Modeling Mercury Transport and Transformation along the Sudbury River, Massachusetts (USA) with Implications for Regulatory Action

ADDENDUM: Sensitivity Analysis

Prepared for:

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Region I

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Introduction

Sensitivity analysis is typically performed on computer models to asses the degree to which the output (i.e., model predictions) are sensitive to different input parameters. This sensitivity analysis was completed based on peer review and subsequent discussion with others at EPA familiar with numerically solved differential mass balance environmental fate and transport models. The computer model that was the focus of this analysis has been described previously in USEPA (2010).

The parameters investigated in this analysis are:

1. Base resuspension velocity
2. Diffusion rate for pore-water to surface water interactions
3. Erosion rates associated with critical shear stress of cohesive sediment
4. Flow rates associated with evaluating a 100-year storm event

As described in Volume 1 of Modeling Mercury Transport and Transformation along the Sudbury River, with Implications for Regulatory Action" (USEPA, 2010), the "Base Case" represents the final calibration of the model used to represent mercury fate and transport within the Sudbury River. The Base Case is a combination of both a "Clean" case, which simulates mercury that enters the river from atmospheric sources, and a "Contaminated Sediments" case, which simulates mercury that is associated with historic discharges attributable to the Nyanza Chemical site. For more information regarding the Base Case refer to Volume 1 (USEPA, 2010).

1. Parameterization

The following table details the values used in the June 2010 final model as well as the values used in conducting this Sensitivity Analysis.

Parameter Investigated	Unit	Original Value	Sensitivity Value(s)
Base Resuspension Velocity	v_r [m/s]	1×10^{-6}	0
Dispersion Rate	D [cm^2/s]	5×10^{-5}	6×10^{-6}
Critical Sheer Stress for Cohesive Bed	τ_c [Pa, N/m^2]	0.6	0.2, 6
High Flow	Q [m^3/s]	March 31, 2010: 2.38 April 1, 2010: 2.19	March 31, 2010: 45.2 April 1, 2010: 8.61

The variation in the parameters included an upper and lower bound for τ_c, 0.2 Pa and 6 Pa, where the Base Case used τ_c = 0.6 Pa. Base resuspension velocity was set to 0, where the Base Case used $1\text{x}10^{-6}$ m/s. Dispersion rate for pore-water to surface water was set to $6\text{x}10^{-6}$ cm^2/s (the molecular diffusion for mercury), where the base case was $5\text{x}10^{-5}$ cm^2/s (the common molecular dispersion value used to incorporate bioturbation of sediments).[1] To evaluate the impact of a high flow event, a 100-year storm was evaluated by changing the upstream flow entering Reservoir 2 on March 31, 2010 and April 1, 2010. The base case had flows of 2.38 and 2.19 m^3/s for these dates, and the 100-year storm event used 45.2 and 8.61 m^3/s for these dates. A 100-year storm event occurred on these dates and was recorded by USGS, the higher flows associated with this event lasted for these two days (USGS, 2010).

2. Results

In completing this Sensitivity Analysis, the simulated results were plotted for total mercury, HgT (unfiltered); total methyl mercury, MeHg (unfiltered); total dissolved mercury (filtered); and dissolved methyl mercury (filtered) along with the observed values using the first five years of each simulation for each parameter that was modified (for which each parameter's sensitivity was evaluated). The results of the critical shear stress sensitivity simulations compared to the base case were plotted in Figure 1 - Figure **4**. The resuspension velocity and diffusion rate with the base case were plotted in Figure 6 – 8. The results of the high flow event simulation compared to the base case were plotted in Figures 9 – 12.

3. Discussion

3.1. Critical Shear Stresses

Figures 1 - 4 depict the sensitivity of the model simulations to changes in the critical shear stress for erosion of a cohesive bed. For all mercury species, when a higher critical shear stress was used, the result were identical to the Base Case indicative of a low sensitivity to increasing values of critical shear stress. However, when the critical shear stress was decreased, the results were more variable indicating an increasing sensitivity to lower critical sheer stress values. In the plots showing the unfiltered HgT and MeHg, the lower critical shear stress resulted in predicted spikes of higher mercury concentrations during the periods of high flow.

The critical shear stress is a threshold parameter that describes when erosion of a cohesive bed begins. Shear stress is a parallel stress applied to the sediment surface due to water flowing above it; the faster the velocity of the water, the larger the shear stress. When the shear stress on the sediment is below the critical shear stress value, there is no

[1] From Schnoor (1996), this table represents values for different dispersion coefficients.

Condition	Dispersion Coefficient, cm^2/s
Molecular diffusion	10^{-5}
Compacted sediment	$10^{-7} – 10^{-5}$
Bioturbated sediment	$10^{-5} – 10^{-4}$

The molecular diffusion rate of Hg(II) in water is estimated as $D = \frac{22x10^{-5}}{MW^{2/3}}\frac{cm^2}{sec}$ = 6 x 10^{-6} cm^2/s, where MW is the molecular weight of Hg(II) (USEPA, 1997).

erosion of the sediment; however, upon exceeding the critical shear stress value, the sediment starts to erode. Shear stress of bed sediment is directly related to the velocity of the moving water above it.

The sensitivity analysis results for the critical shear stress value are reasonably expected and readily explained. The model did not demonstrate sensitivity to increases in the critical shear stress value; however, the model demonstrated sensitivity to decreases in the critical shear stress. As the critical shear stress is decreased, the frequency of shear stress going over the critical shear stresses increases. If the critical shear stress were lowered so much that the shear stress in the system always exceeded the critical shear stress, then the system would not be sensitive to further decreases in the critical shear stress value, because the cohesive bed would undergo continual erosion (this does not reflect the conditions at the Sudbury River, because the system is observed to have a positive burial sediment rate, which does match with a system undergoing continual erosion).

In the lower critical shear stress case, the model results demonstrate that flow velocities in the river result in shear stress levels that are higher than the critical shear stress, resulting in the simulated spikes in concentrations. For the filtered HgT, there is little sensitivity to the critical shear stress. For the filtered MeHg, there are spikes of MeHg concentration during the high flow/ high velocity events, demonstrating sensitivity to these parameters. In Reservoir 1 and 2, the model predicts spikes in concentrations when a lower critical shear stress is used yet the simulations return to the base case concentrations during periods of lower flow velocities. In the Great Meadows National Wildlife Refuge, the model shows higher concentrations more often with the lower critical shear stress, but, except for the spikes for a short time, the concentrations are not much different than the base case. Even for the spikes in concentration, these end up being two to four times higher than the base case.

The model simulation results demonstrate a non-linear sensitivity to the critical shear stress value. At values higher than the base case critical shear stress, there is no sensitivity to increases in the critical shear stress value. As the value is lowered, instances of increased erosion occur, showing spikes in the concentrations. After the spike is passed, however, the model simulated concentrations return to the base case simulations, suggesting that the sensitivity is limited primarily to the events.

