant concentrations associated with these inflows along with time-variable flows. The temporally-constant concentrations were calculated using data collected in 1994-1995 (HydroQual, 2007).

4.3.3 Second River, Third River, and MacDonald Brook

Due to lack of suitable measurements of algal and detrital OC, and given the limited watershed of these tributaries, the runoff and OC loadings from these tributaries are expected to be dominated by stormwater runoff. Therefore, the OC loadings from these tributaries was calculated using time-variable river flows paired with the constant detrital OC concentrations used for stormwater outfalls.

4.3.4 Marine Boundaries

Algal and detrital OC loadings at the Arthur Kill and Kill van Kull tidal boundaries were defined using the results of a eutrophication model of NY harbor developed under the CARP program (HydroQual, 2007). The boundary conditions are specified as daily average concentration at these locations, with the loadings calculated internally by the model based on the tidal inflow volumes.

4.4 Model Parameterization

The parameterization of the OC model includes the inputs necessary for the fate and transport of algal and detrital OC. These inputs include the hydrodynamic model linkage, the sediment transport model linkage, the settling velocity for algal OC, inputs for DOC, and an input specifying a lower limit on bed POC calculated by the model. These are briefly described next.

4.4.1 Hydrodynamic Model Linkage

The linkage files necessary to perform OC model calculations derive from the ECOM hydrodynamic model. These are saved as 15-minute averaged quantities over the same horizontal and vertical resolution as the ECOM and OC model grids. The linkage files include quantities describing the advection and dispersion rates, salinity, and temperature (in 3D), and water depths. The OC model subsequently reads the saved hydrodynamic model output and uses these for its fate and transport computations.

4.4.2 Sediment Transport Model Linkage

The linkage files necessary to perform OC model calculations derive from the ECOM-SEDZLJS sediment transport model. These are saved as 15-minute averaged quantities over the same horizontal and vertical resolution as the ECOM and OC model grids. The linkage files include quantities describing the suspended sediment concentrations, erosion and deposition fluxes, bed thickness, and the mass and composition of the active and archive layers. The OC model subsequently reads the saved sediment transport model output and uses these for its fate and transport computations. In particular, since the AOC framework associates all detrital OC with fine sediments (fraction of sediments <63 μm), the erosion and deposition rates computed by the sediment transport model for fine sediments is used by the OC model to calculate the erosion and deposition rates of detrital OC.

4.4.3 Settling Velocity for Algal Carbon

As mentioned previously, the settling velocity of algal OC is an input to the OC model. It is used to solve for the settling of algal OC through the water column followed by deposition to the bed. Settling represents the only adjustable process in the OC model. Model inputs for this term were based on ST-SWEM model inputs. As mentioned in Section 3, the ST-SWEM model includes a temperature-dependent settling velocity for algal OC. This was approximated in the OC model using a temporally constant value of 0.2 m/d. This is a typical representative value for algae and is over an order of magnitude lower than that of the slowest-settling sediment class in the ECOM-SEDZLJS sediment transport model.

4.4.4 DOC

As described in Section 2, DOC is not a state variable in the OC model. Rather, it is treated as an input to the OC model; the input DOC is written to the OC linkage file containing the OC model results passed to the contaminant fate and transport model.

DOC inputs to the OC model were developed from an analysis of DOC measurements from various surveys. The data sources include the PVSC and NJHDG surveys which included several stations within the LPR and NB (PVSC 2002; NJHDG 2006), the PWCM program (AECOM 2009), the CWCM program (AECOM 2011), as well as a few other minor

monitoring programs. Figure 23 shows a location map of the stations sampled during the various monitoring programs. The various monitoring programs include several stations in common.

In the interest of assessing the DOC in the LPR to determine representative inputs, the available data have been grouped into spatial bins and assessed for mean values, temporal trends, and spatial gradients. Figure 24 shows the results of this analysis. This analysis was also performed by segregating the data seasonally into the summer months (May-September) and non-summer months when the impacts of eutrophication would be expected to be lower. However, the analysis showed only a ~10% difference in mean DOC values in any given bin; therefore, seasonal trends were not included in the remainder of this analysis.

The data are presented probabilistically in Figure 24, with the measurements within a given spatial reach (pink, black, and blue symbols) compared against measurements at Dundee Dam (grey symbols) for an assessment of spatial trends. Mean and median values along with the sample size in each bin are also tabulated. The spatial bins extend from Dundee Dam through the LPR and into NB. The presentation also includes the boundaries of NB - the Hackensack River entrance, Arthur Kill, and Kill van Kull. In general, the data show a spatial trend of decreasing DOC from Dundee Dam through LPR and NB, and towards Kill van Kull, mainly driven by lower DOC water entering from NB with the flood tide. Mean DOC ranges over a relatively small range from 5.06 mg/L at Dundee Dam to 3.96 mg/L towards the mouth of the LPR and about ~3.1 mg/L within NB. Within NB, the available data was segregated into two zones above and below RM -1.5 (located just north of the Port Newark terminals). DOC within any given spatial bin also exhibits relatively small variability, with the variation from -1 to +1 standard deviation around the median limited to about a factor of three. In addition, the relatively low DOC values, on average, also suggest relatively small impact on contaminant fate and transport from partitioning to DOC. Therefore, DOC was defined as a spatially variable but temporally constant input to the OC model. Since most of the data within a given bin is from the PVSC/NJHDG dataset, the mean calculated for each spatial bin was assigned to the location of the PVSC/NJHDG station, with DOC at intermediate locations calculated by interpolation. The DOC assigned to given location or model grid cell was also assigned as a constant vertically in the water column.

4.4.5 *Minimum POC*

To ensure numerical stability, especially in the use of the OC model results in RCATOX, a minimum bed POC value is defined as an input to the OC model. This value is based on the measured POC presented in Figure 18 and Figure 19 (bottom panels). POC values within the LPR and NB range over nearly two orders of magnitude, starting from 1000 mg/L (although there is one measured POC value of ~500 mg/L it has been treated as an outlier for purposes of this evaluation). Therefore, a minimum POC of 1000 mg/L is defined in the model. In other words, the model limits the calculated POC in the active and archive layers from decreasing beyond this value at any point during the simulation.

4.5 Summary

The OC model was set up and parameterized for application to the LPR. Model inputs were derived from various sources. Initial conditions in the water column and boundary conditions (OC loadings) were set to the same values as Region 2's ST-SWEM model application (USEPA 2016). Initial conditions for detrital OC in the sediment bed were derived based on an analysis of sediment TOC measurements from various surveys conducted as part of the remedial investigation. Finally, the ECOM hydrodynamic model summarized in Appendix L, and the ECOM-SEDZLJS sediment transport model summarized in Appendix M provide the remainder of inputs necessary to perform OC model simulations. The next section describes the model validation metrics and datasets, validation period, validation process, and performance.

5.0 OC MODEL VALIDATION PERFORMANCE

Following the development and testing of the OC model described in Section 2 and Section 3, respectively, the model was setup, initialized, and parameterized for application to the LPR as described in Section 4. Subsequently, the performance of the OC model was assessed against several metrics over various spatial and temporal scales. This section describes the validation metrics and datasets for the OC model, the validation period, validation process, and model performance relative to data.

5.1 Validation Target Metrics and Datasets

As mentioned previously, the state variables for the OC model include algal and detrital OC. Therefore, the OC model validation metrics include Chl-a (after converting the algal OC using a C:Chl-a ratio), and measures of detrital carbon in the water column (POC) and in the bed (f_{OC}). The data for these metrics was developed from several sources as listed below:

- Water column, Chl-a: PVSC and NJHDG data extending from 2003 through 2013
- Water column, POC: PWCM collected during 2009 and 2010, and CWCM data collected between 2011 and 2013
- Bed, f_{OC} : Various datasets described previously in Section 4 in association with the development of the initial conditions for detrital carbon in the bed.

The sample locations for Chl-a and POC are shown in Figure 23 and for bed carbon in Figure 17.

5.2 Validation Period

The period for assessing the OC model performance consists of a long-term continuous simulation starting at the beginning of WY1996 and proceeding through WY2013. This also corresponds to the calibration period for the ECOM hydrodynamic and ECOM-SEDZLJS sediment transport models, and the linkage files generated by these models were used for performing OC model simulations over this long-term period.

5.3 Validation Process

As described previously, the AOC framework represents a simplified eutrophication model without algal growth kinetics, nutrient dependencies, and sediment diagenesis. In other words, the AOC model is an OC fate and transport model, with very limited parameters for calibration. The only fate and transport processes relevant for algal and detrital OC in the AOC is erosion and deposition. For detrital OC, the parameterization of the erosion and deposition processes are based on erosion and deposition rates calculated by the ECOM-SEDZLJS sediment transport model. For algal carbon, the settling/deposition rate was

defined based on calibration established by Region 2 for their ST-SWEM model application (USEPA, 2016). This parameter value (0.2 m/d) was not altered during the OC model application to the LPR and NB since the model performance using this parameter value was judged to be acceptable and reasonably good in reproducing various validation metrics as discussed in the following text. In other words, the OC model application to the LPR and NB was not subject to additional calibration.

5.4 Validation Performance

Model performance has been assessed for the validation metrics discussed previously by examining the model results for spatial and temporal trends apparent in data, by comparing the model results and data probabilistically, and using cross-plots of model results plotted against measured values. In addition, for POC, model performance has also been assessed by reviewing the trend of POC versus suspended sediment concentration (SSC) in both the model and data. Model performance for each of these metrics and trends is described next.

5.4.1 Water Column, Chlorophyll-*a*

Algal growth in natural systems such as the LPR varies on a seasonal basis, with the summer months subject to more algal growth and algal levels than winter months. Therefore, model performance for algal OC has been assessed spatially as well as seasonally, with summertime considered to be May through September, and wintertime as October through April. Furthermore, as mentioned previously, the OC model simulates the fate and transport of algal OC, with summertime and wintertime phytoplankton groups modeled separately. These were converted to Chl-*a* concentrations using the C:Chl-*a* ratio used in ST-SWEM and summed for comparison to measured Chl-*a* concentrations.

Figure 25 and Figure 26 show cross-plots of measured Chl-*a* and model-calculated Chl-*a* at the corresponding location and time for summertime and wintertime periods, respectively with the individual panels showing comparisons for individual locations. Lines corresponding to perfect correspondence between model and data, as well as +/- factor of 5 are also shown. Note that at Dundee Dam, the model results correspond to results in the very first grid cell downstream of Dundee Dam rather than the boundary condition, and so may reflect some influence of advection from downstream locations. However, advection affects only a relatively minor fraction of the dataset; most model results match with measured values, as expected. Moving downstream from Dundee Dam, the general trend of decreasing Chl-*a* apparent in the data is reproduced by the model. However, the model results tend to be less variable than measured values. Nonetheless, most model-calculated values are within a factor of 5 of measured values. These general trends in model performance are true of both summertime and wintertime comparisons.

Figure 27 and Figure 28 show the same information as Figure 25 and Figure 26 except plotted probabilistically. In general, the measured and model-calculated Chl-*a* distributions agree well in terms of the range of values as well as the shape of the distribution at all locations. The only notable difference is in the spatial trend of Chl-*a* within the LPR. During the summer months, measured Chl-*a* increases with distance downstream from

Dundee Dam, reaching a maximum at RM 8.1 and decreasing thereafter. The increase in Chl-a within the LPR likely reflects algal growth due to seasonal temperature variations as well as longer residence time due to lower river flows during the summer months. However, the OC model, because it does not incorporate algal growth, does not reproduce the increase in measured Chl-a within the LPR. Nonetheless, the difference between the mean measured and model-calculated Chl-a is only 37% at RM 8.1, the location showing the largest impact of algal growth in the LPR. This suggests that the impact of neglecting algal growth on OC dynamics is somewhat limited. In contrast to the summertime trends, mean measured Chl-a during the winter months shows a decreasing trend with distance downstream from Dundee Dam likely due to loss due to settling and dilution with lower Chl-a water entering from Newark Bay. The OC model successfully reproduces these trends.

Figure 29 shows another comparison of the spatial and temporal trends in the data and model results. Both model and data are shown for the period WY2010 to WY2013 (since this is also the period with POC data). The box and whisker symbols indicate statistics for the data (in black) and for model results (in red) at the same location and time as the measured values. The mean and range of model results over the entire period WY2010 to WY2013 are also shown with the black line and grey shaded region. The spatial and temporal trends described previously are also apparent in this figure. The increase in measured Chl-a seen in the upper few miles of the LPR during the summer months is not reproduced by the model. Rather, during both summer and winter months, the model calculates a decrease in Chl-a moving downstream from Dundee Dam. As mentioned previously, the impact of algal growth is limited in the domain both spatially and temporally. The impact of this bias can be further assessed quantitatively by examining model performance for POC in the water column, as well as in the bed. Since deposition of OC (both algal and detrital) from the water column represents the primary source of OC in the bed, any impacts due to the lack of algal growth in the OC model could potentially affect the calculations of bed OC over the long term. Therefore, the long-term assessment of model performance for bed OC presented subsequently represents an additional check on any potential artifacts from the lack of algal growth in the OC model.

5.4.2 *Water Column, POC*

Measurements of water column POC typically measure OC on the particulate matter retained after filtering whole-water samples. Therefore, measurements of POC reflect the presence of detrital as well as algal OC. Therefore, model results for algal and detrital OC were summed for purposes of comparison to measured water column POC. Model performance for POC has been assessed in the same fashion as presented for Chl-a using spatial, temporal, and probabilistic comparisons. An additional metric (trend of POC versus TSS) is also presented.

Figure 30 and Figure 31 show cross-plots of measured and model-calculated POC at the corresponding location and time for summertime and wintertime periods respectively, with the individual panels showing comparisons for given spatial reach. Lines corresponding to perfect correspondence between model and data, as well as +/- factor of 5 are also shown.

Note that at Dundee Dam, the model results correspond to results in the very first grid cell downstream of Dundee Dam rather than the boundary condition. Moving downstream from Dundee Dam, the general trend of increasing POC up to RM 6-10 and decreasing thereafter is reproduced by the model. Most model-calculated values are within a factor of 2-3 of measured values. These general trends in model performance are true of both summertime and wintertime comparisons.

Figure 32 and Figure 33 show the same information as Figure 30 and Figure 31 except plotted probabilistically. In general, the measured and model-calculated POC distributions agree well in terms of the range of values as well as the shape of the distribution at all locations. However, the predicted POC tends to be biased higher than data in the stretch between RM 0 and RM 4 both during summer-time and winter-time. This trend is not as noticeable upstream or in NB. One potential reason for this bias might be an over-prediction of the corresponding suspended solids by the sediment transport model (for example, as seen in Appendix M, Figure 60) leading to an over-prediction of the detrital POC. At the same time, a corresponding bias in the cohesive content of the suspended sediments could be another potential reason for this observed trend. The over-prediction of POC at this location could in turn potentially influence the contaminant fate and transport model's predictions by affecting contaminant partitioning in the water column and the relative strengths of dissolved and particulate fluxes.

On average, mean POC at all locations is higher during the summer months than winter months, likely reflecting the contribution of algae to water column POC. However, in contrast to Chl-a, the relative increase in measured POC within the LPR occurs during both summer and winter months, indicating that the increase in POC is not solely due to algal growth. Rather, the increase in POC reflects the influence of tidal and estuarine hydrodynamics on SSC which results in somewhat higher SSC within the estuarine turbidity maximum (ETM; a spatial zone, the exact location of which depends on the tidal phase, and river flow). During the low-moderate river flow conditions under which most of the POC data were collected, the ETM is expected to be located approximately upstream of RM 4. This likely explains the relative increase in POC (compared to locations upstream or downstream) seen between RM 6-10 during the summer months, and between RM 4-6 during the winter months. This relation between POC and SSC is further assessed subsequently.

Figure 34 shows another comparison of the spatial and temporal trends in the data and model results for POC. Both model and data are shown for the period WY2010 to WY2013. The box and whisker symbols indicate statistics for the data (in black) and for model results (in red) at the same location and time as the measured values. The statistics for both model and data were calculated over 1-mile spatial bins. The mean and range of model results over the entire period WY2010 to WY2013 are also shown with the black line and grey shaded region. The spatial and temporal trends described previously are also apparent in this figure – both model and data during summer as well as winter months shows a gradual increase in POC moving downstream from Dundee Dam, reaching a maximum in the vicinity of RM 6 and decreasing thereafter towards lower values near the mouth of the LPR.

In order to examine the trend of POC with SSC mentioned previously, POC was paired with SSC, and the paired values plotted over various spatial bins. Figure 35 and Figure 36 show the resulting correlations of POC with SSC, for measured data (upper row), for the model results (middle row), and for the model results with the concentration of algal dry matter added to the SSC results from the ECOM-SEDZLJS model (bottom row). The model results were plotted in the latter fashion because algal solids are expected to be captured in the analytical methods for SSC which also relies on the water sample filtration procedure mentioned previously. However, the ECOM-SEDZLJS model does not simulate an algal solids class; the slowest settling class in the ECOM-SEDZLJS model has settling velocity an order of magnitude higher than associated with algal solids (OC) in the OC model. Therefore, adding the concentration of OC model results for algal dry matter (estimated using algal OC concentration and cellulose stoichiometry) to the ECOM-SEDZLJS results for SSC approximates the net concentration of particulate matter. The impact of this adjustment is primarily in areas associated with relatively lower SSC such as upstream of RM 13. The remainder of this discussion only considers the model results for SSC including algal dry matter.

Due to the tidal setting of the LPR and NB, there is gross erosion and gross deposition of sediments every tidal cycle, most prominently in the tidal and estuarine portion of the LPR and in NB. Consequently, detrital OC is also expected to be eroded and deposited over the same time-scales. Therefore, in general, data at all locations show a positive correlation between SSC and POC, a qualitatively reasonable relationship since POC which is predominantly composed of detrital OC, can be expected to scale with SSC. This general trend is also reproduced by the OC model at all locations. The model however appears to predict less of a reduction in f_{OC} at higher solids concentrations than suggested by the data at some locations. This could potentially be due to a slight model bias towards prediction of suspended solids with higher cohesive content and apparent f_{OC} , and influence the contaminant fate and transport model's predictions by affecting contaminant partitioning in the water column and the relative strengths of dissolved and particulate fluxes. The finding that the OC model produces generally similar trends as noted in the data with respect to POC and SSC serves as a validation of the SSC and OC erosion and deposition dynamics in the ECOM-SEDZLJS and OC models.

5.4.3 *Bed, f_{OC}*

OC model results for f_{OC} in the bed has been compared against measured values as an assessment of the long-term model performance. Due to the high spatial variability of bed f_{OC} data and since these data were also used in developing model initial conditions, this assessment of model performance is performed only qualitatively. In other words, the data have not been compared against model results at the exact time and location of measurement. Rather, the objective was to perform a comparison of measured values to model results and assess model performance over large spatial and temporal scales.

Figure 37 shows one such comparison – an assessment of spatial patterns of f_{OC} in the active layer in the OC model against measured bed f_{OC} data presented previously in the context of developing model initial conditions. The cross-sectionally averaged mean initial

condition is shown (with a black line), as well as the cross-sectional range and the cross-sectionally averaged mean model result at the end of the validation period are also shown (with shaded red area and red line). Comparisons for the apparent f_{OC} on fines as well as bulk sediment f_{OC} against corresponding data are shown on the upper and lower panels, respectively.

Comparing the cross-sectional mean initial and final model results for bulk sediment f_{OC} , in general, the OC model preserves the initial values for bed f_{OC} . Notable exceptions include a decrease upstream of RM 13, and an increase between RM 5-6. Review of the model performance of the spatial pattern in the apparent f_{OC} on fines suggests that the two exceptions in model results for bulk sediment f_{OC} noted in the LPR may be an artifact of the model framework assumption that all OC in the bed is associated with fine sediments. Even though the model is initialized with a spatial gradient in the apparent f_{OC} on fines, over the course of the validation period, the model tends to redistribute OC from high concentration areas to low concentration areas, leading to a relatively uniform spatial gradient (decreasing from upstream to downstream). This likely explains the decrease in apparent f_{OC} on fines upstream of RM 13, between RM 8-9, and the increase in bulk sediment f_{OC} between RM 5-6.

The temporal changes in apparent f_{OC} on fines noted above are likely related to the model framework assumption that all OC in the bed is associated with fine sediments. Natural sediments can be expected to have some OC associated with sandy sediments, albeit at order of magnitude lower concentrations than fine sediments. For instance, measurements from the Housatonic River (Weston, 2004) of OC on various sediment size fractions showed OC to be distributed across various size fractions, not just within the fine sediment classes. In the portion of the river characterized by coarse sediments, f_{OC} directly measured on non-cohesive particles averaged approximately 0.3%. In the muddier portions of the Housatonic River, the f_{OC} of the larger particles was over 10% in many cases; however, this was attributed to large pieces of organic matter, including sticks and leaves. Macro-organic material typically has lower particle densities and behaves differently than the large sand particles represented in the OC model of the LPR. The initial estimate of the model f_{OC} on fines is therefore likely overestimated, which might be responsible for the observed change in its value over time. It is possible that including OC on the sand fraction in addition to the fine fraction of the sediments may improve model performance in this regard.

