Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and Suisun Marsh

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Chapter 1
Improvements to the DSM2-Qual: Part 1

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1 Improvements to DSM2-Qual: Part 1

1.1 Summary

An important property of numerical models is that the simulation gets better as time and spatial steps are refined, with the model eventually "converging" to a solution determined by the underlying physics and equations. In qualitative testing, Delta Simulation Model II-Water Quality Model (DSM2-Qual) was found to converge slowly and to exhibit erratic behavior with very small (1 minute) steps. The poor qualitative convergence results from 2 ad hoc features of the code: parcel recombination in the Lagrangian advection scheme, and a spatially dependent mixing scheme for dispersion. Corrections are proposed here to minimize both problems. Tests show that with these changes, DSM2-Qual's qualitative convergence is much improved.

1.2 Advection and Parcel Recombination

DSM2 uses an adapted version of the Branched Lagrangian Transport Model (BLTM) (Schoellhammer and Jobson 1986).

The original BLTM and DSM2-Qual models rely on a Lagrangian scheme for advection. Every time step, they introduce a new "parcel" of water into each channel reach; then the models track the parcels as they move over time. The process of parcel creation is shown in Figure 1-1. The size of the parcel at creation time is the length of channel occupied by all the water coming in over one step Δt. This relationship binds the spatial discretization (parcel size) to the temporal discretization (time step).

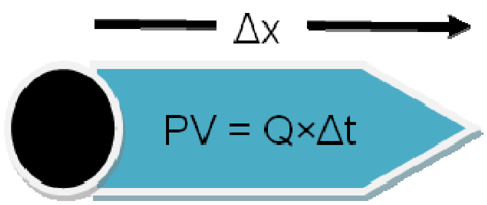

Figure 1-1 New parcel formed by inflow over a single time step

The parcel size Δx depicted in Figure 1-1 is the local parcel size at formation time. The parcel will deform over time as the parcel moves and occupies part of the channel with different cross-sectional area. DSM2-Qual does not track parcel length. The model is written in terms of parcel volume (*PV*), which does not change if not recombined. To estimate Δx, we need information about *PV* and cross sectional area occupied by the parcel $\bar{A}$ (Eq. 1-1):

$$\Delta x = \frac{PV}{\bar{A}} \qquad \text{Eq. 1-1}$$

In practice, PV is tracked exactly, but average area must be estimated from channel-averaged areas. Accuracy of Δx is limited by this approximation.

Due to memory considerations, the original code enforced a maximum number of parcels per channel. Once the number of parcels in a channel exceeded the maximum number (22 was used for DSM2-Qual), the smallest parcel in a channel would be combined with a parcel next to it.

Several problems existed with the original method of parcel recombination. The global maximum parcel number approach does not distinguish longer channels and shorter channels. In very long channels, the maximum might not be adequate to resolve the concentration field. The concept of a maximum number of parcels also introduces step-dependent behavior because of tidal influence. For instance, 22 parcels at a time step of 15 minutes samples 6 hours of flow; once you sample a half tide period, the average parcel size tends to vary less. With a 15 minute step, the maximum parcel number rule is seldom invoked because the parcels are big and travel a long way per time step. In contrast, 22 parcels at a time step of 1 minute are created in 22 minutes. In the absence of recombination, this spacing would tend to make the parcels locally uniform. However, in practice the maximum is always exceeded and recombination leaves small uniform parcels next to monolithic combined parcels.

In version 8.1, the parcel combination approach is altered. At every time step, the new parcel entering a reach is checked. If the new parcel is smaller than a user defined minimum size and the parcel on the interior side is also smaller, the parcels will be combined (Figure 1-2 and Figure 1-3). This has the effect of holding the parcel adjacent to the beginning of the reach until it has met a minimum size criterion. As far as time stepping, the scheme acts somewhat like an adaptive time step at the point of parcel creation: time steps are combined (made longer) when flow is gentle and parcels are small.

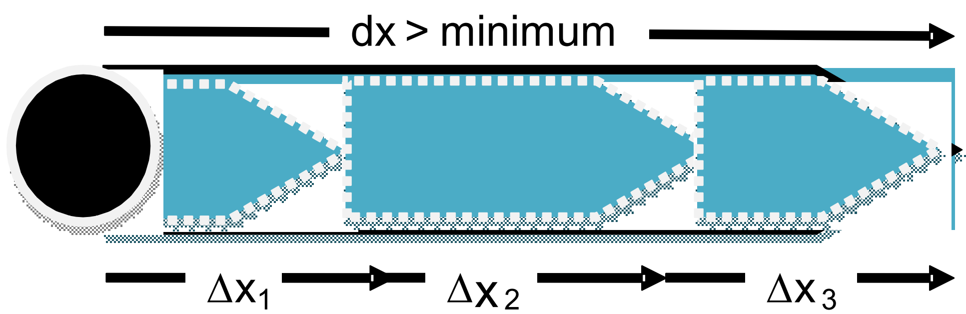

Figure note: The estimated parcel lengths of 3 existing parcels are bigger than the minimum. Next time step the parcels will advect freely and a new parcel will start forming behind it.

Figure 1-2 Parcel recombination strategy example

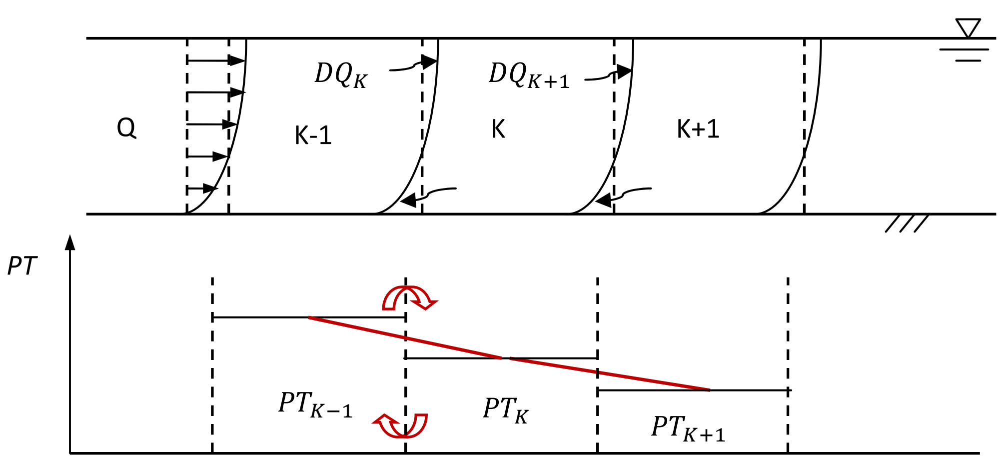

Figure 1-3 Explanation of mixing between parcels

The goal of the new parcel recombination scheme is to keep neighboring parcels similar in size and close to the defined minimum. The scheme is actively used: the minimum parcel size is set large enough compared to typical new parcels that the recombination scheme controls parcel size and number. The maximum parcel number (the one that used to be 22) is set to a large value (e.g. 100), and is almost never reached. In the rare case where the maximum parcel number is reached, the model reverts to the original method and the smallest parcel will be combined with a parcel next to it.

This modification appears to work well, comparing the old model results (Figure 1-4 through Figure 1-7) in the new model advection-only test results (Figure 1-8 to Figure 1-11[1]). Results at Collinsville and Jersey Point show the model converges well at 5-, 3-, and 1-minute time steps (Figure 1-8 and Figure 1-9, and Figure 1-10Figure 1-11). Figure 1-12 shows sensitivity test of minimum parcel sizes. The difference between 1,000 ft and others are obvious, while 600, 500, and 400 ft results are very close. We believe that numerical diffusion in advection previously attributed to mixing at nodes was actually due to parcel recombination.

Figure 1-13 shows the full scheme after advection fix, including advection and dispersion. The odd behavior with a time step of 1 minute is fixed and the model is qualitatively much more convergent. Some of the remaining issues are addressed in the next section.

1.3 Dispersion Changes

1.3.1 Discretization Issue

The BLTM dispersion equation was derived from an “exchange flow” mixing concept. The exchange flow rate between parcels (volume of exchange per time) was defined as a fraction of the river discharge (illustrated in **Error! Reference source not found.**) (Eq. 1-2):

$$DQ = DQQ * Q \qquad \text{Eq. 1-2}$$

in which *DQ* is the exchange flow rate, *DQQ* is the ratio of exchange flow to river discharge, and *Q* is the river discharge. DQQ is defined by user in the input file for every reach. The mixing equation for parcel K is thus (Eq. 1-3):

$$\Delta PT = DT * (DQ_K PT_{K-1} - DQ_K PT_K + DQ_{K+1} PT_{K+1} - DQ_{K+1} PT_K)/PV_K \qquad \text{Eq. 1-3}$$

where Δ*PT* is the change in parcel concentration and *DT* is the simulation time step. In the original BLTM programmer’s manual (Schoellhammer and Jobson 1986), it was indicated (Eq. 1-4):

$$DQQ = \frac{D_x}{U\Delta x} \qquad \text{Eq. 1-4}$$

in which D_x is the classic longitudinal dispersion coefficient, *U* is the mean cross-sectional velocity. This shows *DQQ* is a function of the size of a parcel Δx.

[1] Figures 1-4 through 1-23 are presented at the back of this chapter.

This involvement of Δx in the physics of mixing is problematic. Changing the time/spatial step doesn't just change the accuracy of the solution; it changes the physical description of the problem. Moreover, in DSM2-Qual, the parcel size varies from parcel to parcel and changes with time step; how big a parcel depends on the time step and velocity at the time the parcel entered the channel.

In terms of standard diffusion analogs models of mixing, the DSM2-Qual scheme appears to discretize something akin to the following (Eq. 1-5):

$$\frac{\partial C}{\partial t} = \frac{1}{A}\frac{\partial}{\partial x}\left(\Delta x DQ\frac{\partial C}{\partial x}\right) \quad \textbf{Eq. 1-5}$$

in which *C* is concentration, *t* is the time coordinate, *x* is the longitudinal axis, *A* is the cross sectional area, Δx is grid size in a finite difference scheme or parcel size in DSM2-Qual—usually people use ξ to represent the Lagrangian longitudinal axis, but the equations are similar and we feel this notation is more familiar for discussion.

