

Multiple tracers to evaluate travel time through a multi-layered aquifer using a novel transport approximation

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Table S1. Time split during each phase of the multi-tracer investigation. Units are in days.

Phase	Start Time	End Time	Total Length	Recharge	Shutdown	Pumping
1	05/15/18 14:15	08/02/18 17:00	79.11	54.06	24.34	0.71
2	08/02/18 17:00	08/21/18 14:45	18.91	-	2.01	16.90
3	08/21/18 14:45	11/21/18 01:15	91.44	58.79	31.98	0.67
4	11/21/18 01:15	04/26/19 08:00	156.28	0.17	155.59	0.52
5	04/26/19 08:00	04/29/19 07:00	2.96	0.01	0.07	2.87
6	04/29/19 07:00	12/25/20 17:15	606.43	338.79	246.91	20.56
7	12/25/20 17:15	04/09/21 13:15	104.83	0.77	104.06	-
8	04/09/21 13:15	04/14/21 12:00	4.95	0.18	0.89	3.86
9	04/14/21 12:00	11/02/21 02:15	201.59	133.19	60.22	8.04

Table S2. General description of operating conditions for each phase of the SWIFT Research Center demonstration phase (duration of multi-tracer investigation).

Phase	General Description of Operating Conditions
1	Normal operations with steady recharge and intermittent backflush. An initial ramp-up process was completed before recharge steadied at 700 gallons per minute (gpm) (1MGD).
2	Extended backflush for removal of injectate with high nitrite concentrations.
3	Normal operations with steady recharge and intermittent backflush.
4	Well shutdown for rehabilitation due to clogging caused by the presence of iron corrosion products in injectate.
5	Post-rehabilitation extended backflush.

Phase	General Description of Operating Conditions
6	Normal operations with steady recharge and intermittent backflush. Two extended shutdowns (each ~ 1 month) occurred due to issues in the treatment process that had to be addressed before the SWIFT Research Center could return to recharge
7	Well shutdown for rehabilitation to increase injectivity.
8	Post-rehabilitation extended backflush.
9	Normal operations with steady recharge and intermittent backflush.

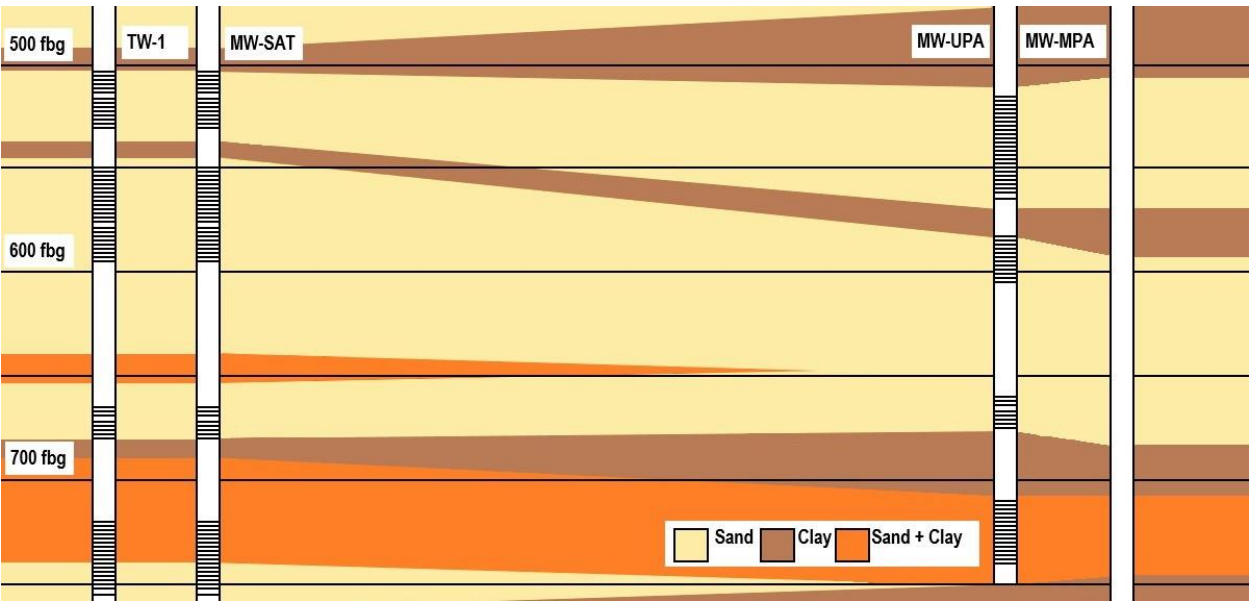


Fig. S1. Well locations and screen depths of wells at the SWIFT Research Center. Screen depths range from 500 to 1400 ft (152 to 427 m) below grade, but this study focuses on the UPA, which contains screens 1-4. Horizontal distance between wells is not shown to scale.

Upper Potomac Aquifer (UPA)

First, a breakthrough model for sulfate was calculated for each individual screen (Fig. S2). We applied the length and flow weighted distributions using all screens (Fig. S3) and using screens 1 and 2 only (Fig. S4), since we suspected that the upper screens were contributing more. Using screens 1 and 2 proved to be the most effective in all cases.

After flowmeter testing, drawdown at the conventional wells indicated that response in the UPA was decreasing, and the assumption could not be made that the flow distribution measured by the in-situ flowmeter was constant. For the initial comparisons, flow distribution before $t=344$ days (right before the restart of recharge after rehabilitation) is equal to the pre-rehab flow distribution. From $t=344$ days until $t=445$ days, flow distribution is equal to the post-rehab flow distribution. After 500 days, we assume that flow distribution returns to the original pre-rehab flow distribution, since there was not a direct measurement of flow distribution, but we know that it decreased.