In contrast to the model performance in the active layer, as shown in Figure 38, model performance in the archive layer shows only minor changes from the initial condition. This is largely due to the larger volume of the archive layer and the relatively small changes due to erosion and deposition. The only notable changes in the archive layer relate to apparent f_{OC} on fines upstream of RM 13, and between RM 5-6, with both locations showing a slight decrease, a trend similar to that seen in the active layer. The reason for this result is the same as explained for the active layer.

In addition to the qualitative assessment of spatial trends presented above, model performance has also been assessed probabilistically, by comparing the initial and final

results for bed f_{OC} in the active layer of individual cells to measured values in given spatial reach. Figure 39 shows the results of this comparison, with each panel including model results and data from given spatial reach. In most reaches, the range of values, and the shape of the distribution showing final results tends to similar range and shape as measured values. The only notable exception includes model results upstream of RM 12 which is characterized by predominantly sandy substrate and therefore susceptible to model framework assumption of no OC associated with sands. The differences between the measured and final results in this stretch could also be due to the data being biased towards pockets of fines with higher apparent f_{OC} within coarser areas at a scale that the model grid cannot capture. It is also noted from Figure 39 that the values representing the initial f_{OC} conditions tend to fall into a finite number of discrete levels. This is a consequence of the specification of the apparent f_{OC} as a function of the sediment cohesive fraction, and the finite number of initial representative sediment cores with a specified characteristic cohesive fraction in the sediment transport model.

5.5 Summary

The OC model performance was assessed by comparing model results for the various state variables in the OC model – water column algal OC (Chl-a), water column detrital OC (POC), and sediment bed (f_{OC}). The model was not calibrated beyond the parameter value for the settling rate of algal OC established as part of the ST-SWEM model calibration. The model was applied to and its performance evaluated over a continuous long-term simulation from WY1996 through WY2013. Model performance was evaluated over various spatial and temporal scales. Overall, the model reasonably reproduces the range of values, trends, and processes apparent in the data. Minor artifacts related to the lack of algal growth, OC loadings at the Arthur Kill and Kill van Kull boundaries, and related to the framework assumption of no OC on sands may affect model performance.

6.0 SUMMARY

A proposal was made to replace the eutrophication model component ST-SWEM from the LPR/NB Modeling Program by a data driven approach for the specification of organic carbon behavior in the LPR/NB modeling area. Since none of the remedial measures under consideration to address sediment contamination are expected to influence primary production, the simplification of the ST-SWEM eutrophication model component serves to reduce the modeling scope and schedule (by avoiding the effort involved in data collection, model development, and model calibration), and also eliminate associated modeling uncertainties.

After review of the proposal made by the CPG, the scientific discussion between Region 2 and the CPG modeling team led to the consensus that ST-SWEM was best replaced by the modeling of two substances: 1) algal carbon that behaves as a conservative substance with a relatively low settling rate, and 2) sediment-bound particulate carbon that settles and resuspends at the settling/deposition and erosion rates calculated by the sediment transport model. Furthermore, the organic carbon content in the sediment bed is based on a mass balance with the erosion and deposition fluxes of OC. This replacement is called the Alternative Organic Carbon approach (AOC).

The OC model was implemented following the description above. A non-calibrated and non-validated one-year test simulation with ECOM-SEDZLJS – ST-SWEM – RCATOX for the LPR/NB model area provided by Region 2 was run by the CPG modeling team using the ECOM-SEDZLJS – OC – RCATOX model sequence. Non-negligible differences were found. The main causes for the differences were identified to be: 1) the temperature-dependent particle mixing in the active layer of the bed used by ST-SWEM as opposed to the constant particle mixing used by the OC model, and 2) differences in archive layer administration. Differences in algal POC were also found for the summer months in the lower miles of the LPR. They had minor effect on the overall model outcome.

Next, the OC model setup for the LPR was refined from its initial application (which used inputs developed for ST-SWEM), primarily to reflect changes to boundary conditions made by Region 2, and for the initial condition for OC in the sediment bed. The OC model was then applied to a long-term period (from WY1996 through WY2013), and its performance assessed by comparison to water column Chl-a and POC data, and bed POC data over various spatial and temporal scales. In general, the OC model performs quite well in reproducing various trends, features, and processes apparent in the data. A few minor discrepancies evident between model and data are expected to be minor in terms of its impact on contaminant fate and transport processes. The OC model has subsequently been incorporated into the standard CPG modeling sequence ECOM-SEDZLJS – OC – RCATOX for use in RI/FS simulations.

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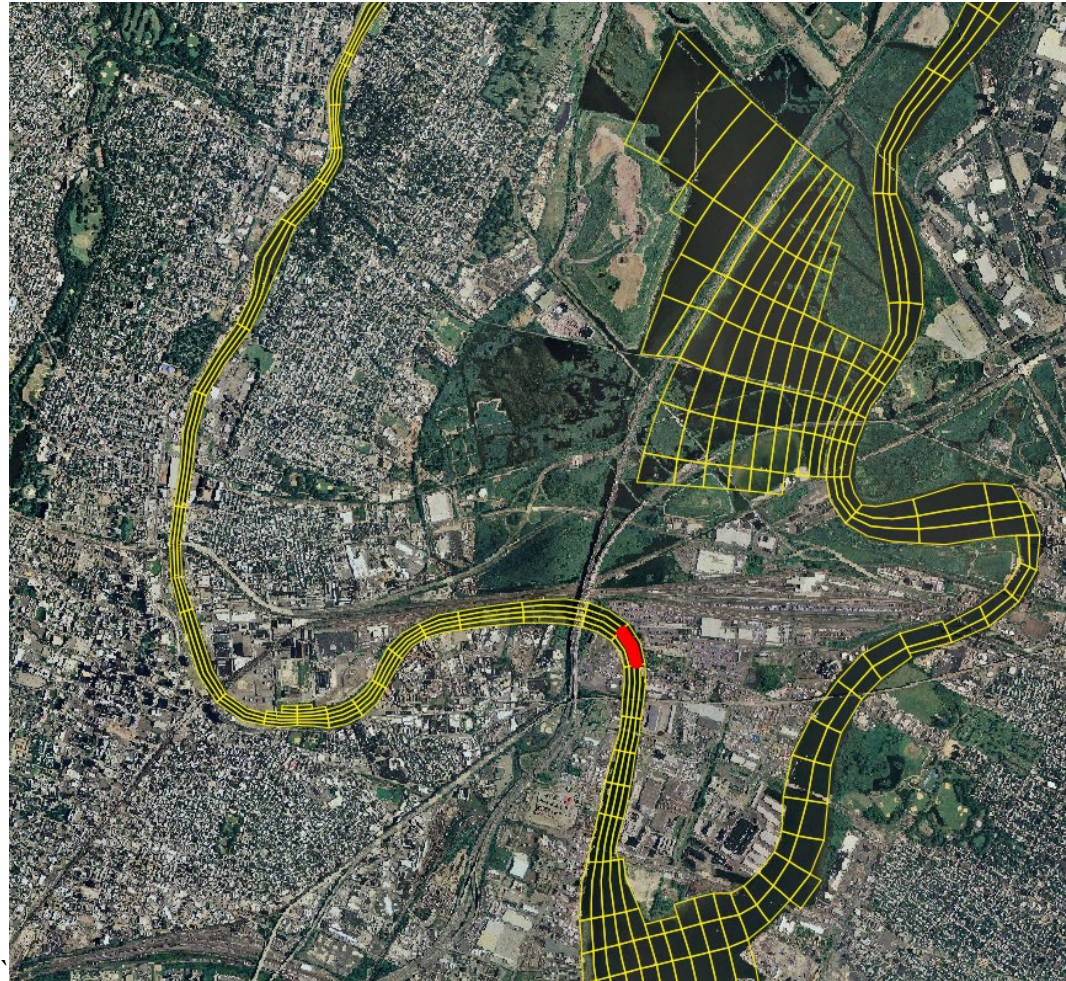


Figure 1 Lower Passaic River and NB confluence with cell (18,42) at RM 2.0

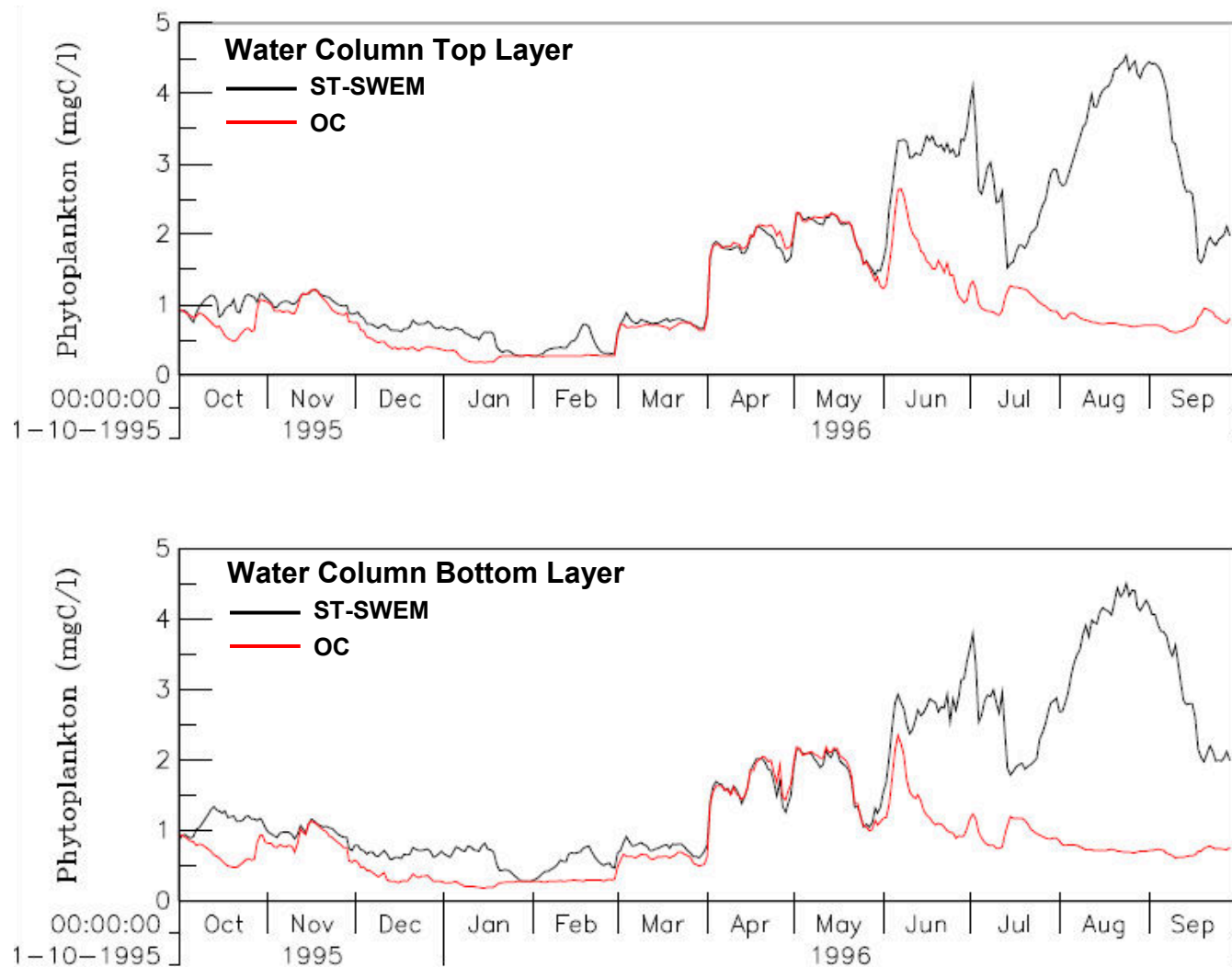


Figure 2. Phytoplankton carbon at RM 2.0, from ST-SWEM and OC models

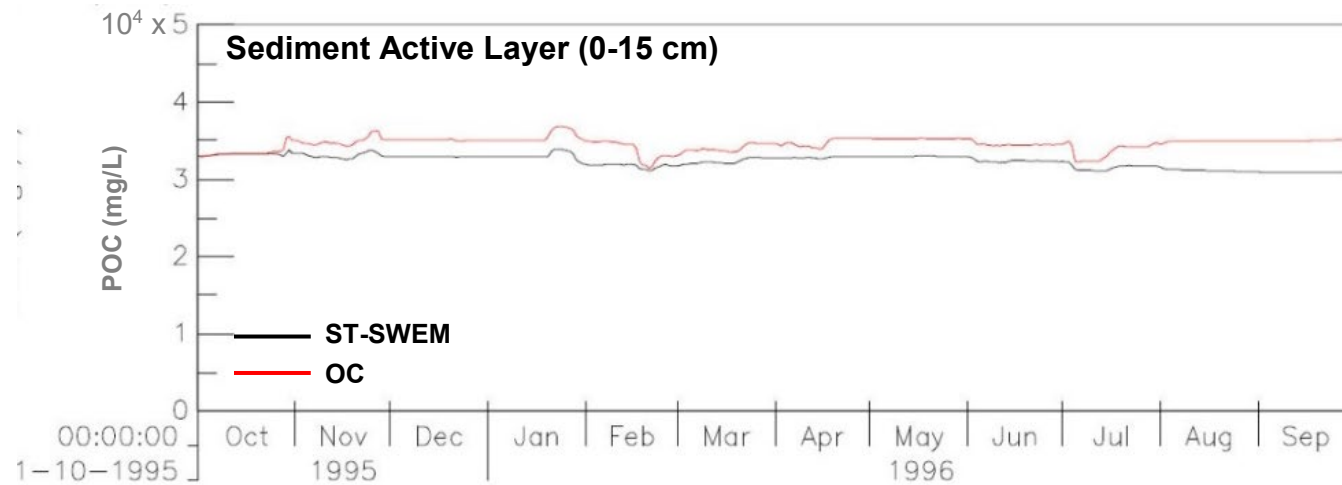


Figure 3. Accumulation of POC in the bed with ST-SWEM and OC models at RM 2.0

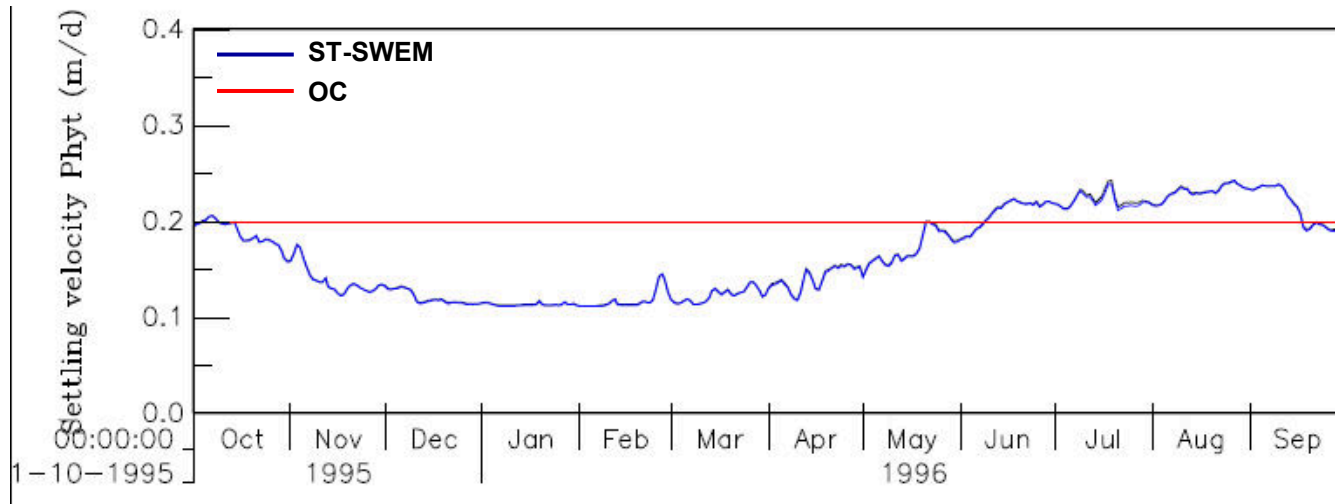


Figure 4. Phytoplankton settling rates at the water column surface at RM 2.0

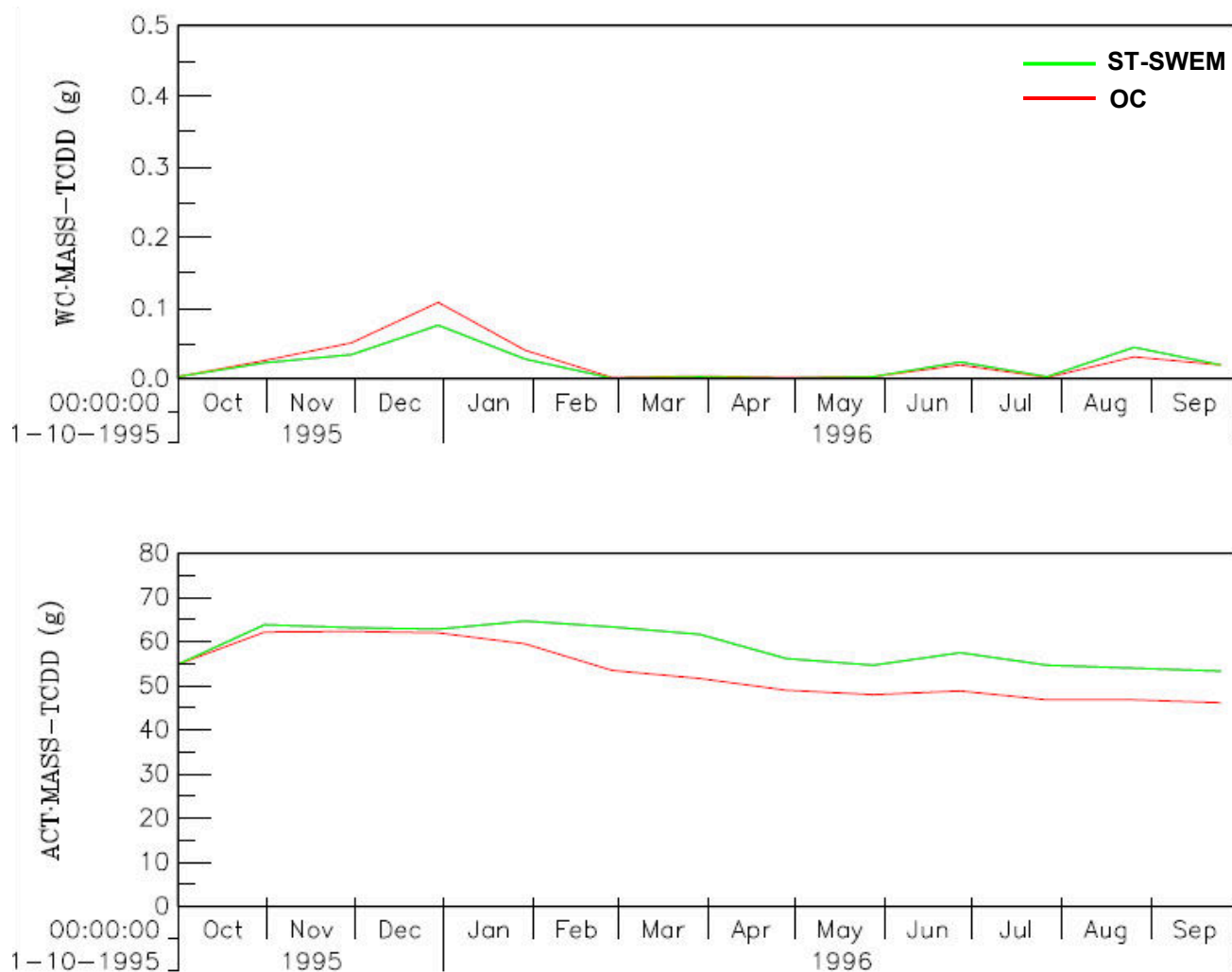


Figure 5. Total mass in the water column (upper panel) and the active layer (lower panel) in RM 8-17 using the ST-SWEM and OC models

