

## Methods

For this research, to characterize the spatiotemporal structure of residence times via a numerical model of the bay dynamics, several iterations of model and data systems were necessary before a final model parameterization and data set were obtained. The first runs utilized an existing model, having a coarse grid, no evaporation or precipitation at the surface boundary, and only a few of the major river discharge inputs. In this first modeling effort, the particle tracking was handled externally to ECOM-3D and the validation data was solely the PORTS data set. This early attempt at coupling a particle tracking model with ECOM-3D will be denoted as First Model/Data Set (FMDS). To improve model accuracy, a finer grid and an internal particle tracking subroutine were developed; precipitation, evaporation, and more detailed river input to ECOM was added. To this end, the Second Model/Data Set (SMDS) was again constructed using PORTS data, but it was augmented with the detailed river, evaporation, and precipitation data. Finally, a Third Model/Data Set (TMDS) was developed using the model from the SMDS, and data from the TOP study, allowing the most thorough calibration of the various parameters, particularly salinity.

The methods used at each stage of refinement followed a standard pattern. First, a preliminary skill assessment was conducted for the model in hind-cast mode

using available data. This consisted of varying some of the “tunable” model parameters, including the Smagorinsky horizontal mixing coefficient (HORCON), the bottom friction coefficient (BFRIC), bottom roughness coefficient (ZOB), scaling of the bathymetry, and/or groundwater input. Once a best fit was obtained, the configuration was fixed for subsequent validation simulations. A test of the particle tracking routine was then conducted to determine the accuracy of short-term particle runs. Concurrent with residence time simulations, a check was conducted to determine the ability of the model to capture the residual (30 day averaged) flow field.

Each model was considered to be adequately validated when the fit to the data obtained was comparable to the FMDS. The tests for fit included, lag of highest cross correlation and cross correlation on both water level and current data from the available stations, as well as the statistics computed by the method of Hess and Bosley (1992). For the latter method, each parameter (i.e., water level or currents) is defined as:

Mean extrema range,  $R$  is given by

$$R = 2/M \sum_{j=1}^M | Y_j | \quad 16$$

Root mean square difference between the model and data,  $D_{rms}$  is given by

$$D_{rms} = [1/n \sum_{i=1}^n (y_i - \hat{y}_i)^2]^{1/2} \quad 17$$

The *Drms* non-dimensionalized via  $R$ ,  $Dp$  is given by

$$Dp = D_{rms}/R \tag{18}$$

Gain ratio of model extrema to data,  $Gw$  is given by

$$Gw = R/R \tag{19}$$

Root mean square difference of extrema values,  $Arms$  is given by

$$Arms = [1/M \sum_{j=1}^M (Y_{T_j} - Y_j)^2]^{1/2} \tag{20}$$

Mean time lag of extrema,  $Lm$  is given by

$$Lm = 1/M \sum_{j=1}^M (T_{T_j} - T_j) \tag{21}$$

Root mean square extrema lag,  $Lrms$  is given by

$$Lrms = [1/M \sum_{j=1}^M (T_{T_j} - T_j)^2]^{1/2} \tag{22}$$

Here extrema are defined as maxima or minima that are separated by more than two hours. The primed variables are from the model, and  $M$  is the number of

extrema while  $n$  is the total number of model/data points. Defining  $Ap = A_{rms}/R$  and  $Lp = L_{rms}/6.21$  where 6.21 hours approximates the mean time between extrema, then

$$SD = 1 - Dp \tag{23}$$

$$SA = 1 - Ap \tag{24}$$

$$SL = 1 - Lp \tag{25}$$

where  $SD$  is the 6 minute difference skill;  $SA$  is the extrema amplitude skill;  $SL$  is the extrema lag skill.  $SD$ ,  $SA$ , and  $SL$  are the primary test statistics that were used by this method to evaluate the model.

The FMDS was used as a lower bound on  $SD$ ,  $SA$ , and  $SL$  and for an upper bound on the short-term particle tracking ability,  $MD$  (described below), for subsequent model and data sets.

The particle tracking component of the modeling effort was also independently verified. Since there is no feedback from the particle tracking routine to the ECOM-3D -in fact the FMDS was constructed with the particle tracking program external to ECOM-3D- the only calibration and validation possible were by comparing real drifter position to modeled trajectories and tuning of the single parameter for the horizontal dispersion of the modeled particles.