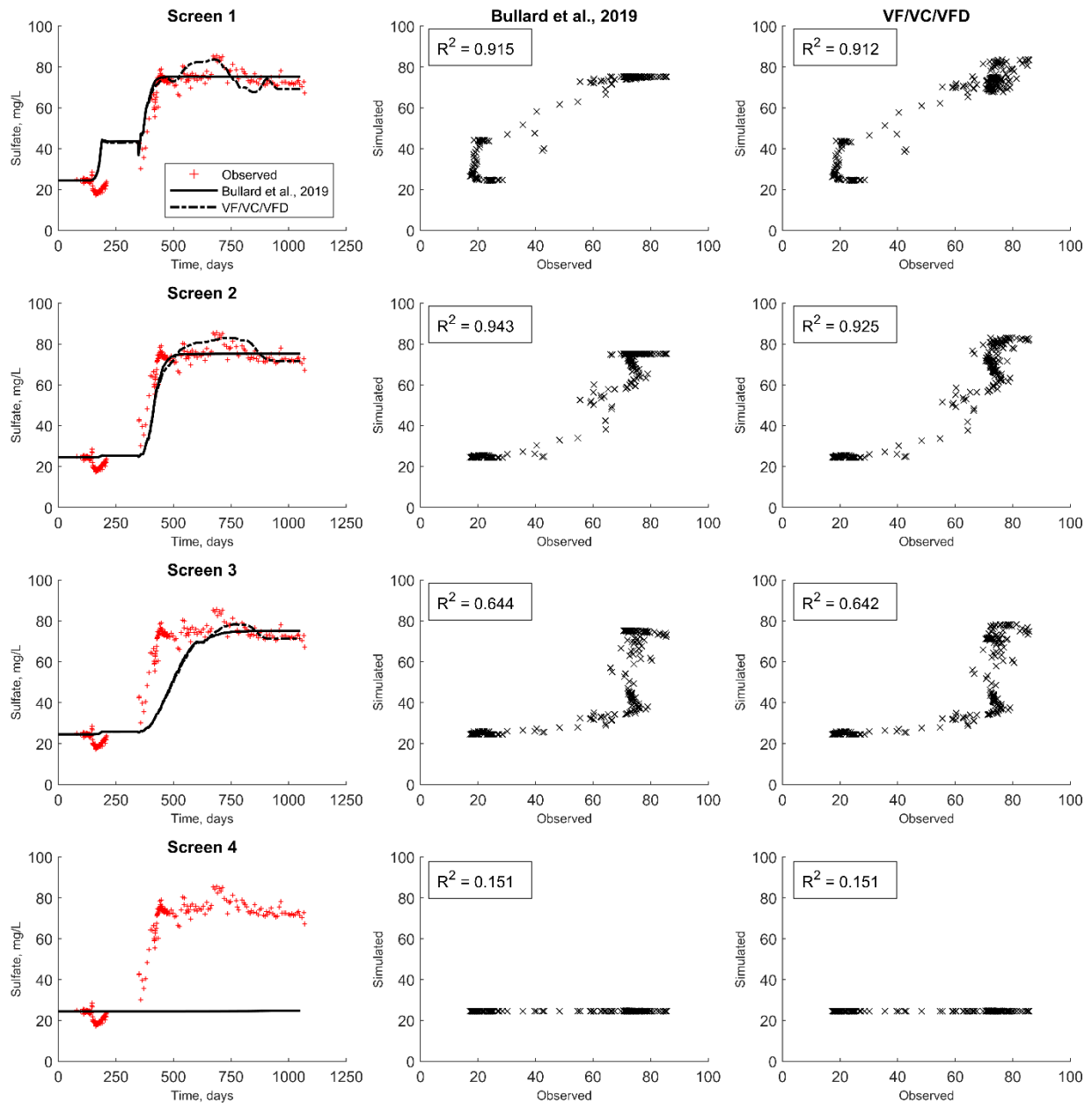


Fig. S2. Breakthrough calculated at each screen using aquifer characteristics (n and α) determined in Bullard et al. (2019). Coefficients of determination are shown for the constant concentration model (labeled Bullard et al. 2019) and the variable concentration model (labeled VF/VC/VFD). Both models account for variable flow and variable flow distribution.

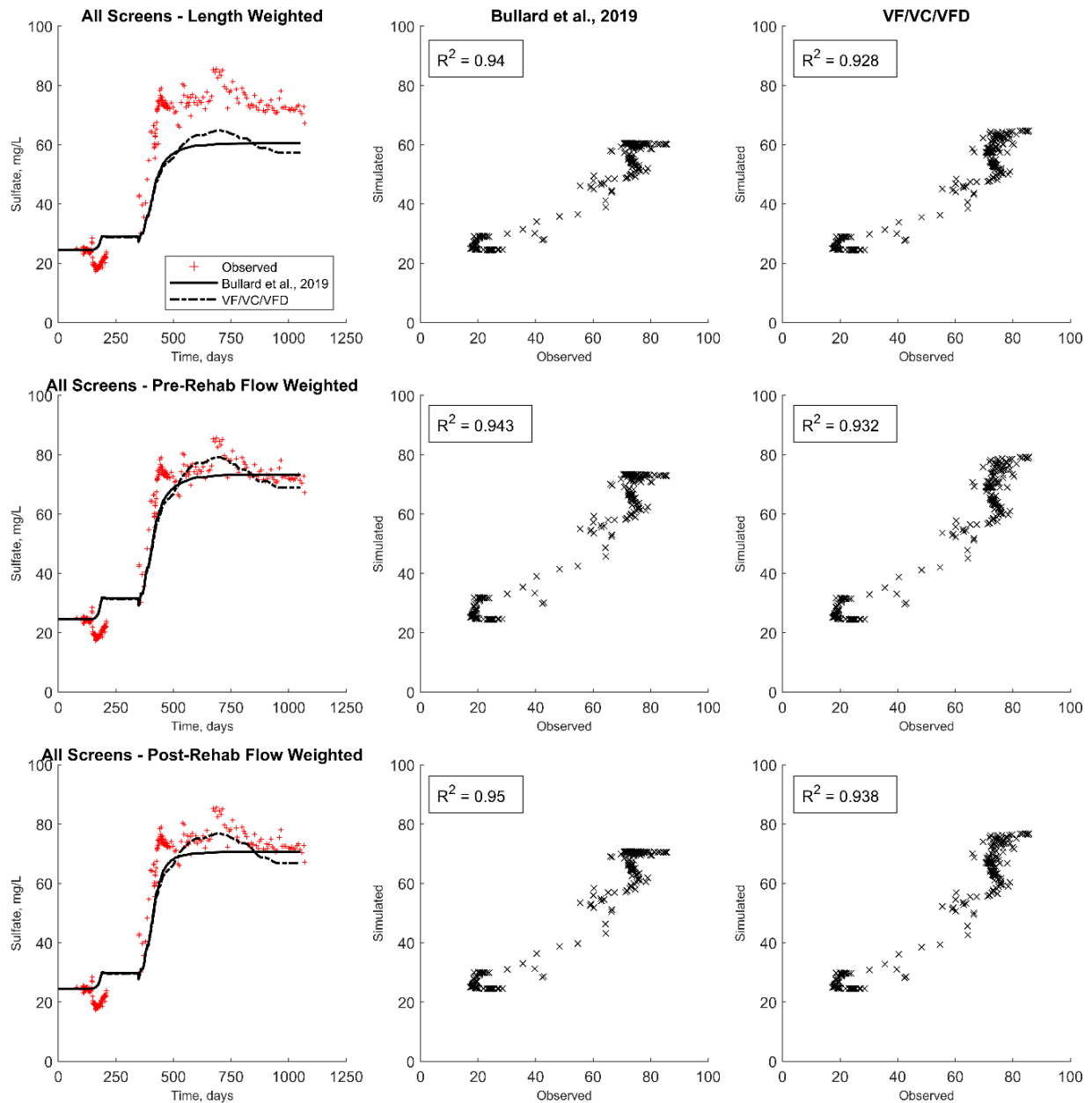


Fig. S3. Flow- and length-weighted models using screens 1-4. Coefficients of determination are shown for the constant concentration model (labeled Bullard et al. 2019) and the variable concentration model (labeled VF/VC/VFD). Both models account for variable flow and variable flow distribution.

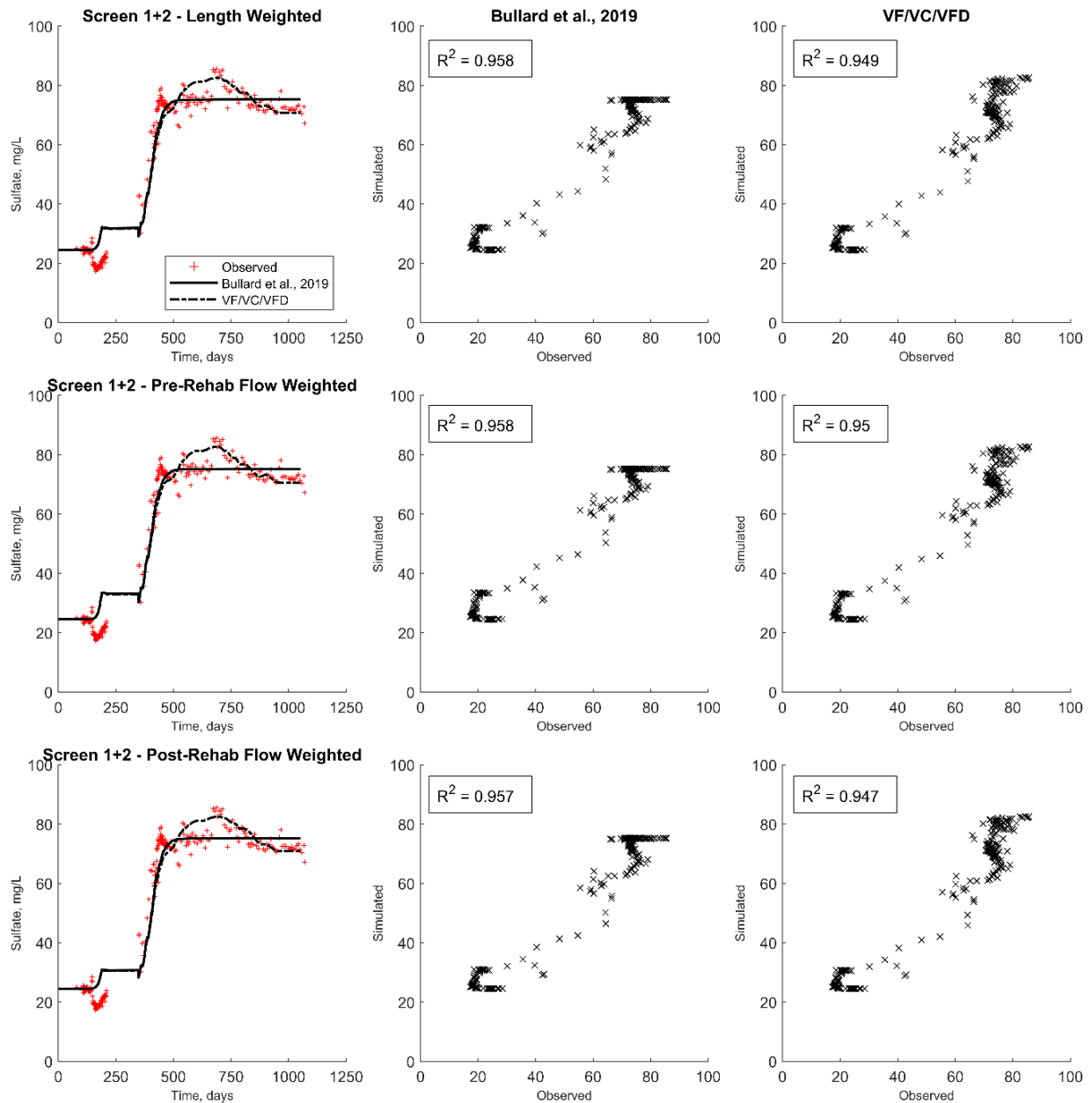


Fig. S4. Flow- and length-weighted models using screens 1 and 2 only. Coefficients of determination are shown for the constant concentration model (labeled Bullard et al. 2019) and the variable concentration model (labeled VF/VC/VFD). Both models account for variable flow and variable flow distribution.

