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Title: Transport in the Hudson Estuary: A Modeling Study of Estuarine Circulation and Tidal Trapping

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Abstract: The effects of estuarine circulation and tidal trapping on transport in the Hudson Estuary are investigated by a numerical model simulation of a tracer release. The data set used is from a large-scale SF₆ tracer release experiment conducted during July/August 2001. It consists of over 2,000 measurements taken over a period of two weeks and a distance of 100 km with a typical resolution of 400 meters. The model is based on the three-dimensional, time-variable, estuarine and coastal circulation modeling framework (ECOM), and consists of over 10,000 mass balance segments with a 600 m horizontal and 1 m vertical resolution in the study area. The modeled and measured longitudinal profiles of surface tracer concentrations (plumes) differ from the ideal Gaussian shape in two ways: (1) On a large scale the plume is asymmetric, with the downstream end stretching out farther. (2) Small-scale (1-2 km) peaks are present at the upstream and downstream ends of the plume. A number of diagnostic model simulations are performed to understand the processes responsible for these features. The model forcing functions (e.g., freshwater flow, boundary salinity, geometry) and process parameterizations (e.g., gas transfer velocity) are systematically modified and the resulting tracer profiles are compared to those from the unmodified model (base case). These comparisons show that the large-scale asymmetry is related to salinity. The salt causes an estuarine circulation, which (a) decreases vertical mixing (vertical density gradient), (b) increases longitudinal dispersion (increased vertical and lateral gradients in longitudinal velocities), and (c) increases net downstream velocities in the surface layer. Since salinity intrusion is confined to the downstream end of the tracer plume, only that part of the plume is affected by those processes, which leads to the large-scale asymmetry. The small-scale peaks are due to tidal trapping. Small embayments along the estuary trap water and tracer as the plume passes by in the main channel.

At a later time, when the plume in the main channel has passed, the tracer is released back to the main channel, causing a secondary peak in the longitudinal profile.

Introduction

Understanding the transport characteristics of the Hudson Estuary is important for predicting the fate of contaminants discharged in the past (e.g., polychlorinated biphenyls (PCBs)), present (e.g., pathogens from combined sewer overflows (CSOs)) and future (e.g., spills). Estuarine transport can be studied by observation as well as analytical and numerical modeling. Whereas either of these approaches can be used alone, the combination of data and model is the most effective approach because observational and modeling strategies complement each other. Data can be used to calibrate and validate a model and models help understand the physics governing natural systems and extrapolate data to areas and times with little or no coverage.

Continued improvements in analytical techniques provide us with the capability to observe tracers released into a water body at much higher temporal and spatial resolution. This allows for a much more sophisticated model calibration. At the same time computational power increases, and with it the spatial resolution of numerical estuarine models. The result is greater realism, but also increased complexity, which makes models more difficult to understand. High-resolution models of complex natural systems, such as the Hudson Estuary, frequently produce features that are intuitively difficult to explain, and diagnosing such features is important for

understanding the model and the real system. Advanced model diagnostic tools that allow for the visualization of computed parameters (e.g., animations of surface currents) are crucial for understanding the behavior of models. They are, in essence, tools for observing the model system, as data collection is a tool for observing the natural system. Another diagnostic strategy, which is typically not possible with the natural system, is to modify the model forcing functions and coefficients systematically and observe the effect on the simulated variables. Salt, for example, can be removed to understand its effect on the transport of constituents dissolved in the water. This technique is commonly used to understand the sensitivity of model results to the values of various input parameters (e.g., uncertainty analysis). However, it can also be used to identify and understand the mechanisms controlling the behavior of models. Here, such diagnostic simulations are used to understand the behavior of a model and the physical processes operating in the Hudson Estuary.

In this contribution a numerical simulation of a tracer release into the Hudson Estuary is presented. The study combines high-resolution tracer sampling (over 2,000 samples, 400 m resolution) and modeling (over 10,000 mass balance segments; 600 m horizontal, 1 m vertical resolution in the study area). An existing model presented by Blumberg et al. (2003) is used to simulate the fate and transport of SF₆ released in a field study presented by Ho et al. (2002).

Study Area

The Hudson River starts at Lake Tear of the Clouds in the Adirondack Mountains and ends in New York City. The 248 km stretch below Troy, NY is commonly referred to as the Hudson Estuary (Fig. 1). Freshwater inflow into the estuary occurs predominantly from the Upper Hudson River at Troy, NY at an average rate of $392 \text{ m}^3 \text{ s}^{-1}$. Smaller tributaries, like Wappinger Creek ($7 \text{ m}^3 \text{ s}^{-1}$), also discharge downstream of that point. The flow of the Upper Hudson River is seasonal, highest during winter and spring and lower in the summer. As a result the salinity intrusion is also seasonal. In the spring the salt front is located near Yonkers, NY and in the summer it is located by Newburgh, NY. The hydrodynamics of the Hudson Estuary have been studied by Steward (1958), Pritchard et al. (1962), Busby and Darmer (1970), Abood (1974), Posmentier and Rachlin (1976), Hunkins (1981) and Geyer et al. (2000).

Data

In the summer of 2001 a large-scale SF_6 tracer release experiment was conducted in the Hudson Estuary (Ho et al. 2002). On 7-25-01, roughly 4.3 moles of SF_6 gas were injected at 5 m depth near Newburgh, NY (Fig. 2; KMP 98; distances are referenced to the Battery at the southern tip of Manhattan) from a boat while twice traversing the estuary laterally over a period of 28 min. The release time (12:14-12:42) approximately corresponds to slack before flood (SBF) at Newburgh, NY. Based on subsequent concentration measurements, Ho et al. estimated that of the 4.3 moles injected ca. 1.1 moles dissolved in the water, whereas the remainder escaped to the atmosphere in the form of bubbles. SF_6 is an inert gas and consequently is lost from the water column only by gas exchange across the air-water interface. On the basis of a

mass balance, Ho et al. estimated an average gas transfer velocity for SF₆ (K_{L,SF_6}) of 1.4 m d⁻¹ for the duration of the experiment.

SF₆ concentrations were measured over a period of two weeks following the release. Measurements were taken daily at 2 m depth with a fully-automated continuous analysis system from a boat while traversing the plume longitudinally. The typical sample interval was 2 min in time and 400 m in space. The resulting 12 longitudinal profiles contain an average of 172 measurements for a total of 2,060 data points. On certain days SF₆ concentrations were measured at several depths at various locations (Fig. 2).

Model

The model, described in detail by Blumberg et al. (2003), is based on the three-dimensional, time-variable, estuarine and coastal circulation modeling framework (ECOM). It is an estuarine and coastal version of the Princeton Ocean Model (POM; Blumberg and Mellor 1987), incorporating the Mellor-Yamada 2.5 level turbulent closure model that provides a realistic parameterization of vertical mixing processes. A curvilinear horizontal segmentation allows for smooth and accurate representation of shoreline geometry, and a sigma-level vertical coordinate system permits better representation of bottom topography. The model solves a coupled system of differential, prognostic equations describing the conservation of mass, momentum, salinity, temperature, turbulent energy, and turbulence macro scale. Recent applications of the model to St. Andrew Bay, FL and Pensacola Bay, FL are presented by

Blumberg and Kim (2000) and Ahsan et al. (2003), respectively. A detailed description of the model's governing equations can be found in Blumberg et al. (1999) and HydroQual (2001).

The model covers 209 km of the Hudson Estuary from Hastings-on-Hudson, NY, to Troy, NY (Fig. 1). It consists of 1,191 horizontal grid boxes, each with 10 layers in the vertical, for a total of 11,910 mass balance segments. The model is forced with discharge from five rivers (Upper Hudson River, Esopus Creek, Rondout Creek, Wappinger Creek and Croton River), atmospheric heat flux and wind stress (based on data at Albany and New York City) and water surface elevation, salinity and temperature at the downstream boundary (Hastings-on-Hudson, NY). In addition, withdrawal and discharge rates and temperature rise of five power plants (Danskammer Point, Roseton, Indian Point, Lovett and Bowline Point) are specified as input. The model was originally set up to simulate the periods 3-11-98 to 4-9-98 (high flow) and 8-1-97 to 8-30-97 (low flow) and validated extensively against field data including water surface elevation, salinity and temperature at various locations, shipboard acoustic Doppler current profile (ADCP) velocity, salinity and temperature measurements and fixed-site ADCP velocity, salinity and temperature measurements as described by Blumberg et al. (2003).

Tracer Simulation

MODEL SET-UP

For the tracer simulation the model forcing functions were updated for the period 7-10-01 to 8-9-01 allowing for 15 days of “spin-up” before the tracer release on 7-25-01. The model boundary conditions (freshwater flow rate, wind speed, wind direction and downstream boundary water surface elevation) were assigned based on data. The mean flow rate for the model period of the Hudson River at Troy was $140 \text{ m}^3 \text{ s}^{-1}$. Salinity and temperature for the start of the simulation (initial conditions) were not available. They were specified based on ship surveys before and after the start date (6-15-01, 7-28-01) and surface measurements at the USGS gage at Hastings-on-Hudson. Power plant intake and outfall data for the new period were not available and were kept the same as for the original low flow period.