3.2. Base Resuspension and Dispersion

Figures 5 – 8 show the results for the resuspension and dispersion sensitivity analysis. The sensitivity to the resuspension and dispersion are included on the same figures because they are similar processes, but each simulation is carried out separately, only changing one of the parameters. For all Hg species, the base case and molecular diffusion case show similar results. For HgT, the base case and molecular diffusion simulations overlay each other. For MeHg, the base case predicts slightly higher concentrations of MeHg for some time periods, but generally the molecular diffusion case is within 10% of the base case simulations. The no resuspension case shows model sensitivity for the total mercury, but only slight sensitivity for the MeHg. Over some time periods, the no resuspension is slightly less than the base case and molecular diffusion case, particularly in the last part of Reservoir 2 (top row, right). There is little sensitivity of MeHg to the no resuspension case for Reservoir 1 and the Great Meadow Wildlife Refuge. For HgT, in Reservoir 2 the higher concentrations of observed mercury and the larger peaks are removed in the no resuspension case. This is particularly seen in the middle and end of Reservoir 2 (top row, middle and right) and the main lobe of Reservoir 1 (middle row, middle); where the no resuspension case results in lower HgT concentrations, with a much less dynamic response. The Great Meadow Wildlife Refuge did not show this level of sensitivity.

3.3. 100-Year Storm Event (high flow event)

Figures 9 – 12 show the results of the sensitivity analysis for a high flow event. The high flow event is evident in the figures as a sharp spike in the concentration in some of the figures. For the upper left plot in Figure 9, a sharp rise and drop in concentration is seen, which occurs at the same time as the high flow (March 31, 2010, and April 1, 2010). The concentration then immediately returns to match the base case (the base case line cannot be seen because it lies directly beneath the 100-year flood case), demonstrating that the overall model results are not sensitive to a 100-year storm event, and that a 100-year storm even does not cause a large disruption in the system itself. (Because the x-axis runs from 0 – 8, year six occurs on the figures from 5 to 6.) The impact of the high flow event diminishes with distance down Reservoir 2, the largest concentration is in the upper portion of Reservoir 2, is less in the middle, and is on the same scale as the concentration changes over time at the end of Reservoir 2. The spike in concentration in Reservoir 1 and the Great Meadows Wildlife Refuge is within the base case variability of the concentration range.

4. Conclusions

Sensitivity analysis on critical shear stress, resuspension velocity, dispersion rate, and flow field were completed. Through this analysis, model simulations were found to have little sensitivity to most of these parameters. Of the parameters evaluated, the model simulations were found to be most sensitive to the critical shear stress. Higher critical shear stress had no effect, but decreasing the critical shear stress resulted in events where erosion occurred due to lowering the threshold where the shear stress was higher than the critical shear stress. These events resulted in higher concentrations of mercury and methylmercury in surface water during these events, but the rest of the simulation remained relatively insensitive to the change in critical shear stress. If shear stress were further lowered, the occurrence of erosional events would increase, but given that a site-specific critical shear stress was used, using a parameter much less lower than what was measured by others (US ACoE, 2001) may not accurately reflect the system.

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FIGURES

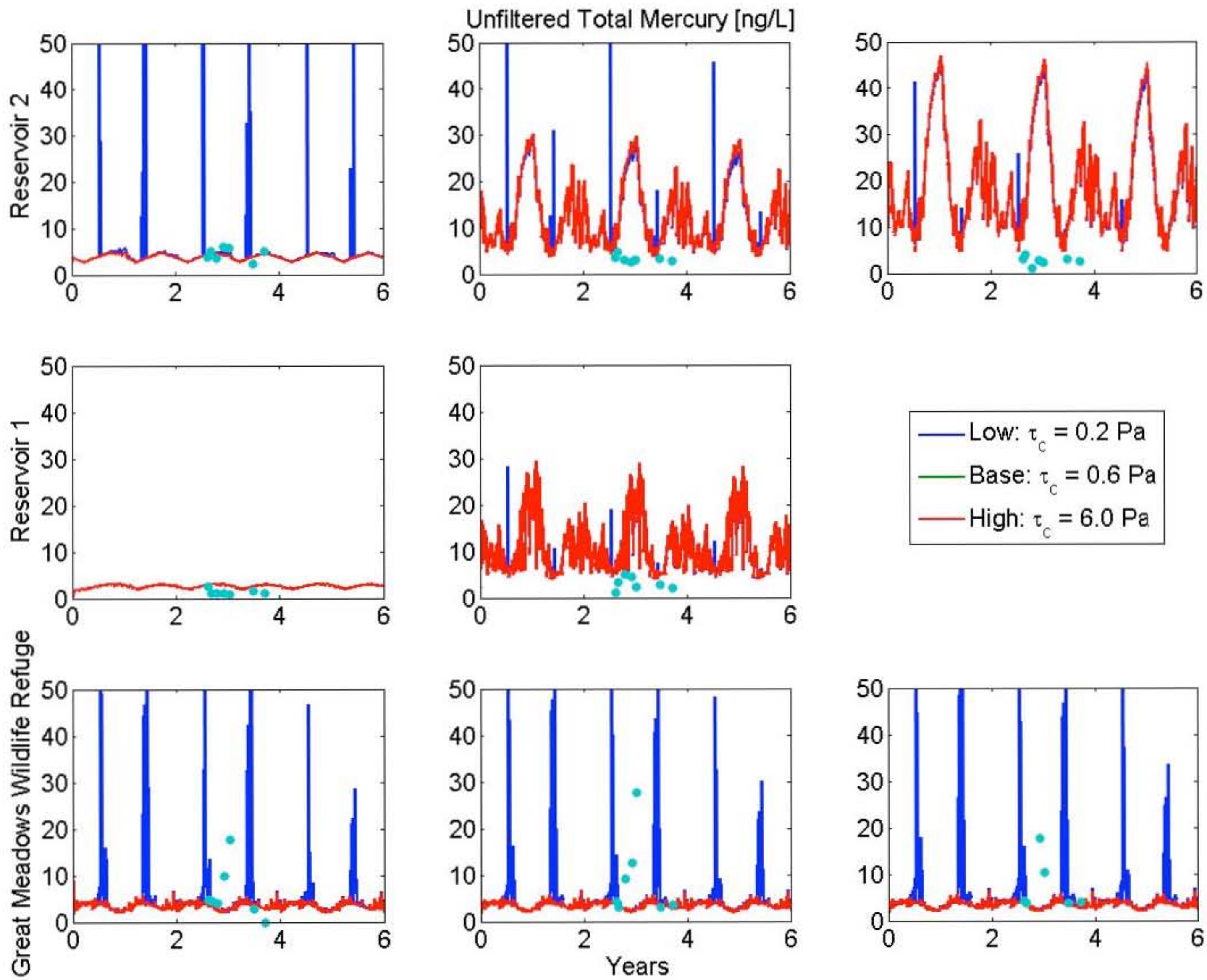

Figure 1. Unfiltered Total Mercury Concentrations over first six years for different critical shear stresses: low = 0.2 Pa, high = 6.0 Pa. The base case was run using critical shear stress of 0.6 Pa.