Once it was determined that a combination of screens 1 and 2 was most accurate, a secondary investigation was conducted to determine whether the length of time that the model used the post-rehab flow distribution impacted the fit of the model. This involved varying the

transition day for post-rehab flow distribution back to pre-rehab flow distribution from 400 days to 600 days and measuring the coefficient of determination for the variable influent concentration model. Because the difference in fit between the length and flow weighted models were minimal, only the length weighted model was used for this part of the analysis. The optimal switchback time to pre-rehab flow distribution was 445 days, which produced a R^2 value of 0.9566.

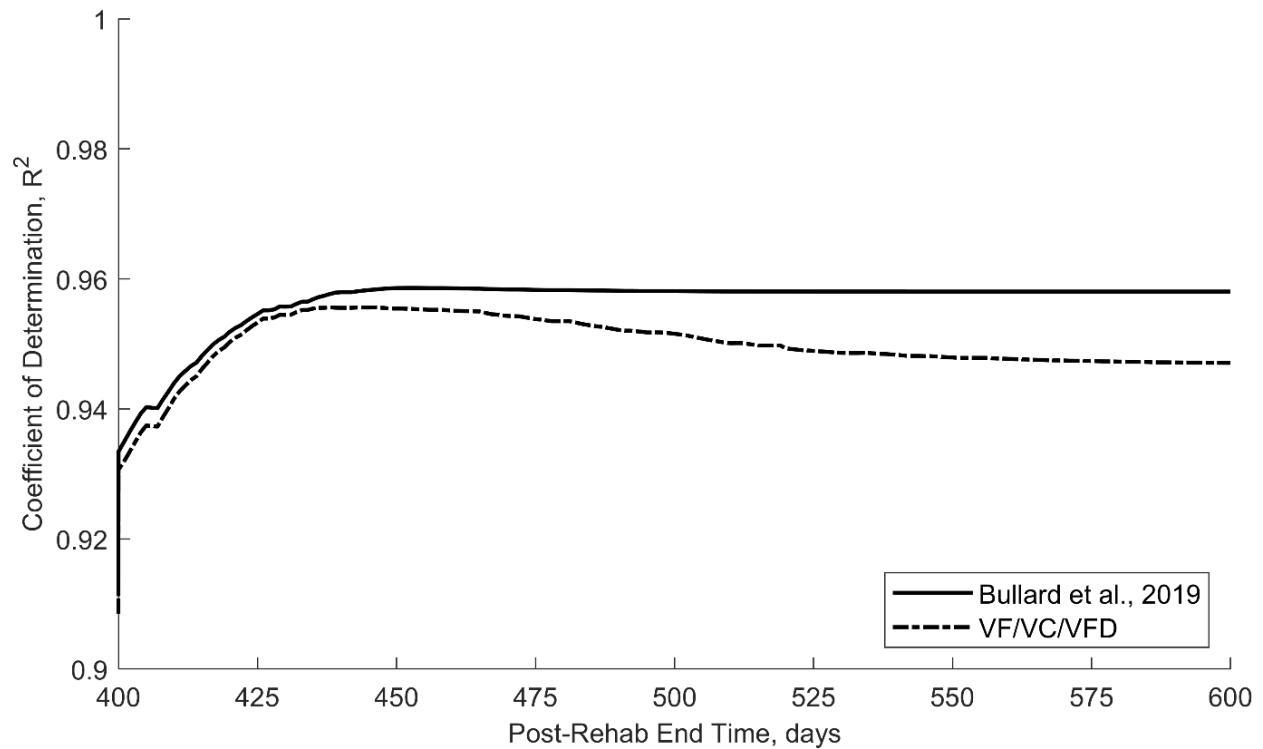


Fig. S5. Coefficient of determination.

Following the determination of the optimal switchback time, the full model was run for all constituents using screen 1 and 2 length weighted, pre-rehab flow weighted, and post-rehab flow weighted values (Fig. S6, Fig. S8, Fig. S10). Coefficients of determination were calculated for each constituent over each model run (Fig. S7, Fig. S9, Fig. S11). Since the results were not significantly different, the pre-rehab flow-weighted model was chosen for inclusion in the article.

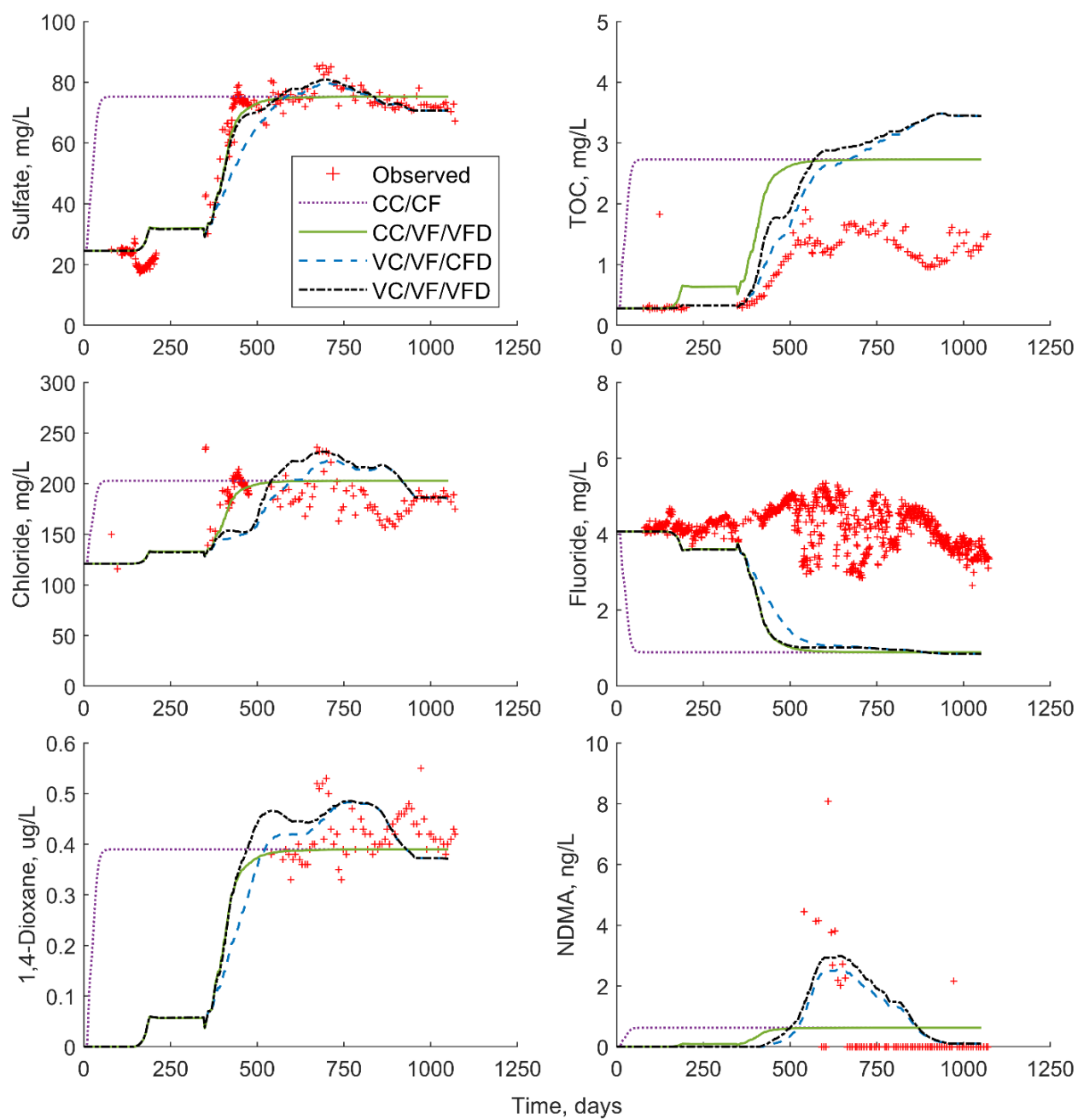


Fig. S6. Length-weighted model using screens 1 and 2.