SF₆ was added to the model at a constant loading rate (mol s^{-1}) over a period of 28 min at KMP 98, distributed equally over the 10 lateral grid boxes (Fig. 2) and top 5 vertical layers (corresponding to approx. 5 m). Ho et al. (2002) injected 4.3 moles, of which they estimated 1.1 moles dissolved. Their estimate was based on subsequent SF₆ inventory estimates, and in a similar manner the total mass added to the model was adjusted here to match the SF₆ concentration profiles, resulting in an addition of 1.6 moles to the model. To simulate SF₆ gas exchange a constant gas transfer velocity (K_{L,SF_6} , m d^{-1}) was specified. This velocity was divided by the depth of the top layer, to yield a first-order decay rate, which was applied to the top layer. This assumes the atmospheric gas concentration is negligible, which is a safe assumption for this study. The approach is relatively crude, in that it neglects the effect of varying wind speed on the gas transfer velocity and assumes the tracer is vertically uniformly mixed over the top layer. A constant gas transfer velocity of $K_{L,\text{SF}_6} = 1.4 \text{ m d}^{-1}$ as estimated by Ho et al. (2002) was used.

The horizontal dispersion used by Blumberg et al. (2003) was based on calibration to relatively small horizontal gradients in salinity. Initial simulations of the SF₆ tracer release using the same coefficient of dispersion, $C_S = 0.10$ (C_S is the constant in the dispersion formulation by Smagorinsky 1963), as Blumberg et al. (2003) resulted in an underestimation of the dispersion of SF₆. The C_S coefficient was therefore recalibrated to match observed tracer concentrations resulting in a value of 0.01. This is within the range of other applications (HydroQual 2001; Ezer and Mellor 2000), but at first glance, it is surprising that such a large change is required. To illustrate the effect of the C_S coefficient (and to validate the model performance), a model-data comparison using both C_S values is presented for salinity and SF₆ in Figs. 3 and 4, respectively. A more extensive model-data comparison for SF₆ concentrations will be presented in the following section. For salinity (Fig. 3), the simulation with $C_S = 0.10$ under-predicts salinity at KMP 83 and 88. The simulation with $C_S = 0.01$ is in good agreement with those data points, but over-predicts salinity at the downstream end (KMP 73). Overall, the effect of C_S on salinity is relatively weak and considering the uncertainty in initial conditions the calibration with either C_S value can be considered acceptable. For SF₆ concentrations (Fig. 4), the choice of C_S has a larger effect. The simulation with $C_S = 0.10$ clearly underpredicts the dispersion of the tracer. It should be noted that the dispersion of SF₆ is indirectly affected by salinity (which is also affected by dispersion), as described in detail later in the paper. The difference in SF₆ dispersion observed in Fig. 4 is therefore not just a direct effect of the C_S coefficient. The difference in sensitivity of the two tracers (salinity and SF₆) to horizontal dispersion is due to differences in the spatial gradient. The spatial gradient of salinity is relatively small and as a result it is not

very sensitive to horizontal dispersion. In the complete absence of a spatial gradient (i.e. constant salinity) the dispersion would have no effect on the predicted salinity. The SF_6 concentration has a much higher spatial gradient and is therefore more sensitive to dispersion. This comparison highlights (a) the utility of deliberately introduced tracers for model calibration, and (b) the importance of dispersion in the transport of substances with high spatial gradient (i.e. spills).

MODEL-DATA COMPARISON

General Considerations

The tide can cause an injected tracer to travel upstream and downstream within the tidal cycle, as illustrated in Fig. 5. The distance traveled by a water parcel between low and high water (tidal excursion) is typically about 8 km in the study area. As a result the tracer concentrations at a given location can vary significantly in time. The model-data comparison is therefore a very stringent test, because it not only tests the ability of the model to reproduce the shape of the plume but also tests the timing. In this contribution, tracer concentrations will generally be presented on a logarithmic scale for two reasons. First, the concentrations vary over four orders of magnitude and a logarithmic scale allows for the visualization over a large range. Second, as described in the Appendix, the logarithmic scale is most appropriate for skill assessment of fate and transport models, especially for conservative substances.

Quantitative Model Skill Assessment

To quantitatively assess the skill of the model, a real-time comparison was performed. This involved matching measured and model computed values in three dimensional space and time. The comparison, presented in Fig. 6, shows that the model can predict the observed SF₆ concentration over four orders of magnitude. Several statistics are presented in the figure. As described in detail in the Appendix, the most appropriate statistics for skill assessment of models of conservative substances are the mean relative deviation (MRD), mean relative bias (MRB) and explained variance in log space (EVL). For this application the MRD is 1.9, indicating that on average the relative agreement between the model and data is about a factor of two (i.e., 50 vs. 100 fmol L⁻¹). Although the agreement between model and data is generally good, a bias is evident with the model generally over-predicting higher concentrations and under-predicting lower concentrations. Also, the distribution of modeled concentrations is less dispersed indicating that the model under-predicts dispersion.

Longitudinal Profiles

Longitudinal profiles of surface SF₆ concentration for data and model simulations are compared for 12 days in Fig. 7. Note that the figure only covers a portion (KMP 60-120) of the full model domain (KMP 36–248). A comparison of spatial profiles is most useful if it is synoptic, meaning a “snapshot” of concentration values at one point in time. Also, to evaluate

the day-to-day progression of the tracer plume it is desirable to eliminate the variability introduced by tidal movement. This is done by plotting each subsequent day at the same time in the tidal cycle (SBF at Newburgh, NY). For model results this is not a problem, because a virtually continuous representation of concentrations is available for each grid box. However, for the data, which were collected at different times over the course of a sampling cruise and at a different time in the tidal cycle at subsequent cruises, a correction has to be applied. Here the data were made synoptic and corrected to the same time in the tidal cycle as described by Ho et al. (2002) and any errors in this transformation are therefore also reflected in this model-data comparison.

Figure 7 shows that the SF₆ concentrations decreased with time due to gas exchange and dispersion. At the same time dispersion increased the length scale over which the tracer was spread out. The peak tracer concentrations decreased from more than 10,000 to less than 1,000 fmol L⁻¹ during the 14 days following the release. After 4-5 days the concentration at KMP 115 reached 10 fmol L⁻¹ and remained at approximately that value for the remainder of the study period. The tracer continuously spreads in the downstream direction. The model reproduces these features. Downstream of KMP 70 the model under-predicts the tracer concentration by up to about a factor of two (at KMP 60). The model boundary is located far enough downstream (KMP 36; tidal excursion ~ 8 km), for this not to be a boundary effect.

On the large scale, the data and model both show an asymmetric longitudinal concentration profile. Downstream of KMP 80 the tracer spreads out faster. Since the

asymmetry starts at about KMP 80, this feature is most evident at later times when the tracer has reached that location. The data and model show small-scale features (peaks) on the upstream and downstream sides of the plume. These features are most pronounced early in the experiment (e.g., 7-27-01) when the longitudinal concentration gradient is high, but they are present throughout the simulation (e.g., 8-6-01, KMP 101). The spatial scale of these features is as low as 1-2 km and they are resolved because of the high resolution of the data and the model. The cause of these large- and small-scale features will be discussed in the next section.

Location of Peak Concentration and Center of Mass

The location of the peak concentration and the center of mass as a function of time for model and data are compared in Fig. 8. The trajectory of the peak concentration is highly variable, because it is defined by a single point. The trajectory of the center of mass is a more robust measure, because it is based on all points. It moves downstream at a velocity corresponding to approximately the net estuarine flow, but the peak concentration travels downstream at a significantly lower velocity. This is evident in the data and model, and the cause of this behavior will be discussed in the next section.

Vertical Profiles

Vertical profiles of SF₆ concentration for three locations and four days are presented in Fig. 9. Depending on the depth at the sample point, the model depth can be lesser (e.g. Iona

Island, 7-31-01) or greater (e.g. World's End, 7-29-01) than the data depth, because the depth in the model is the average for the grid box. The model reproduces the vertically averaged concentration at Storm King, but underestimates the concentrations at World's End and Iona Island. At Iona Island the model under-predicts the concentration by up to about a factor of two, consistent with the longitudinal profiles. Although SF₆ mixes to great depths, a weak concentration gradient remains with concentrations generally higher at the surface than at the bottom. The average ratio of surface to bottom concentration for data and model is 1.7 and 1.6, respectively, indicating that the model reproduces the vertical mixing.

Horizontal Distribution

Most of the data were collected along one-dimensional longitudinal transects and therefore cannot be used to resolve any two-dimensional features of the tracer plume. However, limited lateral surveys performed by Ho et al. (2002) did show significant lateral structure with concentrations on the banks as low as half of those in the channel. The model also predicts significant two-dimensional structure in the plume. This is illustrated by the horizontal SF₆ concentrations in Newburgh Bay, presented as contours in Fig. 10. The modeled concentrations in the channel, which approximately corresponds to the sample locations, can be higher (KMP 107) or lower (KMP 102) by a factor of about 2 than on the banks. This pattern is variable in time, depending on the tidal condition (i.e., flooding or ebbing).

Discussion

ANALYSIS STRATEGY

The model-data comparison illustrates that the model can reproduce many features of the observed SF₆ fate and transport in the Hudson Estuary. In this section the model is analyzed with the objective to learn how different features of the system (e.g., freshwater flow) affect the fate and transport of dissolved constituents. Also, the cause(s) of the (a) large-scale asymmetry, (b) small-scale secondary features in the longitudinal concentration profile, and (c) difference in downstream velocity of the peak concentration and center of mass are investigated. To answer these questions, a number of diagnostic model simulations were performed. Rather than visualizing parameters computed by the model (e.g., plot surface velocities) the model forcing functions (e.g., reduce freshwater flow) and parameterizations of processes (e.g., double gas transfer velocity) are modified and the effect on the simulated concentration is examined. The concentrations computed by the modified model are compared to that of the unmodified model (base case). The longitudinal profile ten days after the release (8-4-01) is used for comparison.