The relationship of the parcel mixing scheme to Eq. 1-5 is easy to demonstrate when the spatial grid is uniform (which in the original DSM2-Qual usually implies steady uniform flow). Ignoring the mix of discrete and continuous quantities, Eq. 1-5 can be discretized using central finite differences (Eq. 1-6 through Eq. 1-8):

$$\frac{\Delta C}{\Delta T} = \frac{\Delta x}{A_K}\cdot\frac{\left(DQ\frac{\partial C}{\partial x}\right)^{+} - \left(DQ\frac{\partial C}{\partial x}\right)^{-}}{\Delta x} \quad \textbf{Eq. 1-6}$$

$$\frac{\Delta C}{\Delta T} = \frac{1}{A_K}\left[DQ_{K+1}\frac{C_{K+1}-C_K}{\Delta x} - DQ_K\frac{C_K - C_{K-1}}{\Delta x}\right] \quad \textbf{Eq. 1-7}$$

$$\Delta C = \frac{\Delta T}{PV_K}\left[DQ_{K+1}(C_{K+1}-C_K) - DQ_K(C_K - C_{K-1})\right] \quad \textbf{Eq. 1-8}$$

Eq. 1-8 is identical to Eq. 1-3. The factor of Δx in Eq. 1-5 is not explicitly included in the discretization, but rather arises due to omission—from failing to divide by Δx in the original DSM2-Qual dispersion scheme. This represents the involvement of a discretization artifact in what should be a physical equation. Possible reasons for this in the original formulation are either (1) accurate estimates of Δx are not available or (2) a sentiment that sub-grid mixing processes are greater with larger parcels. The practical consequence for any particular grid is that an "effective average" $\widehat{\Delta x}$ gets built into the estimation of the dispersion factor *DQQ*. This makes the calibrated coefficient less meaningful, a problem that was compounded by the numerical dispersion from advection.

1.3.2 Proposed Scheme

The dispersion flux (rate of mass exchange) in the original scheme was (Eq. 1-9):

$$F = DQ_K(PT_{K-1} - PT_K) \qquad \textbf{Eq. 1-9}$$

The problem is that it is not normalized by parcel size. A new scheme is proposed to fix the problem. The dispersion flux (rate of mass exchange) at each side of the parcel is defined as (Eq. 1-10):

$$F = f\left(Q, \frac{\partial C}{\partial x}\right) = -DC \cdot |Q| \cdot \frac{\partial C}{\partial x} \qquad \textbf{Eq. 1-10}$$

in which *DC* is a coefficient with a length unit. The mixing equation for parcel K can be written as following (Eq. 1-11):

$$\Delta PT = DT * (DC_K|Q_K|\frac{PT_{K-1} - PT_K}{(\Delta x_K + \Delta x_{K-1})/2} + DC_{K+1}|Q_{K+1}|\frac{PT_{K+1} - PT_K}{(\Delta x_K + \Delta x_{K+1})/2})/PV_K \qquad \textbf{Eq. 1-11}$$

where Δx_K is the parcel length estimated based on parcel volume and channel-wide average cross-sectional area (Eq. 1-1).

The parcel exchange in Eq. 1-11 roughly discretizes the following partial differential equation with a simple explicit finite difference scheme (Eq. 1-12):

$$\frac{\partial C}{\partial t} = \frac{1}{A}\frac{\partial}{\partial x}\left(DC \cdot |Q| \cdot \frac{\partial C}{\partial x}\right) \qquad \textbf{Eq. 1-12}$$

The generally accepted form of 1-D river Lagrangian dispersion equation can be written as (Rutherford 1994) (the advection term is not shown here, only the dispersion term for discussion) (Eq. 1-13):

$$\frac{\partial C}{\partial t} = \frac{1}{A}\frac{\partial}{\partial x}\left(A \cdot K_x \frac{\partial C}{\partial x}\right) \qquad \textbf{Eq. 1-13}$$

in which *C* is concentration, *t* is the time coordinate, K_x is the classic longitudinal dispersion coefficient (same as D_x in the original BLTM manual).

Comparing equations Eq. 1-12 and Eq. 1-13, we get (Eq. 1-14 and Eq. 1-15):

$$DC \cdot |Q| = A \cdot K_x \qquad \textbf{Eq. 1-14}$$

$$DC = \frac{A}{|Q|} \cdot K_x = \frac{K_x}{|\bar{u}|} \qquad \textbf{Eq. 1-15}$$

in which $\bar{u}$ is the mean cross-sectional velocity. The coefficient *DC* is used as the input variable for "Dispersion Coefficient" in new versions of DSM2. *DC* can be estimated using Eq. 1-15 and calibrated for each reach. Comparing this formula to Eq. 1-4, it can be seen that the scaling by Δx is not involved anymore[2].

1.3.3 Estimating the Dispersion Coefficient (DC)

A formula for K_x in natural streams by (Fischer, et al. 1979) may be used to estimate DC as a starting value (Eq. 1-16).

$$K_x = 0.011 \frac{\bar{u}^2 W^2}{d u^*} \qquad \textbf{Eq. 1-16}$$

in which $\bar{u}$ is the mean cross-sectional velocity, *W* is river width, *d* is flow depth, and u^* is shear velocity. For a steady uniform flow in a prismatic channel (Eq. 1-17),

$$u^* = \sqrt{\bar{\tau}_0/\rho} = \sqrt{gRS} \qquad \textbf{Eq. 1-17}$$

in which $\bar{\tau}_0 = \gamma RS$ is the average shear stress; γ=specific weight of the fluid; ρ = density; *g* = gravitational acceleration; *R* = hydraulic radius; *S* = friction slope or energy slope, which can be estimated using Manning's equation (Eq. 1-18):

$$Q = \frac{1.486}{n} A R^{\frac{2}{3}} S^{\frac{1}{2}} \qquad \textbf{Eq. 1-18}$$

Combining the 4 equations (equations Eq. 1-15 through Eq. 1-18), we get (Eq. 1-19):

$$DC = 0.011 \frac{1.486}{n} \frac{W^2 R^{\frac{1}{6}}}{d\sqrt{g}} \qquad \textbf{Eq. 1-19}$$

Which shows *DC* is not directly a function of discharge or velocity, although width and depth do change with discharge, but the change is secondary to discharge/velocity change. Eq. 1-19 shows the wider the channel, the larger the coefficient.

Eq. 1-16 has been found to agree with observations within a factor of 4 or so in real streams (Fischer, et al. 1979). The book also listed experimental measurement data for Sacramento River as 15 m^2/s (161 ft^2/s) with depth 4 m, mean velocity 0.53 m/s. *DC* can be calculated as 93 ft. The exact location is not known.

Most part of the Delta is influenced by tidal flow. The tidal flow effects have to be considered. Equations for dispersion coefficient in estuaries (Fischer, et al. 1979) may be used to consider tidal effects. Values of the longitudinal dispersion coefficient in estuaries are approximately in the range of 100-300 m^2/s (1000-3000 ft^2/s) (Fischer, et al. 1979). The book also listed the value for San Francisco Bay as 200 m^2/s.

Dispersion is a complicated process, and is influenced by river irregularity, curvature, and tidal effects, etc. We have not so far been successful using empirical formulas to predict the coefficients. From the

[2] In our prototype code, the user input values for *DC* are scaled down by 1500, i.e., a user input value of 2.0 corresponds to DC=2.0*1500 = 3000. Users might feel more comfortable to calibrate a coefficient between 0 to 2 than 0 to 3000, although they are actually the same. The coefficient is strongly related to river geometry, with bigger value for the wider reaches near downstream. We are still actively discussing the most user-friendly form input for our official release of v8.1.

literature and initial trial runs, the range for *DC* in Delta is most likely between 100 in small channels to about 2000 in the large channels near Martinez, with a strong correlation to channel width. Calibration based on field data should be performed to find the appropriate value for each reach.

1.4 Tests Using DSM2 Historical Setup

The DSM2 historical run setup was used to test the models. The runs are from July 1, 1996 to July 1, 1998. Figure 1-14 to Figure 1-17 show that the new model converges well with various time steps. Figure 1-18 to Figure 1-21 show the new model converges well with different parcel sizes.

A natural question is: what is the bottom line? How much will this change results? The new model needs a fresh calibration to find proper dispersion coefficients for each channel. A trial run by merely rescaling all the original dispersion coefficients by 1500 produced similar results as previously calibrated. Figure 1-22 and Figure 1-23 show historical results for using DSM2-Qual v8.0.5 with a 15 minute time step (red line) compared to DSM2-Qual v8.1 (green line) and field data (blue dots).

We hope to see numerous benefits from the modifications in version 8.1, including a greater tendency to get answers for the "right reason"—apportioning advection and dispersion correctly, eliminating numerical diffusion in the advection scheme, and making the interpretation of calibrated parameters less arbitrary.

With a 5 minute time step, the model runs 9 minutes for the 2 year historical run with 3.2 GHz PC, which means 72 minutes for 16 year planning run. The new model is slower compared to the original model (about 48 minutes for 16 year run with 5 minute time step). Slowness may be due to a greater number of parcels and more subcycles in dispersion calculations.

1.5 Conclusions

- The new model with corrections to advection and dispersion formulation shows good convergence with respect to time step and parcel size.
- Recommended time step is 5 minute, and minimum parcel size 500 feet.
- The new model is expected to do a better job of partitioning transport into advection and dispersion and may be easier to calibrate.
- The prediction of dispersion coefficient using empirical formulas is not recommended. Calibration seems the only feasible way to determine the coefficients.
- The new model is slower compared to the original model (72 minutes for 16 year planning run with 3.2 GHz PC), but still fast enough for planning studies.
- The new model needs to be calibrated before we can compare new results with previous model results thoroughly. However, early indication is that model results can be coerced to be very similar.

1.6 References

Fischer, H. B., E. J. List, R. C.Y. Koh, J. Imberger, and N. H. Brooks. *Mixing in Inland and Coastal Waters.* Academic Press, 1979.