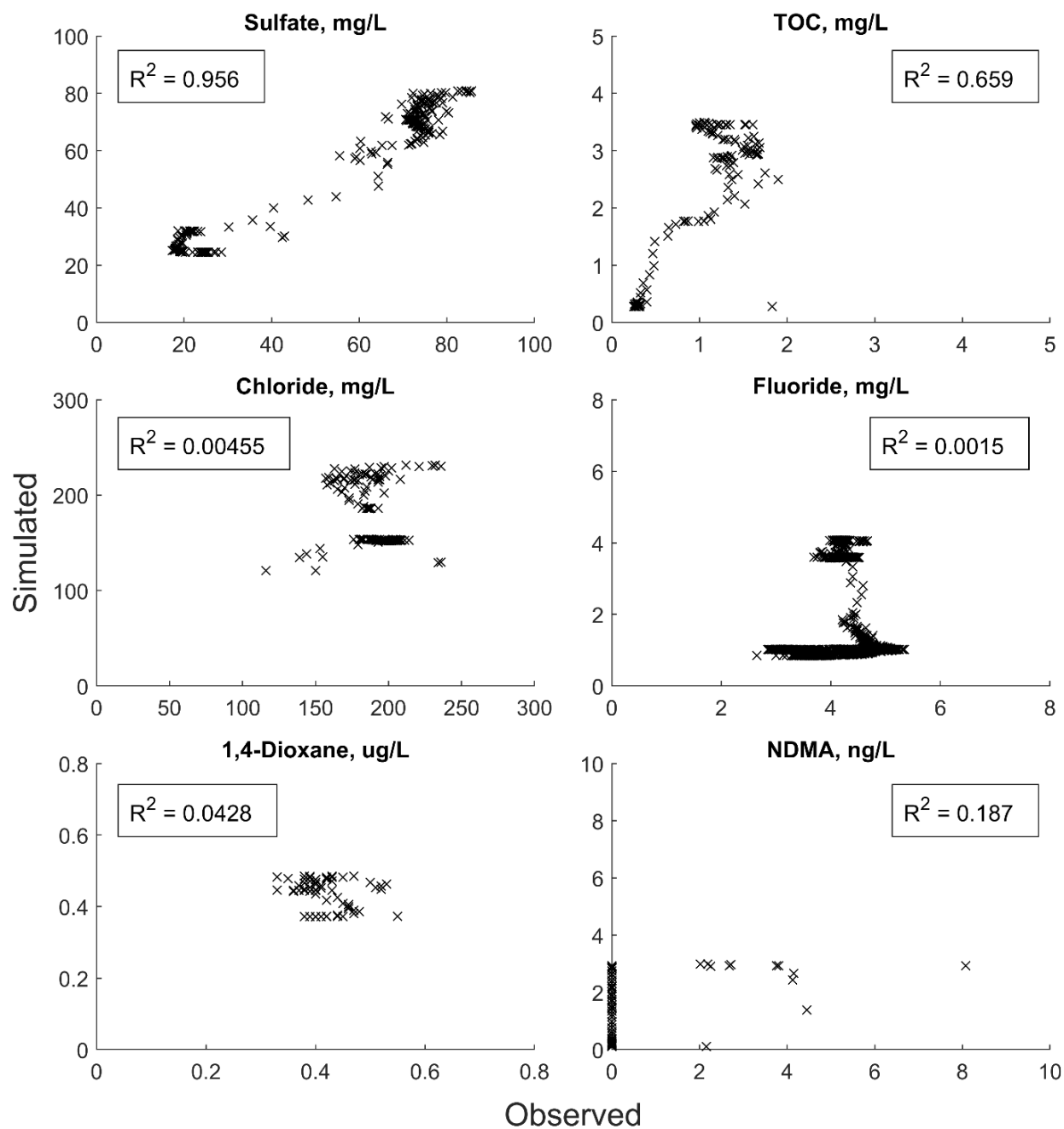


Fig. S7. Length-weighted model coefficients of determination.

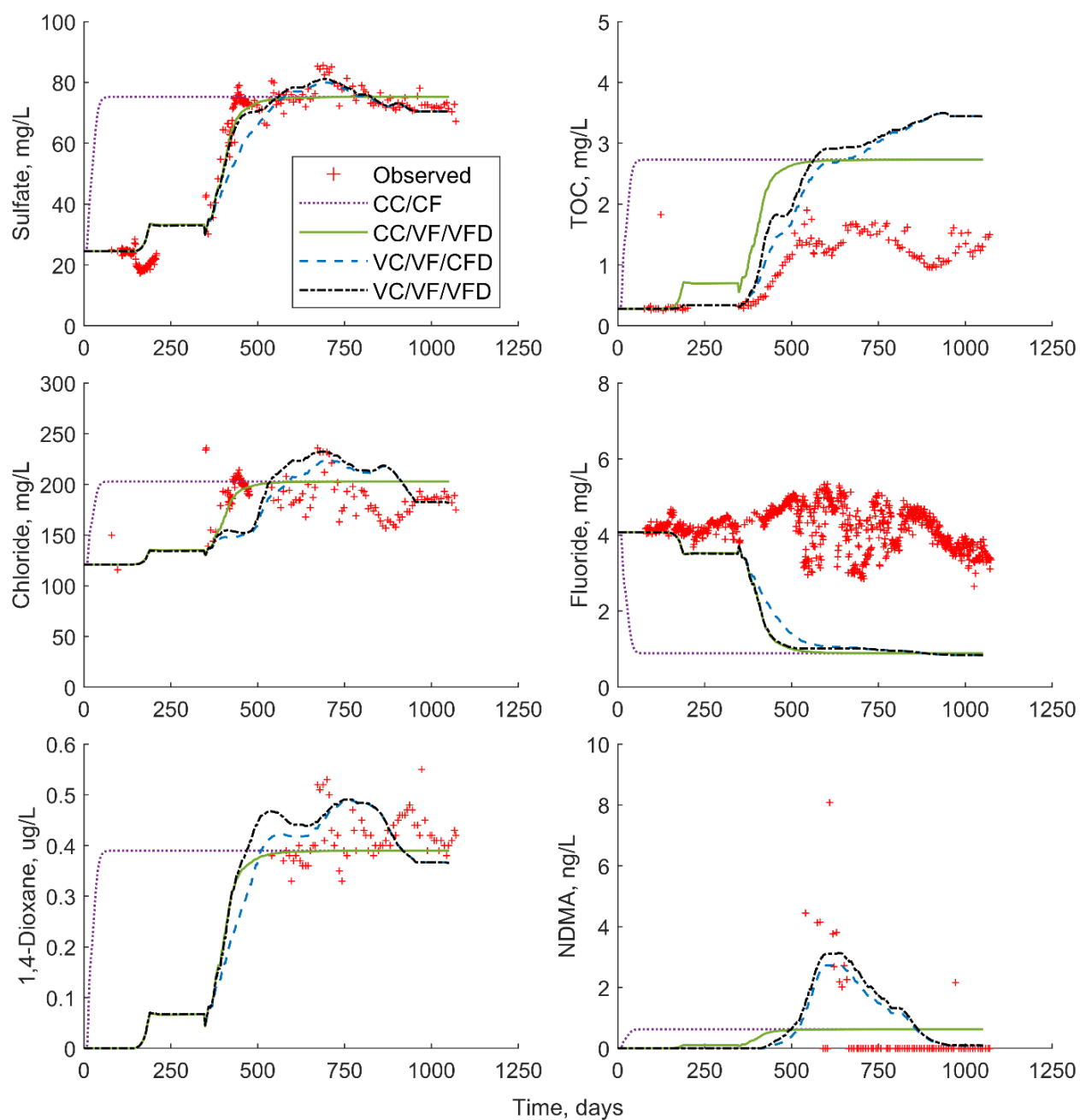


Fig. S8. Pre-rehab flow weighted model using screens 1 and 2.