EFFECT OF AIR-WATER GAS EXCHANGE

Air-water gas exchange is the only sink of SF₆ from the water column and it is of interest how much of the magnitude and shape of the longitudinal concentration profile can be attributed to it. This allows for the results to be related to spills of more or less conservative substances.

Further, it is possible that gas exchange is responsible for the asymmetric concentration profile, because it is a function of the surface area. The width of the estuary significantly decreases downstream of Storm King (KMP 88; Fig. 2) causing a decrease in surface area (on a unit length basis), which could be responsible for the asymmetric concentration profile.

Two simulations were performed with the gas transfer velocity (K_{L,SF_6}) modified from the base case (1.4 m d^{-1}) to zero and twice the base case (2.8 m d^{-1}). The results illustrate that gas exchange is responsible for about half of the decrease in peak SF_6 concentrations over the ten days following the release (Fig. 11a). Gas exchange affects mainly the overall magnitude of tracer concentration. The general shape of the longitudinal concentration profile, including the asymmetry and secondary peaks, is not affected. Those features are therefore not related to gas exchange.

EFFECT OF FRESHWATER FLOW

Freshwater inflow to the estuary affects the transport of constituents in mainly two ways. First, on a time scale of days to weeks, it causes a net downstream movement of water that contributes to the flushing of the estuary. Second, on a time scale of weeks to several months (e.g., seasonal), it affects the salinity intrusion that influences much of the estuarine circulation. Here the short-term effect of freshwater flow is examined. For this purpose the tributary inflows are modified and the initial and downstream boundary salinity concentrations were assigned as in the base case. Several simulations were performed with the Hudson River flow rate at Troy being

modified from the base case ($140 \text{ m}^3 \text{ s}^{-1}$) to zero, mean flow ($400 \text{ m}^3 \text{ s}^{-1}$), typical spring flow ($1,000 \text{ m}^3 \text{ s}^{-1}$) and the 10-year flood ($3,400 \text{ m}^3 \text{ s}^{-1}$).

The results illustrate how freshwater inflow causes a net downstream movement of tracer (Fig. 11b). The modeled concentrations for the 10-year flood simulation are not visible at that scale, because the tracer is flushed out of the estuary by 8-04-01. The no-flow case shows that after 10 days the peak concentration is located upstream of the release point. This is an effect of the different dispersion characteristics in the upstream and downstream direction (to be discussed subsequently). The center of mass shows no temporal trend for that simulation and after 10 days it is located at the release point (KMP 98). As for the base case, the longitudinal concentration profiles for various flow regimes have secondary peaks and are asymmetric, illustrating that neither of these features are related to the short-term effects of freshwater flow.

EFFECT OF SALINITY

The presence of salty ocean water at the downstream end, and freshwater at the upstream end results in a spatial salinity (and hence density) gradient. This causes a gravitational circulation with the salty water moving upstream in the lower layer and right-bank side (looking upstream) and freshwater moving downstream in the surface layer and left-bank side. There is also a small net vertical motion directed from the bottom to the surface layer (Pritchard 1969). The vertical density gradient stabilizes the water column, which inhibits vertical mixing. The

vertical and lateral shear caused by this “estuarine circulation” was recognized by Pritchard (1954) and Fischer (1972) as the main contributor to longitudinal dispersion.

To investigate the effect of salinity, the initial and open boundary salinity concentrations were set to zero and twice the base case. At the downstream boundary the salinity was thus increased from 16 to 32, which represents extremely saline conditions. The tracer concentrations for the zero salinity simulation are similar to the base case at the upstream end of the plume (Fig. 11c). This is plausible, because at that location the salinity is close to zero for the base case as well (see Fig. 3). However, the downstream end of the plume has changed significantly. Most interestingly, the new profile is symmetric, which shows that the asymmetry is related to salinity. For the high salinity simulation the point where the asymmetry starts (80 km in the base case) is further upstream. This shows that the location where the asymmetry starts is determined by dynamics, depending on the salinity and not tied to fixed physical features (e.g., bathymetry).

The presence of salt significantly changes the hydrodynamics at the downstream end of the plume. One effect is reduced vertical mixing. This is evident in the vertical SF_6 concentration profiles in Fig. 12, where concentrations are normalized to that at the surface. As described in the model-data comparison, the base case shows a vertical stratification similar to the data. The “no salt” case is comparatively well mixed throughout the water column. It shows a weak subsurface peak, which is due to tracer being removed from the surface to the atmosphere by gas transfer. The salt also affects the longitudinal velocities, as illustrated by vertical and transverse profiles of residual longitudinal velocities for the “no salt” and base cases presented in

Fig. 13. At Iona Island (Fig. 13a,c) the velocities are significantly different between the two cases. The “no salt” case has relatively uniform vertical and horizontal distributions of longitudinal velocities in the downstream direction. The base case has upstream velocities at the bottom and downstream velocities at the surface. This is the classical estuarine circulation described previously. Also, the lateral distribution of longitudinal velocities is more variable, with west bank velocities in the upstream direction. This is opposite to the typical Coriolis induced horizontal asymmetry, which would predict downstream movement on the west bank. The reason for this discrepancy is that the effect of the apparent Coriolis force is small compared to other factors (i.e. geometry). In Newburgh Bay, near the release point (Fig. 13b,d), the velocities of the two cases are similar. That is because at that location the salinity is close to zero in both cases.

We propose that three mechanisms related to the estuarine circulation at the downstream end of the plume are responsible for the asymmetric SF₆ profile. First, the lesser vertical dispersion over the salt contributes to the asymmetric longitudinal concentration profile of surface concentrations, because less mass is “lost” to the deeper layers by vertical mixing. Second, as pointed out by Pritchard (1954) and Fischer (1972), longitudinal dispersion is enhanced by lateral and vertical gradients in longitudinal velocities. The increased gradients in the presence of salt, enhance longitudinal dispersion at the downstream end of the plume, contributing to the asymmetric longitudinal SF₆ profile. Third, the net downstream velocity in the surface layer, which corresponds to the concentration measurements, increases over the salt

(compare base case in Figs. 13a and 13b). This accelerates the water carrying the tracer at the downstream end of the plume, stretching out the plume.

The above analysis demonstrates that the large-scale asymmetry is related to salinity and three mechanisms are proposed. It is interesting to note that those three mechanisms are different than the two proposed by Pritchard et al. (1962). They suggested that on the downstream side of estuaries increased (1) tidal energy and (2) cross sectional area can lead to an asymmetry. Using numerical and physical models of the Hudson Estuary they showed that the first process leads to an asymmetry of a tracer released in the lower portion of the Hudson Estuary (at the southern end of Manhattan, KMP 3). The second process is not important in this case, because the cross-sectional area is relatively constant in the Hudson Estuary. The relative importance of the various processes proposed here and by Pritchard et al. (1962) depends on the hydrodynamics and all of them should be considered when studying the transport of a tracer in an estuary.

In the model-data comparison it was observed that the center of mass moves downstream at a faster velocity than the peak concentration. Also, in the “no freshwater” simulation, the peak concentration moved upstream, consistent with the base case considering the center of mass remained stationary. The cause for this phenomenon is the difference in the dispersion characteristics in the upstream and downstream directions as pointed out by Pritchard et al. (1962). Mass spreads out faster in the downstream direction, and over time this causes the peak to shift upstream from the center of mass. If there were absolutely no dispersion across a point at

the upstream end of the plume (e.g. KMP 120) and the only loss process was dispersion in the downstream direction, the peak concentration, after a long time, would actually be located at that upstream point.

EFFECT OF GEOMETRY

The geometry of the Hudson Estuary is highly variable containing deep narrow channels (e.g., World's End), wide shallow bays (e.g., Newburgh Bay) and many smaller scale indentations that occur in the form of coves and inlets. The geometry affects the fate and transport of a tracer directly, by trapping water parcels as the tracer plume passes and allowing them to be released later in the tidal cycle. The phase lag between the currents in the nearshore embayments and main channel acts to form “dead zones” that trap and release tracer into the main flow. The effect is to increase longitudinal dispersion of the tracer (Okubo 1973). Besides this “tidal trapping”, the overall dynamics of the circulation are also affected by the geometry, which can have indirect effects on tracer transport.

To investigate the effect of geometry on tracer transport the model grid was modified to a straight rectangular channel with dimensions based on those of the Hudson Estuary covered by the model grid (width = 1.3 km, depth = 9 m). Other factors that introduce two-dimensional effects (tributary freshwater flow, wind, coriolis force and power plants) were kept as in the base case. The model predicts less overall spreading of the tracer plume illustrating that geometry irregularities contribute to the longitudinal dispersion (Fig. 11d). The profile is relatively

symmetric, which is a reflection of reduced salinity intrusion, consistent with the decreased longitudinal dispersion. For that reason it might be more appropriate to compare the straight channel case to the no salinity case (Fig. 11c). Although the profile is not perfectly smooth, there are no pronounced secondary peaks, which illustrates that those features are related to geometry irregularities. Small-scale embayments, like that near Wappinger Creek (KMP 106; Fig. 10) trap tracer mass leading to the secondary peaks in the longitudinal concentration profile.