Rutherford, J. C. *River Mixing.* John Wiley & Sons, 1994.

Schoellhammer, D. H., and H. E. Jobson. *Programmers Manual for a One-dimensional Lagrangian Transport Model.* Manual, U.S. Geological Survey, 1986.

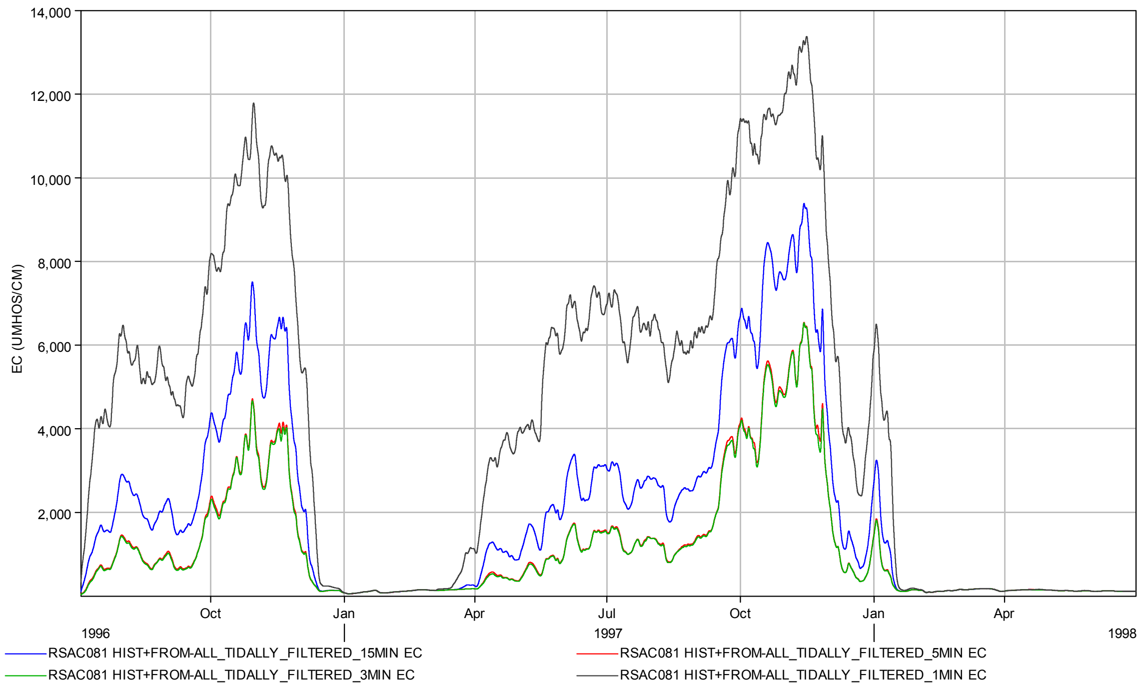

Figure 1-4 Previous model result at Collinsville

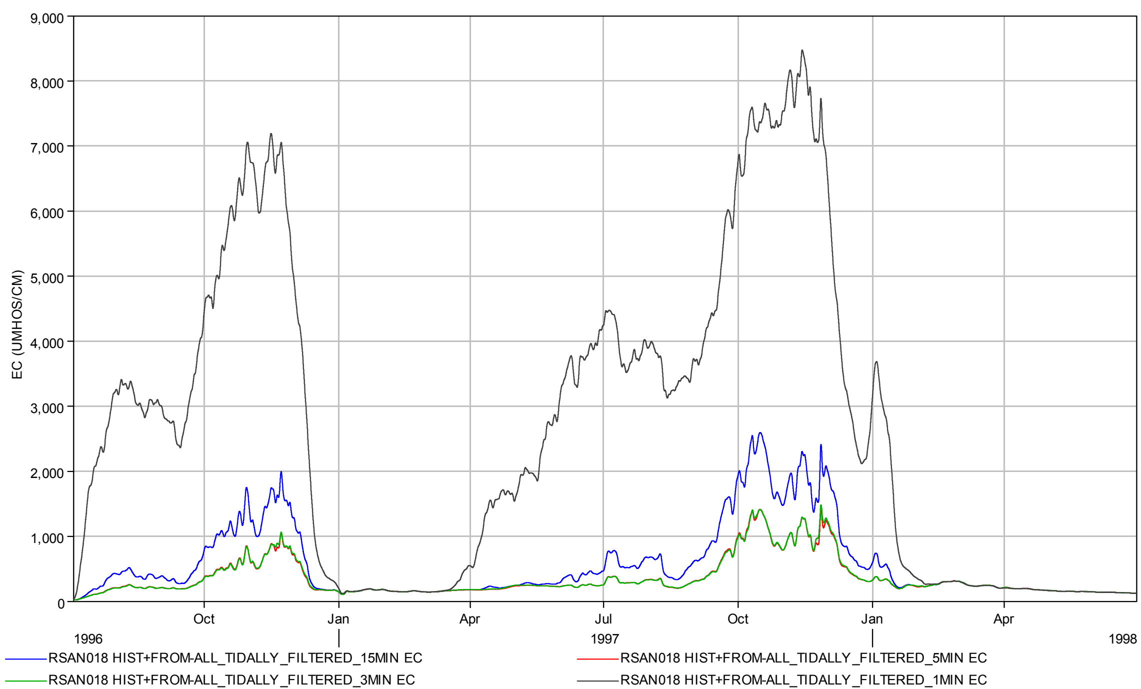

Figure 1-5 Previous model result at Jersey Point

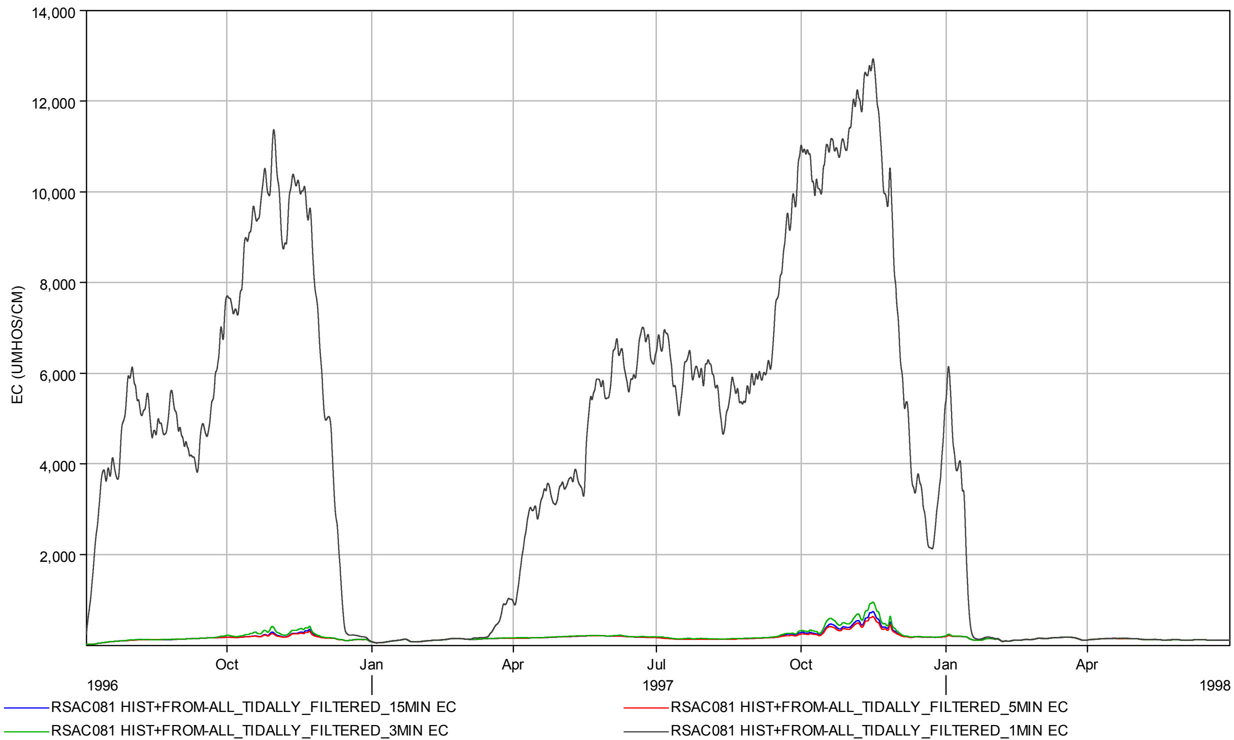

Figure 1-6 Previous model advection only result at Collinsville

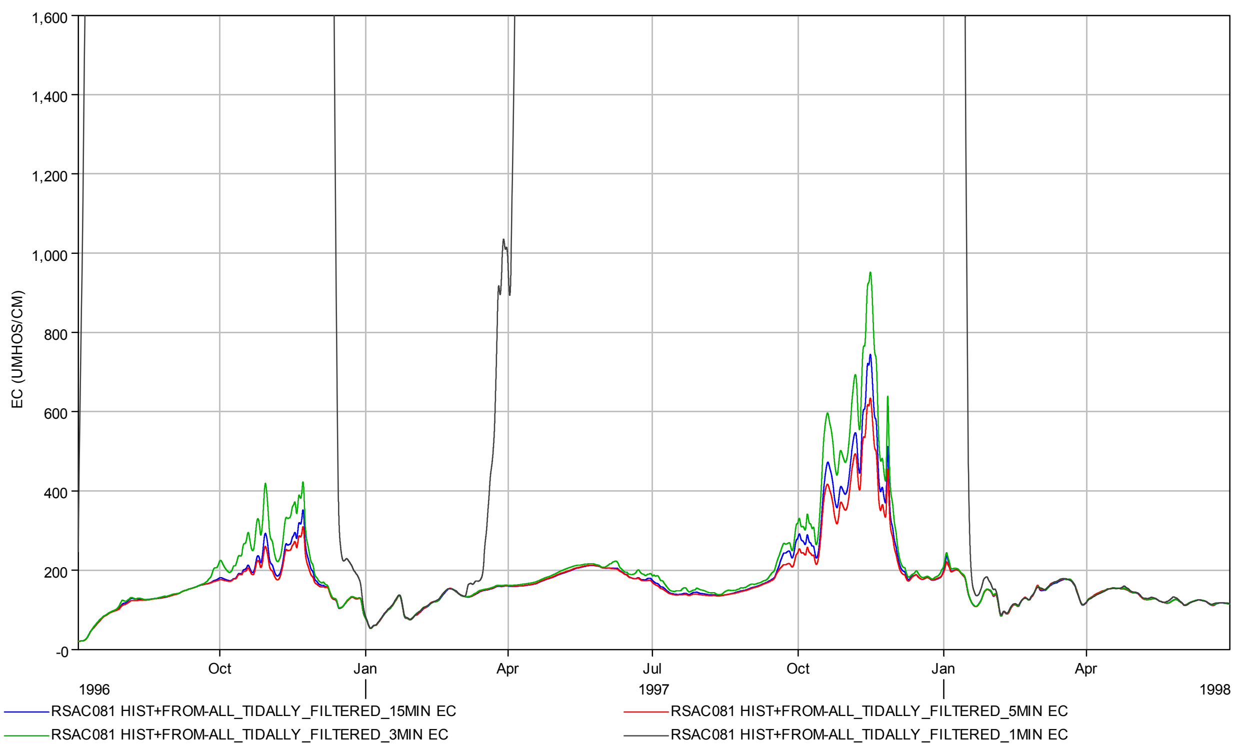

Figure 1-7 Previous model advection only result at Collinsville (zoom in)