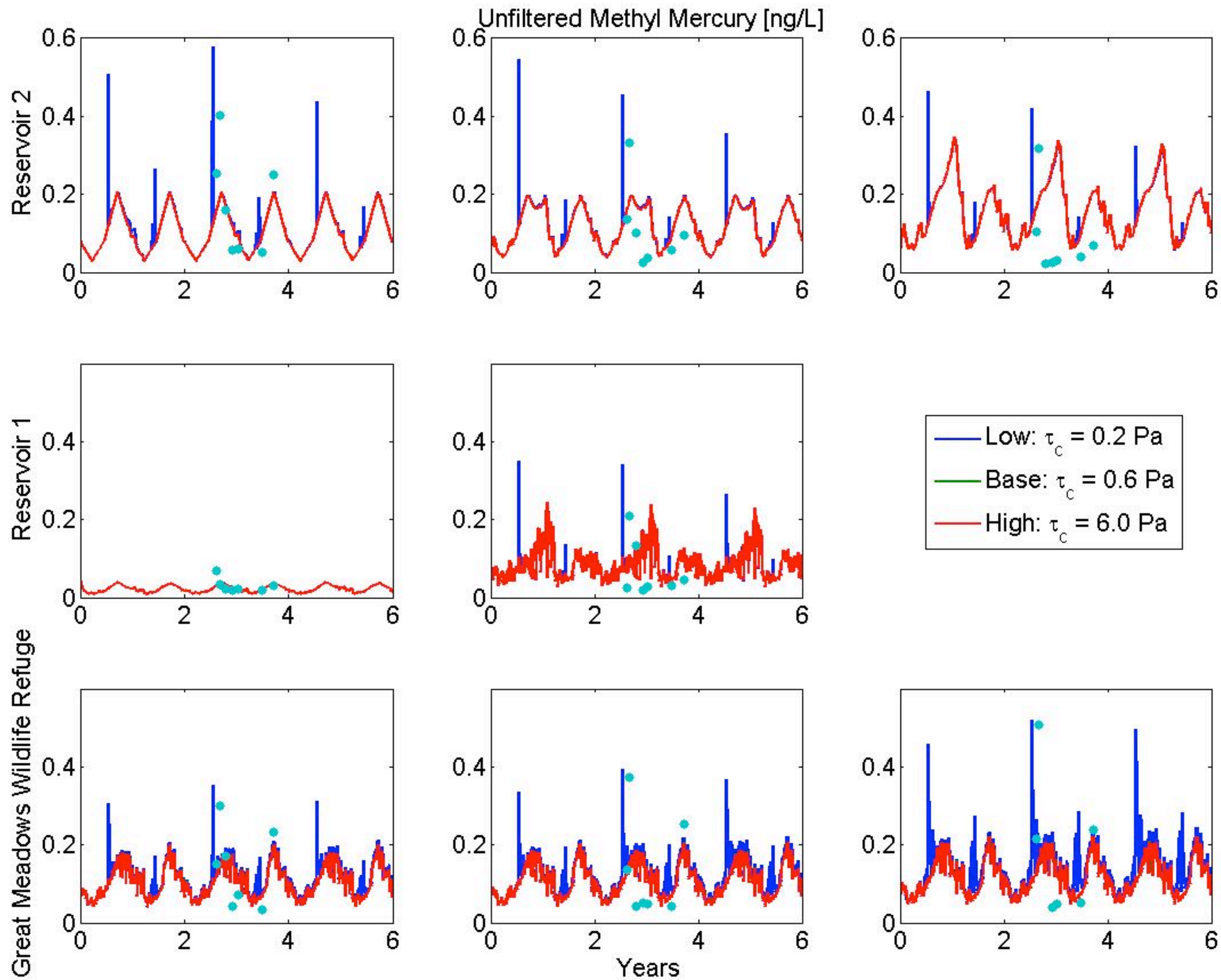

Figure 2. Unfiltered Methyl Mercury Concentrations over first six years for different critical shear stresses: low = 0.2 Pa, high = 6.0 Pa. The base case was run using critical shear stress of 0.6 Pa.

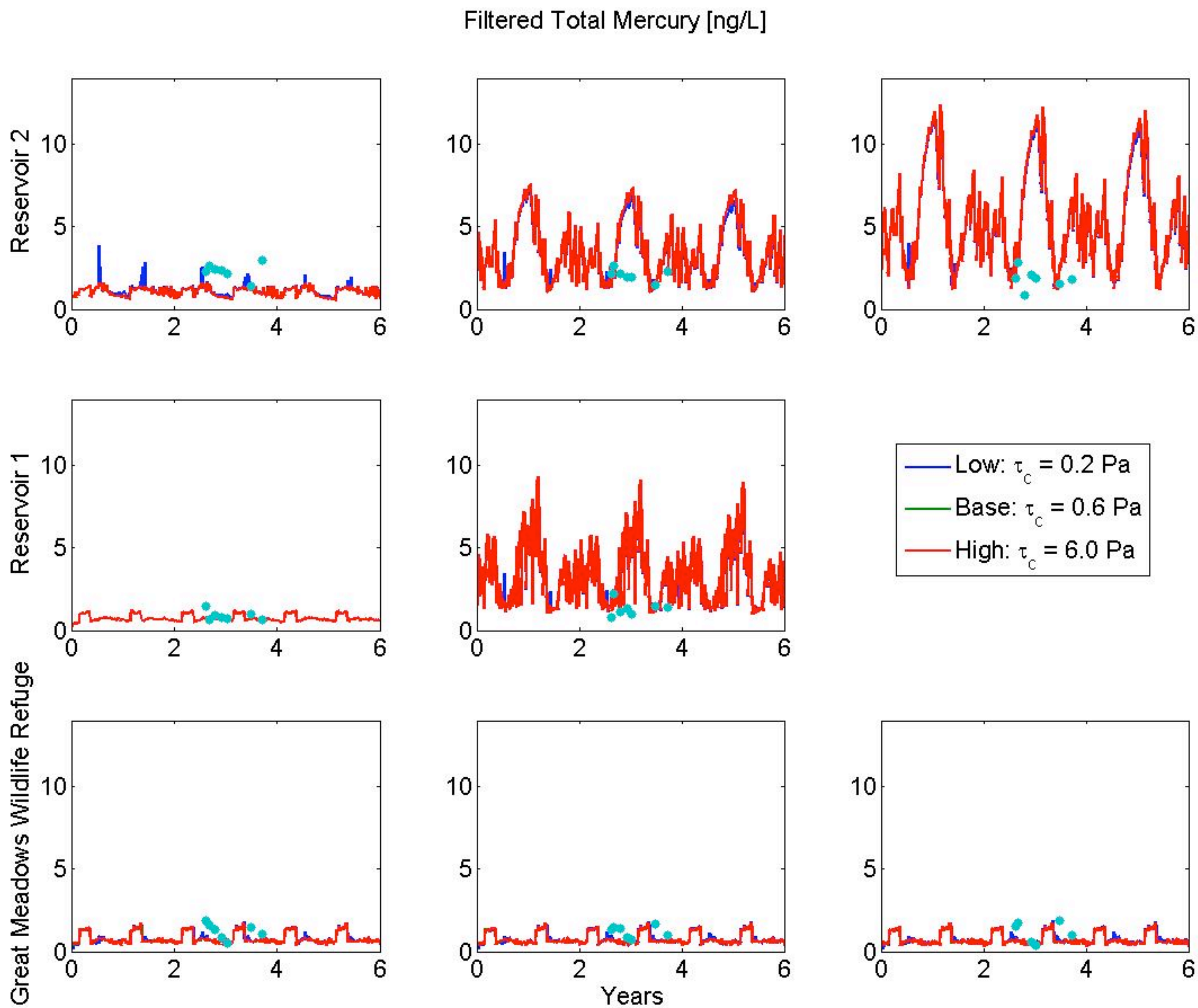

Figure 3. Filtered Total Mercury Concentrations over first six years for different critical shear stresses: low = 0.2 Pa, high = 6.0 Pa. The base case was run using critical shear stress of 0.6 Pa.