Summary and Conclusions

A numerical model was used to simulate a large-scale SF₆ tracer release experiment in the Hudson Estuary. In general, the model reproduces the observed fate and transport of the tracer. The model underpredicts concentrations at the downstream end of the plume, which points to areas for possible improvement. Also, instead of specifying a constant gas transfer velocity it would be desirable to calculate it dynamically based on the wind (Wanninkhof 1992) and/or current speeds (O'Connor and Dobbins 1958).

The data show a large-scale asymmetry in the longitudinal profile of surface concentrations (plume), small-scale secondary features at the upstream and downstream sides of the plume, and a difference in the velocity of the peak concentration and center of mass. The model reproduces these features. To understand the underlying mechanism responsible for these

features, the model forcing functions and coefficients were systematically varied. This leads to the following general conclusions about the fate and transport of a tracer in the Hudson Estuary.

Salinity intrusion causes an estuarine circulation, which leads to larger dispersion. Three mechanisms related to the estuarine circulation are identified. First, increased vertical density stratification inhibits vertical mixing. Second, increased vertical and transverse gradients in longitudinal velocities (estuarine circulation) increase longitudinal dispersion. Third, increased net downstream velocities in the surface layer stretch out that portion of the plume. A constituent released in the freshwater part of the Hudson Estuary will spread more over the saltier water and mix less with the deeper layers leading to an asymmetric longitudinal profile of surface concentrations.

Geometry irregularities significantly increase longitudinal dispersion by tidal trapping. Kilometer scale embayments, like those by Wappinger Creek, temporarily trap water masses. This causes entrainment of water with higher tracer concentrations into water with lower concentrations, and vice versa. Over time this contributes to longitudinal dispersion.

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APPENDIX: MODEL SKILL ASSESSMENT METRICS

A performance statistic is needed to quantitatively describe the skill of a model. Often the Root Mean Square Error (RMSE), the Mean Absolute Error (MAE) or the fractional explained variance (EV) are used. The RMSE and the MAE provide a measure of the average error, while the EV provides a measure of the spread of the errors scaled by the variability of the data. However, the RMSE, MAE and EV computed with model and observations in real space can

often be inappropriate descriptors of the skill (as related to parameter accuracy) of fate and transport models, especially for conservative tracers. This is related to the way in which errors are generated in these types of models. For conservative substances, the mass balance equation is linear in concentration. For non-conservative substances, reactions can introduce non-linearities. However, often reaction equations are also linear (e.g., first-order decay), resulting in a linear mass balance equation for non-conservative substances as well. For linear models, errors in the transport or reaction parameters will lead to errors in concentration that are proportional to the magnitude of the concentration. A parameter error that leads to a concentration error of 50 fmol L^{-1} for a concentration of 100 fmol L^{-1} will lead to an error of 5 fmol L^{-1} for a concentration of 10 fmol L^{-1} . The absolute error in real space varies with concentration (i.e., $150 - 100 \neq 15 - 10$), which makes it an unsuitable measure of model skill. Here, we recognize that the differences in the concentration (100 vs. 10) in the two settings are due to differences in boundary and initial conditions, and the error in the model concentration corresponds to a fixed mis-specification of the model parameters (e.g. dispersion coefficient). Since the model concentrations are linear in the forcing functions (boundary and initial conditions), the concentration errors are proportional. Consider a slug release of a tracer into a model with a dispersion coefficient that is uniformly too high by a factor of 1.5. Since the error is constant, so is the skill of the model. However, the absolute error (difference between modeled and observed concentration) would vary spatially and temporally. A better measure of skill is the ratio of model-predicted to measured values. In the above example this ratio is constant (i.e., $150/100 = 15/10 = 1.5$) and is therefore the preferred statistic. One can use the mean value of this ratio over all observations, as a measure of skill or equivalently compute the traditional skill measures using log transformed values. The

logarithmic scale is best suited to visualize relative agreement, because a constant relative agreement corresponds to a constant distance on a logarithmic scale, regardless of the magnitude of concentration. The resulting skill statistics of interest are:

$$MRD = 10^{RMSE_{\log}} \quad (1)$$

$$MRB = 10^{ME_{\log}} \quad (2)$$

$$EVL = 1 - \frac{MSE_{\log}}{s^2_{d,\log}} \quad (3)$$

where MRD is the mean relative deviation. It is a transform of the RMSE in log space ($RMSE_{\log}$). That is the RMSE computed with the logs of the data and model values. MRB is the mean relative bias. It is a transform of the mean error (ME) in log space ($ME_{\log}$). EVL is the fractional explained variance (EV) in log space computed from the mean square error (MSE) in log space ($MSE_{\log}$) and the variance of the data (σ^2_d) in log space ($\sigma^2_{d,\log}$). The three measures correspond to the RMSE, ME and EV traditionally computed in real space. Jointly, they provide skill scores for aggregate model performance. Note that the explained variance in real space by a model will likely be smaller than that in log space.

FIGURE LEGENDS

Fig. 1. Hudson Estuary from Troy to Hastings-on-Hudson.

Fig. 2. Model grid in the study area. The grid extends from Troy to Hastings-on-Hudson (see Fig. 1) and consists 1,191 horizontal boxes with 10 vertical layers each. The data consist of 12 longitudinal transects of surface (2 m) concentrations with a total of 2,060 data points (small points) and 4 vertical profiles each at 3 stations (large points). Grid boxes corresponding to tracer release are rendered solid.

Fig. 3. Longitudinal profiles of modeled and measured salinity on 8-2-01. Two model lines for top and bottom are presented corresponding to the times of the first and last measurements. Dashed line corresponds to SF₆ tracer release location.

Fig. 4. Longitudinal profiles of modeled (solid lines) and measured (points) surface (2 m) SF₆ concentration on 8-2-01. Two model lines are presented corresponding to the minimum and maximum model concentration during the period of measurements (7AM-5PM). Dashed line corresponds to release location.

Fig. 5. Longitudinal profiles of modeled surface (2 m) SF₆ concentration on 7-27-01 at three different times. Dashed line corresponds to release location.

Fig. 6. Modeled vs. measured SF₆ surface (2 m) concentration (fmol L⁻¹). Solid line is 1:1 and dashed lines are +/- 1 order of magnitude. Data below KMP 60 are omitted due to proximity to the model boundary at KMP 36. Statistics are for model and data in logarithmic space (N = number of data points, RMSE = root mean square error, ME = mean error (bias), R = cross correlation (correlation coefficient), SS = skill score; Kara et al. 2002; MRD = mean relative deviation, MRB = mean relative bias, EVL = explained variance in log space; see Appendix).

Fig. 7. Longitudinal profiles of modeled (solid lines) and measured (points) surface (2 m) SF₆ concentration. Concentrations correspond to the same time in the tidal cycle (slack before flood at Newburgh, NY). Model concentrations correspond to horizontal location of data (i.e., ship track, see Fig. 2). Dashed line corresponds to release location.

Fig. 8. Location of data and model SF₆ (a) peak concentration and (b) center of mass vs. time. Center of mass for model and data were calculated from one-dimensional longitudinal profiles of surface concentration (2 m; Fig. 7) applied to model geometry. Points are data. Heavy line is model. Dashed line corresponds to the release location. Light line corresponds to the net freshwater flow during model period (150 m³ s⁻¹ upstream of Newburgh, NY) and average geometry (depth = 9 m, width = 1.36 km)

Fig. 9. Vertical profiles of modeled (solid lines) and measured (points) SF₆ concentrations at three stations (Storm King, World's End, and Iona Island). See Fig. 2 for station locations.

Fig. 10. Horizontal distribution of modeled surface (2 m) SF₆ concentration (fmol L⁻¹) in Newburgh Bay on 7-27-01 14:28. Gray lines are shoreline. Black lines are concentration contours. Contour values are indicated by label on land. Points are sample locations for that date.

Fig. 11. Longitudinal profiles of modeled surface SF₆ concentration on 8-4-01. Thin lines are for the base case and heavy lines are for various modifications (see text). Dashed lines correspond to the release location.

Fig. 12. Vertical profiles of modeled (solid lines) and measured (points) SF₆ concentrations at World's End on 8-2-01. Concentrations are normalized to that at the surface. See Fig. 2 for station location. Thin line is for the base case and heavy line is for the "no salt" case.

Fig. 13. Residual velocity profiles. (a,b) lateral average vs. depth. (c,d) vertical average vs. lateral distance. Positive velocities are downstream. Thin lines are for the base case and heavy lines are for the "no salt" case. Dashed lines correspond to zero residual velocity. See Fig. 2 for locations.