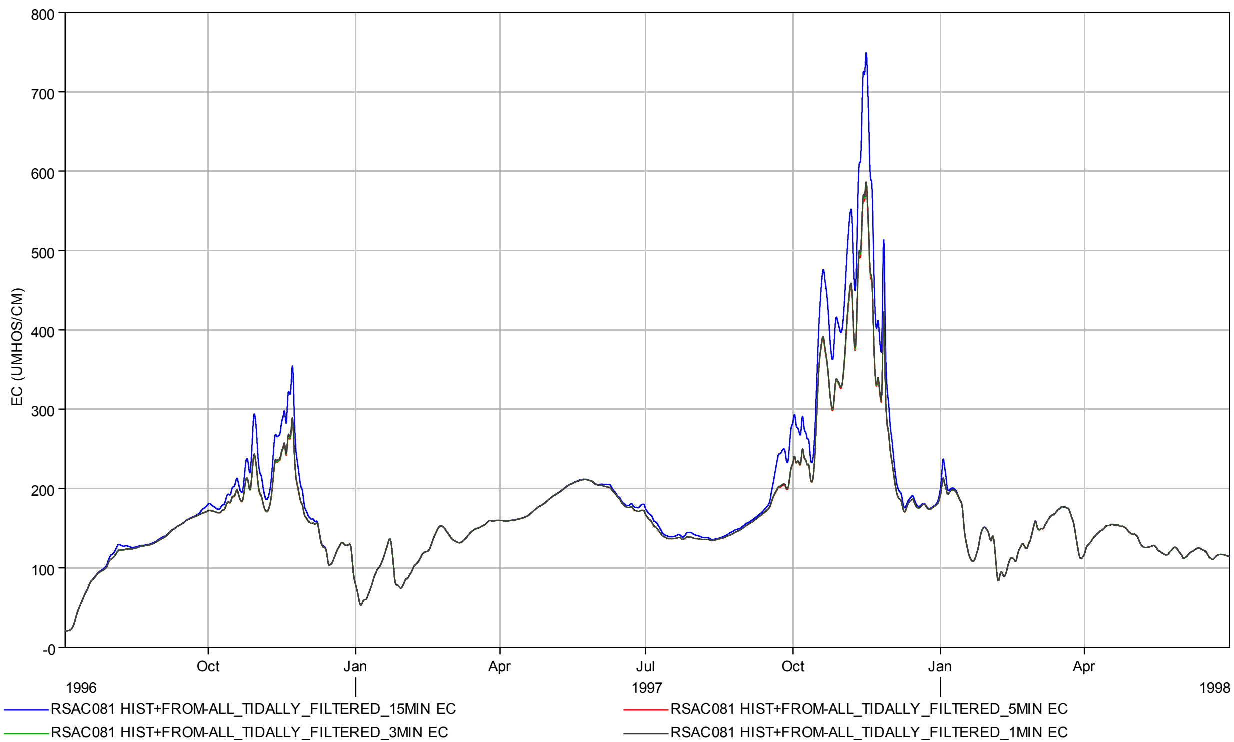

Figure 1-8 New model, advection-only at Collinsville, convergence at 15, 5, 3, 1 min time steps

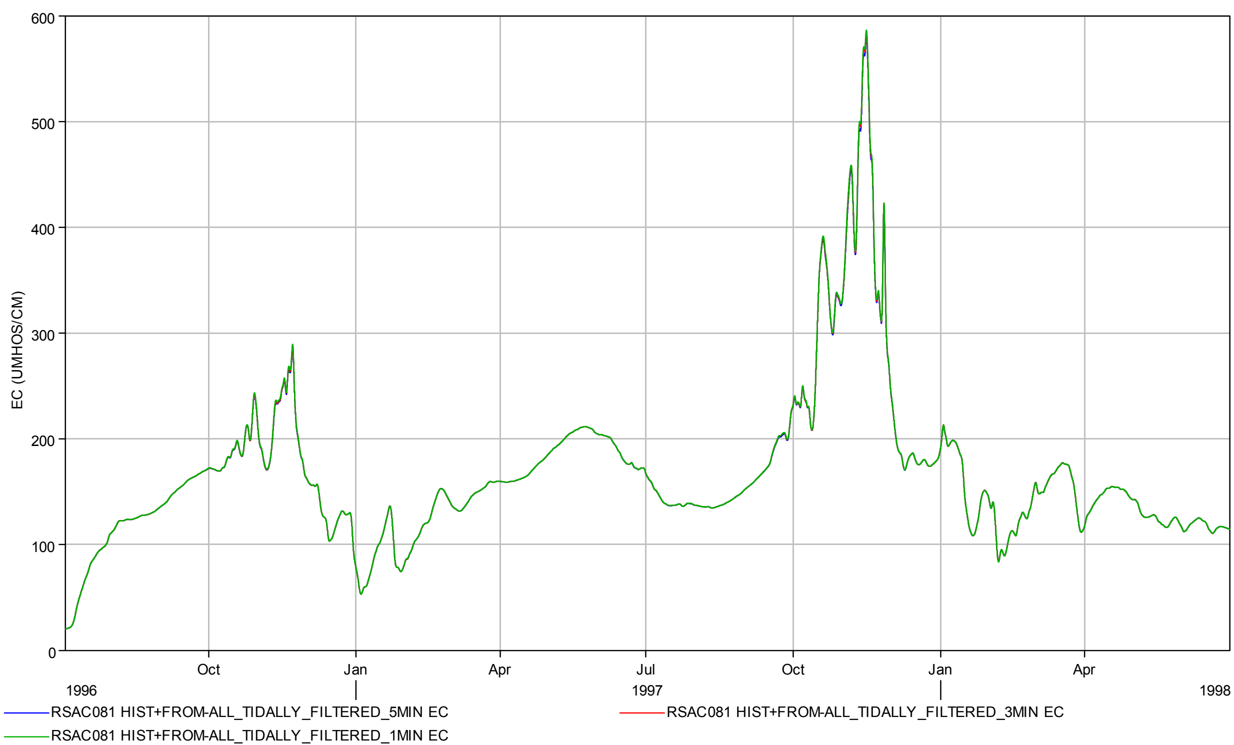

Figure 1-9 New model, advection-only at Collinsville, convergence at 5, 3, 1 min time steps

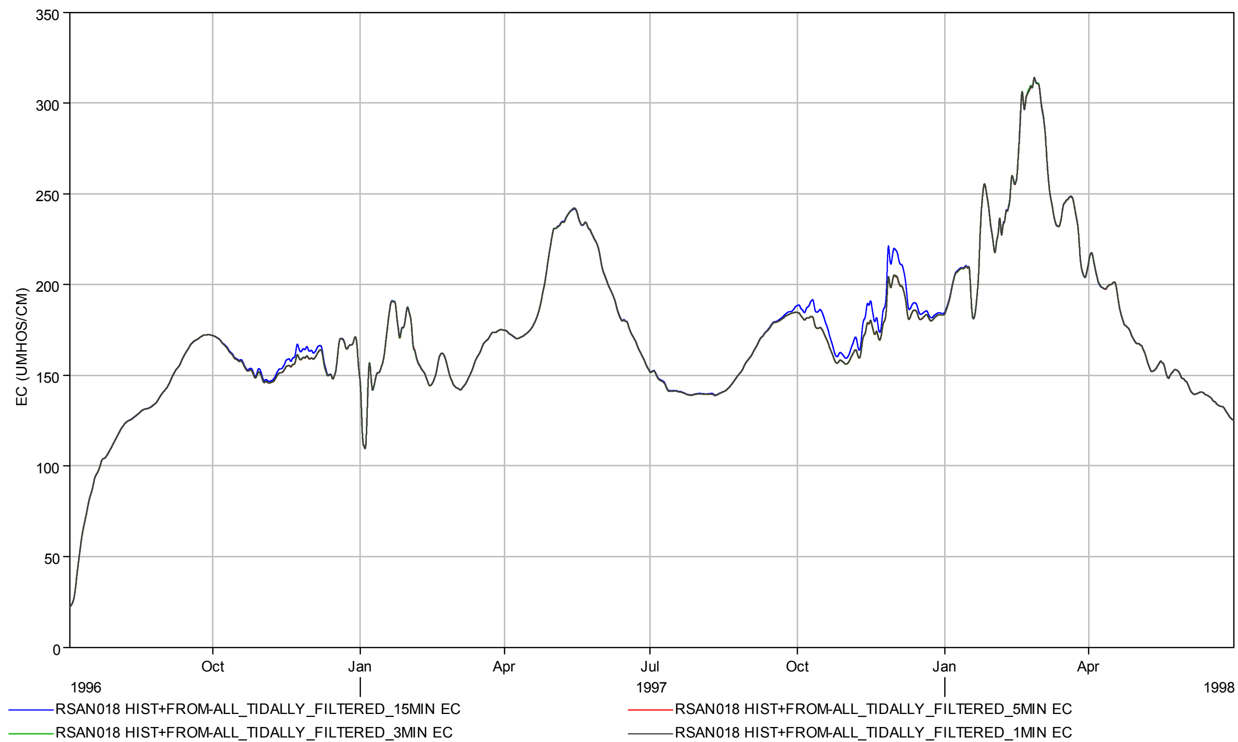

Figure 1-10 New model, advection-only at Jersey Pt., convergence at 15, 5, 3, 1 min time steps