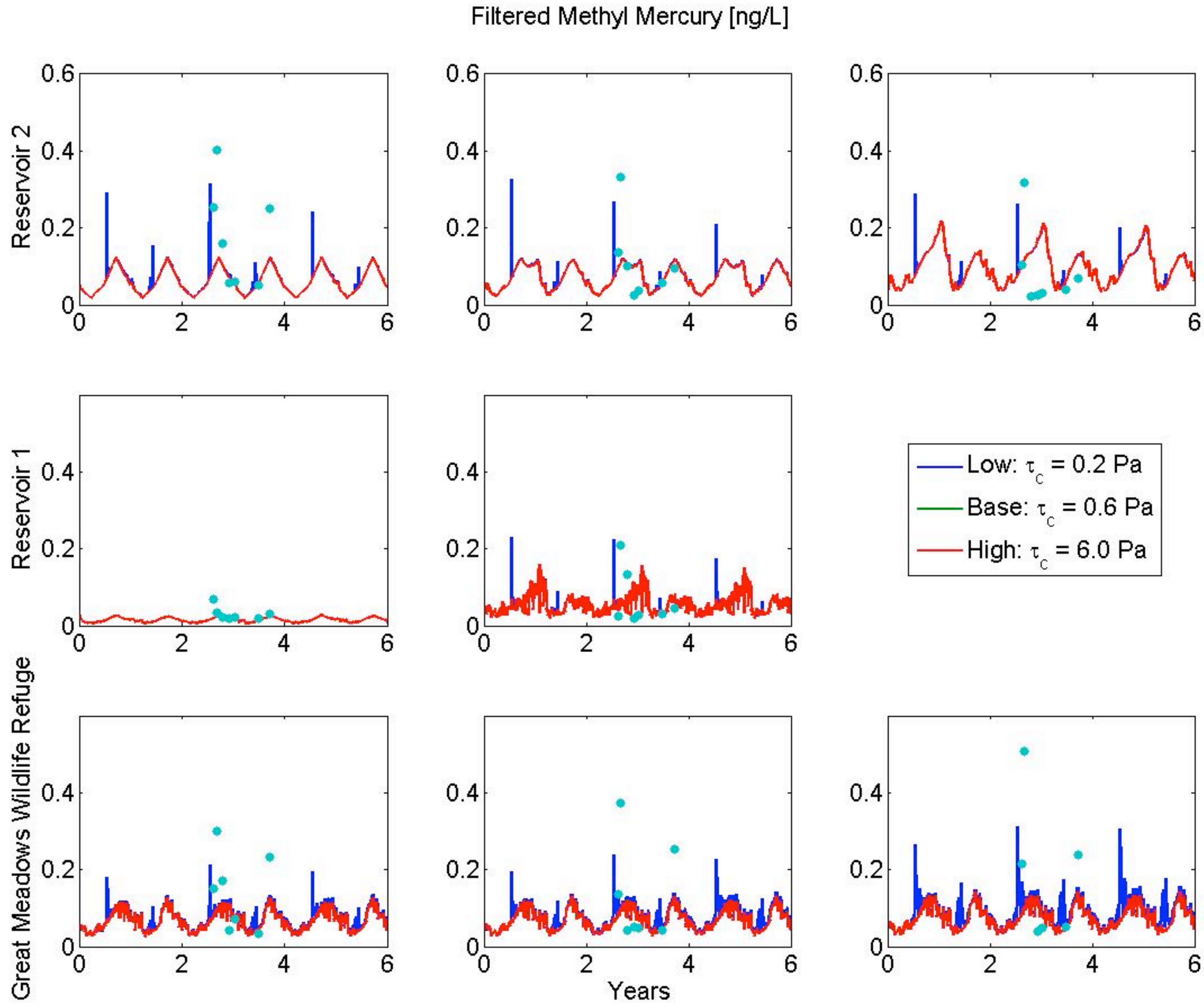

Figure 4. Filtered Methyl Mercury Concentrations over first six years for different critical shear stresses: low = 0.2 Pa, high = 6.0 Pa. The base case was run using critical shear stress of 0.6 Pa.

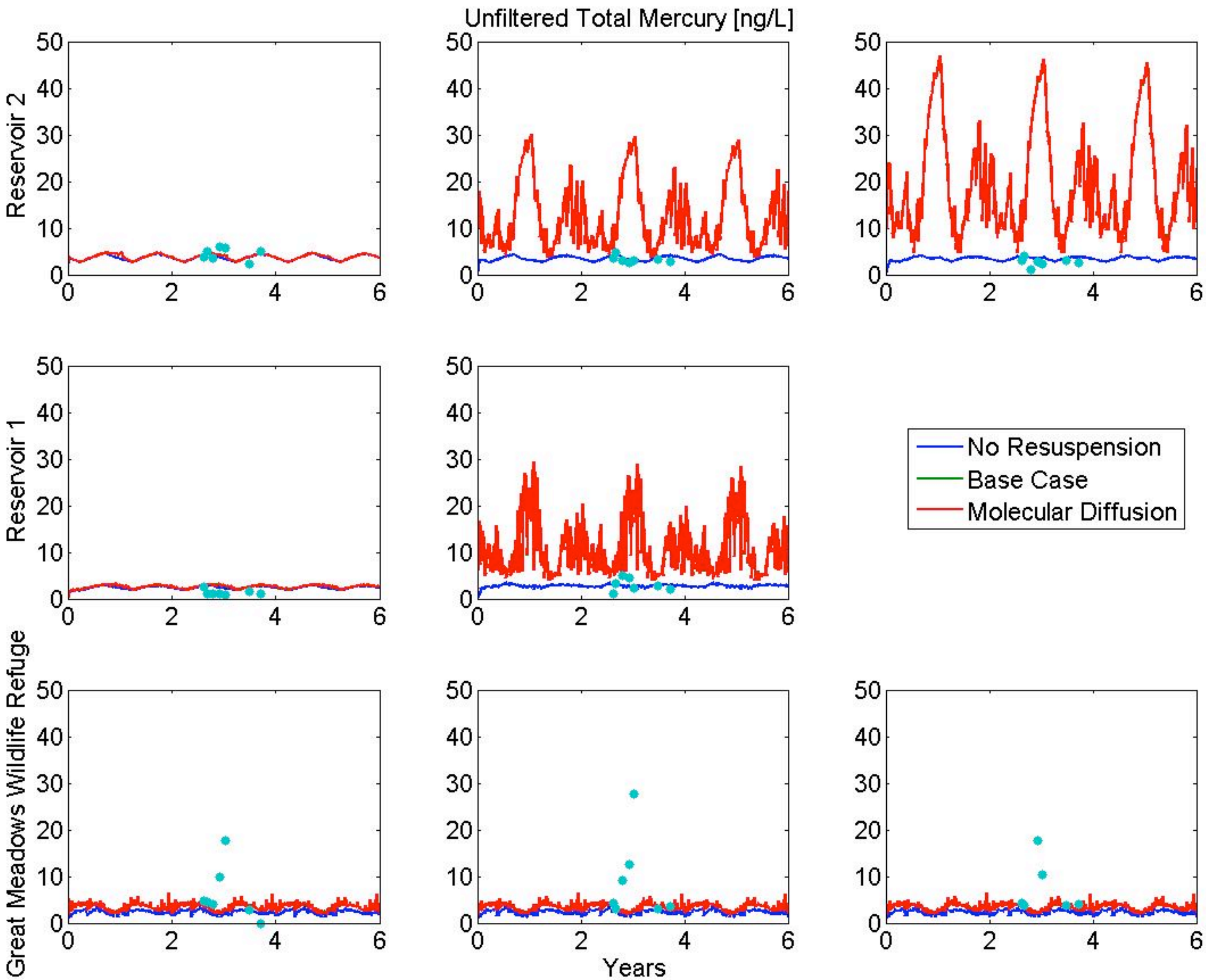

Figure 6. Unfiltered Total Mercury Concentrations over first six years for different resuspension and dispersion. Base Case used a rate of resuspension of 1×10^{-6} m/s, this was set to 0 for "No Resuspension." Base case had a dispersion rate for pore-water to surface water of 5×10^{-5} cm^2/s, this was set to 6×10^{-6} cm^2/s, which is the molecular diffusion rate for mercury in water.