The ideal validation for the particle tracking model would be a longterm (of

the order of months) model run that was concurrent with a neutral tracer release, and a subsequent data collection and mapping program in three dimensions for the tracer. This is similar to, but more intensive than the study done for the Providence River by Asselin and Spaulding (1993). In that study several estimation methods for flushing times were compared, a task that is beyond the scope of this dissertation. It was possible, however, to track surface drifters for short (of the order of hours) runs, and to check that the modeled drifters were approximating the real drifters in position, time, and dispersion. This is a first approximation to a more thorough validation, and quantifies the ability of the particle tracking model to capture the sub-grid scale features. Validation consists of calculations of the separation of the mean modeled particle locations and the drifter locations at regular time intervals,  $MD_t$ , where  $MD_t$  is given by:

$$MD_t = \sqrt{\left(1/N' \left(\sum_{j=1}^{N'} X'_{jt}\right) - 1/N \left(\sum_{j=1}^N X_t\right)\right)^2 + \left(1/N' \left(\sum_{j=1}^{N'} Y'_{jt}\right) - 1/N \left(\sum_{j=1}^N Y_t\right)\right)^2} \quad 26$$

where  $N$  is the number of drifters;  $X_t$  is the drifter longitude at time  $t$ ;  $Y_t$  is the drifter latitude at time  $t$ ; and the primed variables denote the modeled values. For the FMDS a calculation of the mean separation of modeled particles  $MS_t$  was calculated as:

$$MS_t = \sqrt{(1/N_t(\sum_{j=1}^{N_t} X_{jt} - MDX_t))^2 + (1/N_t(\sum_{j=1}^{N_t} Y_{jt} - MDY_t))^2} \quad 27$$

where  $MDX_t$  and  $MDY_t$  are the mean longitude and latitude of the modeled particles at time  $t$  respectively. A similar calculation on the drift buoys was used to set the coefficient of dispersion in the random walk component of the particle tracking subroutine.

The analysis of the residence time runs proceeded as though the model output was accurate in both space and time, i.e., as though the model output was data. Rather than compiling large tables of difference time series, the method of quantifying the spatiotemporal fields of model output chosen was a series of plan view plots showing the loss of concentration and or loss of particle accumulation normalized to the original concentration or accumulation. These spatial distributions are presented at sequential times and also a final pair of plan view plots showing the spatial distribution of the grid cell by grid cell residence time of each method (Eulerian and Lagrangian) is presented as a varying field over the model domain. These final spatial distributions are derived by finding the time in days for each grid to fall below  $1/e$  of the original concentration or accumulation. These results are then considered as a baseline case and the model was modified sequentially by changing the boundary conditions one at a time in five distinct ways, to quantify the effect of these changes on residence time. In the first modification, river inflow was added to the baseline case inflow. The quantity of fresh water was increased to twice the average rainy season inflow for each river, for the entire model

simulation time period. This run was constructed to magnify the density driven flow of the baseline case, and to give a lower bound on bay-wide residence time. The baseline case was started in the dry fall-to-winter transition period. It therefore had relatively low freshwater input from the rivers. The second modification was to use only the astronomical tides instead of the entire tide elevation signal to drive the open boundary. This simulation points to the importance of the sub-tidal variability in residence time. For the third modification, in order to simulate a period with no fresh water inflow, the river inflow was artificially set to zero, while all other parameters were held the same as the baseline case. This simulation effectively eliminates the estuarine circulation and shows the relative importance of fresh water inflow to residence time. The fourth modification is a run with astronomical tides and no winds, which eliminates the major weather-related forcing and ranks the importance of meteorological effects to residence time. The final modification is to remove all forcing to the model except the astronomical tides. All the meteorological inputs (wind, rain, and evaporation at the surface boundary) are set to zero. All the fresh water input from the rivers are set to zero; the model salinity field is set to 34 psu over the domain at startup; and the boundaries are fixed at 34 psu for this simulation. This run, having only harmonic tides, demonstrates the effect of the lack of density-driven or meteorologic-forced flow on residence time, leaving only the tidal excursion and mixing to flush the estuary.

Each of these scenarios is compared to the baseline simulations with plan view plots of the time (in days) required to flush each grid for each of the Eulerian and

Lagrangian methods. The bay-wide residence time is also plotted as a time series for each method and each scenario. These time series point out the effect of the forcing on residence time, as well as, an upper and lower bound on the bay-wide values.