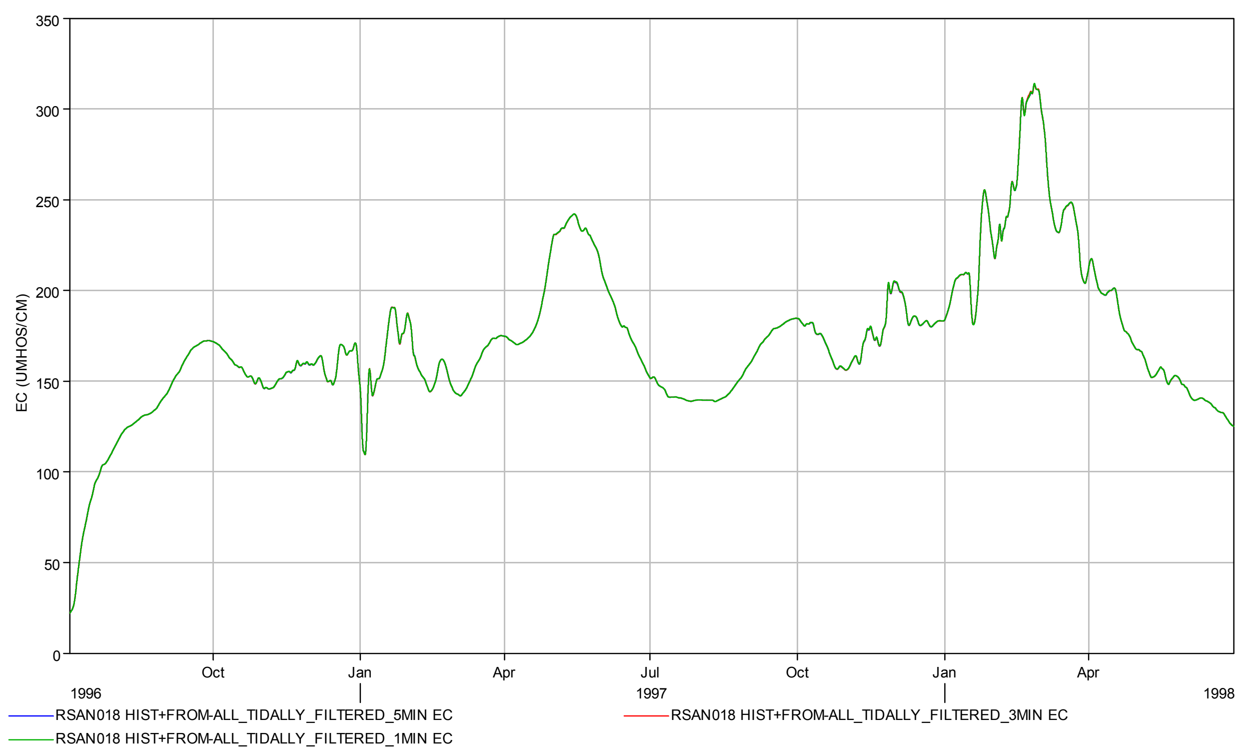

Figure 1-11 New model, advection-only at Jersey Pt., convergence of 5, 3, 1 minute time steps

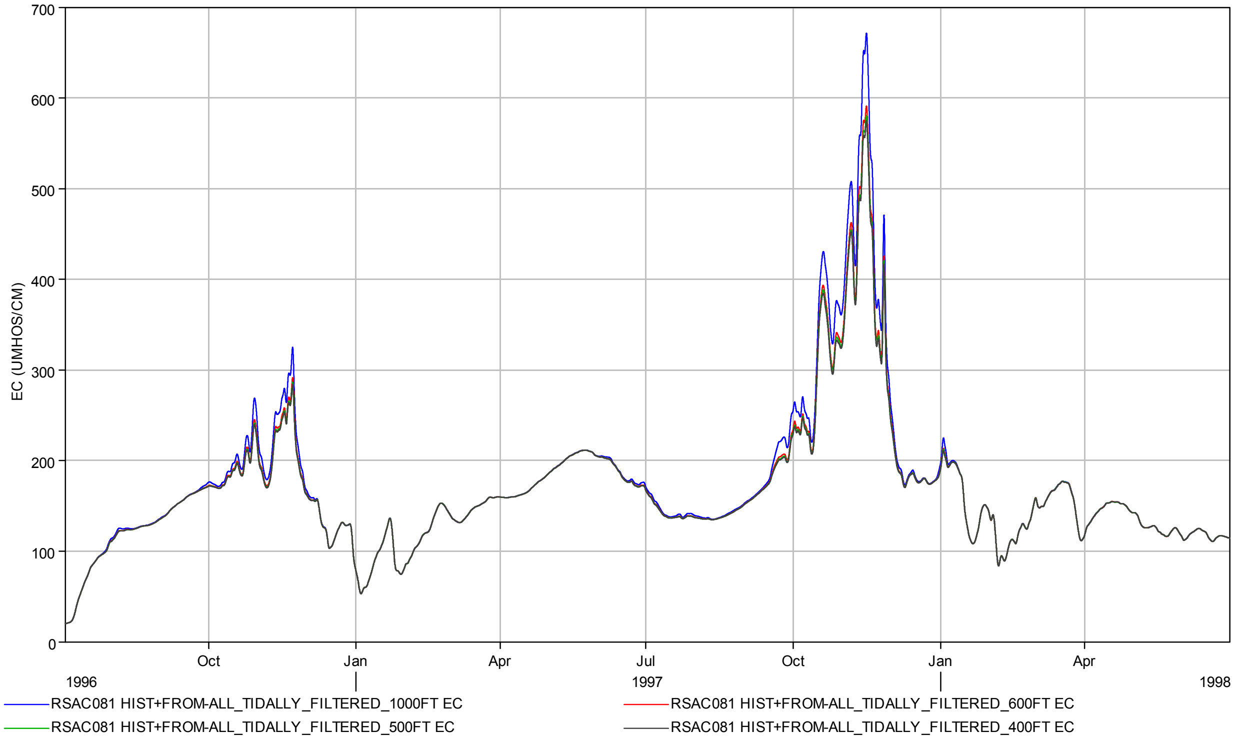

Figure 1-12 New model, advection-only at Collinsville (parcel size sensitivity test, *dt*=5 min)

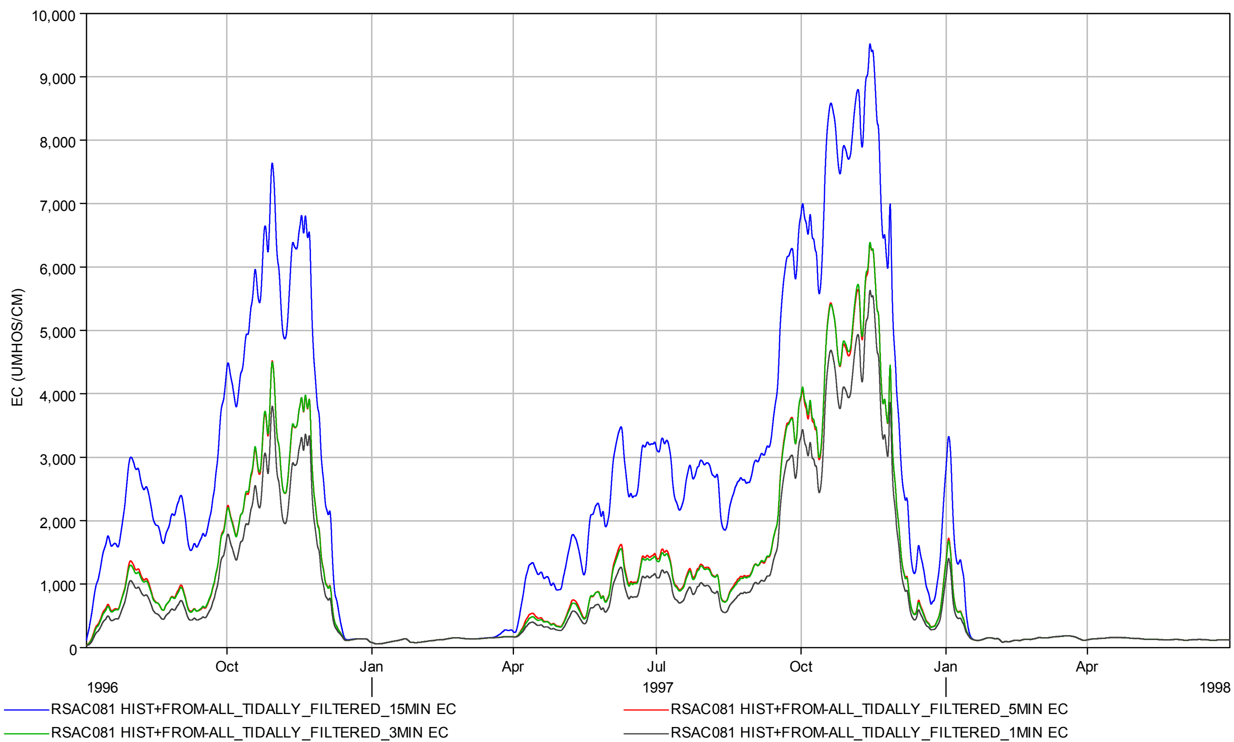

Figure 1-13 Result with previous dispersion model after advection fix at Collinsville