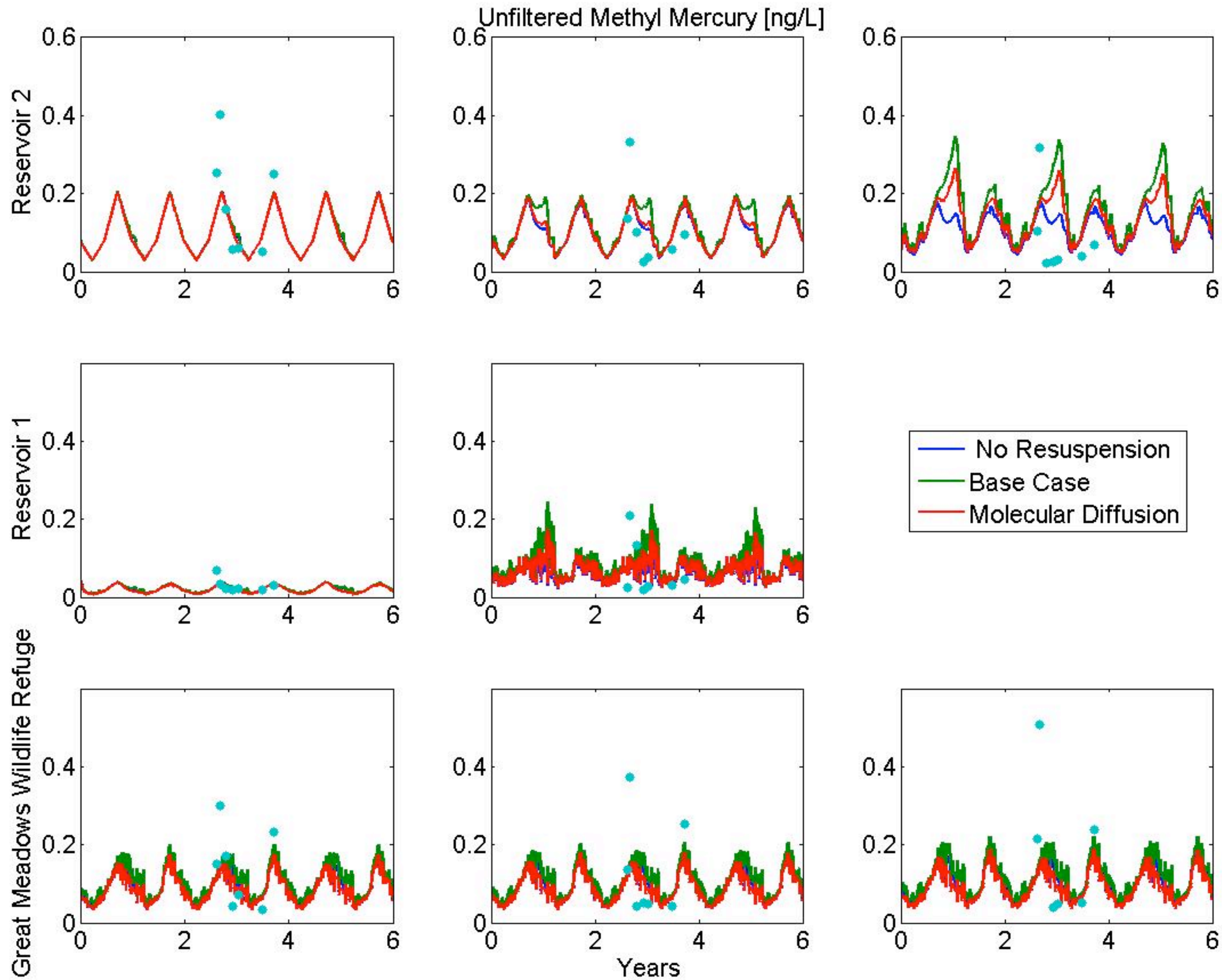

Figure 6. Unfiltered Methyl Mercury Concentrations over first six years for different resuspension and dispersion. Base Case used a rate of resuspension of $1x10^{-6}$ m/s, this was set to 0 for "No Resuspension." Base case had a dispersion rate for pore-water to surface water of $5x10^{-5}$ cm^2/s, this was set to $6x10^{-6}$ cm^2/s, which is the molecular diffusion rate for mercury in water.