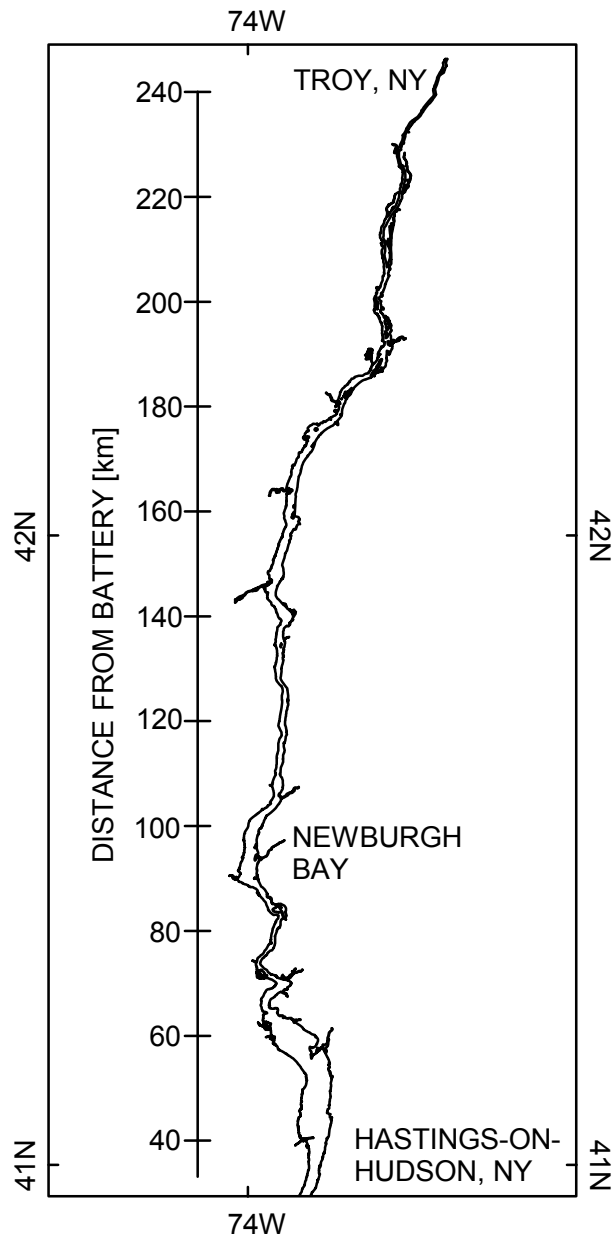


Figure 1
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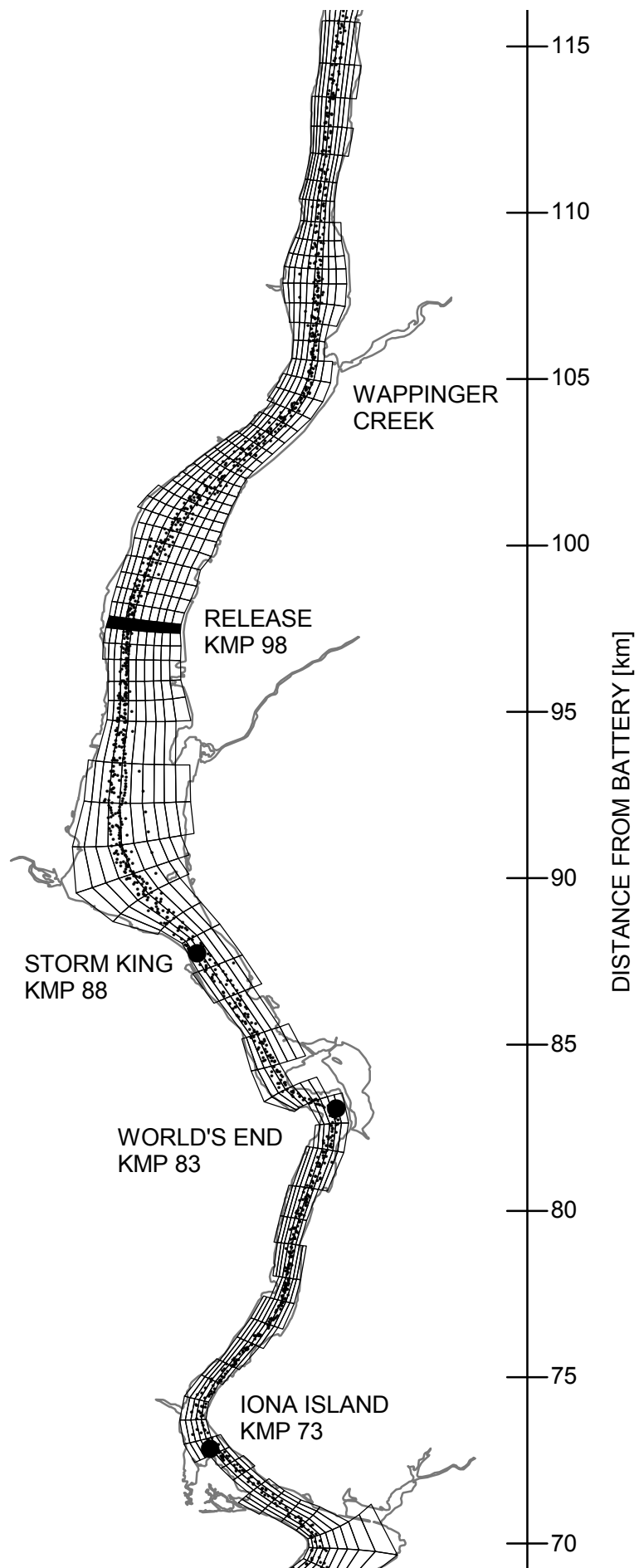
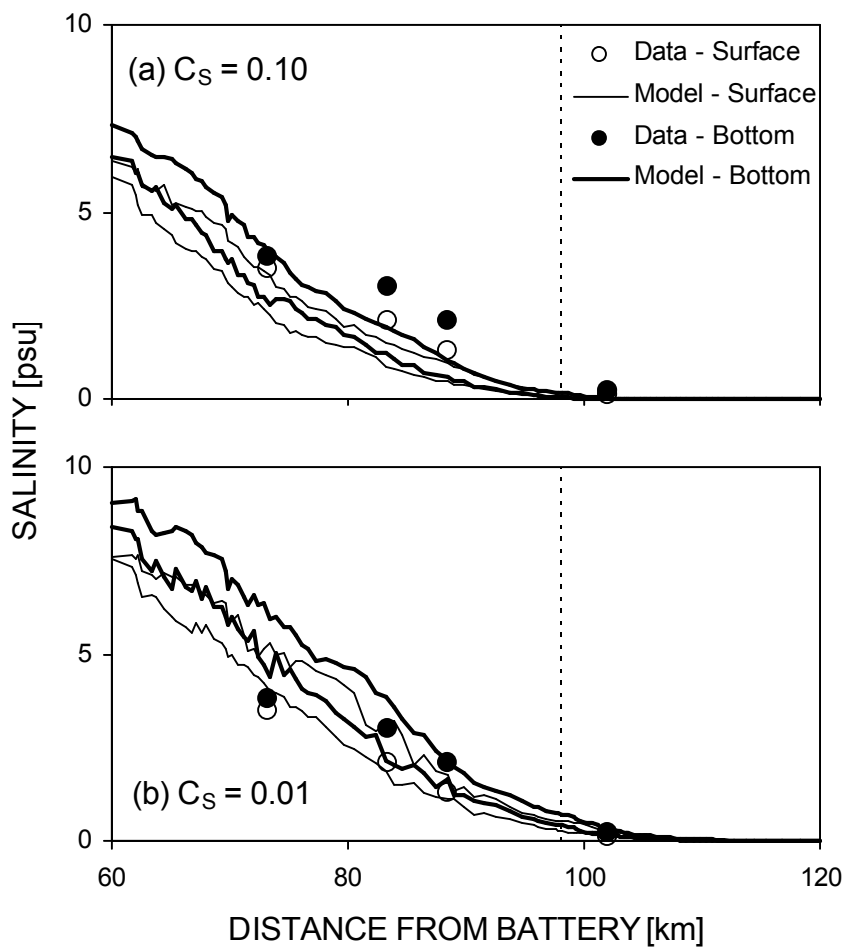
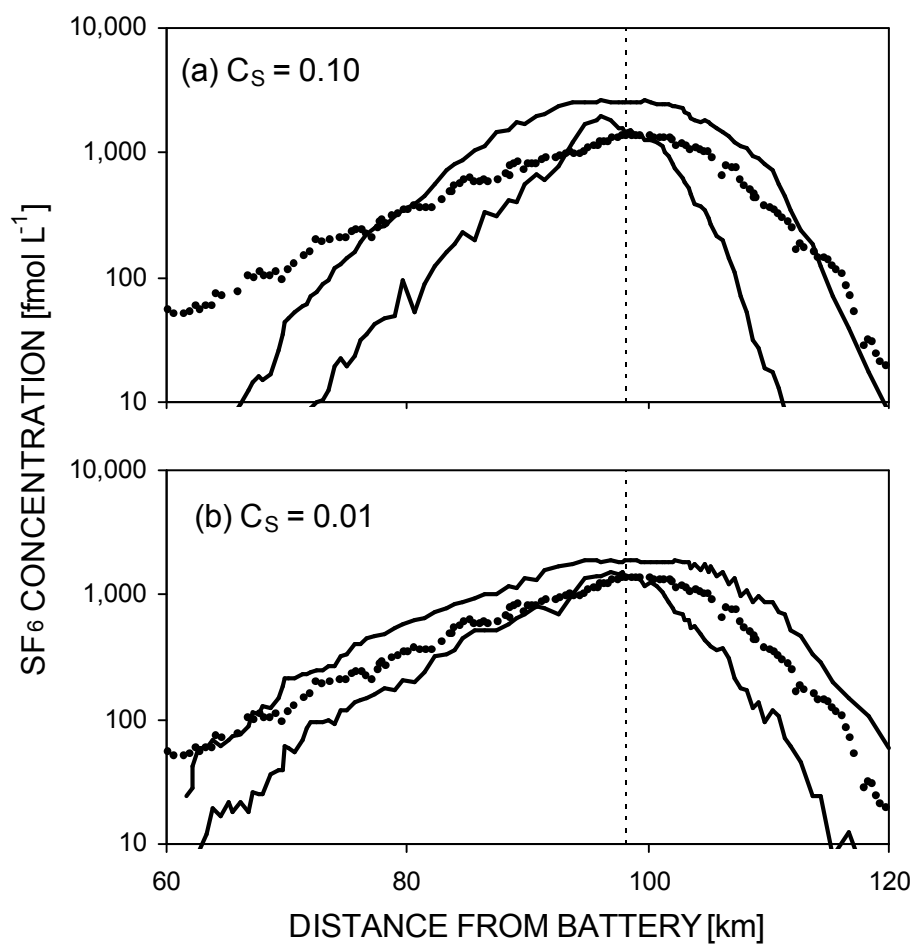
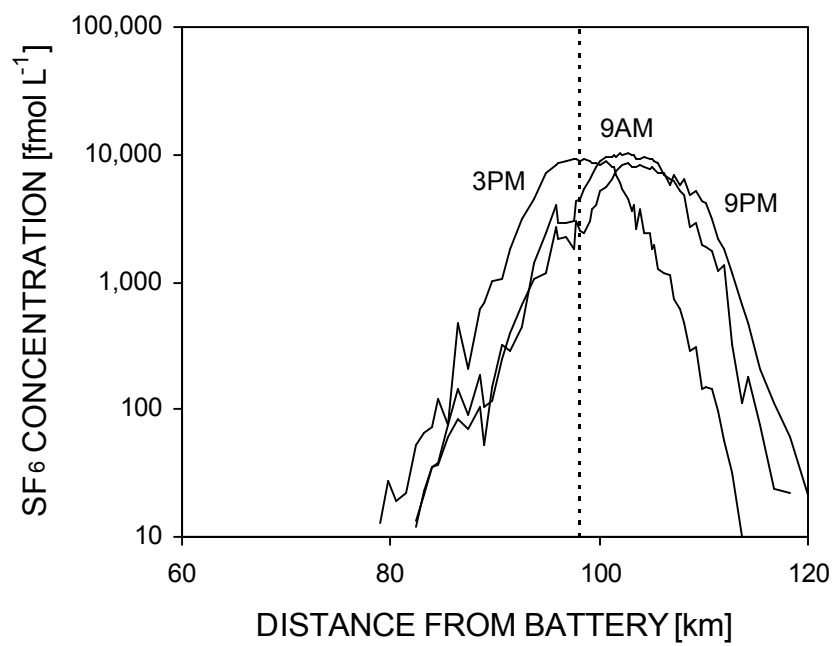
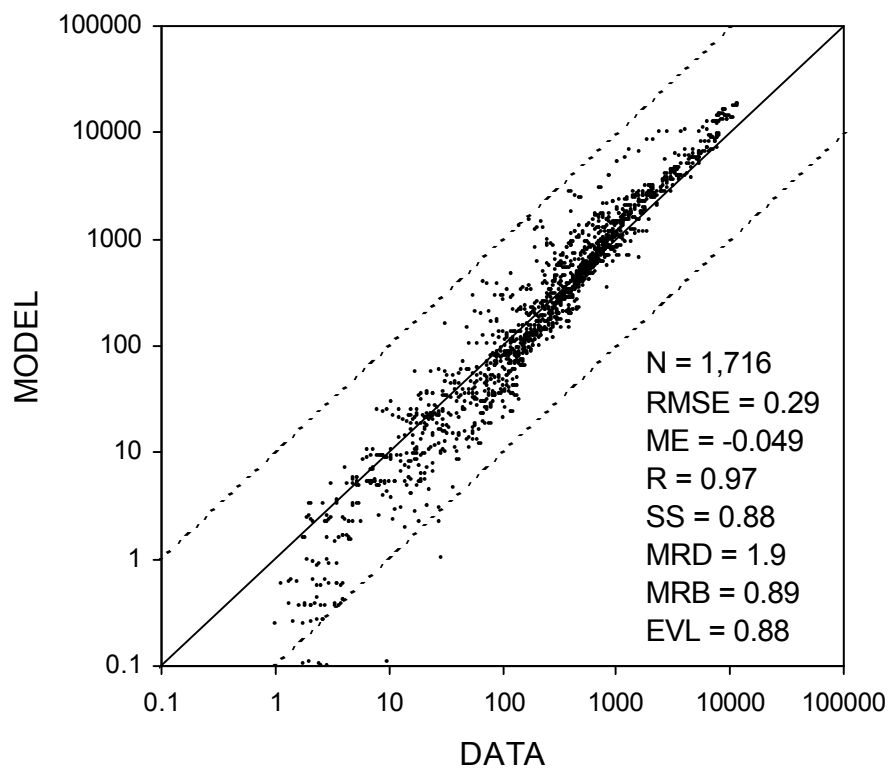