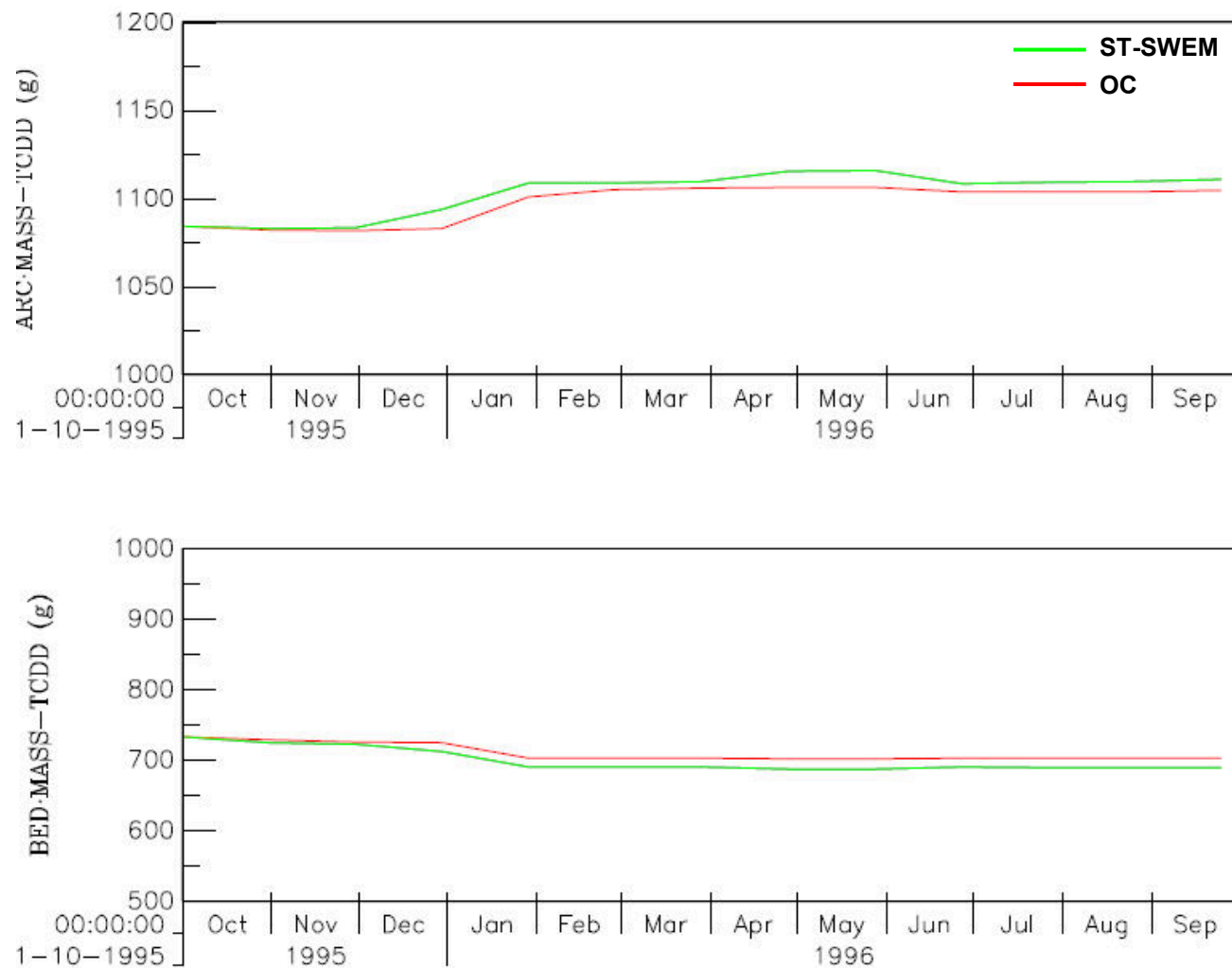


Figure 6. Total mass in the archive layer (upper panel) and in the deep bed (lower panel) in RM 8-17 using the ST-SWEM and OC models

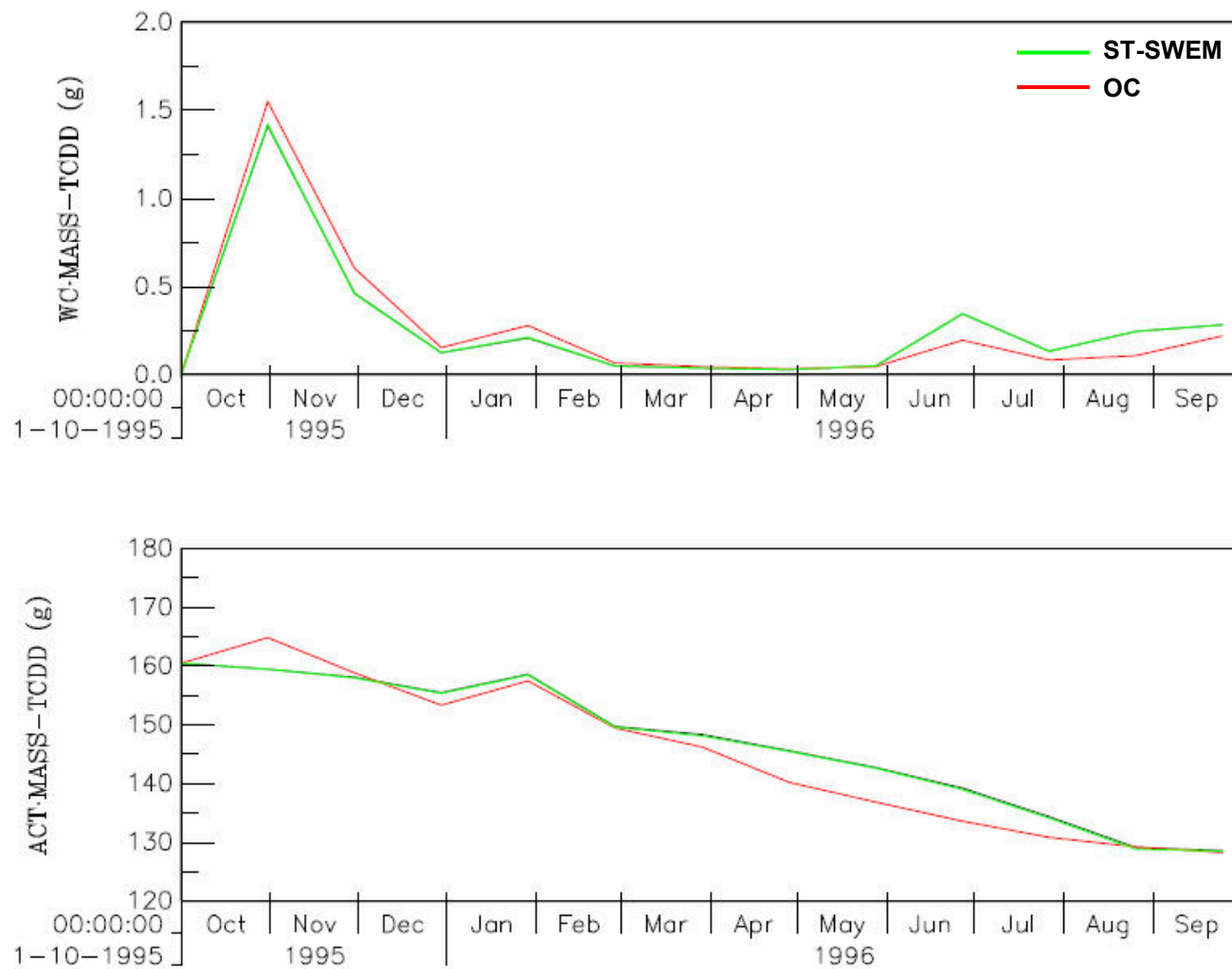


Figure 7. Total mass in the water column (upper panel) and the active layer (lower panel) in RM 0-8 using the ST-SWEM and OC models

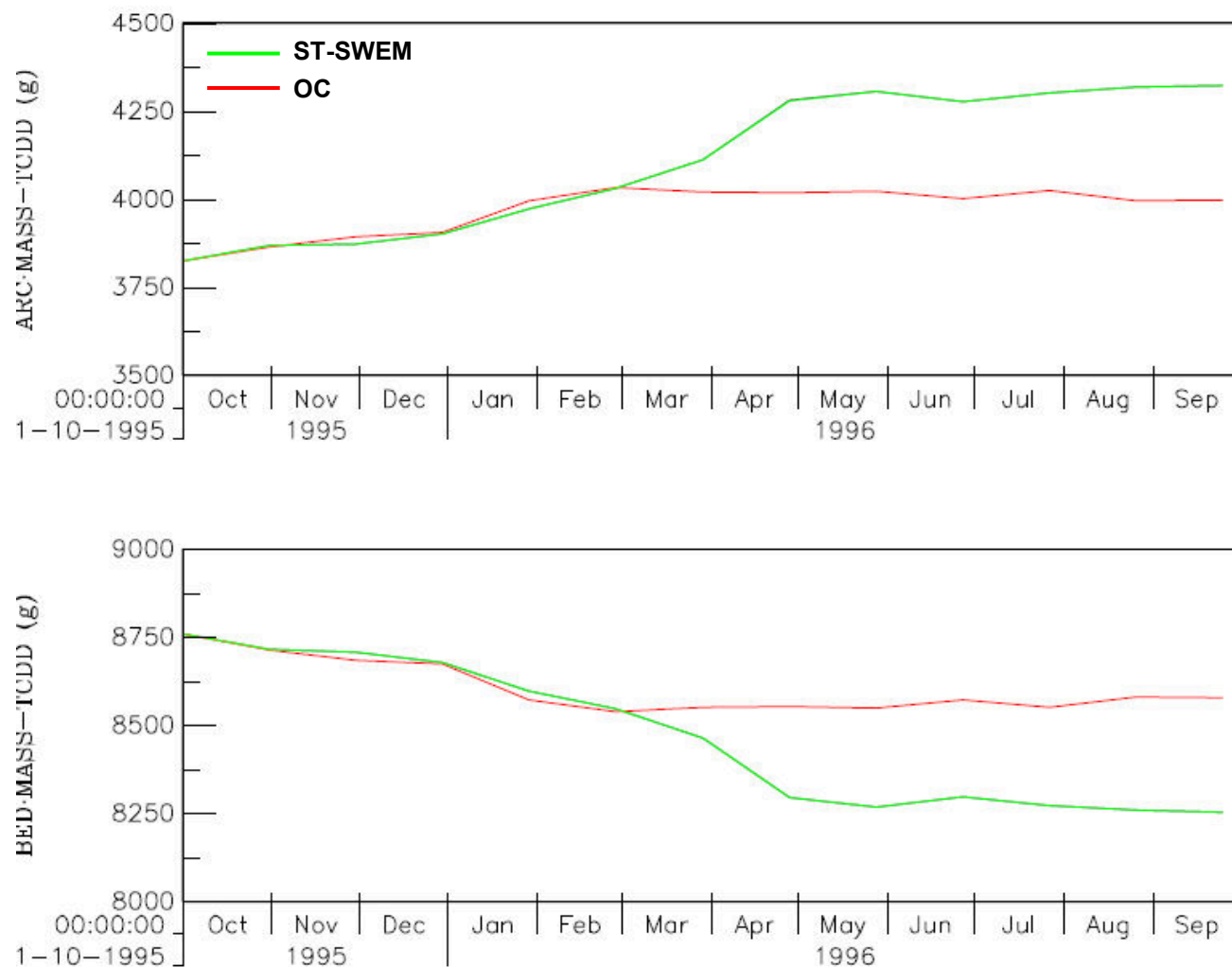


Figure 8. Total mass in the archive layer (upper panel) and in the deep bed (lower panel) in RM 0-8 using the ST-SWEM and OC models

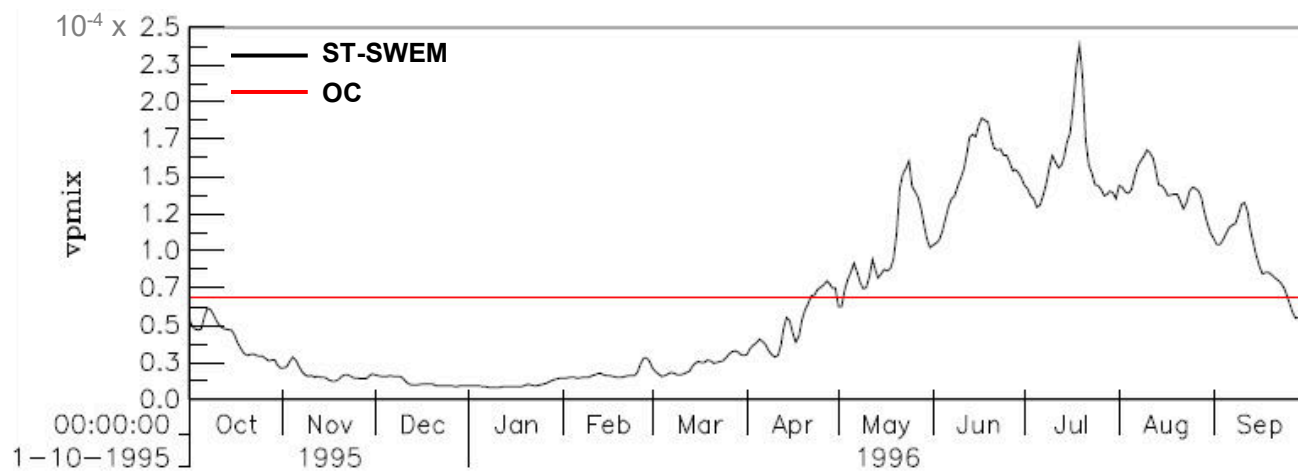


Figure 9. Particle mixing rate (units of m^2/d) within the active layer in ST-SWEM and OC models

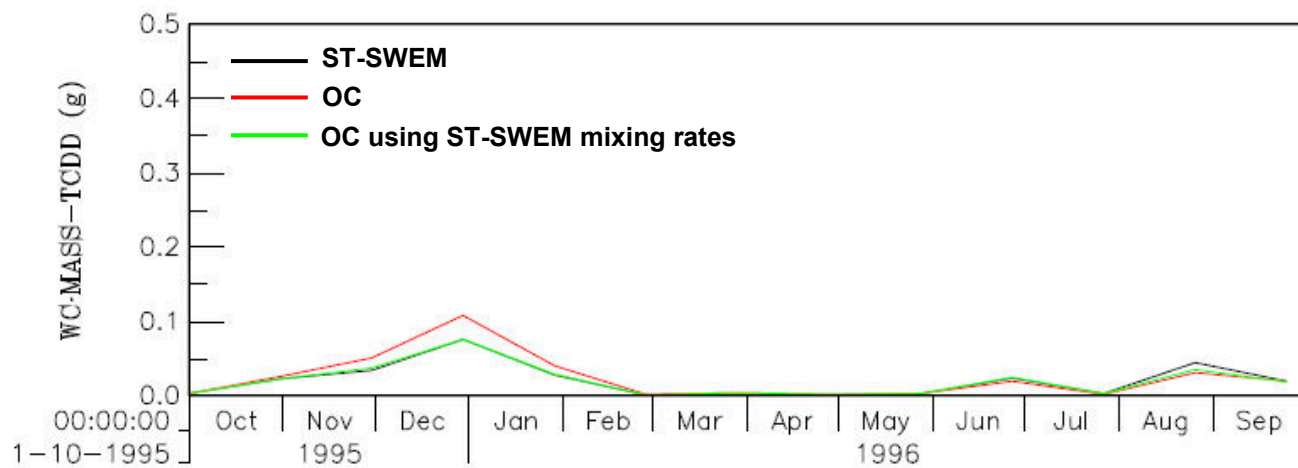


Figure 10. Total mass in the water column in RM 8-17 using the ST-SWEM and OC models, and OC model with ST-SWEM particle mixing rates

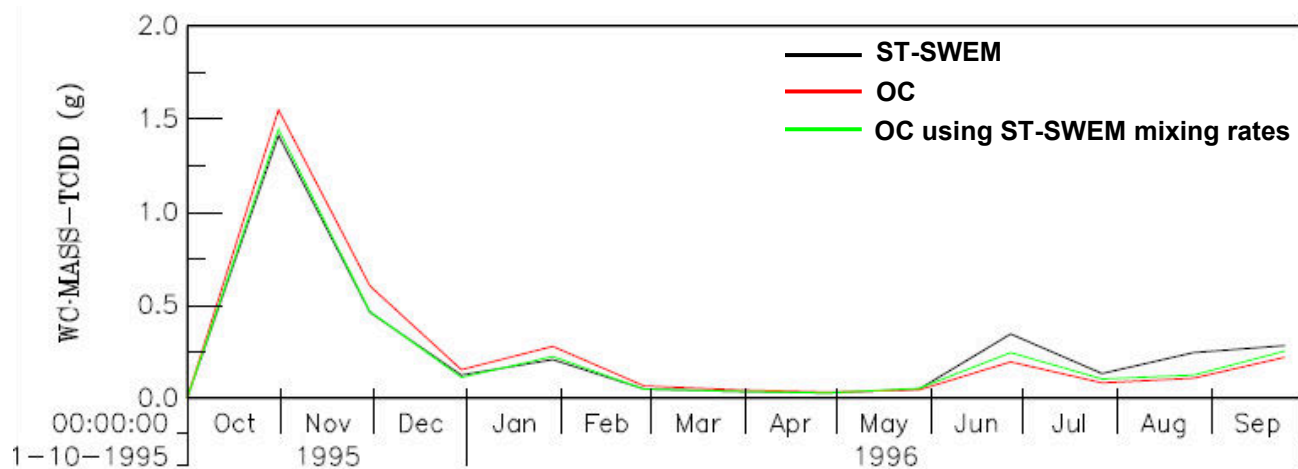


Figure 11. Total mass in the water column in RM 0-8 using the ST-SWEM and OC models, and OC model with ST-SWEM particle mixing rates

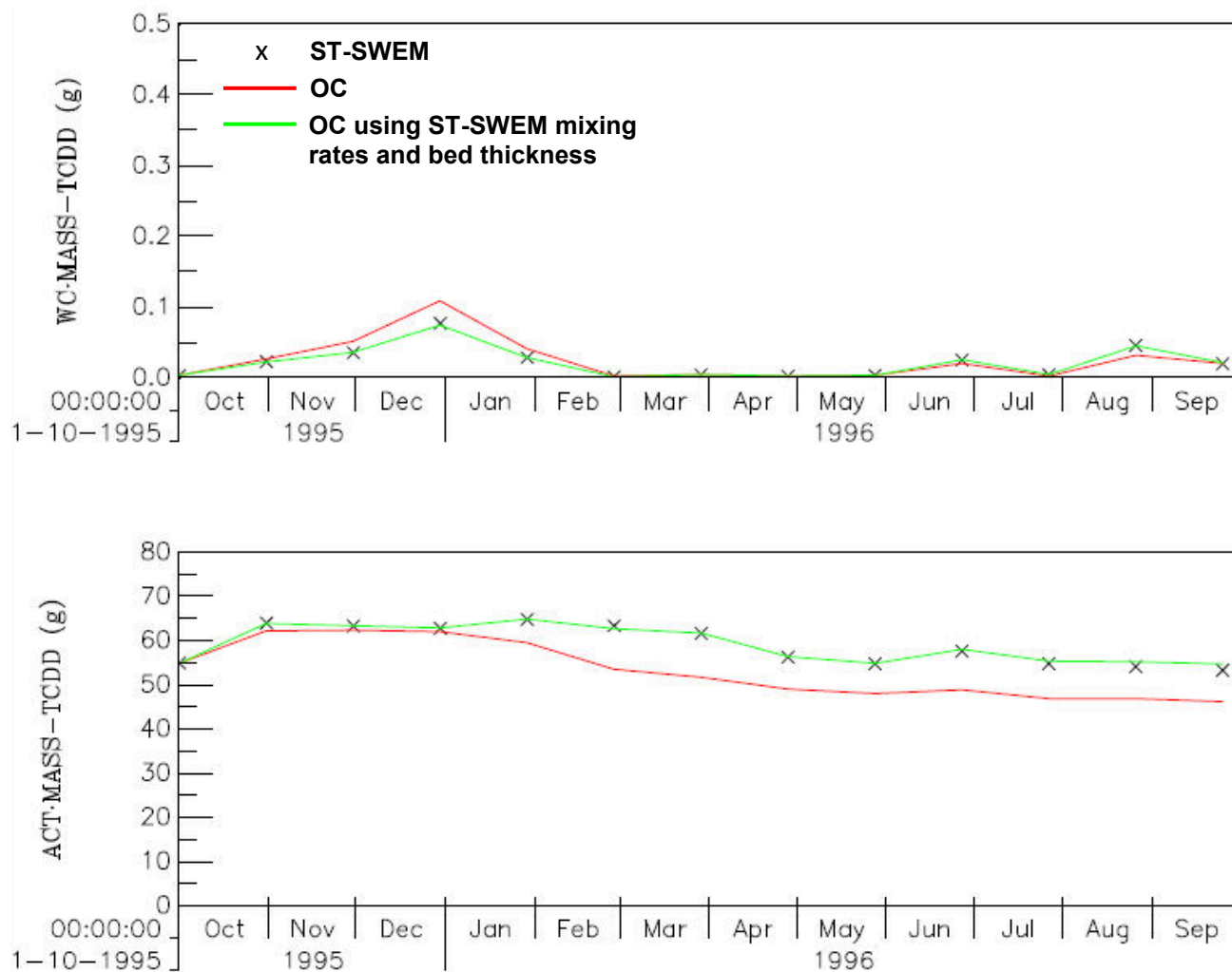


Figure 12. Total mass in the water column (upper panel) and the active layer (lower panel) in RM 8-17 using ST-SWEM, OC, and OC with ST-SWEM mixing and bed thickness