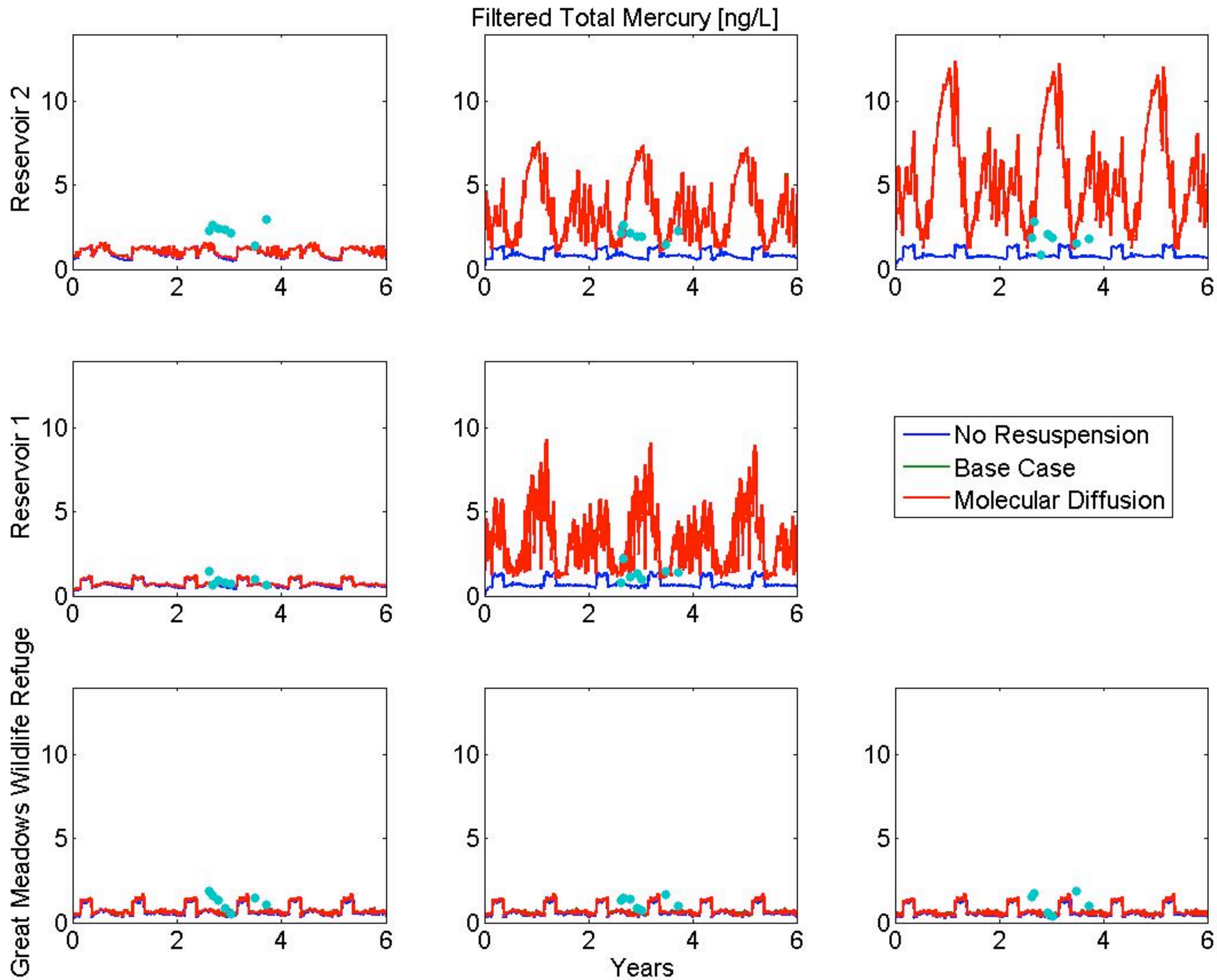

Figure 7. Filtered Total Mercury Concentrations over first six years for different resuspension and dispersion. Base Case used a rate of resuspension of $1x10^{-6}$ m/s, this was set to 0 for "No Resuspension." Base case had a dispersion rate for pore-water to surface water of $5x10^{-5}$ cm^2/s, this was set to $6x10^{-6}$ cm^2/s, which is the molecular diffusion rate for mercury in water.

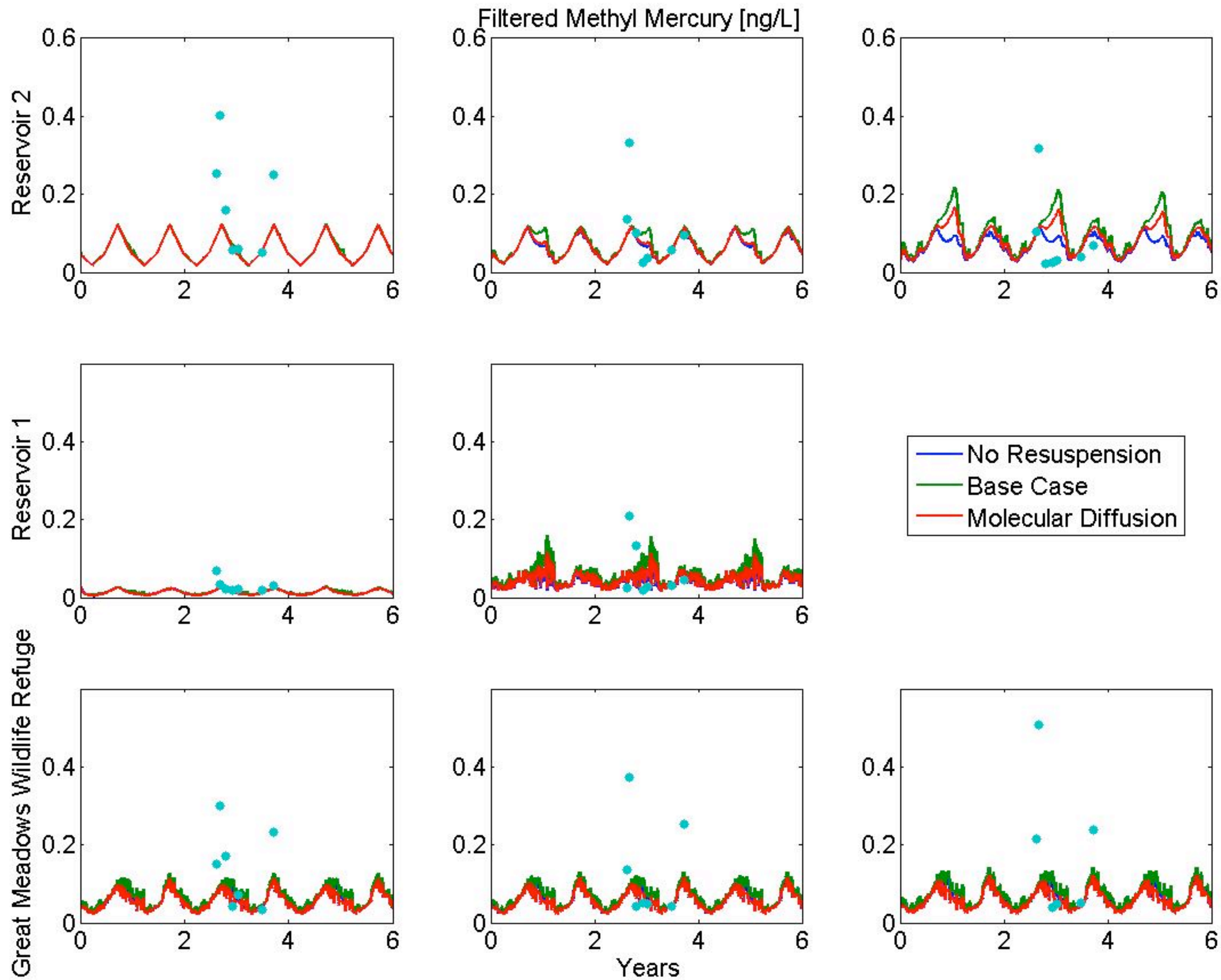

Figure 8. Filtered Methyl Mercury Concentrations over first six years for different resuspension and dispersion. Base Case used a rate of resuspension of $1x10^{-6}$ m/s, this was set to 0 for "No Resuspension." Base case had a dispersion rate for pore-water to surface water of $5x10^{-5}$ cm^2/s, this was set to $6x10^{-6}$ cm^2/s, which is the molecular diffusion rate for mercury in water.