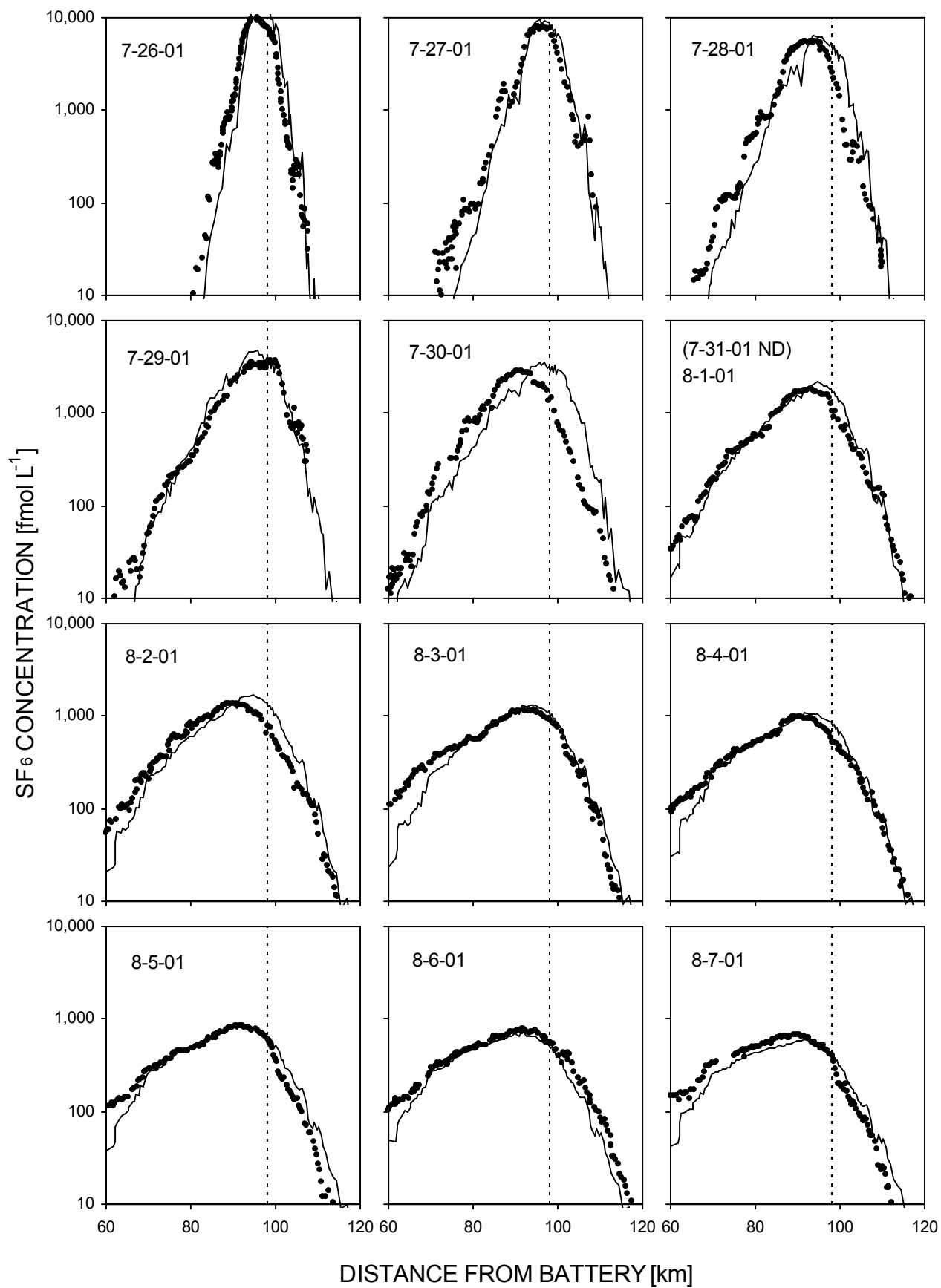
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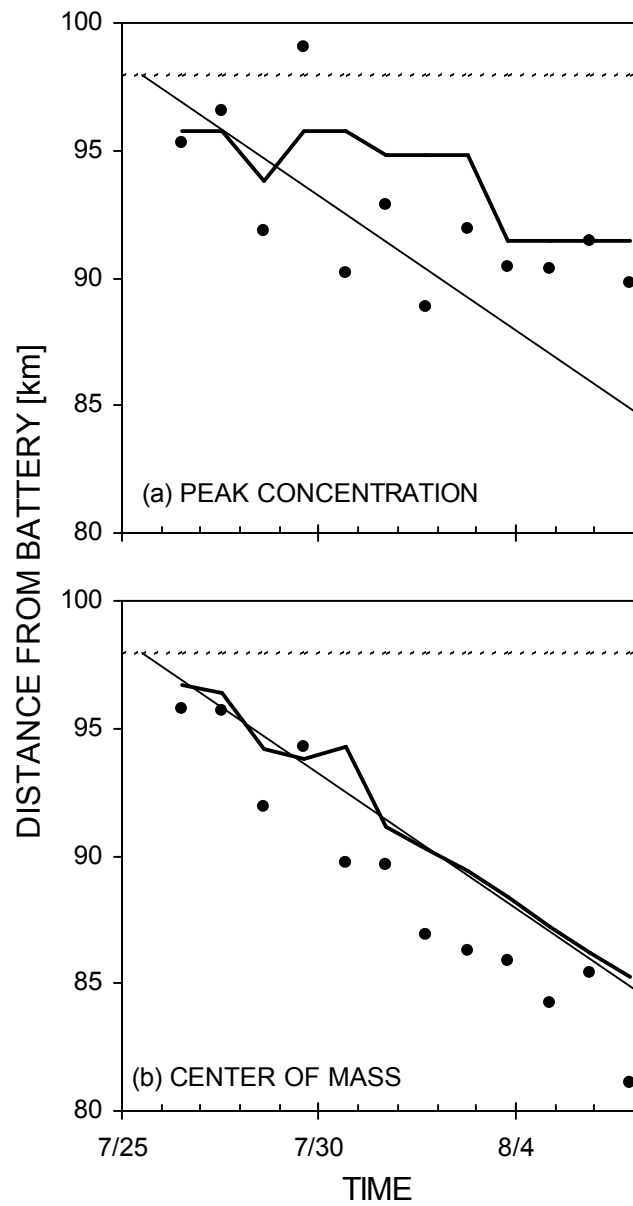