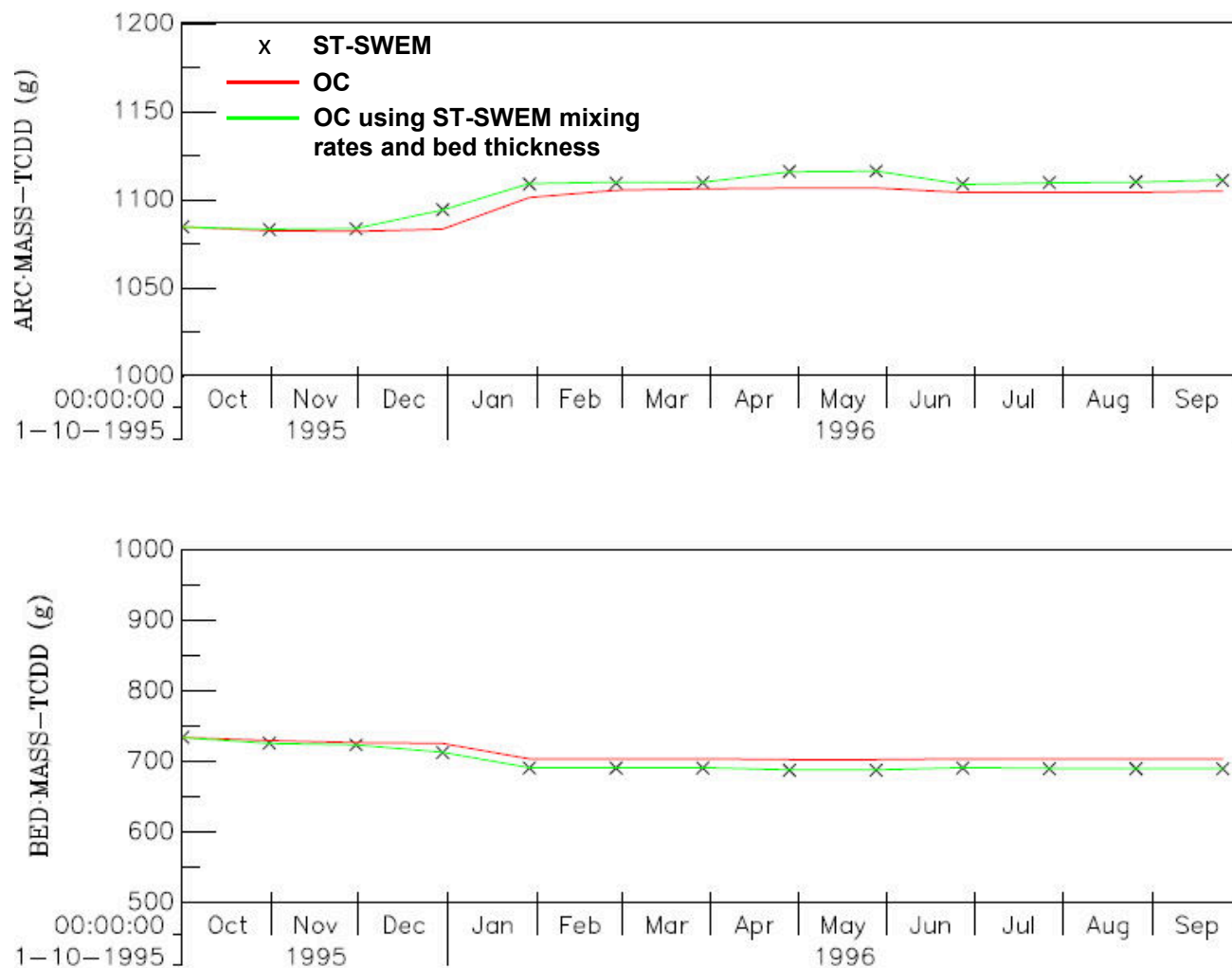


Figure 13. Total mass in the archive (upper panel) and deep bed layers (lower panel) in RM 8-17 using ST-SWEM, OC, and OC with ST-SWEM mixing and bed thickness

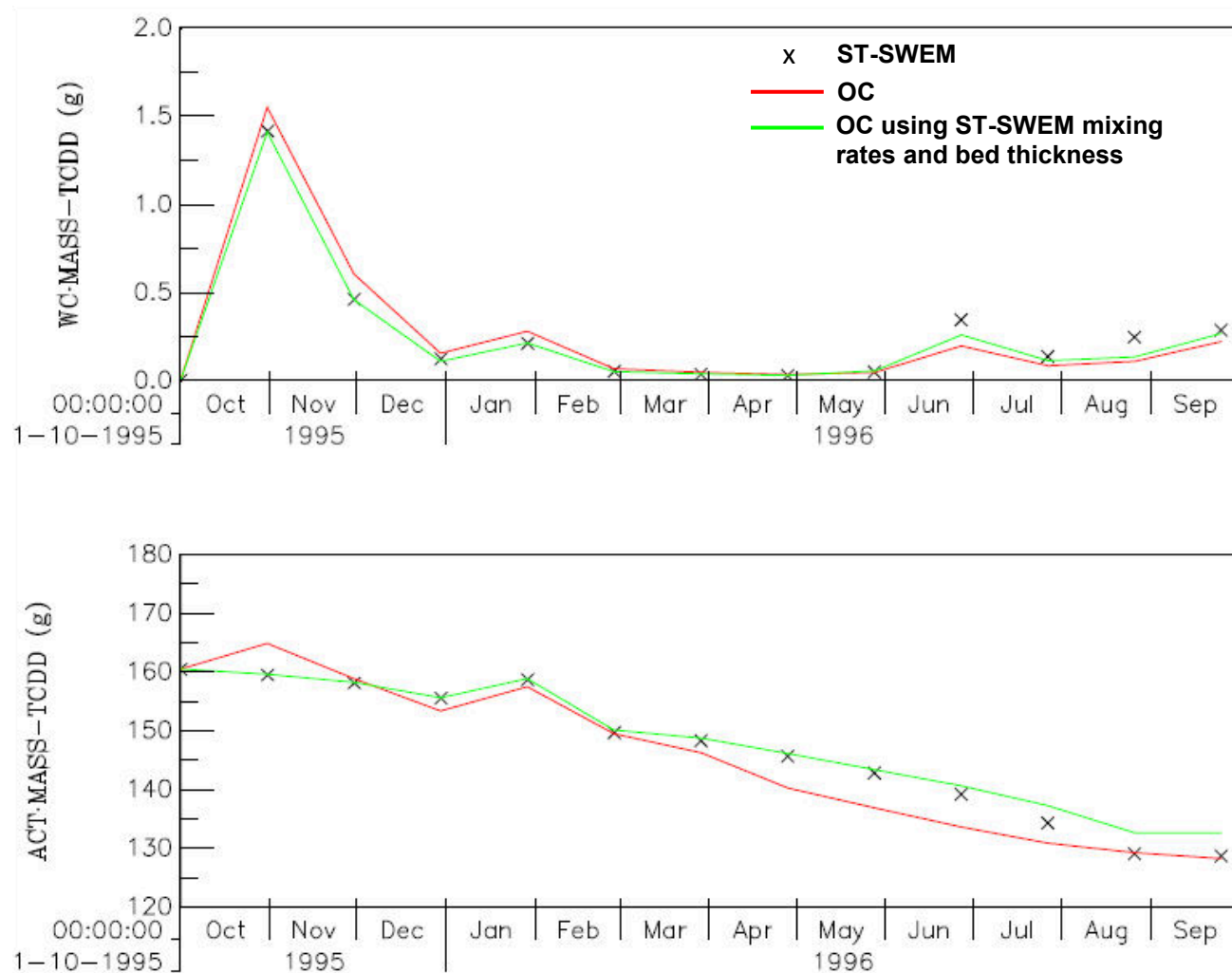


Figure 14. Total mass in the water column (upper panel) and the active layer (lower panel) in RM 0-8 using ST-SWEM, OC, and OC with ST-SWEM mixing and bed thickness

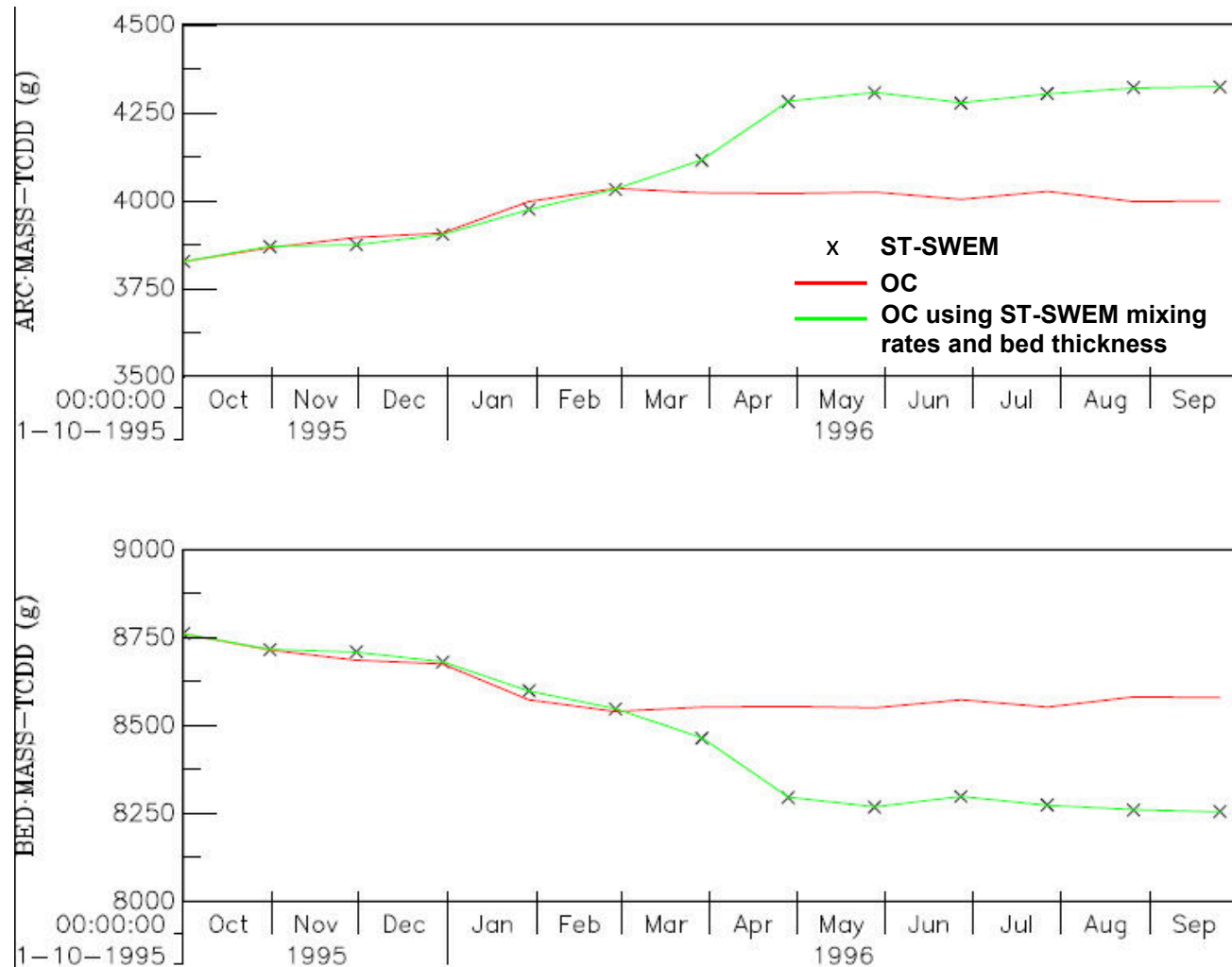


Figure 15. Total mass in the archive (upper panel) and deep bed layers (lower panel) in RM 0-8 using ST-SWEM, OC, and OC with ST-SWEM mixing and bed thickness

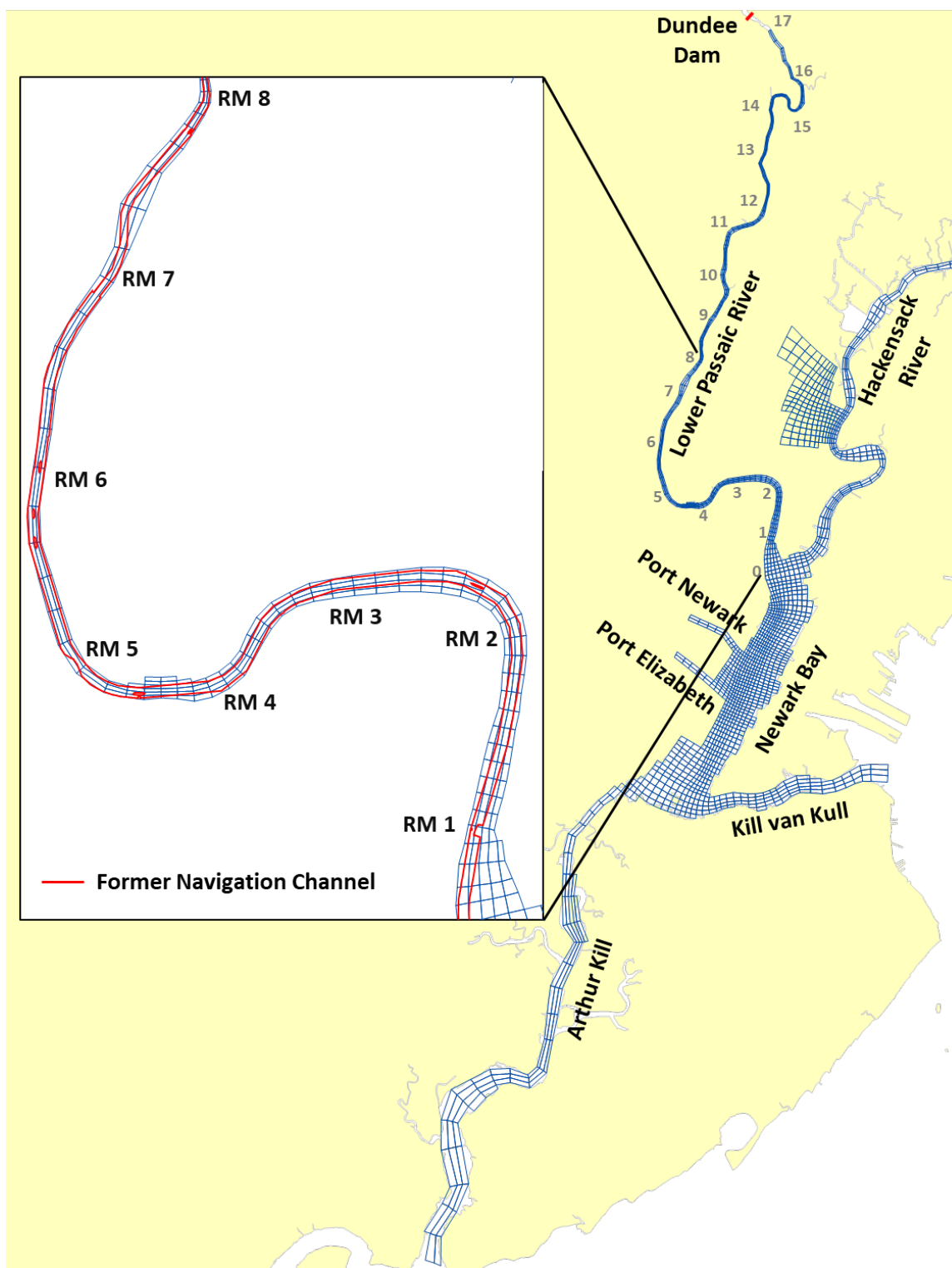


Figure 16. The Lower Passaic River and Newark Bay modeling domains, along with the computational grid for the AOC model

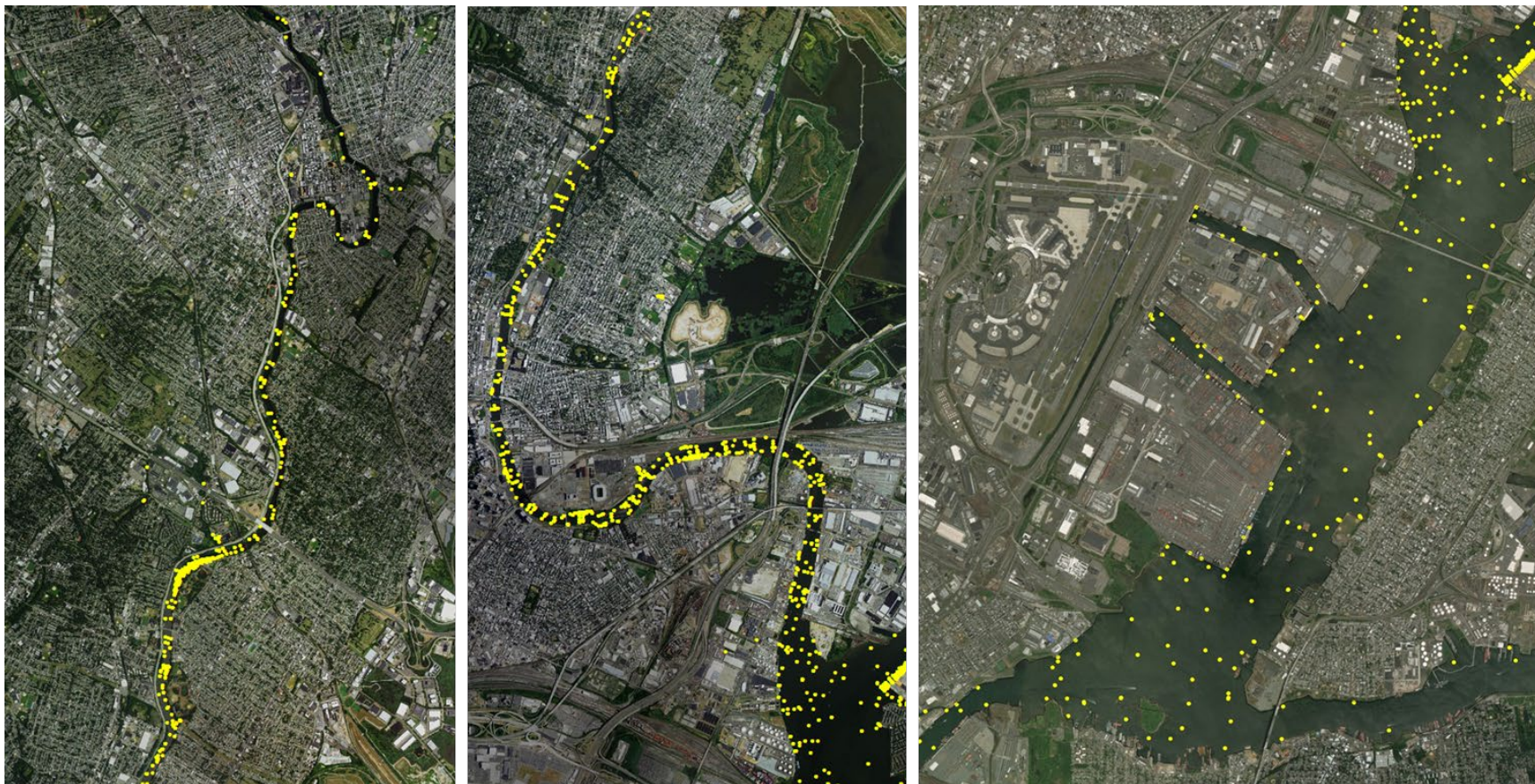


Figure 17. Sediment detrital carbon data between RM 17-10 (left panel), RM 0-10 (middle panel), and Newark Bay (right panel)