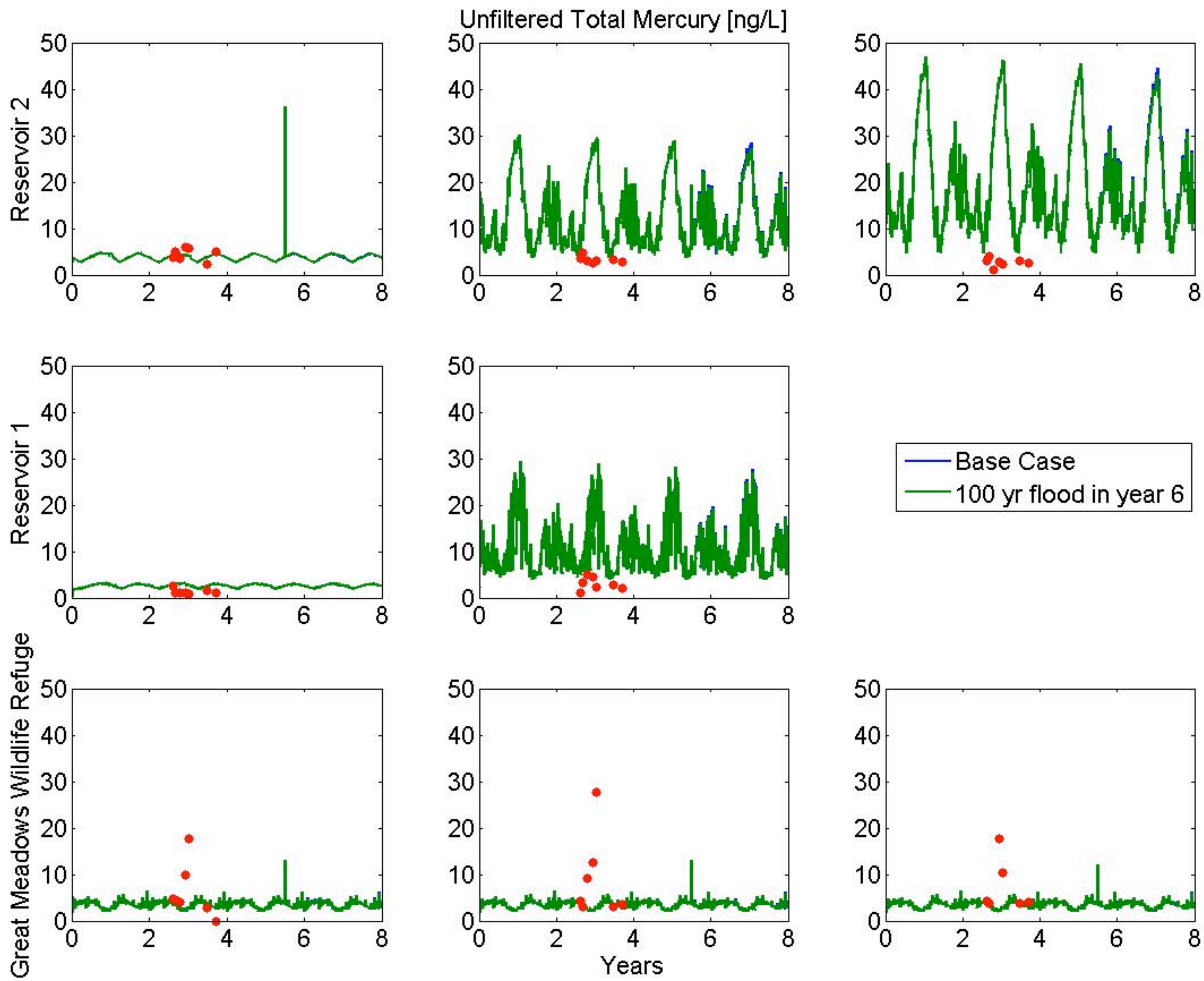

Figure 9. Unfiltered Total Mercury Concentrations over first eight years for a single high flow event simulating a 100-yr storm.

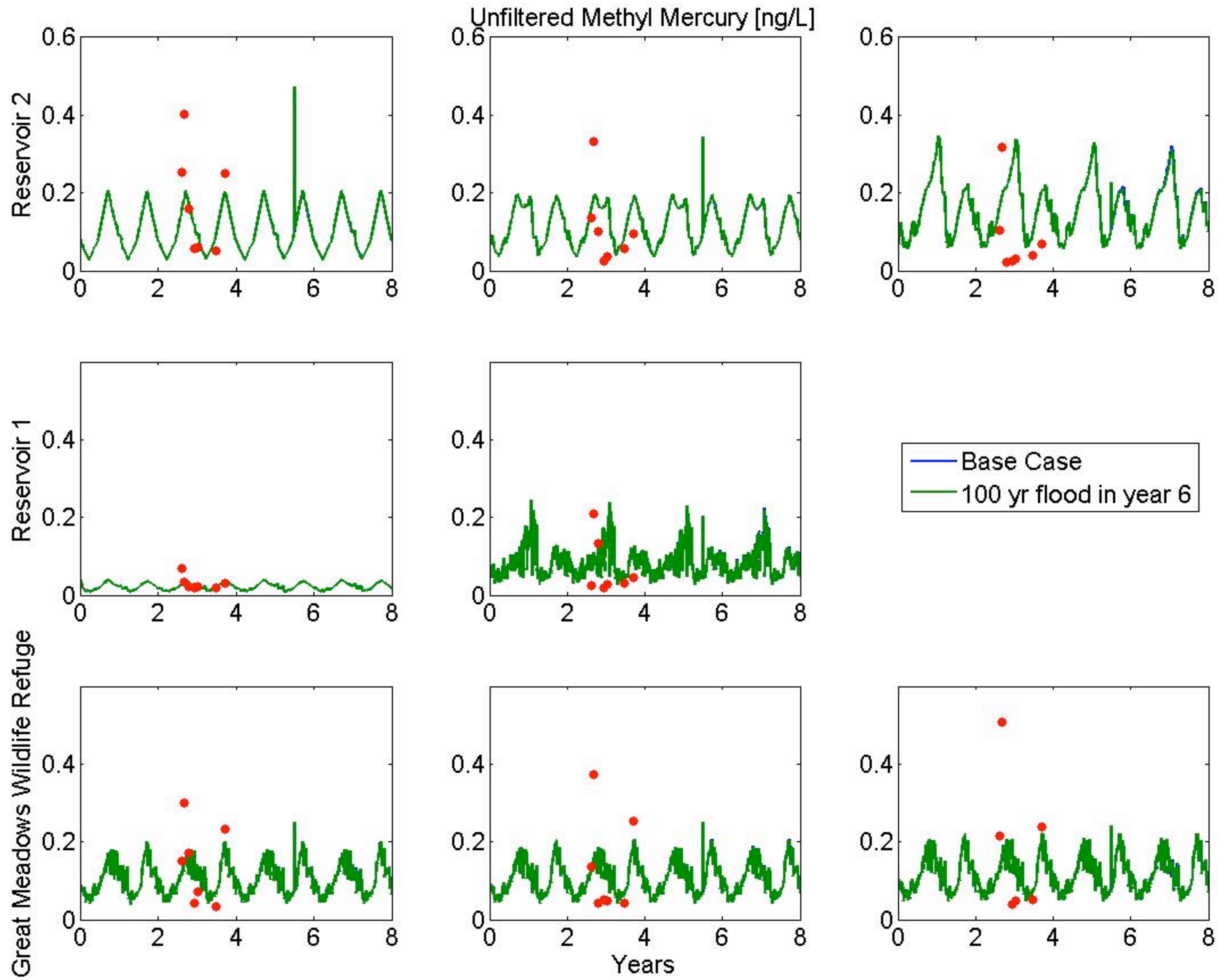

Figure 10. Unfiltered Methyl Mercury Concentrations over first eight years for a single high flow event simulating a 100-yr storm.