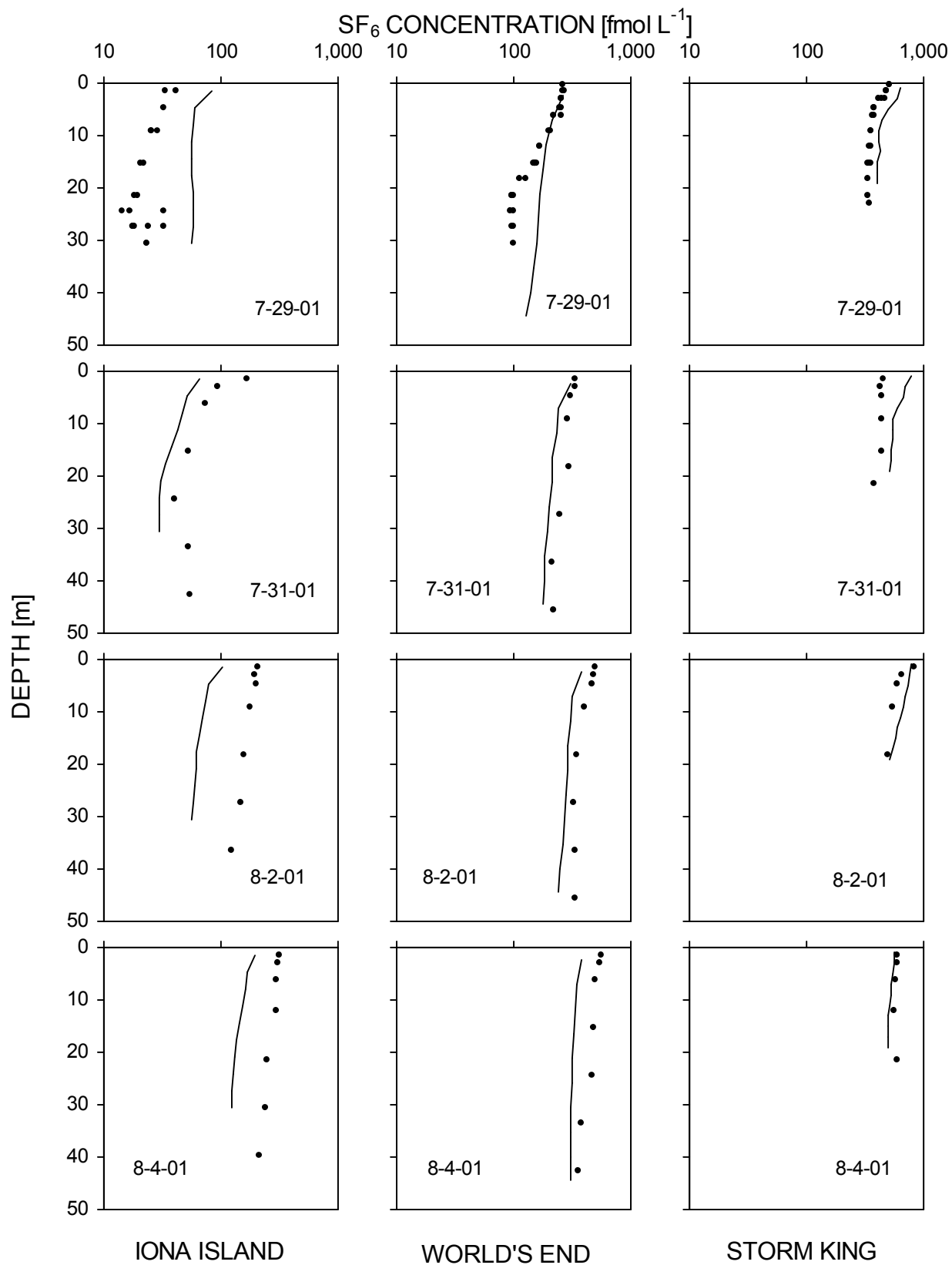






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Fig. 7





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Fig. 9

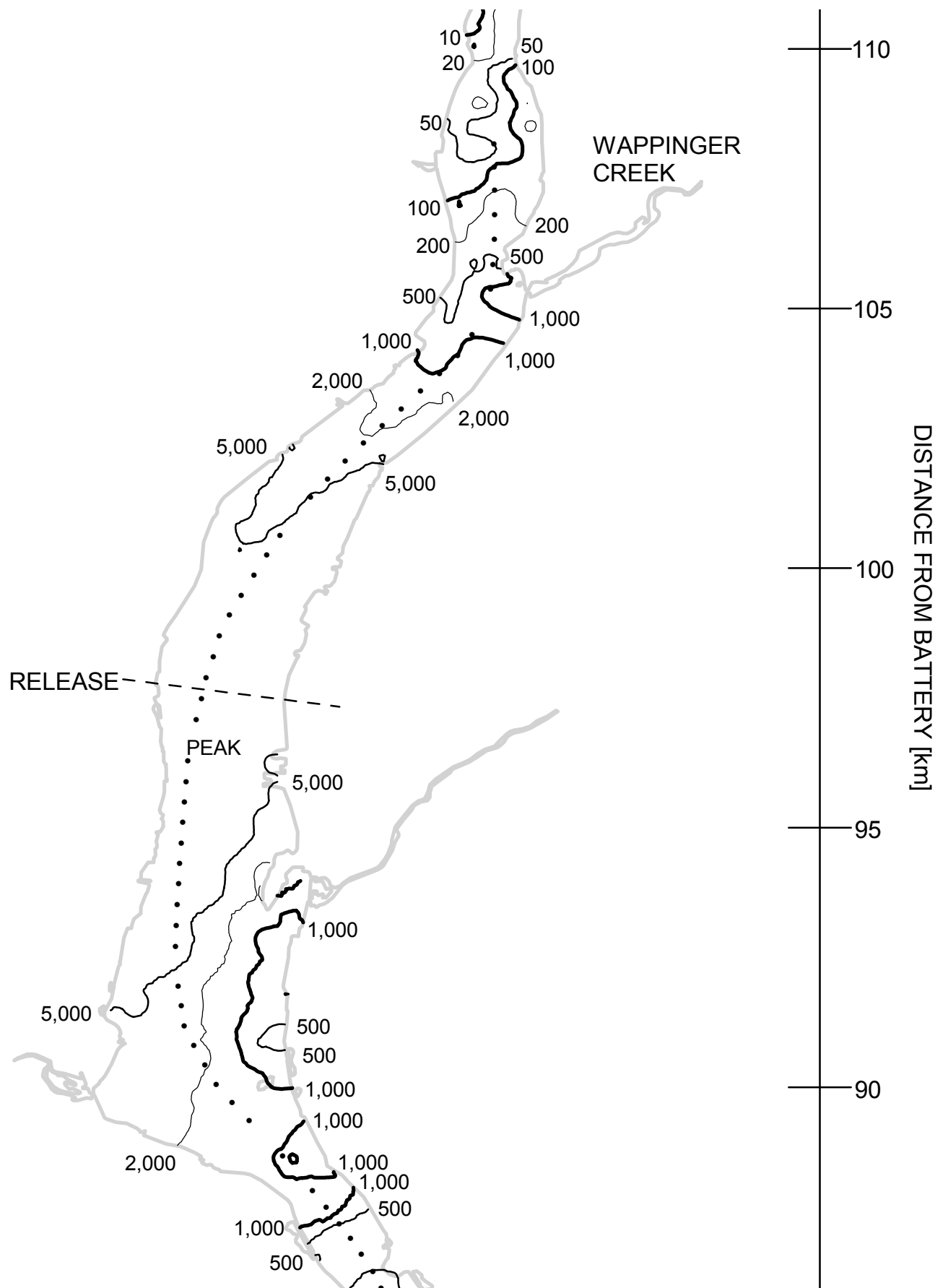
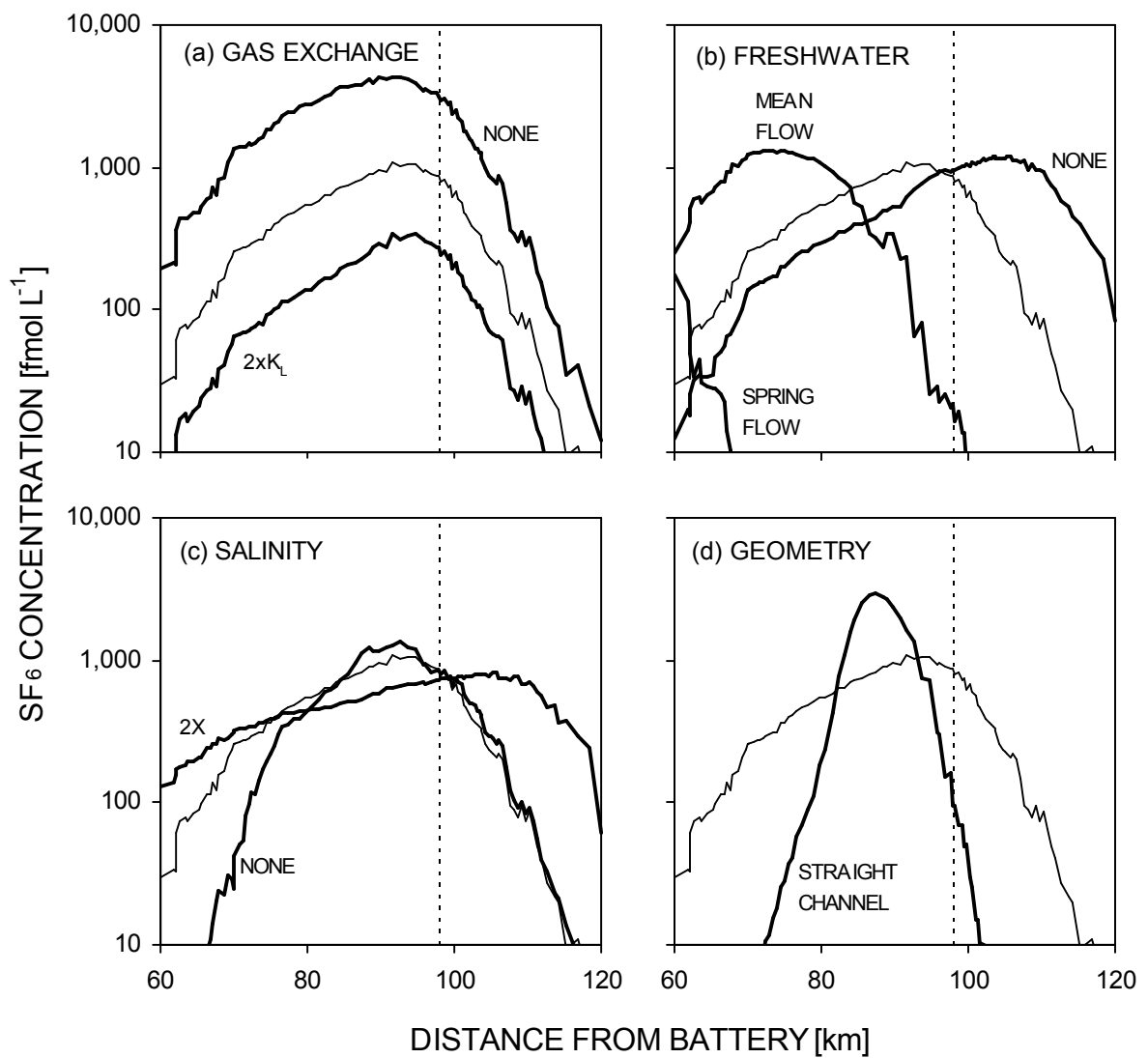