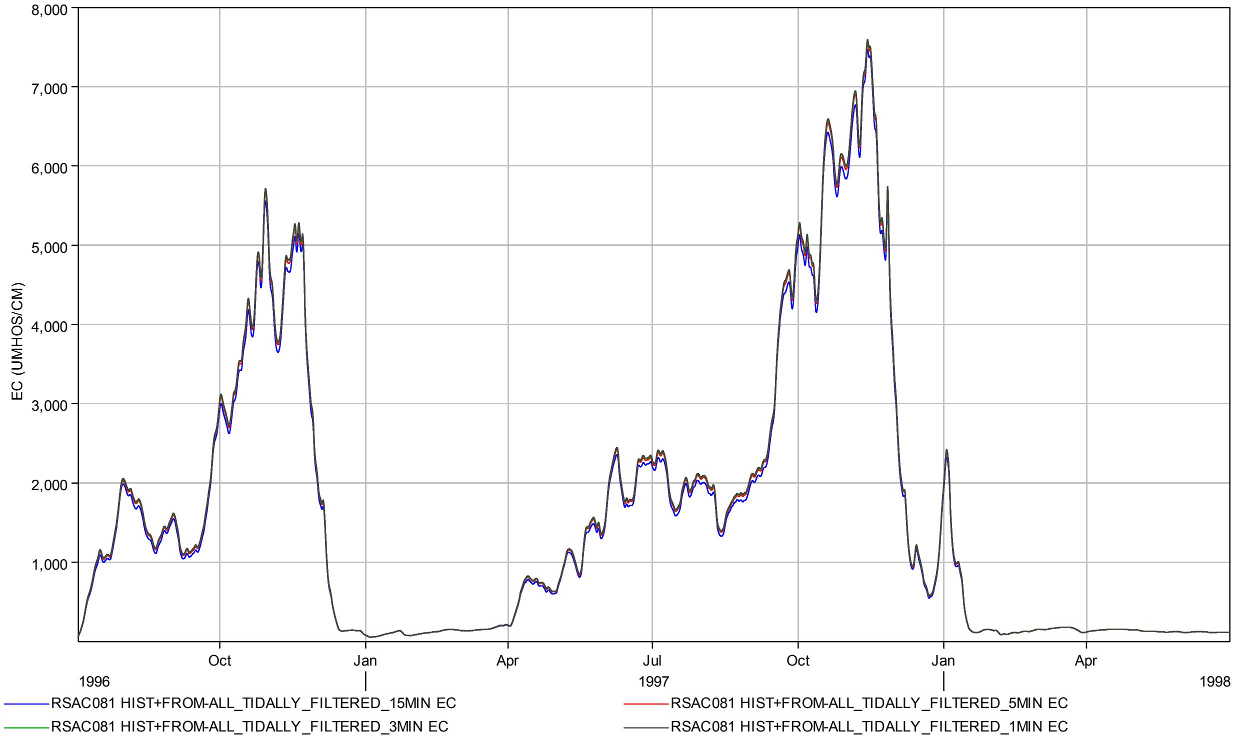

Figure 1-14 New model, result at Collinsville (time step sensitivity test, parcel size 500 ft)

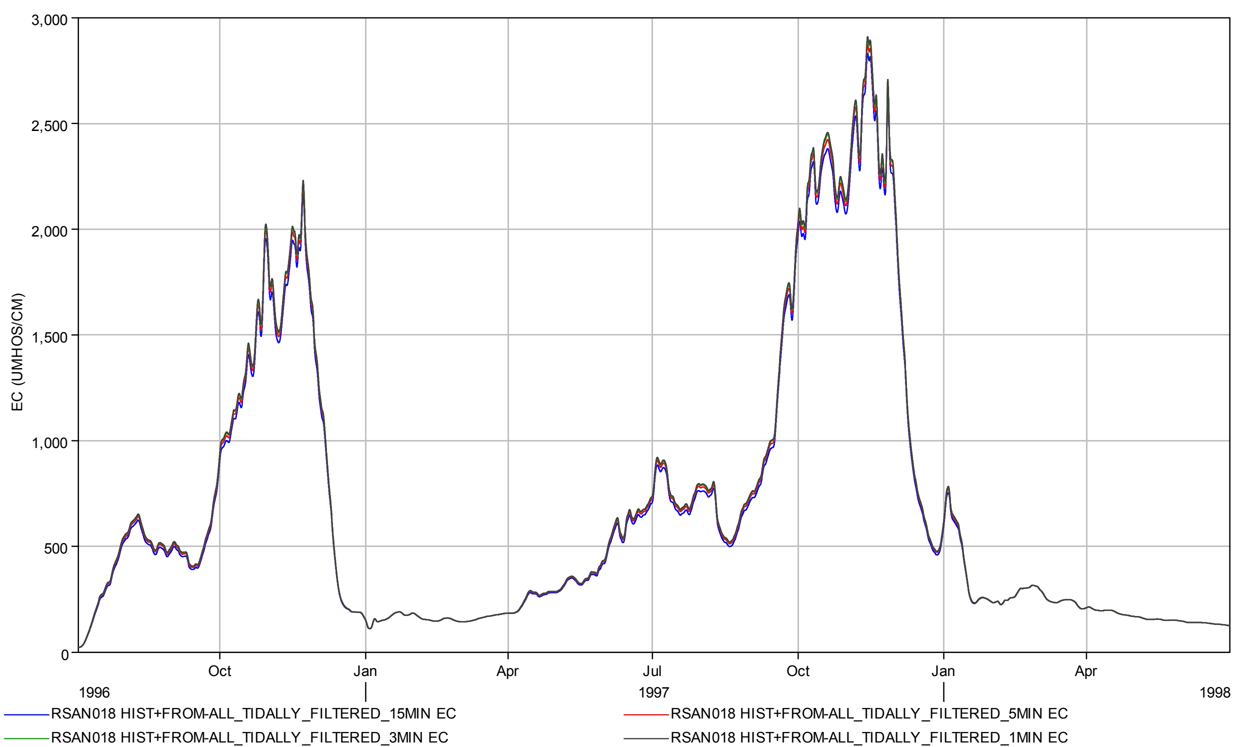

Figure 1-15 New model, result at Jersey Point (time step sensitivity test, parcel size 500 ft)

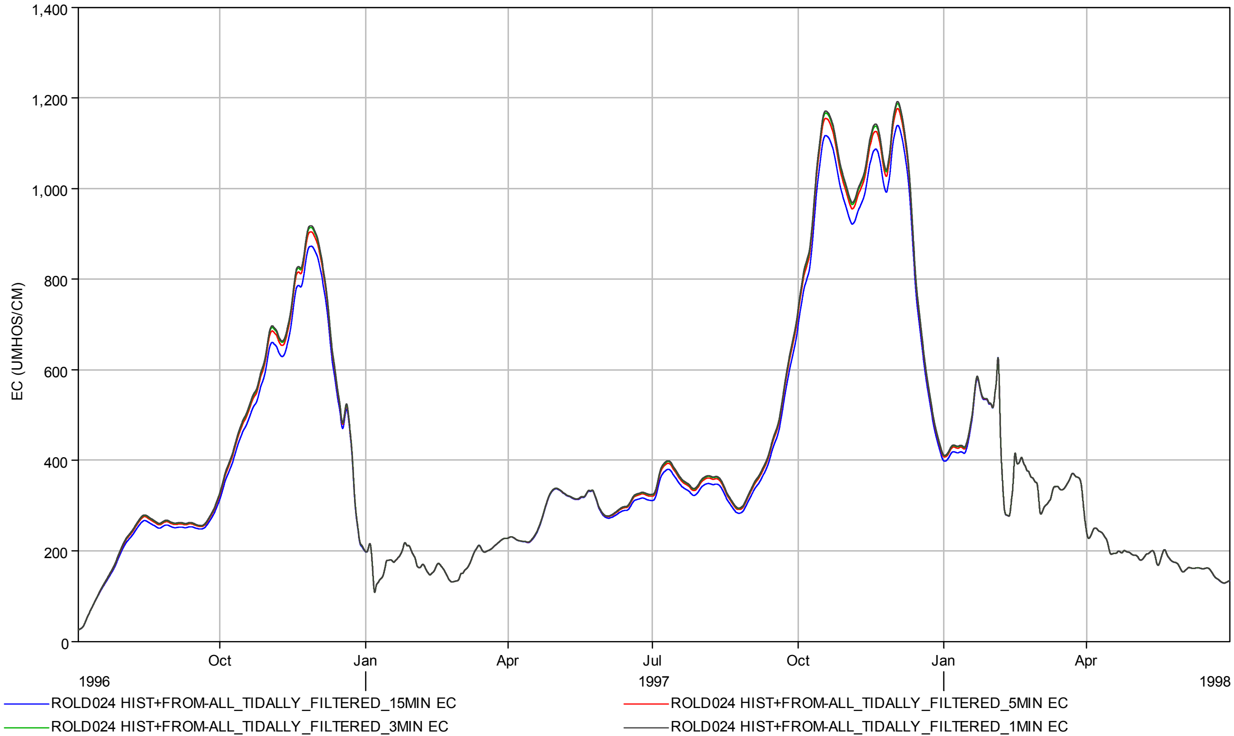

Figure 1-16 New model, result at Bacon Island (time step sensitivity test, parcel size 500 ft)