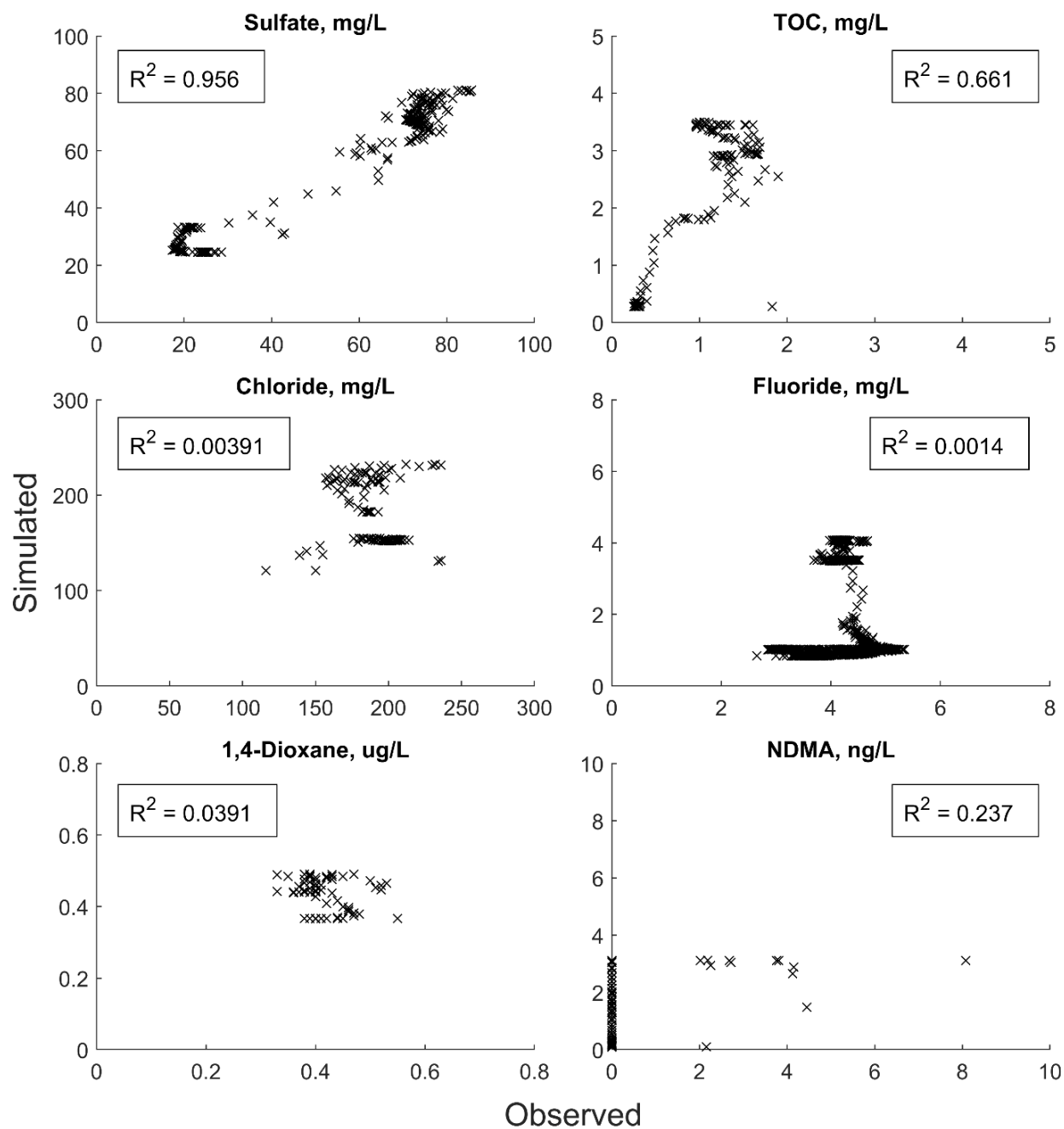


Fig. S9. Pre-rehab flow-weighted model coefficients of determination.

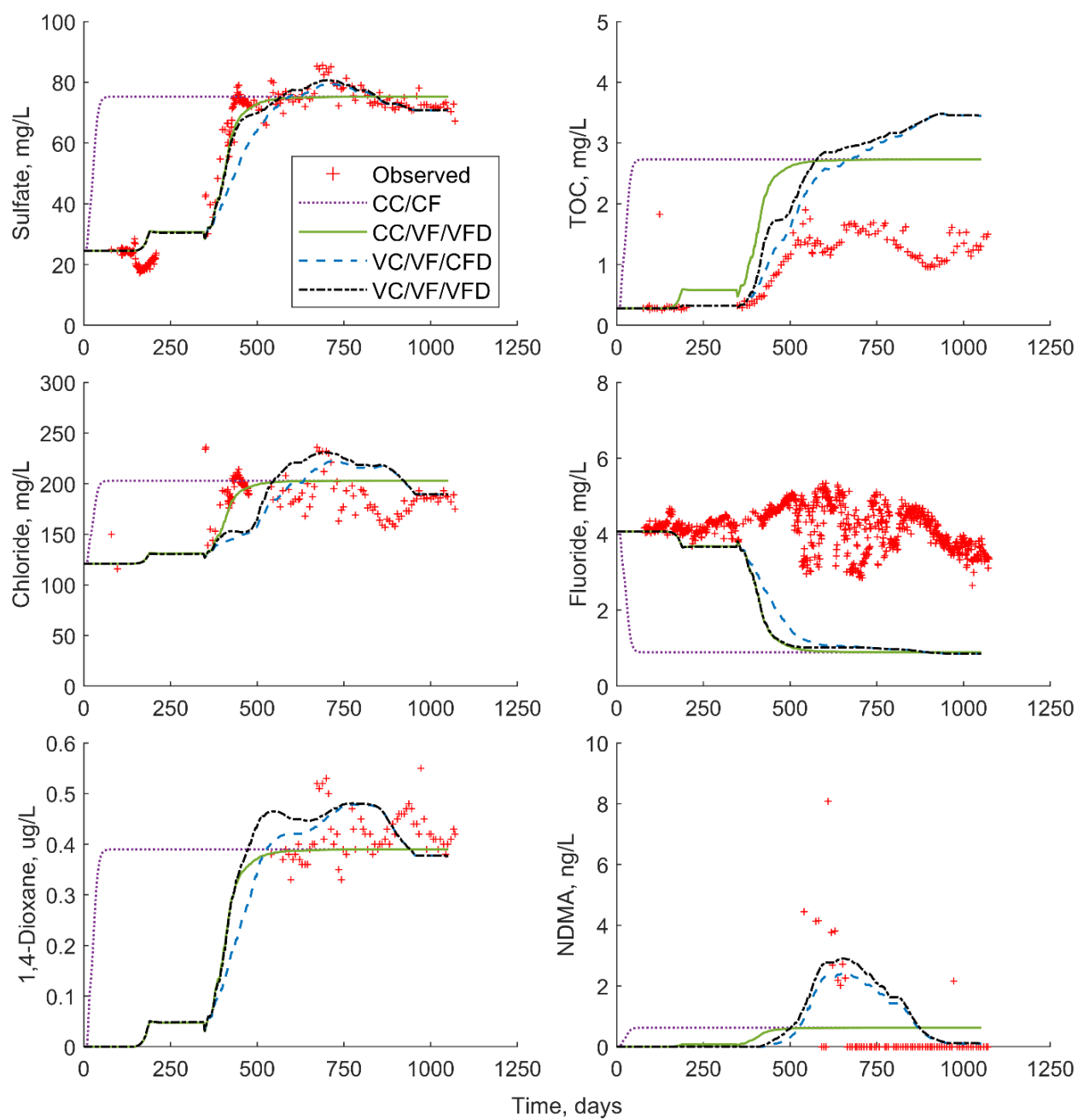


Fig. S10. Post-rehab flow weighted model using screens 1 and 2.