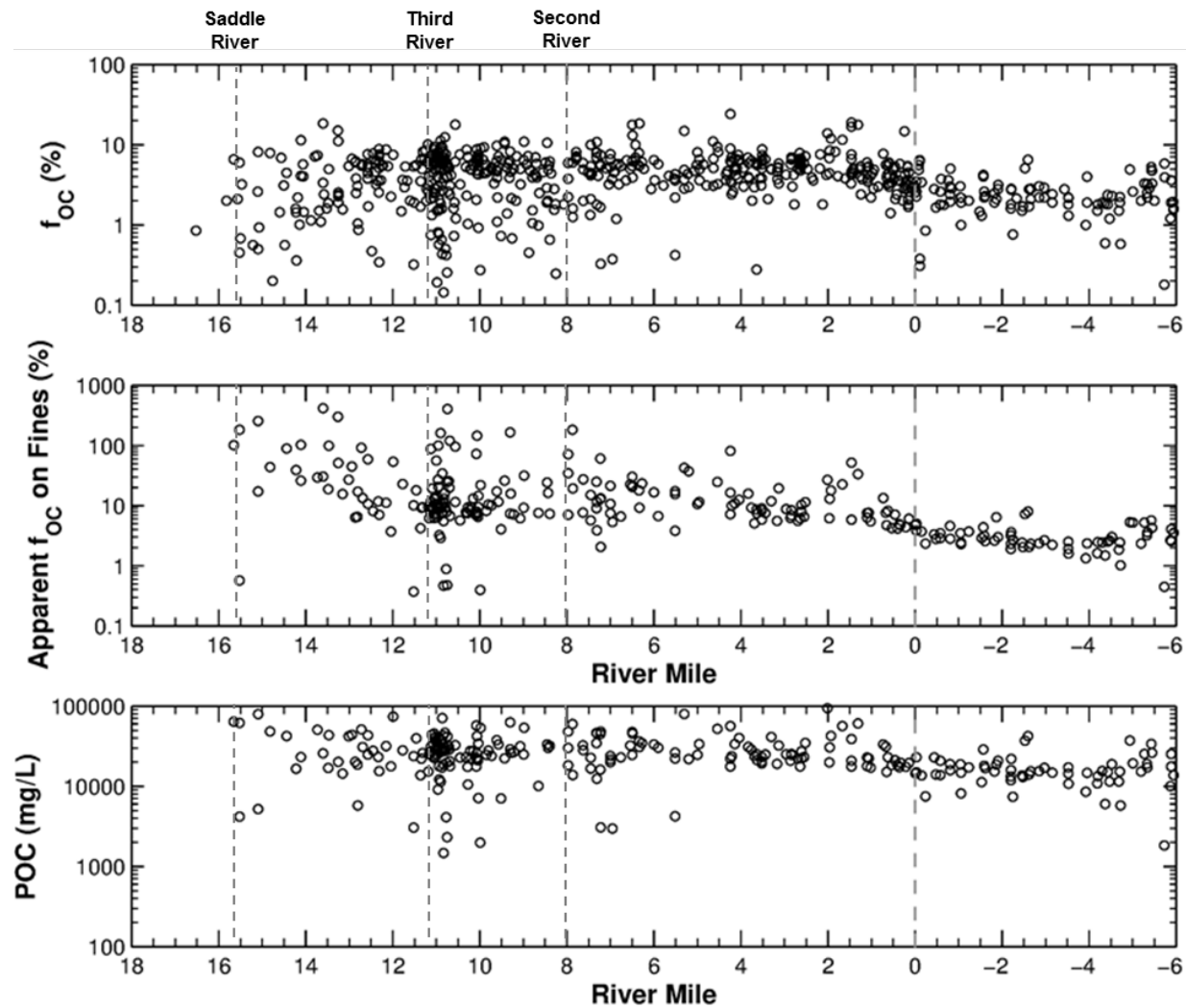


Figure 18. LPR sediment organic carbon measurements in top 15 cm of bed. River Mile 0 represents the boundary between LPR and NB

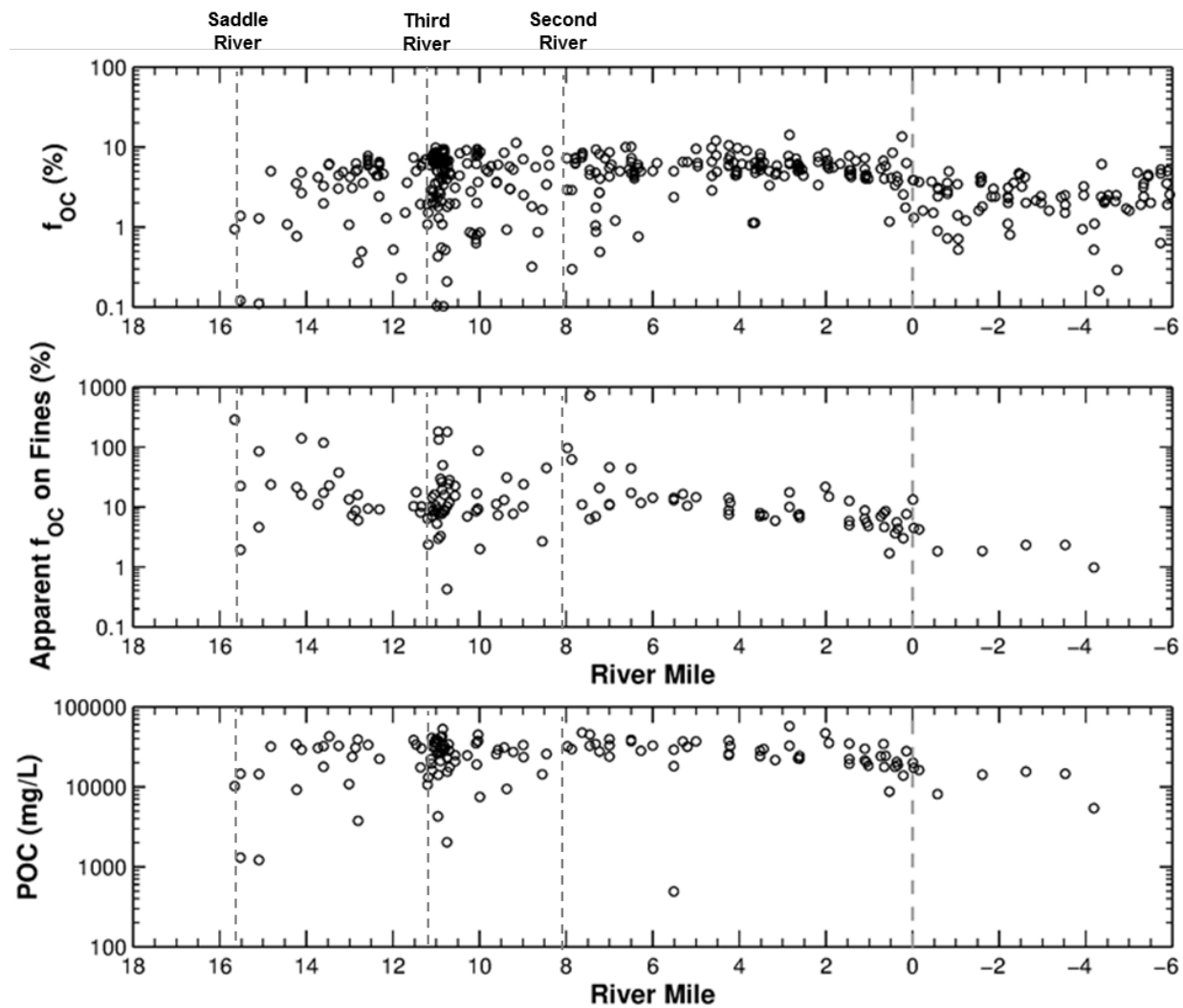


Figure 19. LPR sediment organic carbon measurements below the 15 cm depth-interval in bed. River Mile 0 represents the boundary between LPR and NB

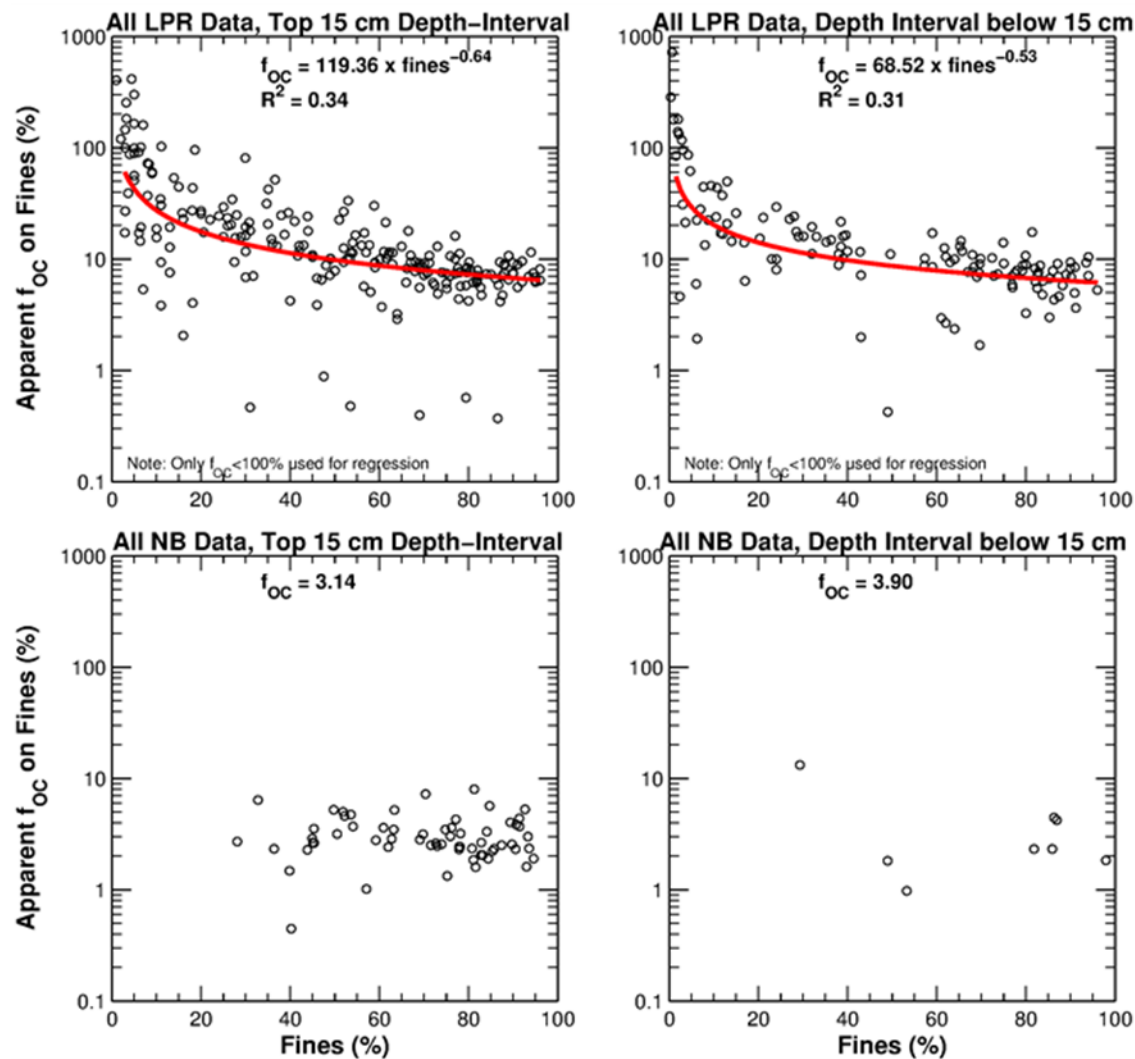


Figure 20. Apparent f_{OC} on fine sediments as a function of sediment fines content.

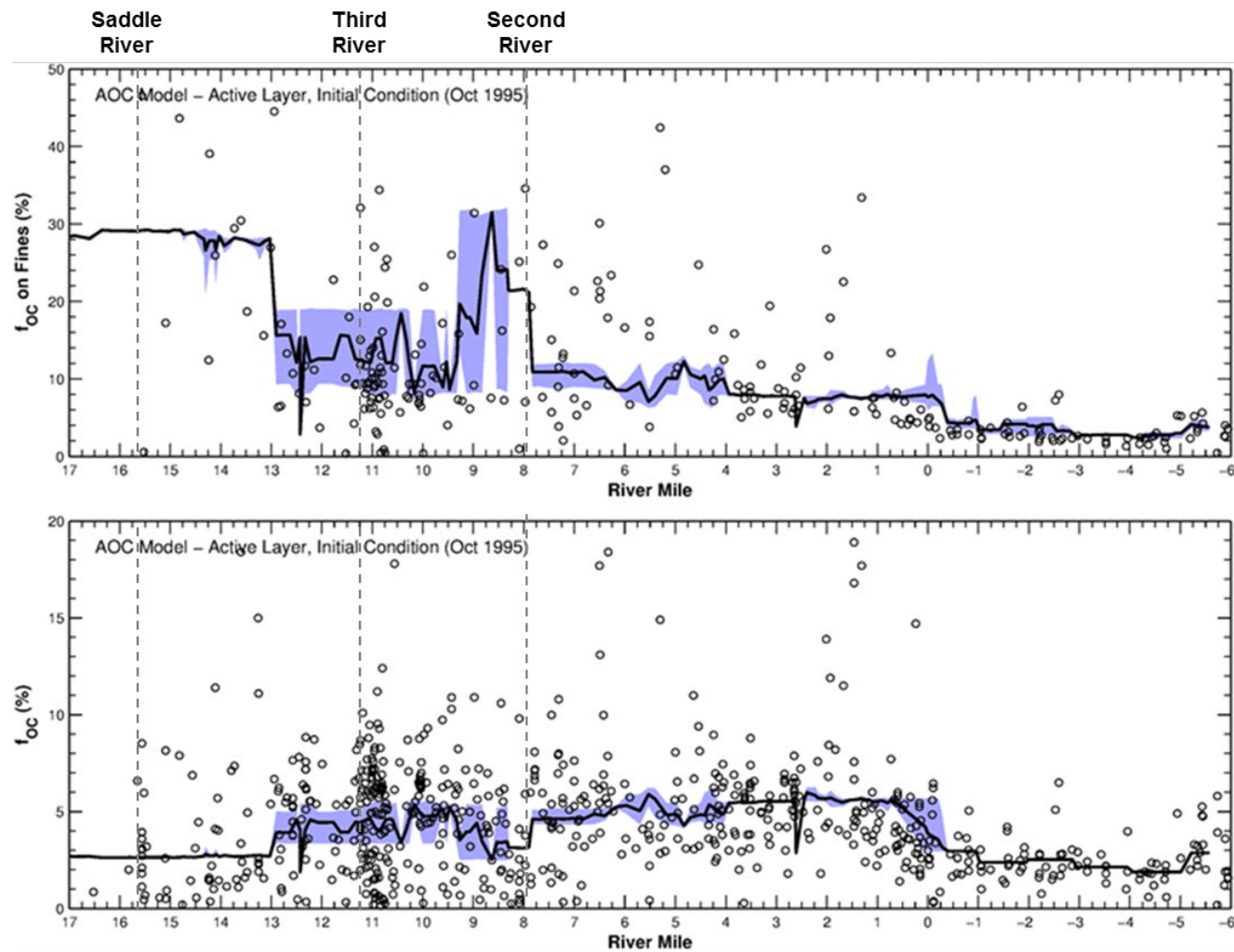


Figure 21. Initial condition for detrital carbon in bed active layer relative to measured values for apparent f_{OC} on fines (upper panel) and bulk sediment f_{OC} (lower panel). Shaded blue region indicates range of values across the river, and black line indicates the mean value.

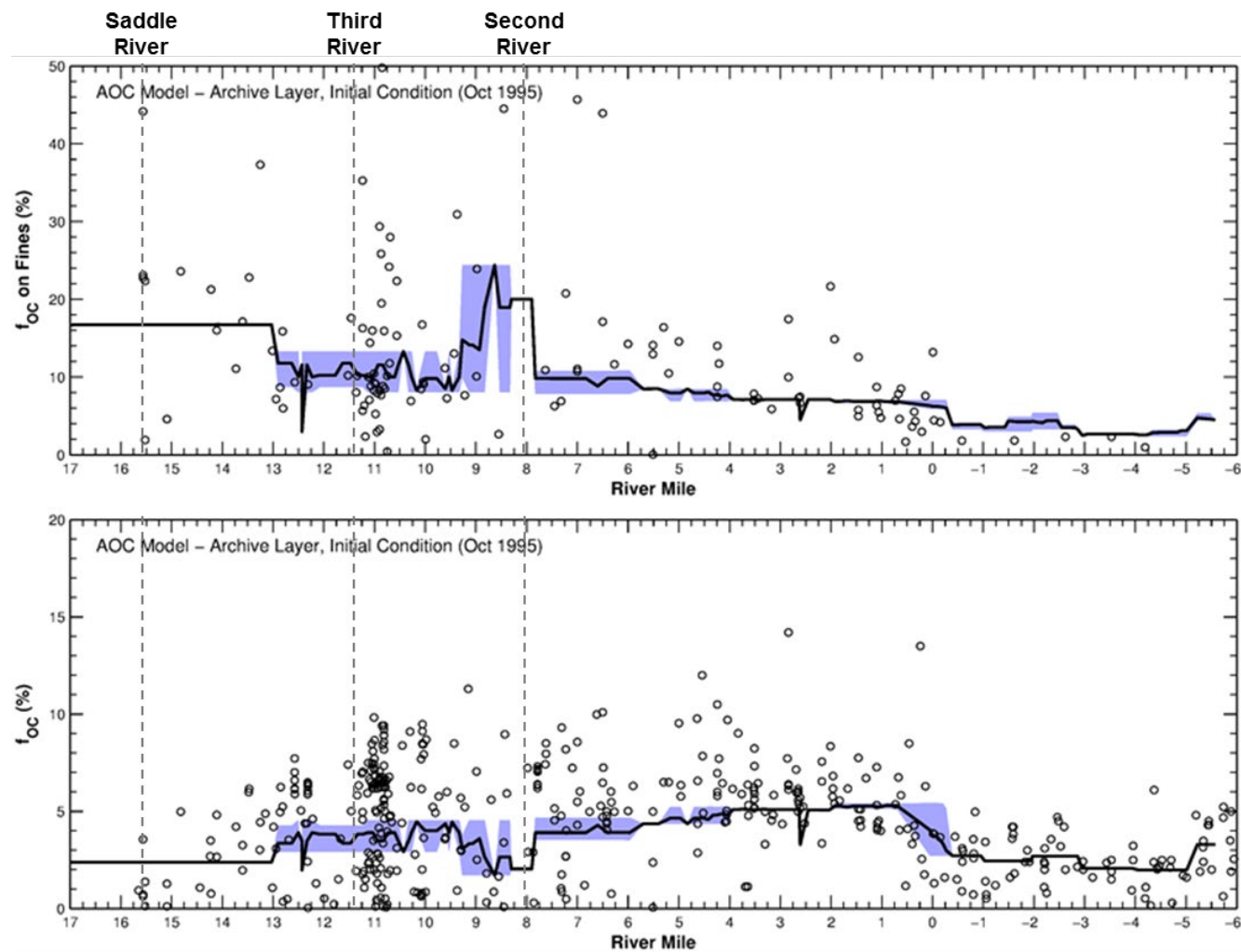


Figure 22. Initial condition for detrital carbon in bed archive layer relative to measured values for apparent foc on fines (upper panel) and bulk sediment foc (lower panel). Shaded blue region indicates range of values across the river, and black line indicates the mean value.