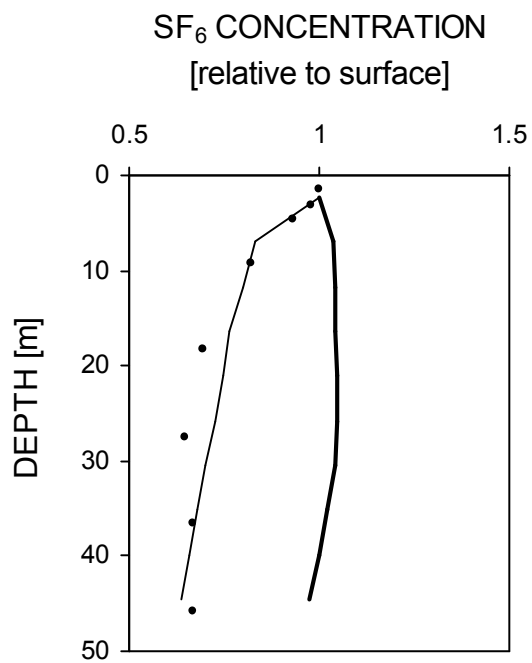
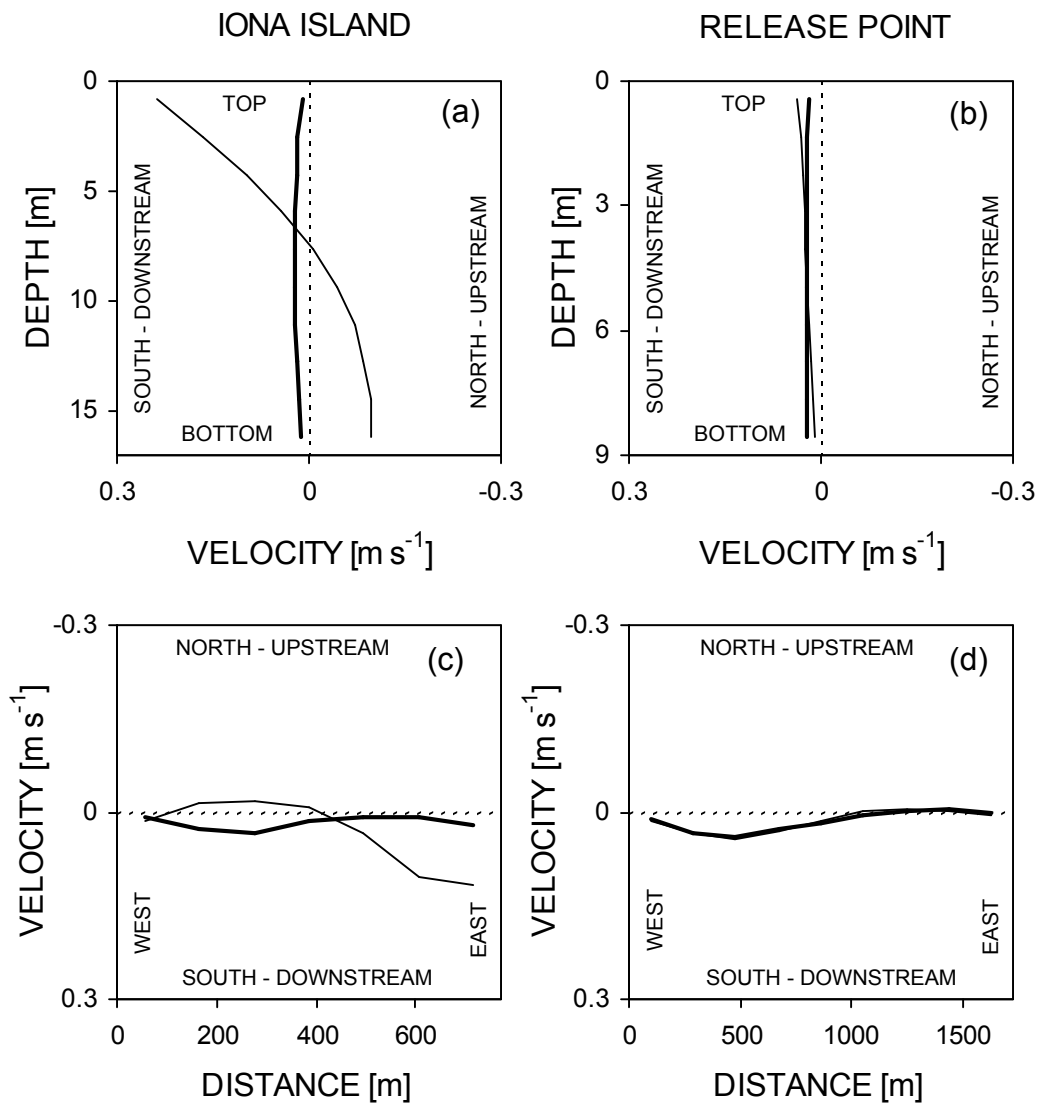


Figure 10
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Fig. 12



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Fig. 13