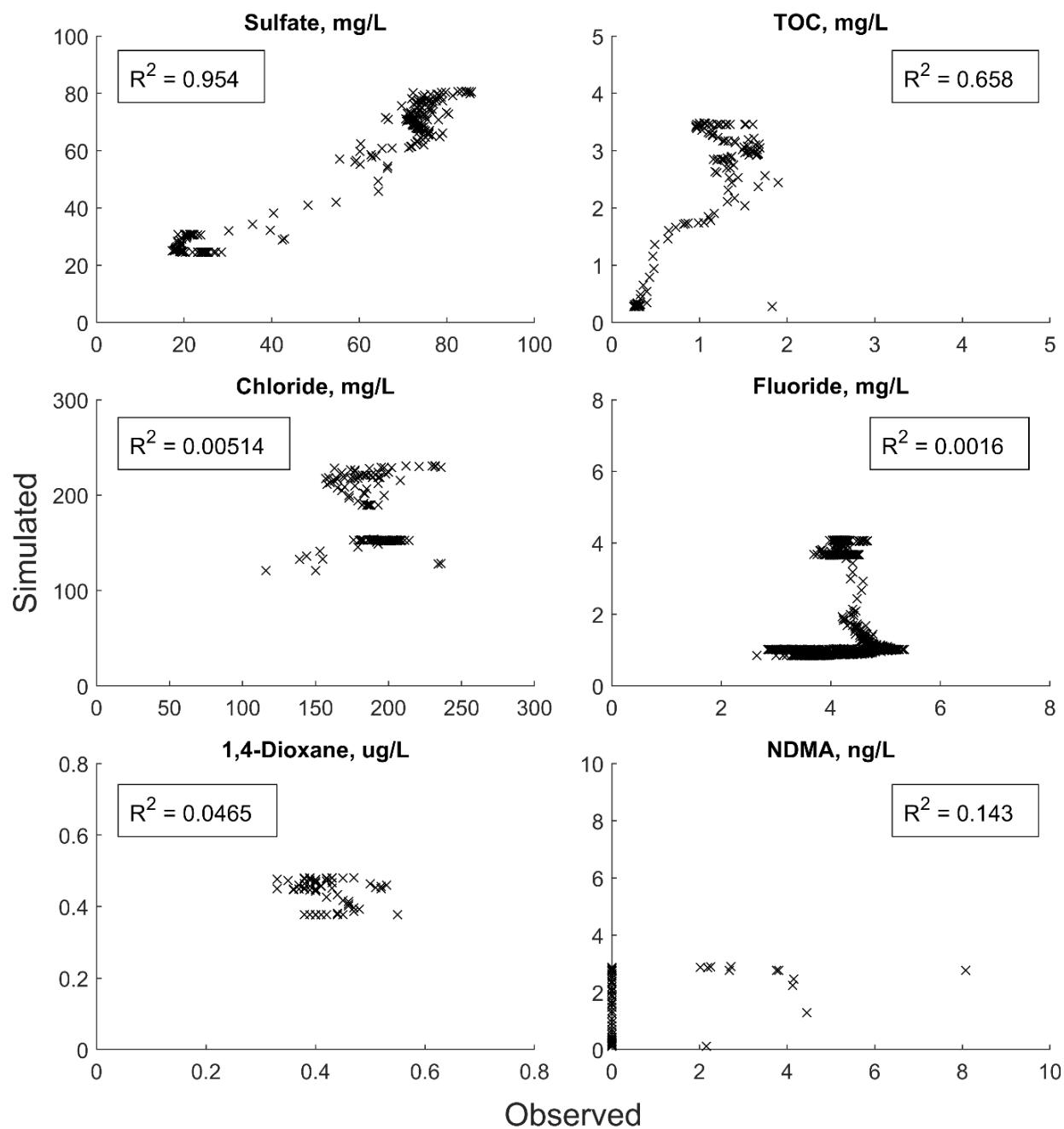


Fig. S11. Post-rehab flow-weighted model coefficients of determination.

Middle Potomac Aquifer

A similar approach was used for chloride breakthrough in MW-MPA. First, a breakthrough model for chloride was calculated for each individual screen (Fig. S2). These models assume that the MPA is solely measuring from that screen alone (only using the screen thickness and aquifer characteristics (n and α) from that screen, as determined from as-built diagrams and the original breakthrough work done in 2018).

Next, length- and flow-weighted averages were calculated using the breakthrough models developed for each screen. Two separate flow-weighted averages were calculated, one based on pre-rehabilitation flow measured during initial conductivity breakthrough (Bullard et al. 2019), the other based on post-rehabilitation flow distribution measured during in-situ flowmeter testing in May 2019. Details regarding pre- and post-rehab flow distribution and individual screen characteristics are documented in Table S3.

Table S3. Pre- and post-rehab flow distributions and aquifer characteristics for MW-MPA.

Screen	Pre-Rehab Flow Distribution (Conductivity Breakthrough)	Post Rehab Flow Distribution (In-Situ Flowmeter)	Porosity	Longitudinal Dispersivity (ft)
5	4.0%	6%	0.25	8
6	3.5%	3%	0.30	20
7	1.2%	2%	0.28	30
8	0.8%	2%	0.32	10
9	31%	11%	0.23	10

The results of the length- and flow-weighted model using all the screens confirms the same conclusion made in the UPA – that sample bias exists within the monitoring well and that the sample collected is not representative of all of the screens (Fig. S13). If the sample was representative of all of the screens, chloride from screen 9 would have caused the breakthrough to occur much faster. The process was repeated for combinations of the remainder of the screens – screen 5 and 6 (Fig. S14), screens 5-7 (Fig. S15), and screens 5-8 (Fig. S16). While these data are

103 preliminary, it seems to confirm the choice of a flow-weighted combination of screens 5-8. The
104 choice of pre- or post-rehab in this case is not important since the difference between the two is
105 insignificant to the results. Further conclusions should not be drawn without continued observation
106 and analysis.

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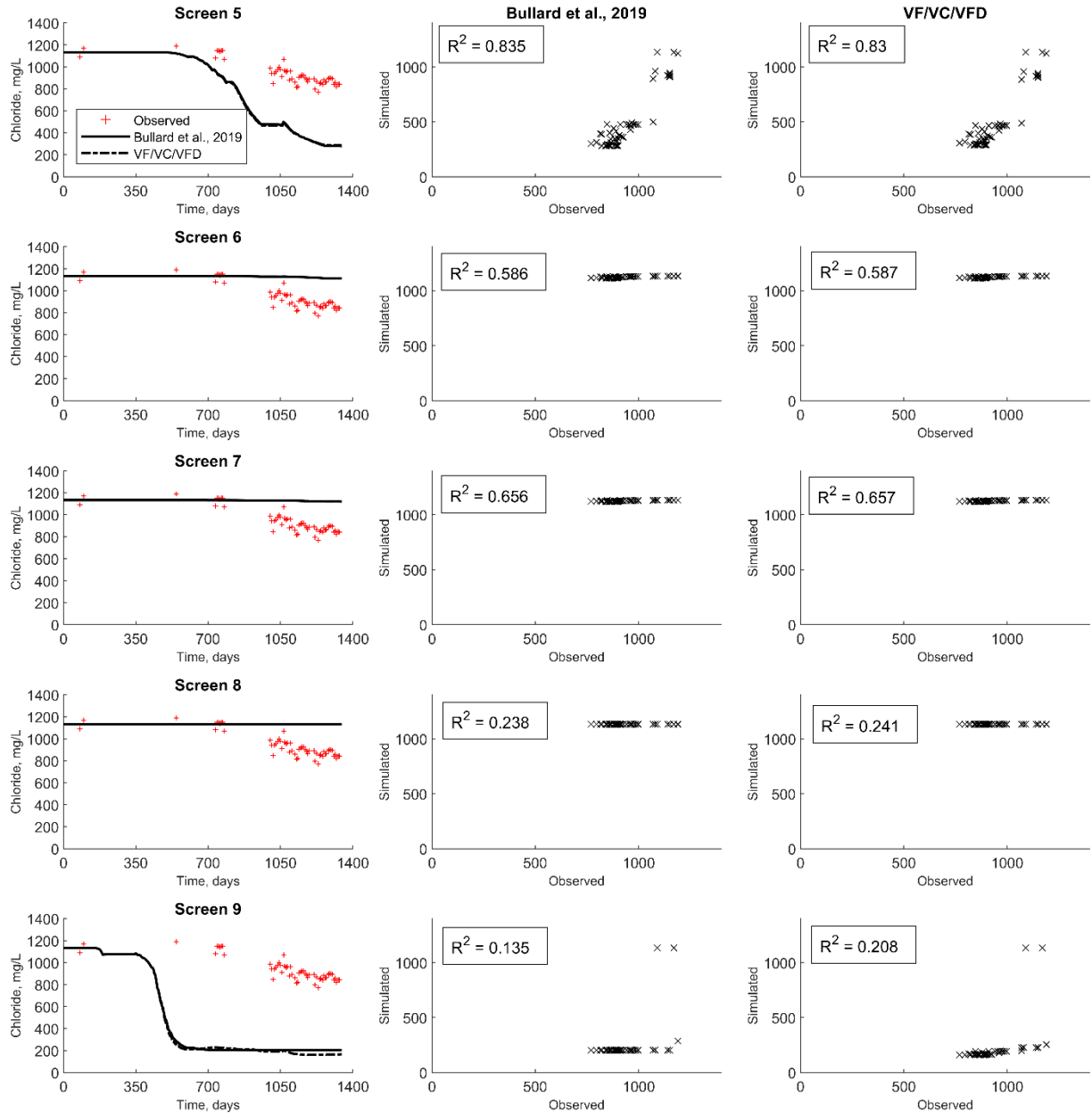


Fig. S12. Breakthrough calculated at each individual screen (5-9) using aquifer characteristics (n and α) determined in Bullard et al., 2019. Coefficients of determination are shown for the constant concentration model (labeled Bullard et al. 2019) and the variable concentration model (labeled VF/VC/VFD). Both models account for variable flow and variable flow distribution.