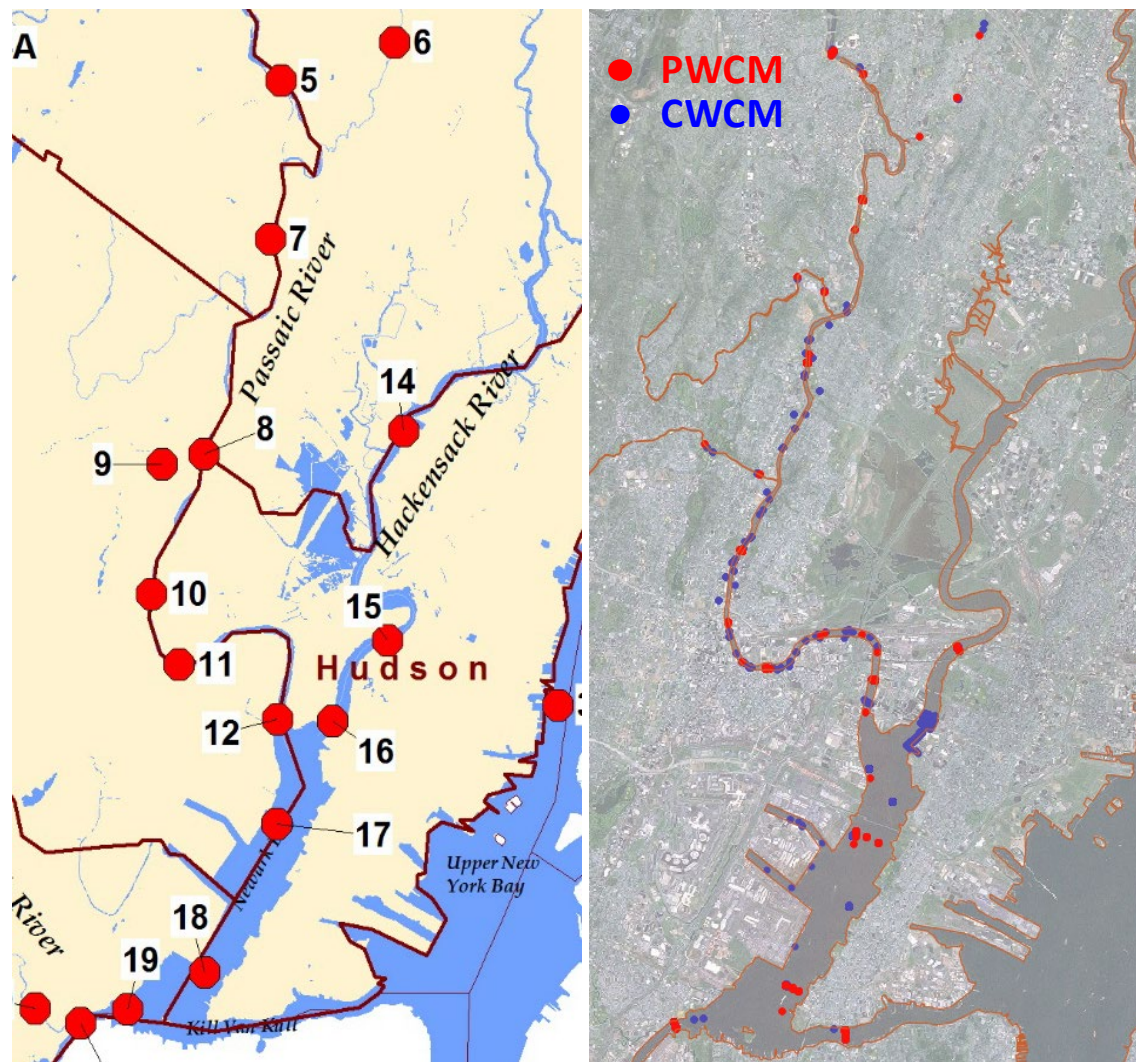


Figure 23. Location map of PVSC/NJHDG sampling stations (left panel; adapted from NJHDG 2006) and PWCM/CWCM (and other minor surveys) sampling stations (right panel)

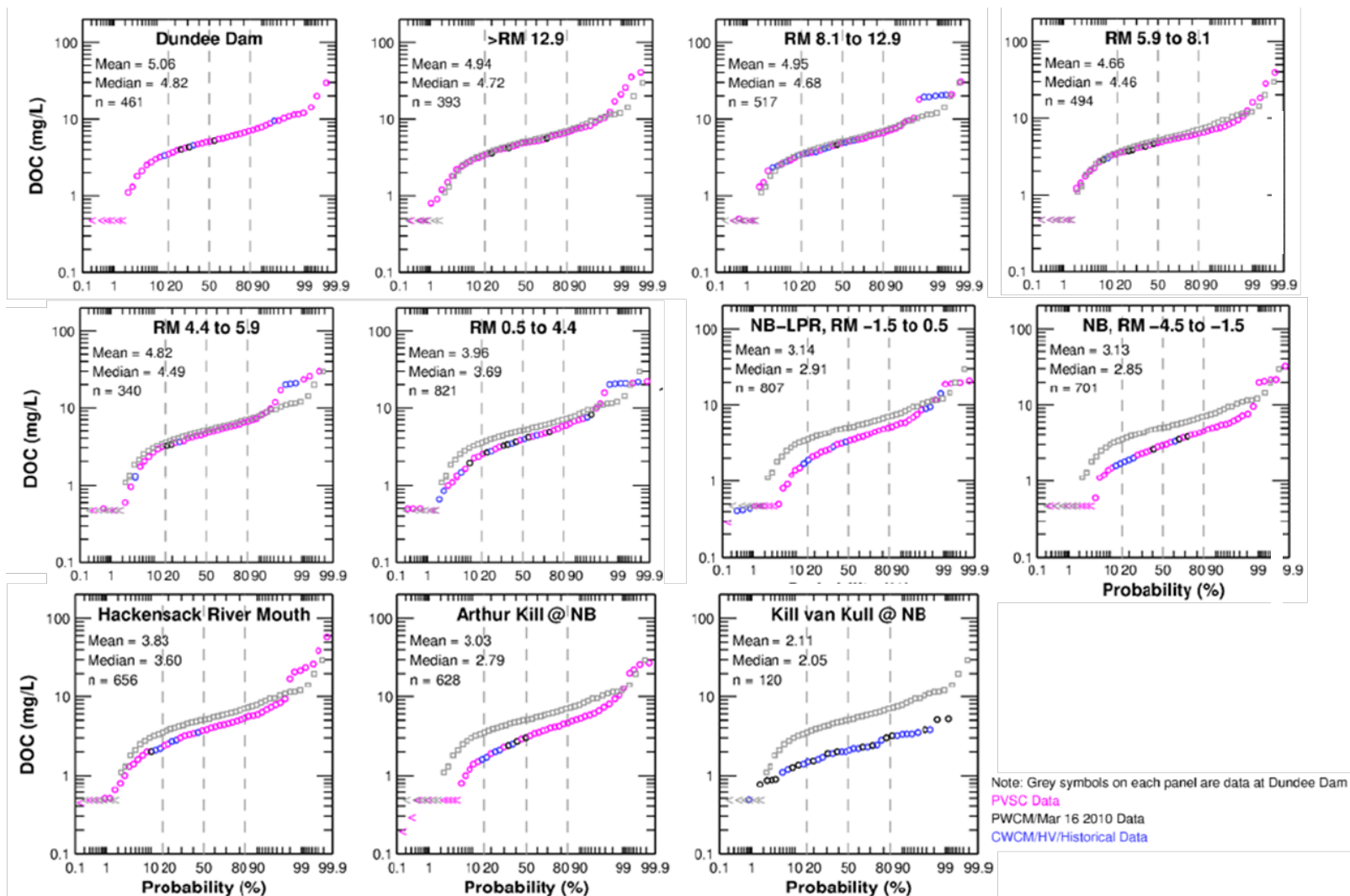


Figure 24. Probabilistic comparisons of DOC measurements in various spatial bins in LPR relative to data at Dundee Dam. Data from all seasons.

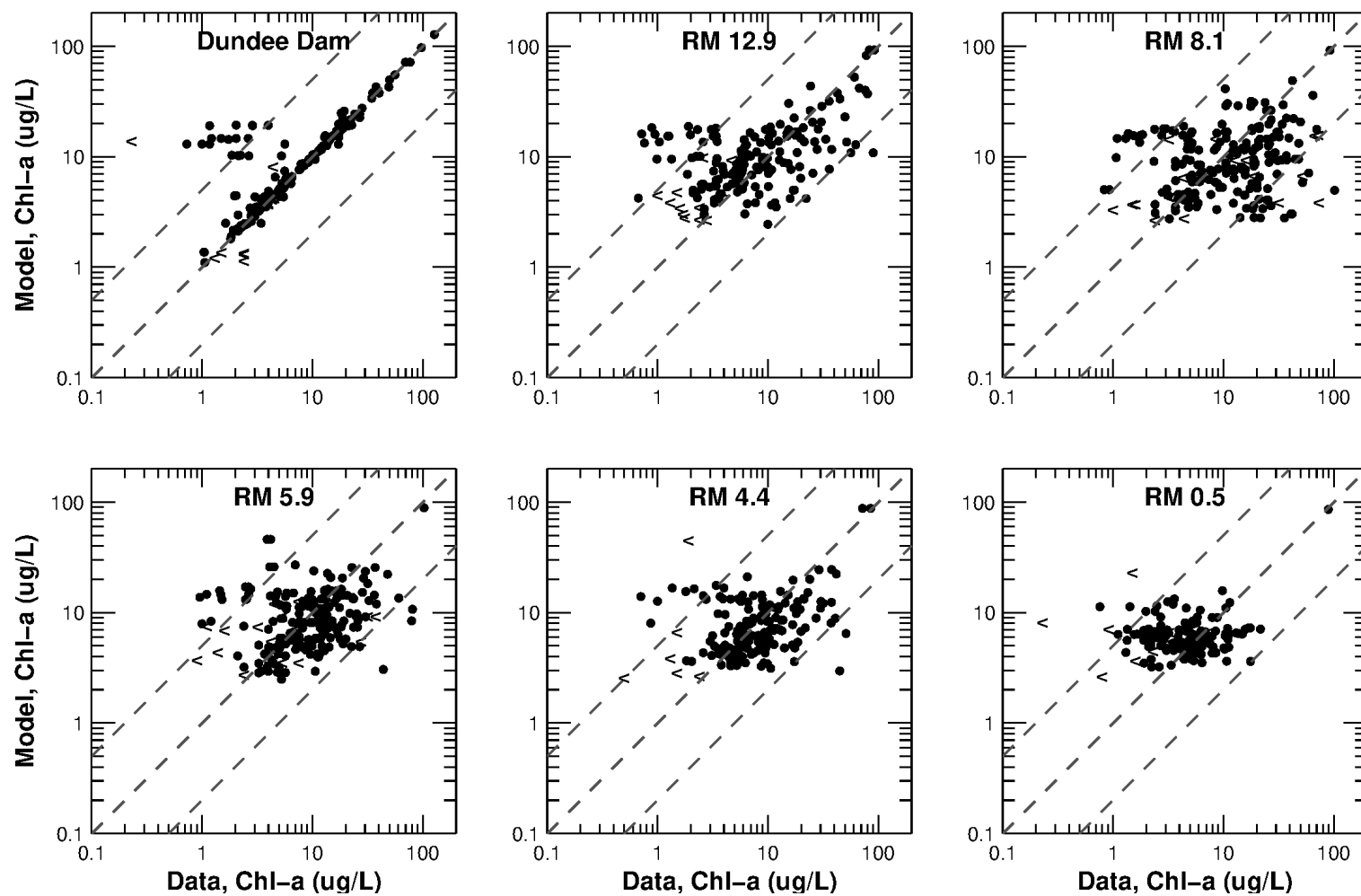


Figure 25. Cross-plot of model results for Chl-a versus measured values for summertime (May-September) data.

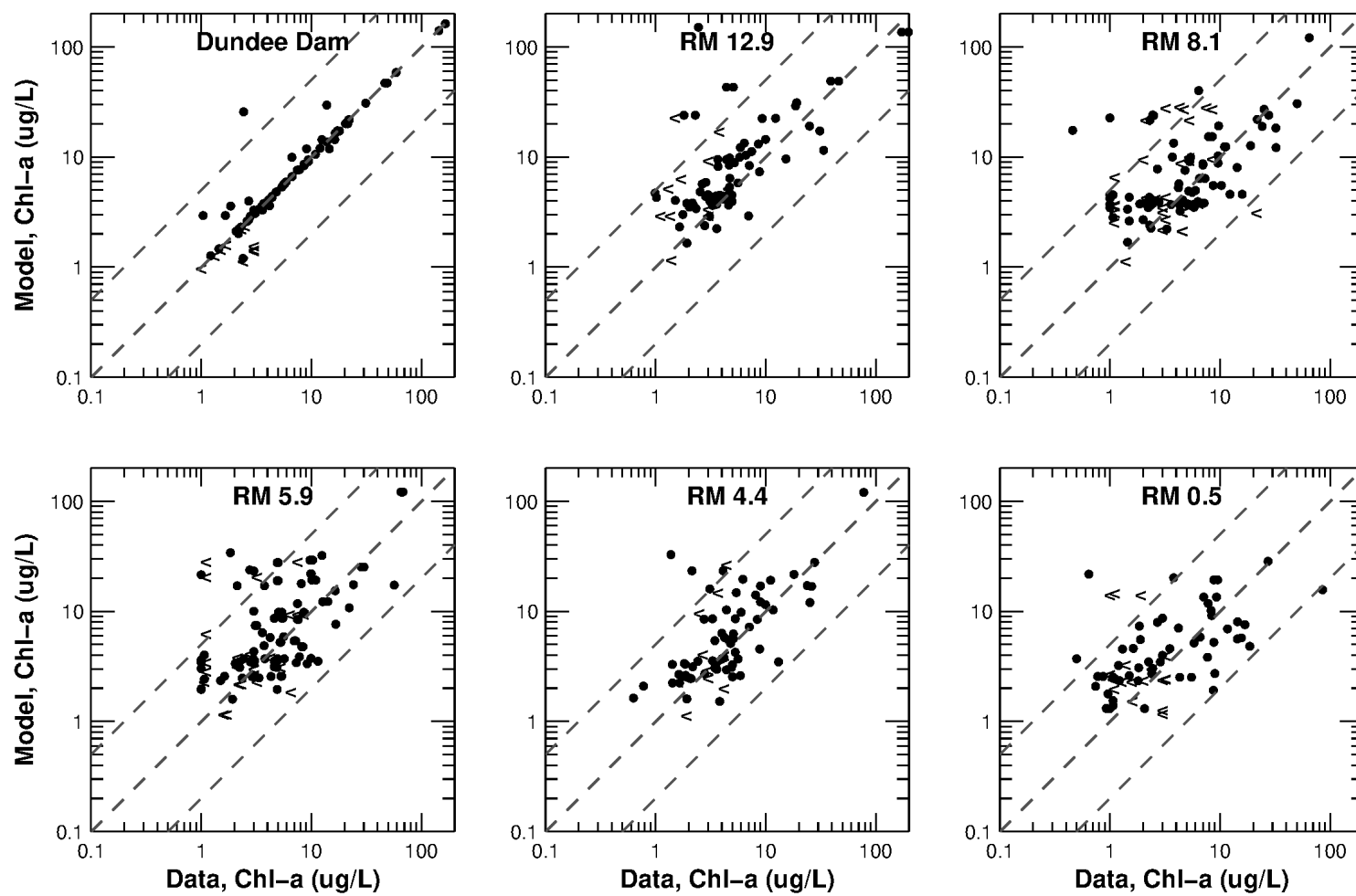


Figure 26. Cross-plot of model results for Chl-a versus measured values for wintertime (October-April) data.

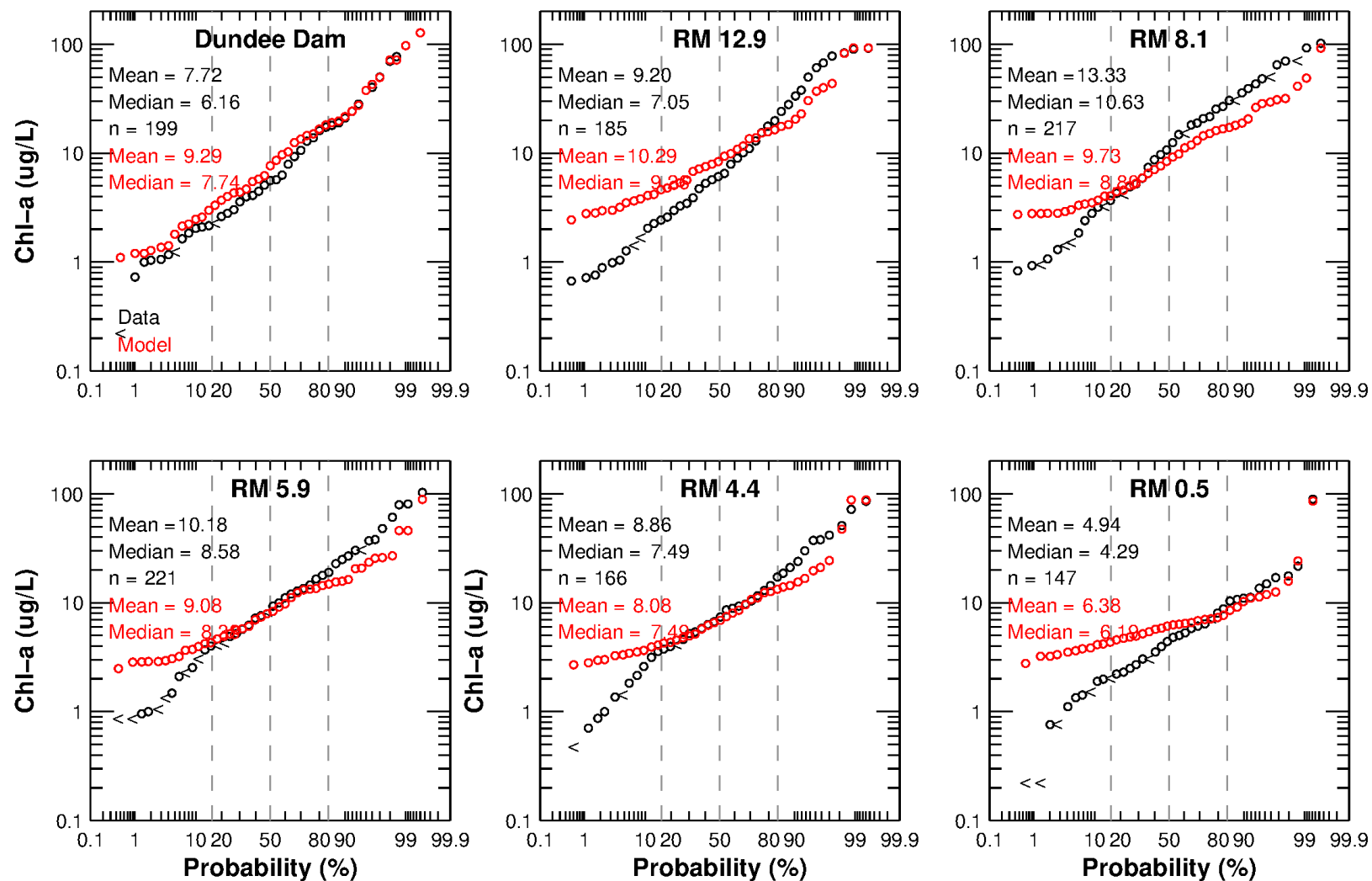


Figure 27. Probabilistic comparison of model results for Chl-a and measured values for summertime (May-September) data.

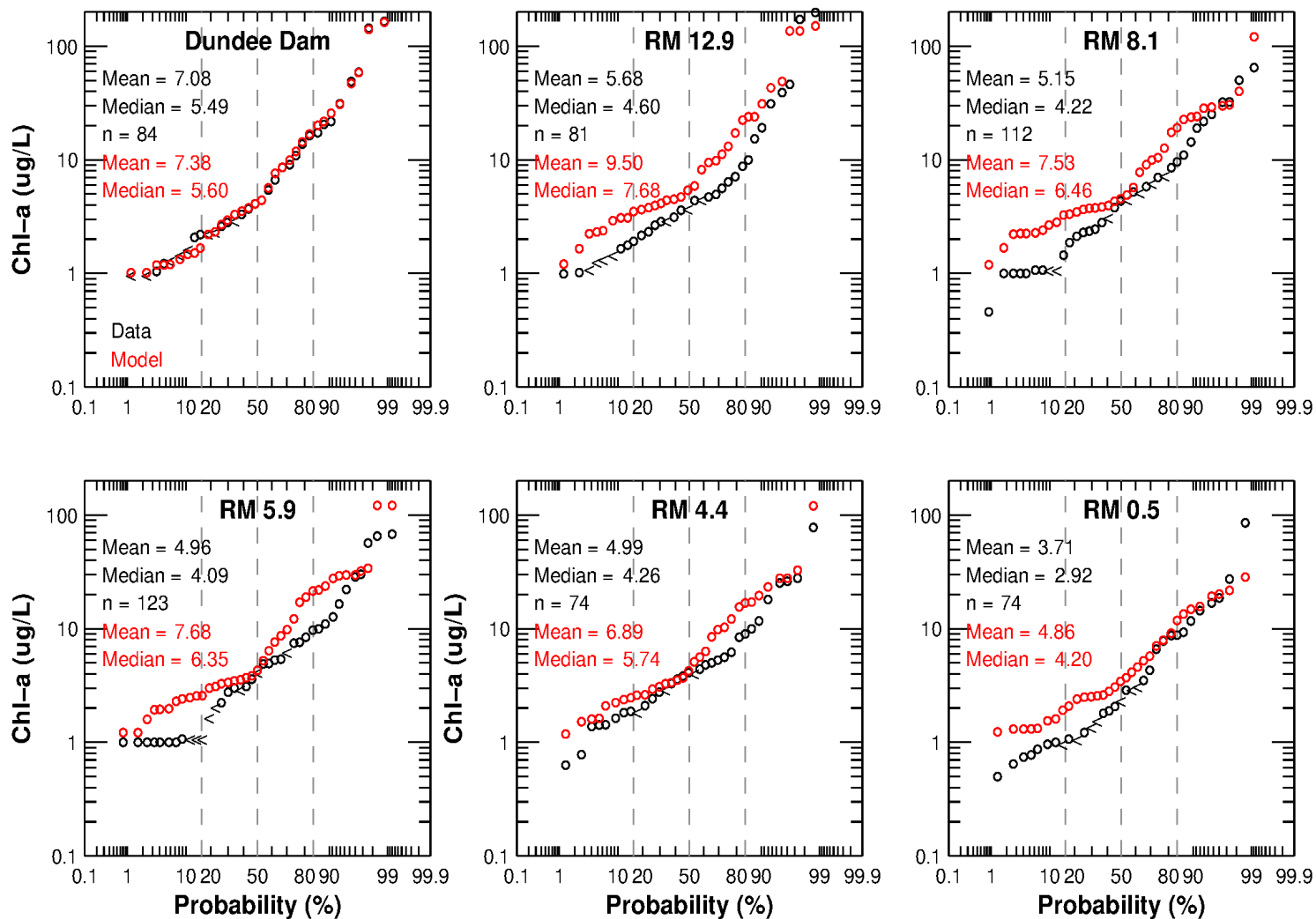


Figure 28. Probabilistic comparison of model results for Chl-a and measured values for wintertime (October-April) data.