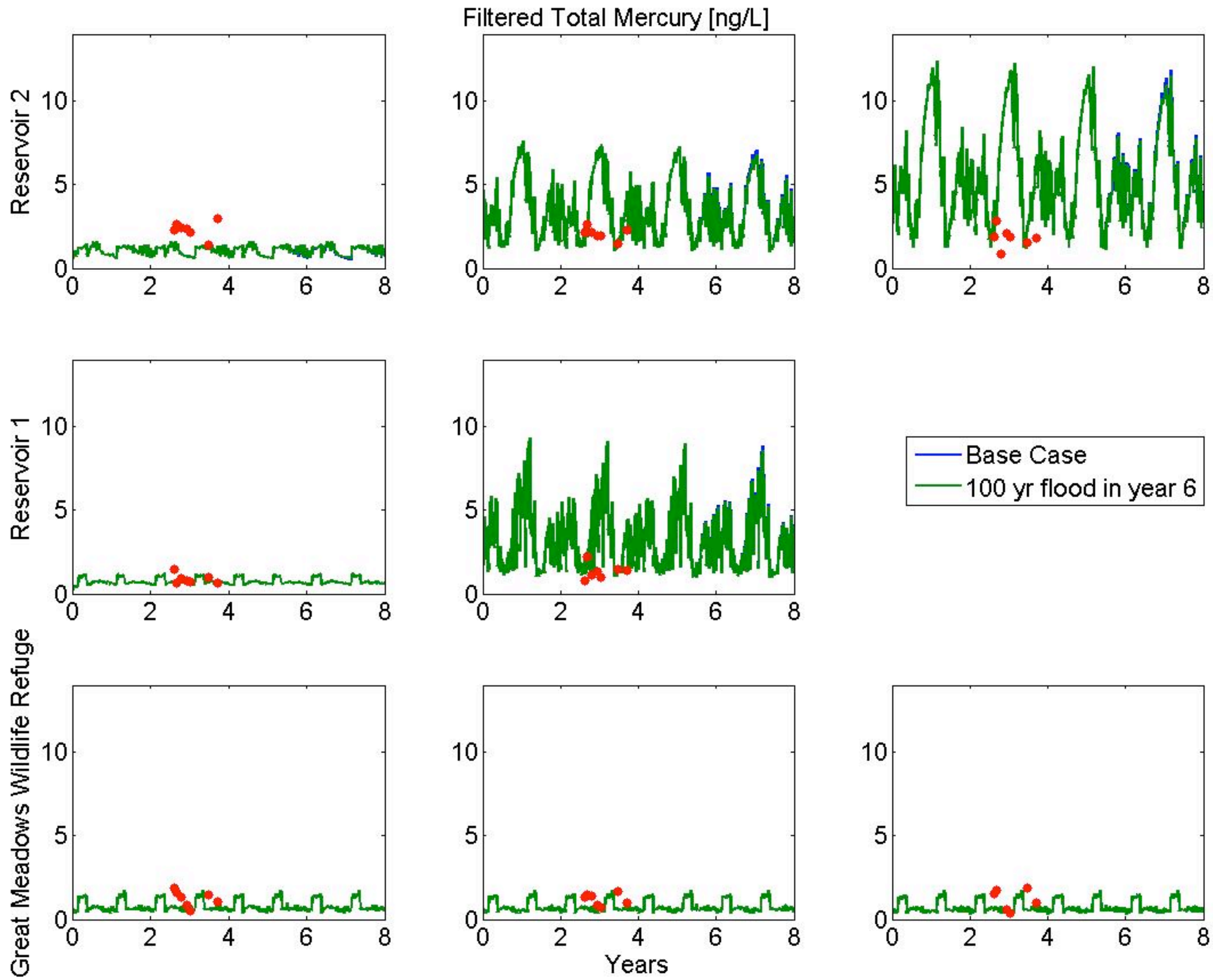

Figure 11. Filtered Total Mercury Concentrations over first eight years for a single high flow event simulating a 100-yr storm.

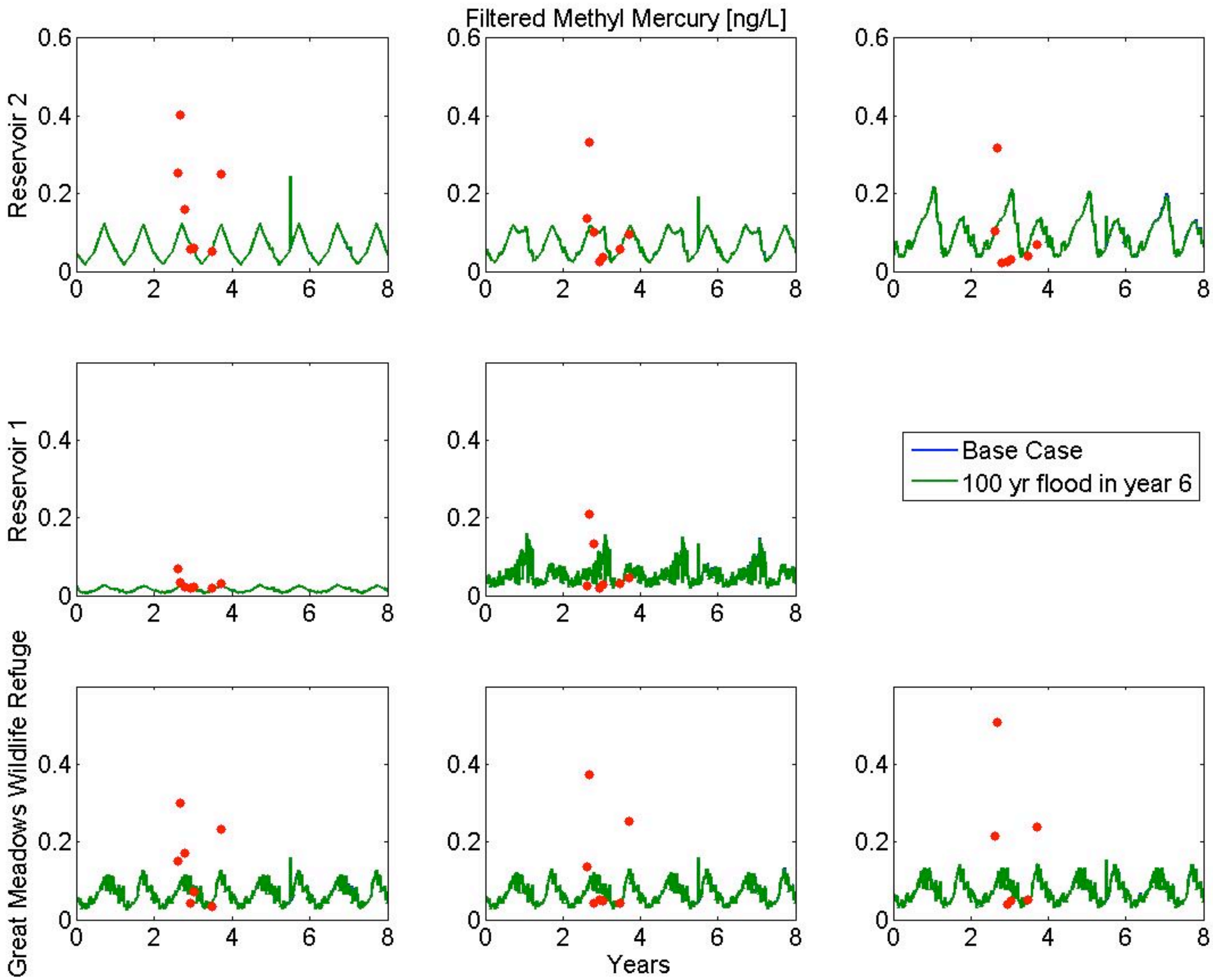

Figure 12. Filtered Methyl Mercury Concentrations over first eight years for a single high flow event simulating a 100-yr storm.