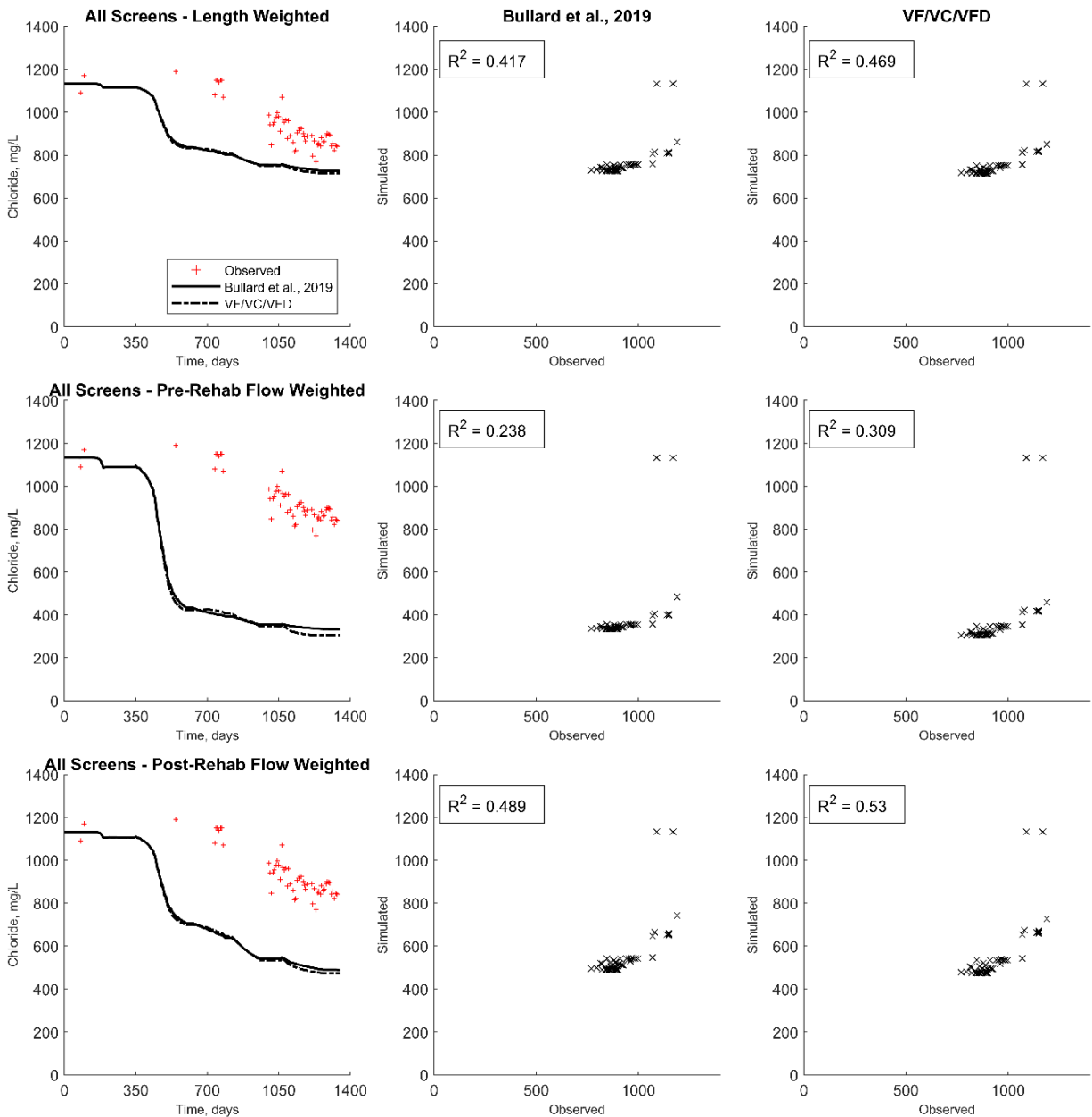


Fig. S13. Flow- and length-weighted models using screens 5-9. Coefficients of determination are shown for the constant concentration model (labeled Bullard et al. 2019) and the variable concentration model (labeled VF/VC/VFD). Both models account for variable flow and variable flow distribution.

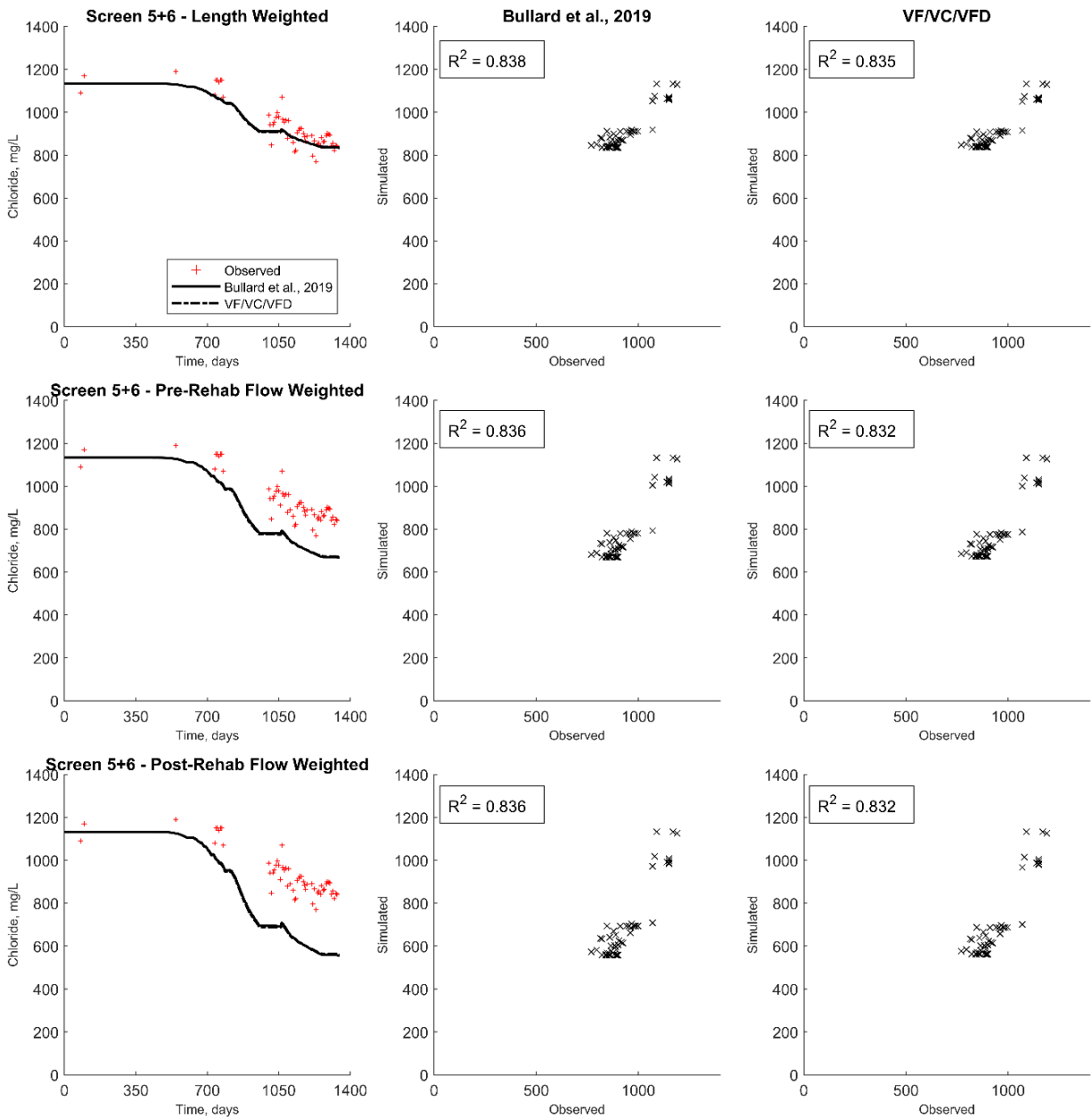


Fig. S14. Flow- and length-weighted models using screens 5-6. Coefficients of determination are shown for the constant concentration model (labeled Bullard et al. 2019) and the variable concentration model (labeled VF/VC/VFD). Both models account for variable flow and variable flow distribution.