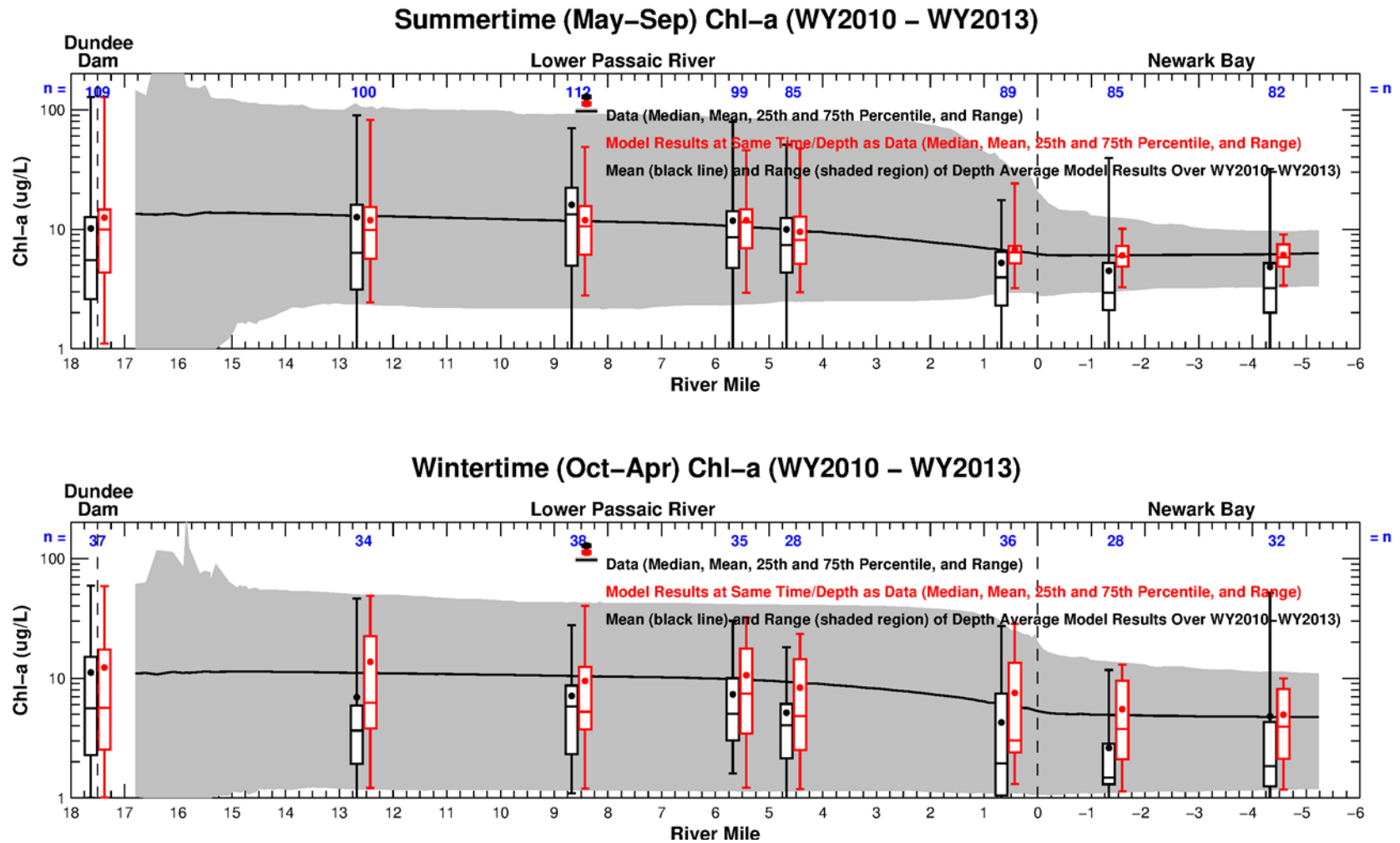


Figure 29. Longitudinal spatial profile of Chl-a data and model results for summertime (upper panel) and wintertime (lower panel) over WY2010-WY2013.

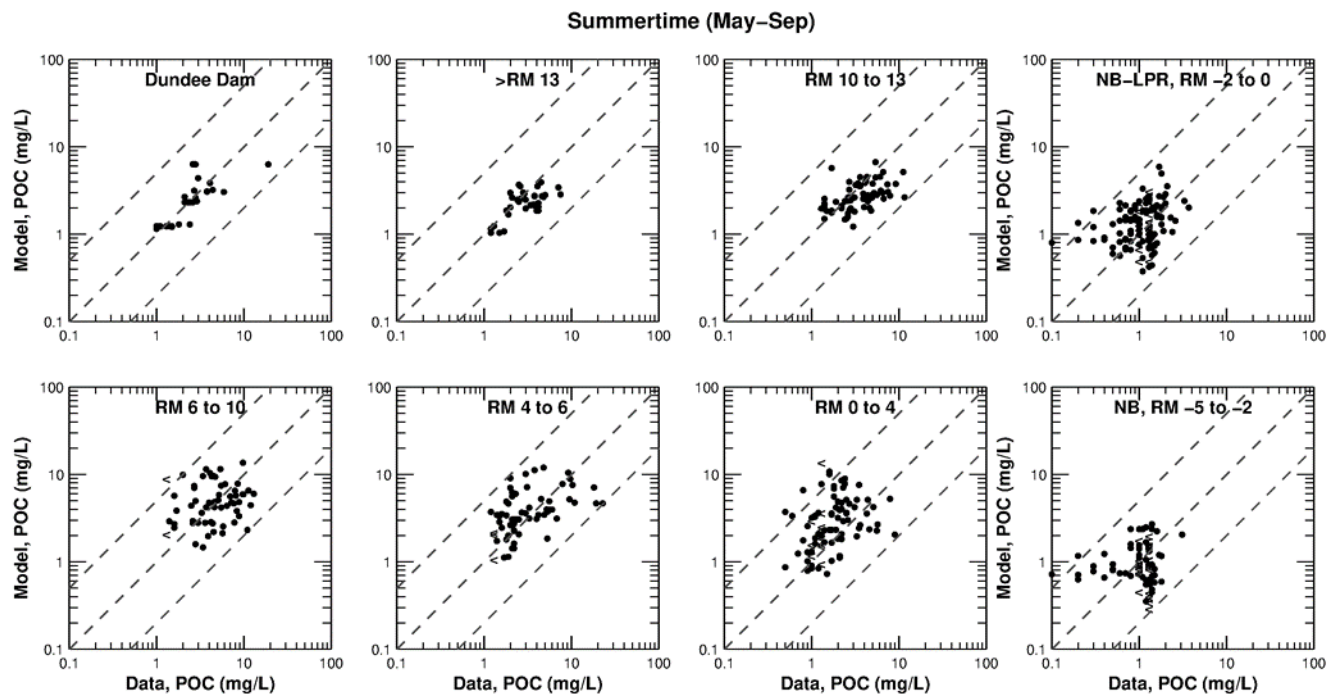


Figure 30. Cross-plot of model results for POC versus measured values for summertime (May-September) data.

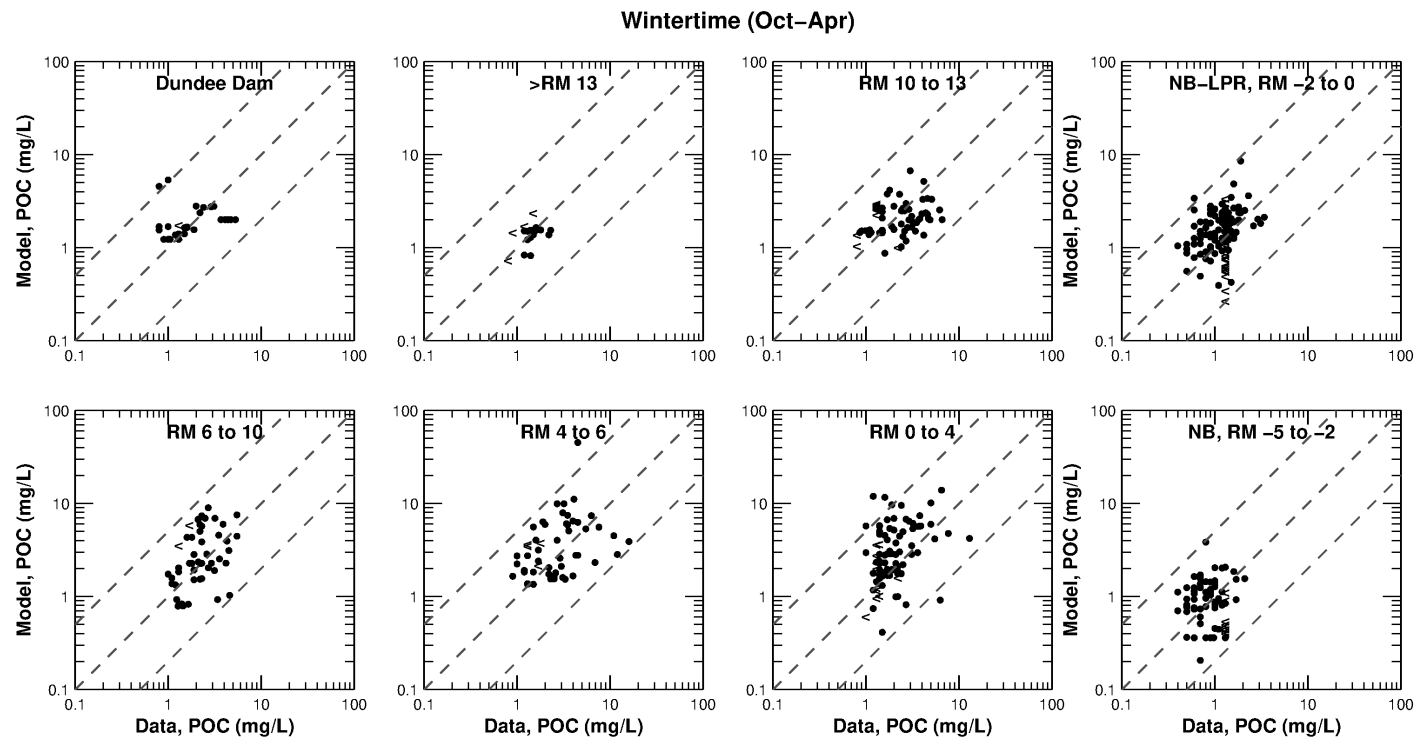


Figure 31. Cross-plot of model results for POC versus measured values for wintertime (October–April) data.

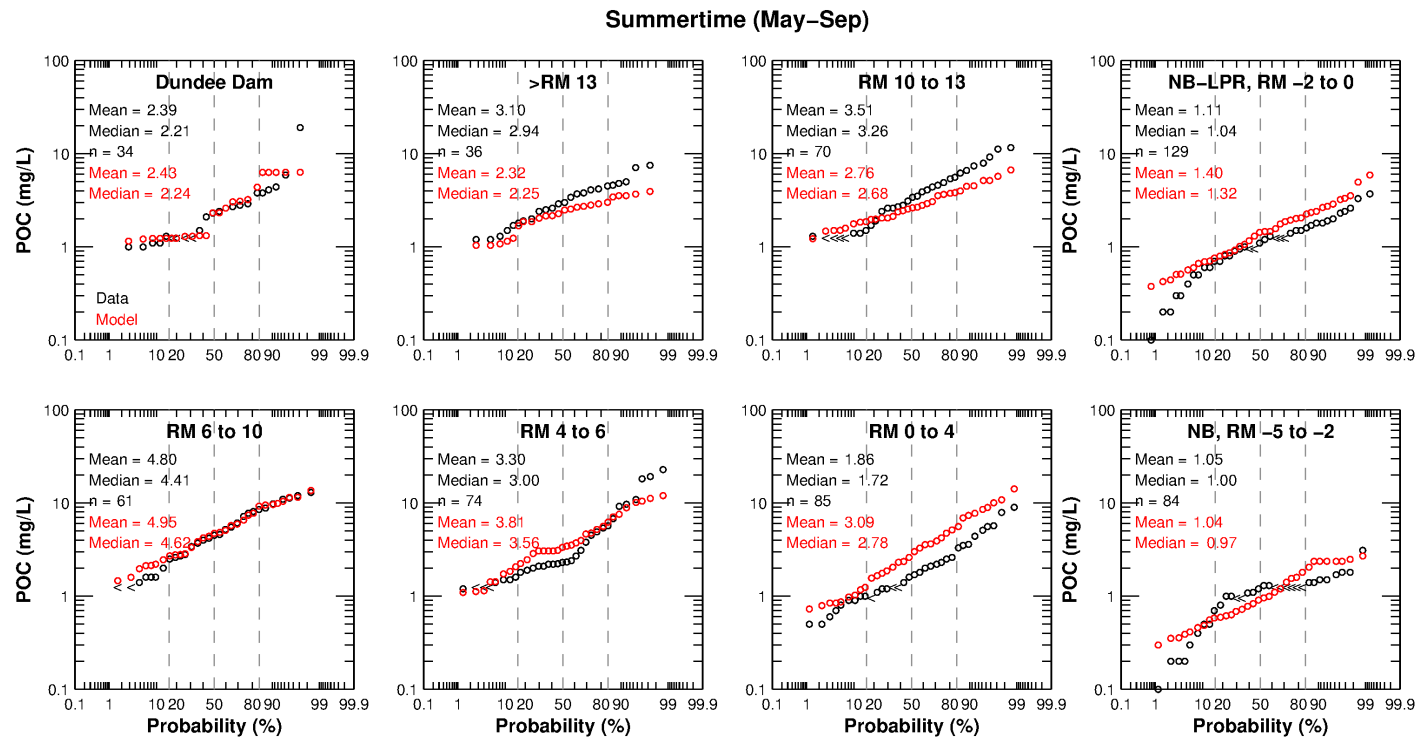


Figure 32. Probabilistic comparison of model results for POC and measured values for summertime (May-September) data:

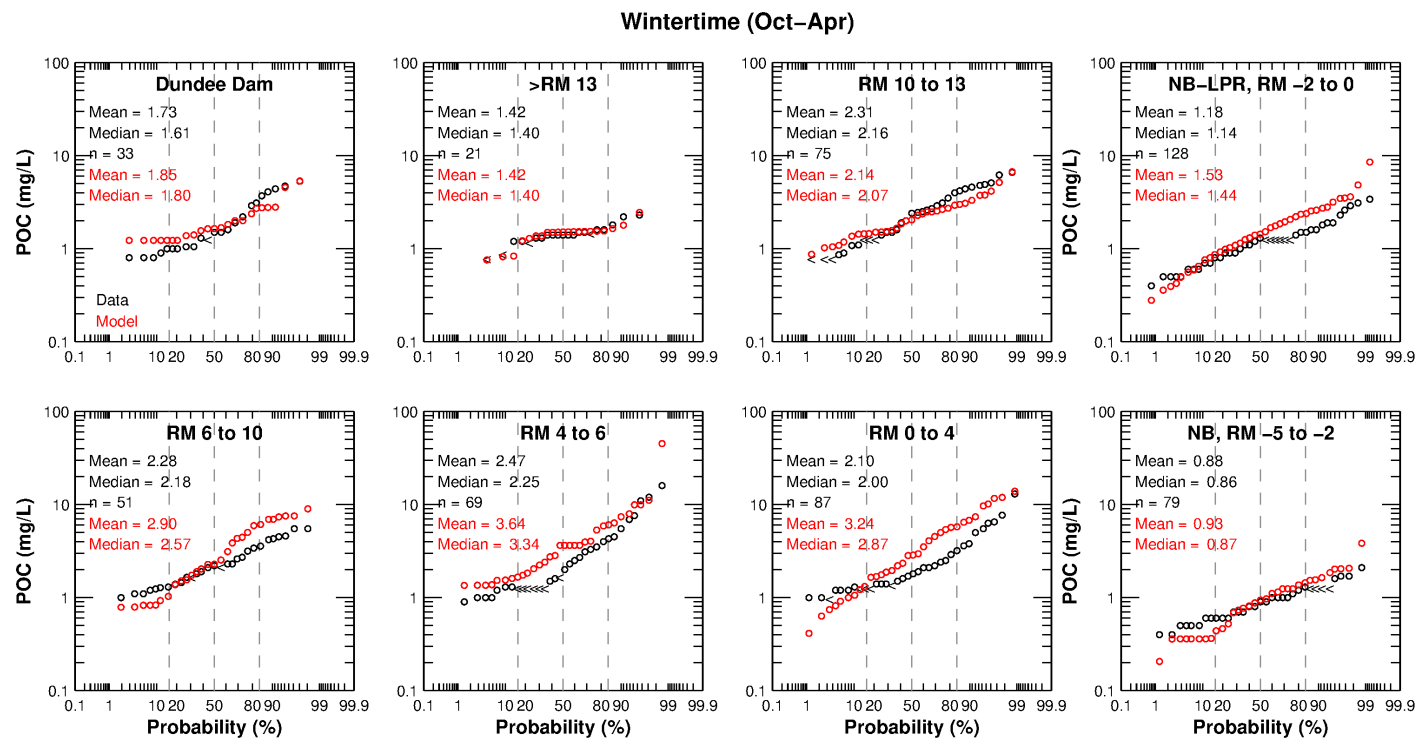


Figure 33. Probabilistic comparison of model results for POC and measured values for wintertime (October-April) data.