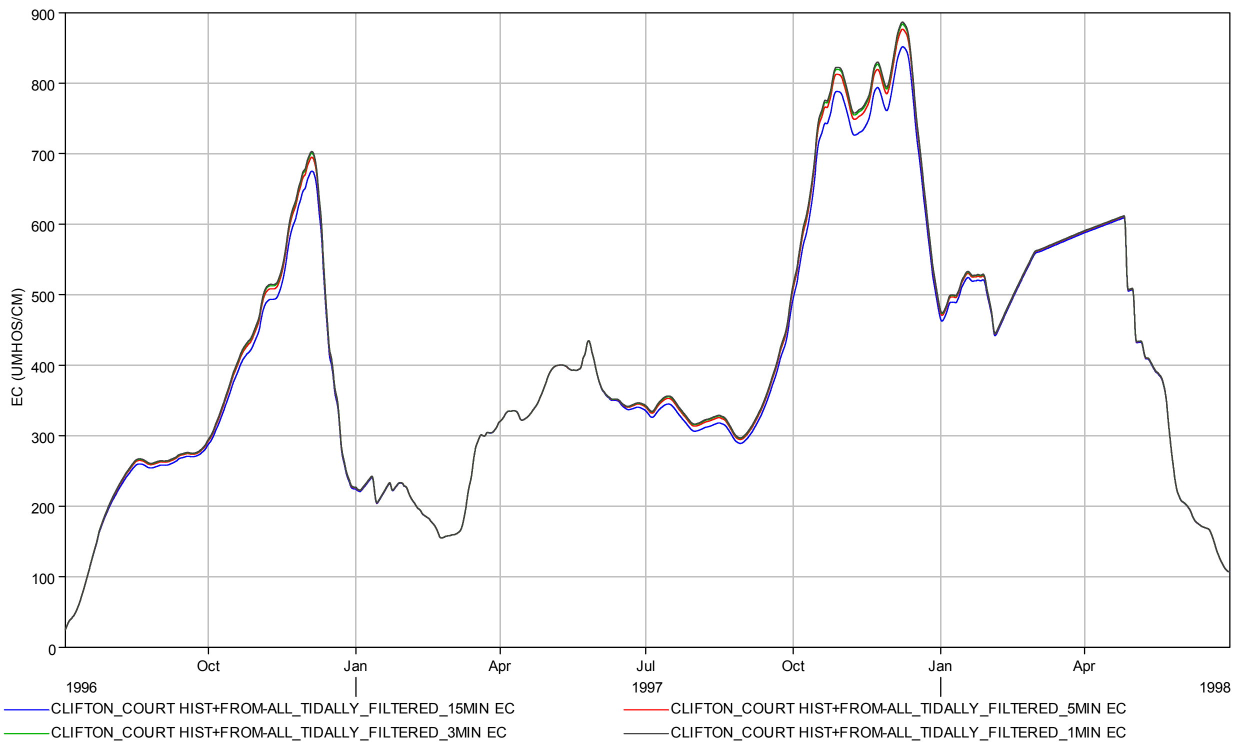

Figure 1-17 New model, result at Clifton Court (time step sensitivity test, parcel size 500 ft)

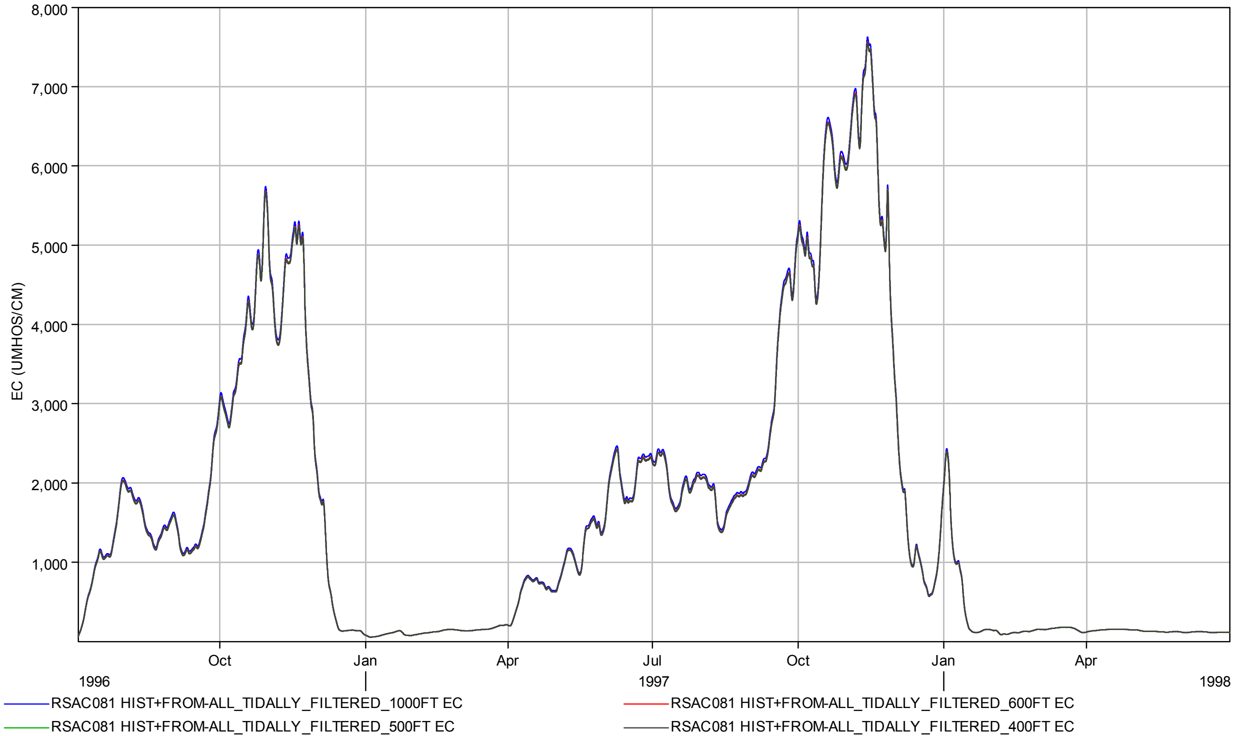

Figure 1-18 New model, result at Collinsville (parcel size sensitivity test, time step=5min)

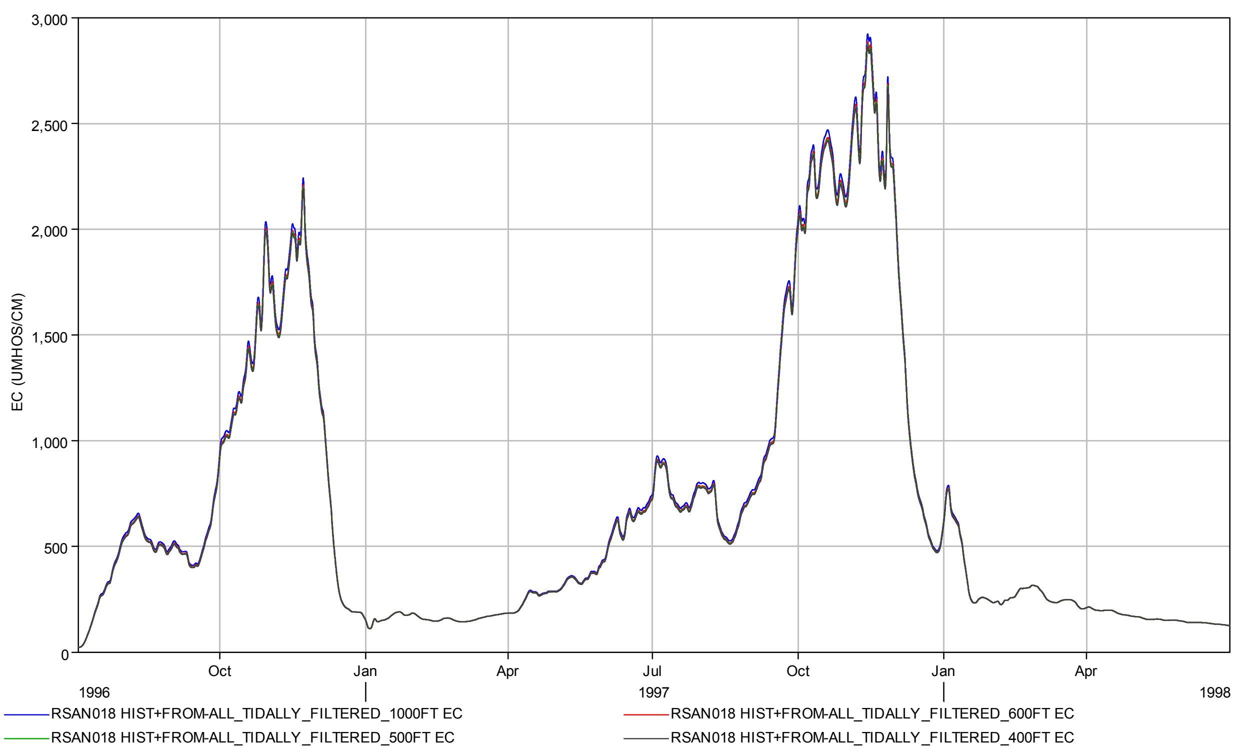

Figure 1-19 New model, result at Jersey Point (parcel size sensitivity test, time step=5min)

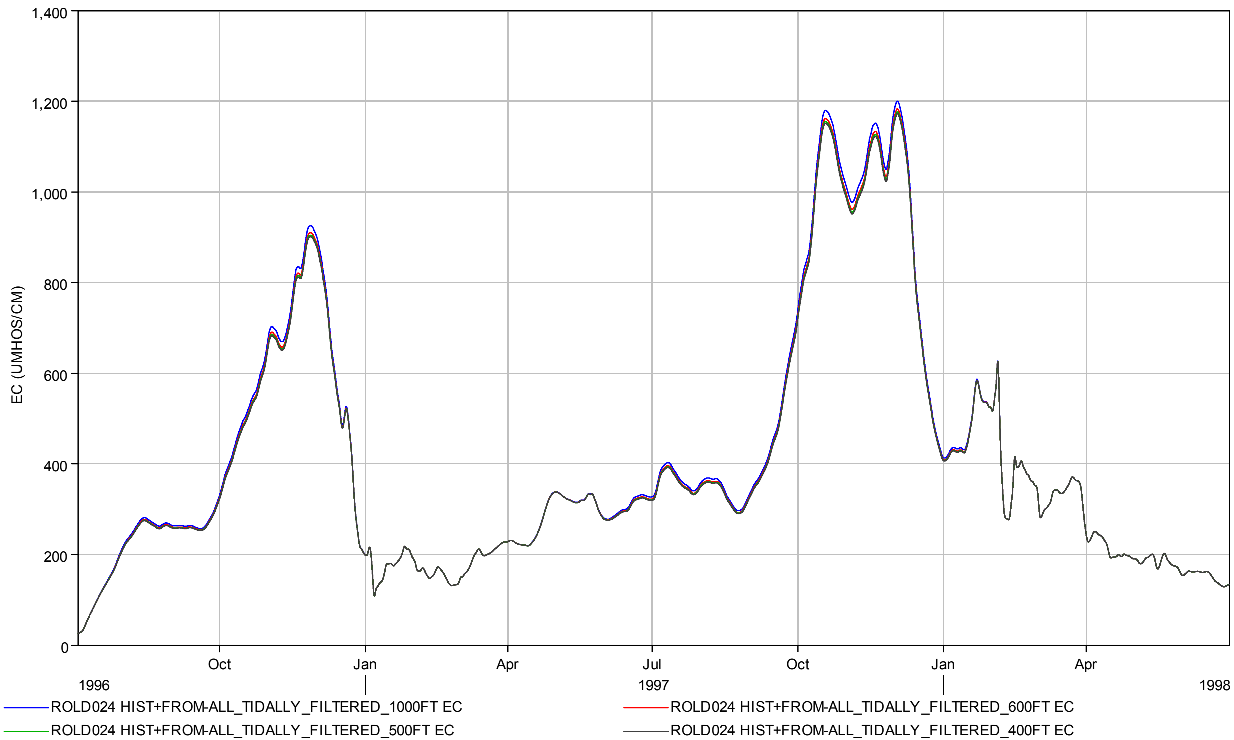

Figure 1-20 New model, result at Bacon Island (parcel size sensitivity test, time step=5min)