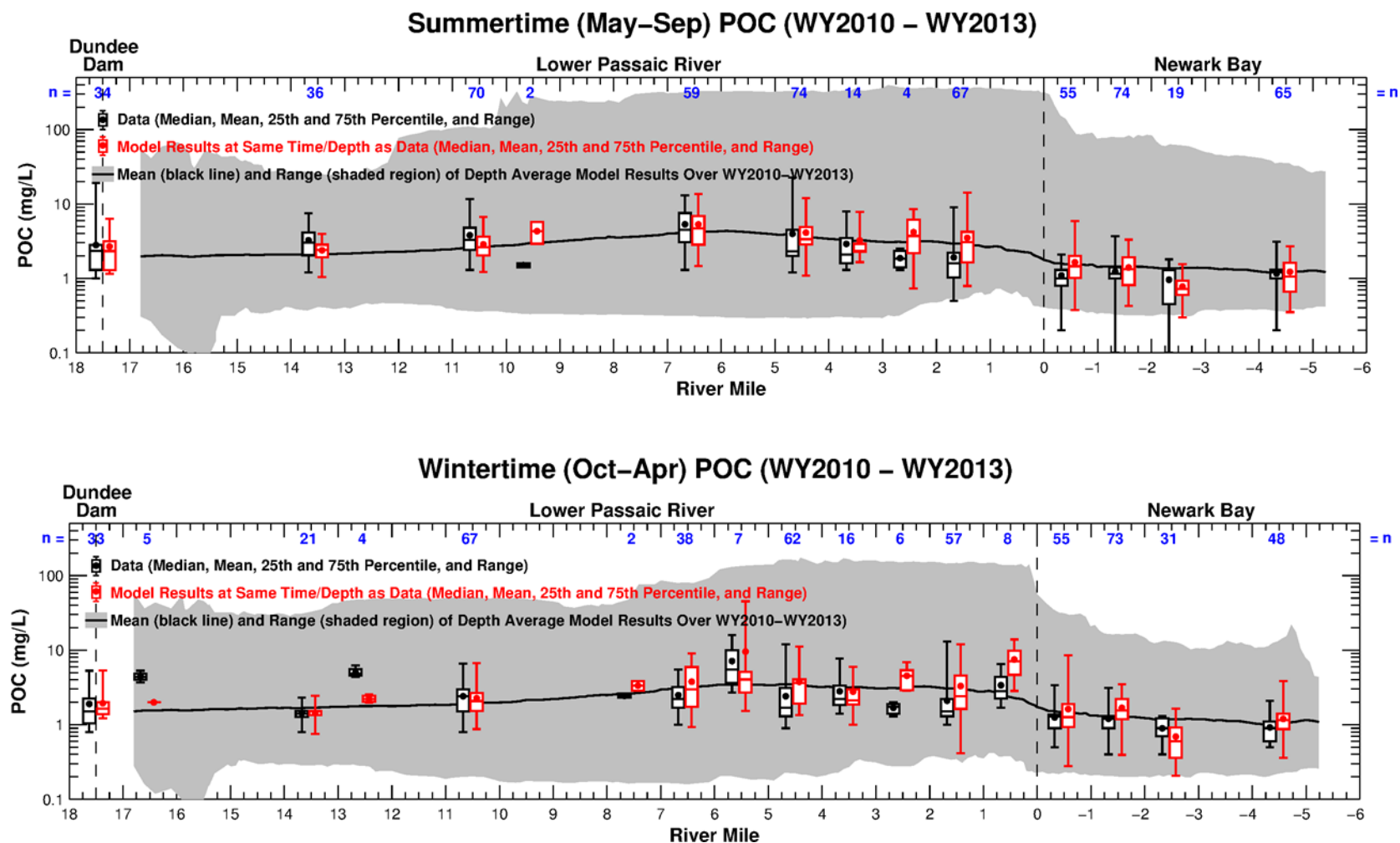


Figure 34. Longitudinal spatial profile of POC data and model results for summertime (upper panel) and wintertime (lower panel) over WY2010-WY2013.

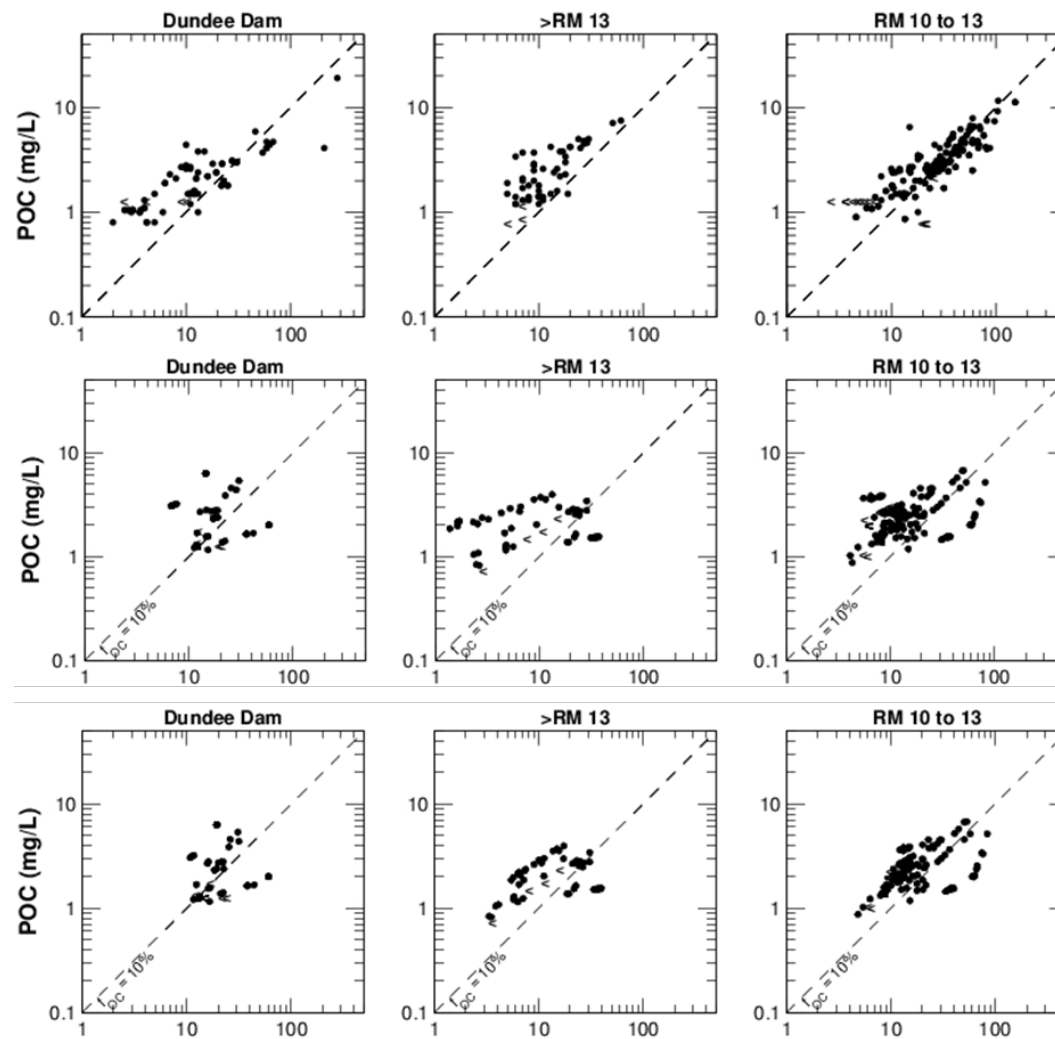


Figure 35. Trend of POC versus SSC in upper LPR for data (upper row), model results (middle row), and model results with algal solids included in SSC (bottom row).

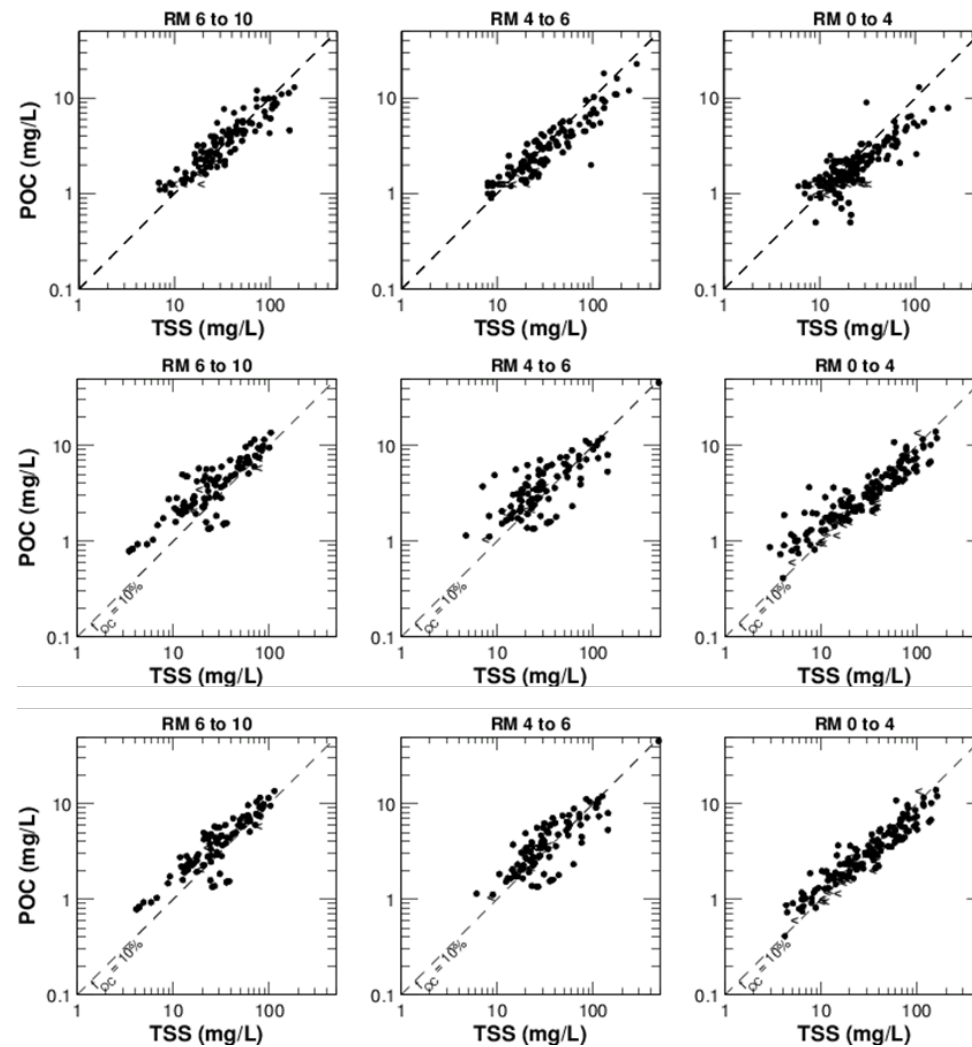


Figure 36. Trend of POC versus SSC in lower LPR for data (upper row), model results (middle row), and model results with algal solids included in SSC (bottom row).

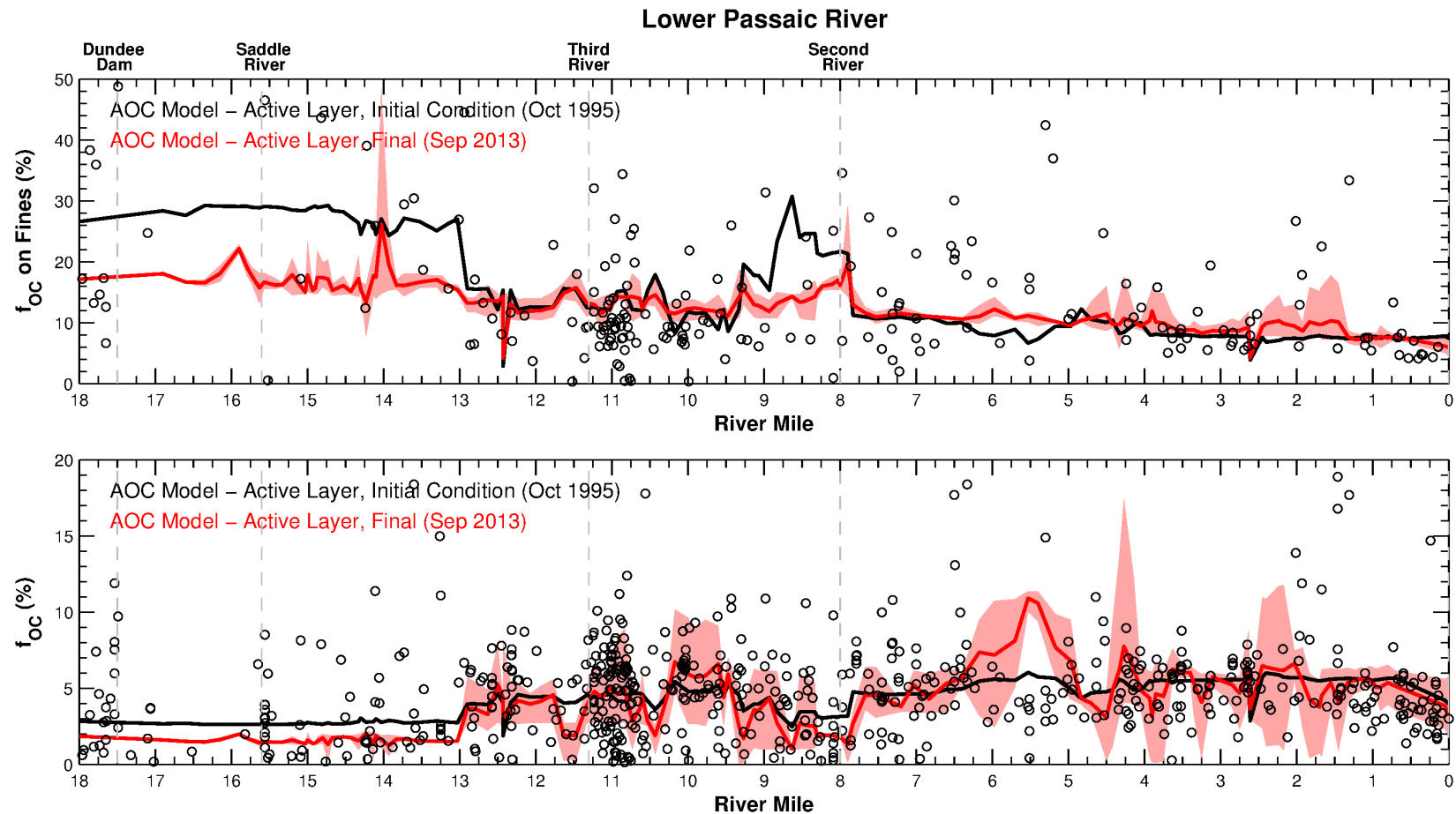


Figure 37. Initial condition (black line) and final results (red shaded area and line) for detrital carbon in bed active layer relative to measured values for apparent f_{OC} on fines (upper panel) and bulk sediment f_{OC} (lower panel). Shaded red region indicates range of values across the river, and red line indicates the mean value.

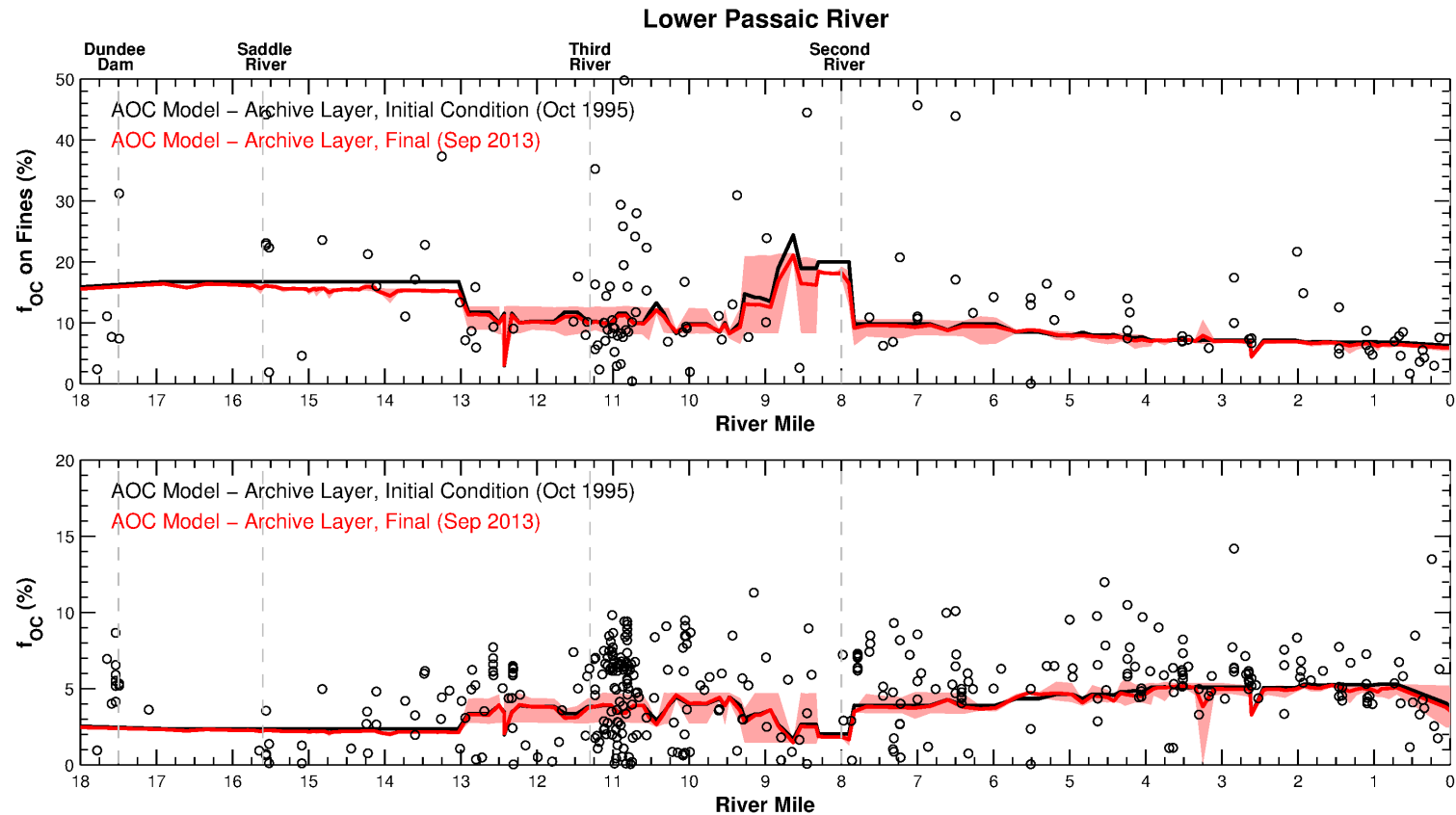


Figure 38. Initial condition (black line) and final results (red shaded area and line) for detrital carbon in bed archive layer relative to measured values for apparent f_{OC} on fines (upper panel) and bulk sediment f_{OC} (lower panel). Shaded red region indicates range of values across the river, and red line indicates the mean value.

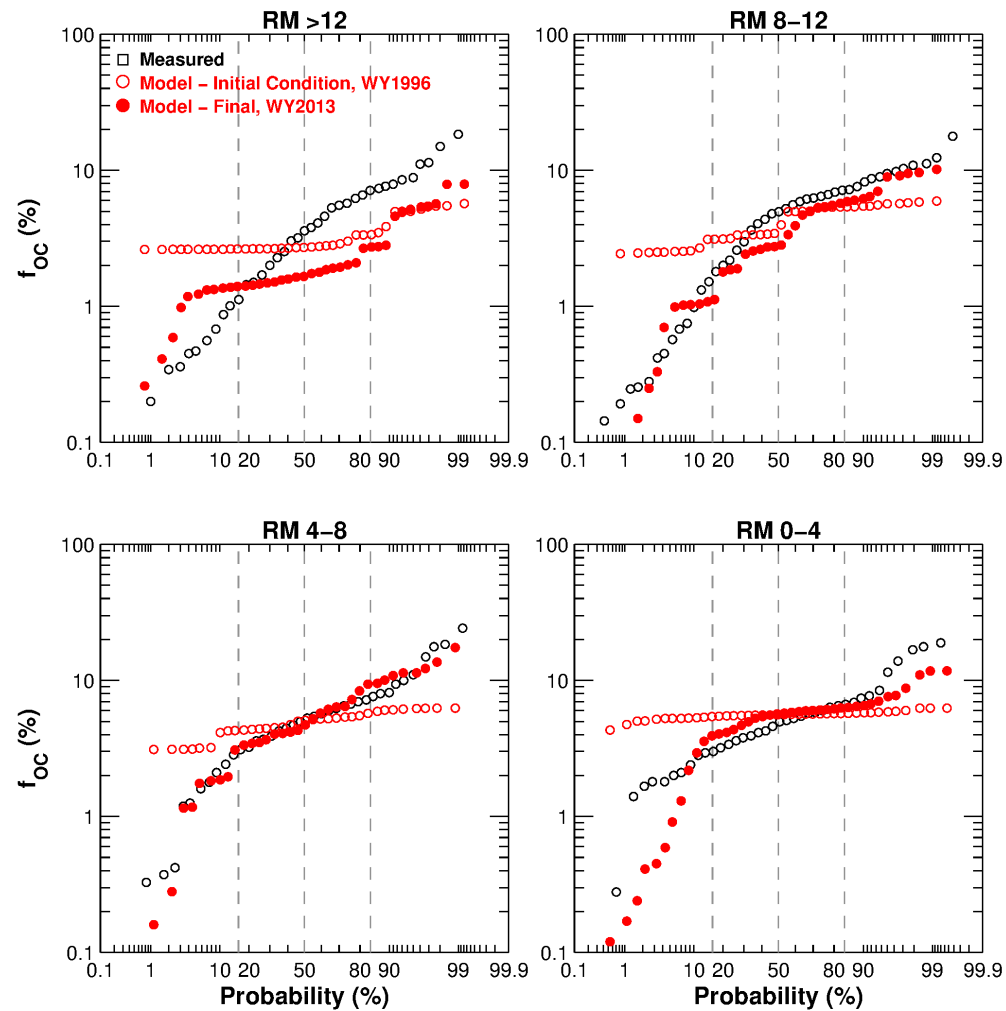


Figure 39. Probabilistic comparison of bed f_{OC} measurements, model initial conditions, and model results at end of calibration simulation for various spatial reaches in LPR.