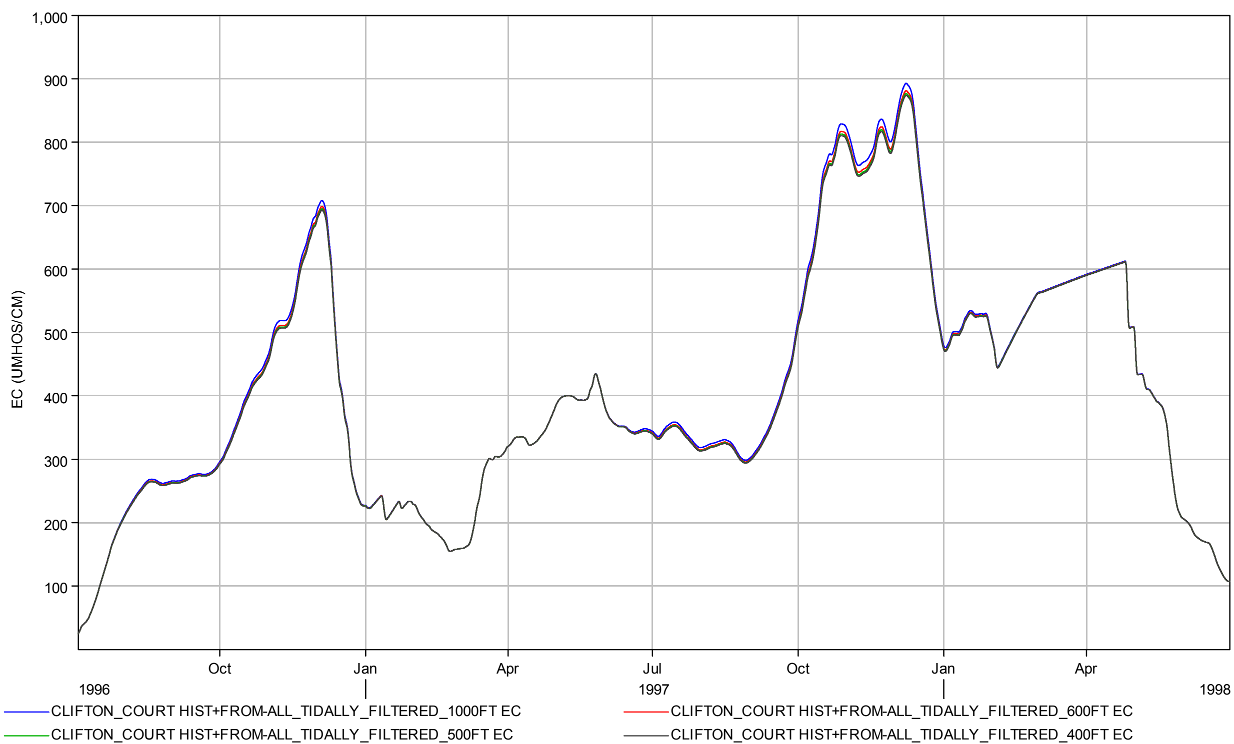

Figure 1-21 New model, result at Clifton Court (parcel size sensitivity test, time step=5min)

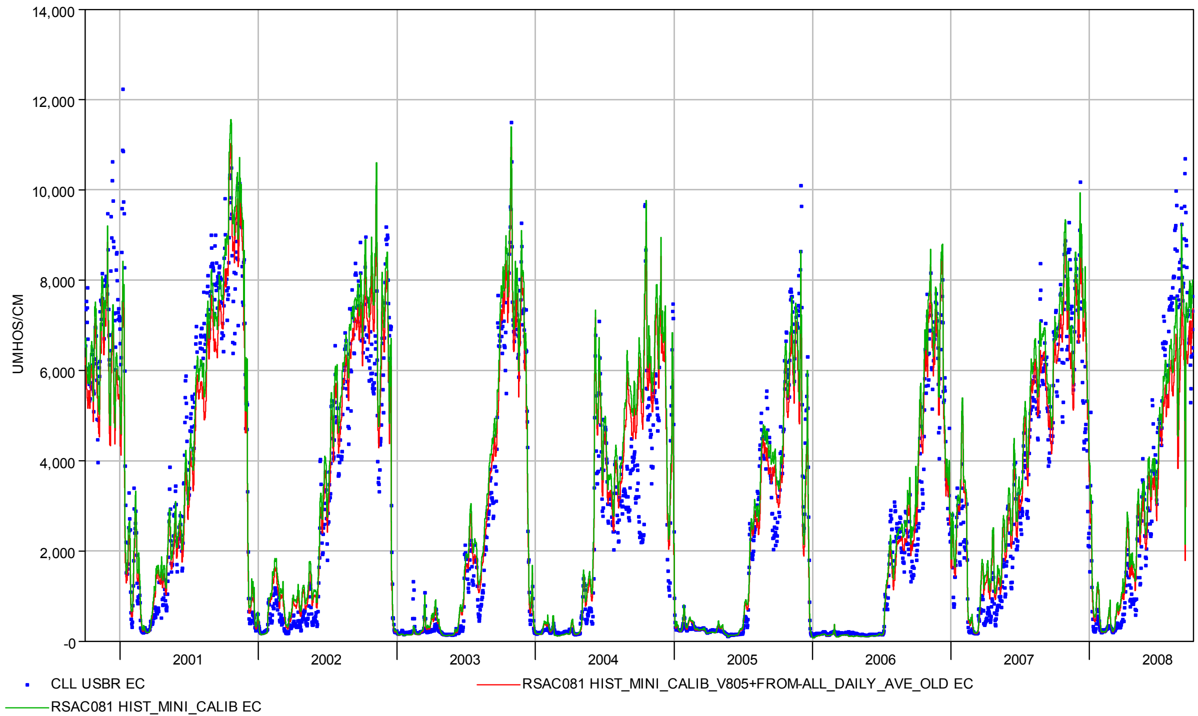

Figure 1-22 Comparison of previous (red line) and new (green) model results with field data (blue dots) at Collinsville

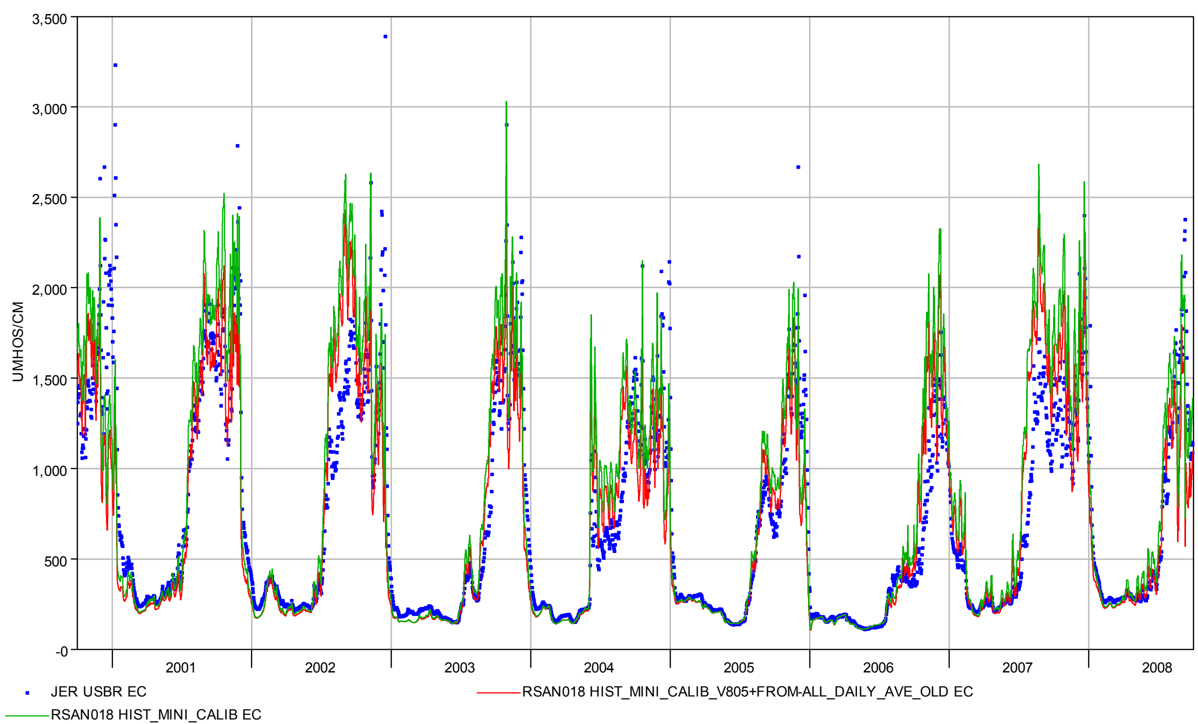

Figure 1-23 Comparison of previous (red line) and new (green) model results with field data (blue dots) at Jersey Point