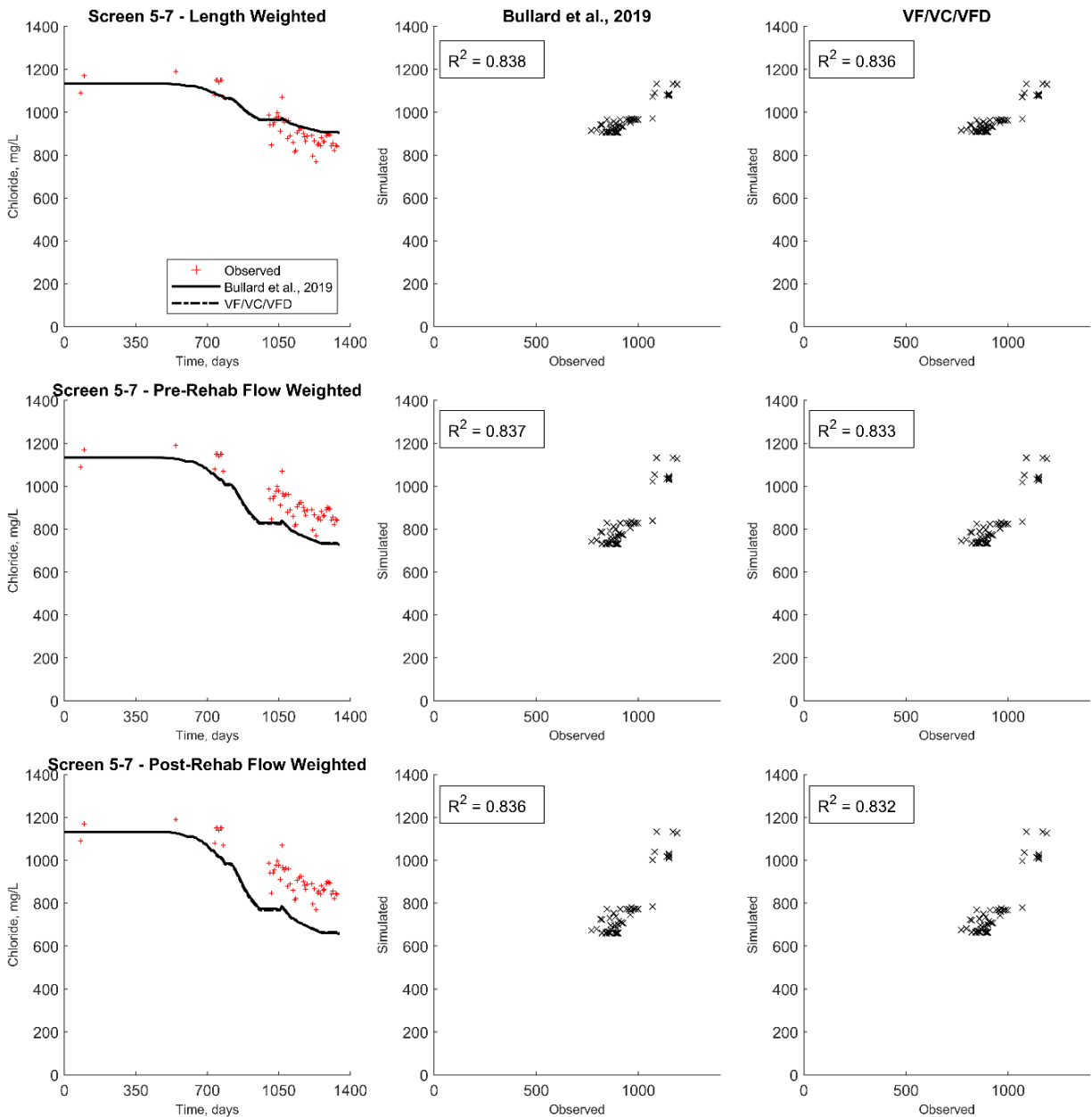


Fig. S15. Flow- and length-weighted models using screens 5-7. Coefficients of determination are shown for the constant concentration model (labeled Bullard et al. 2019) and the variable concentration model (labeled VF/VC/VFD). Both models account for variable flow and variable flow distribution.

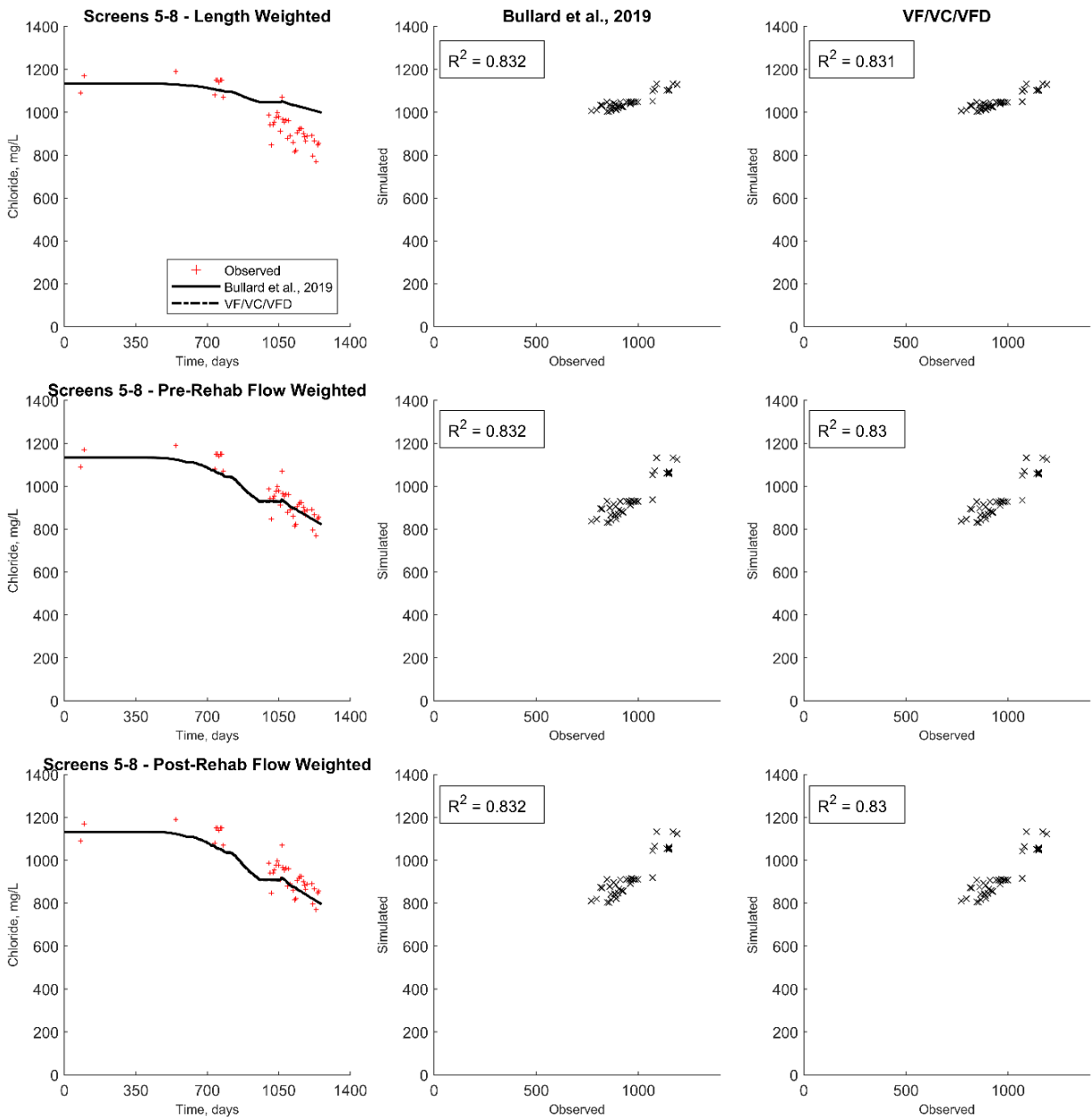


Fig. S16. Flow- and length-weighted models using screens 5-8. Coefficients of determination are shown for the constant concentration model (labeled Bullard et al. 2019) and the variable concentration model (labeled VF/VC/VFD). Both models account for variable flow and variable flow distribution.

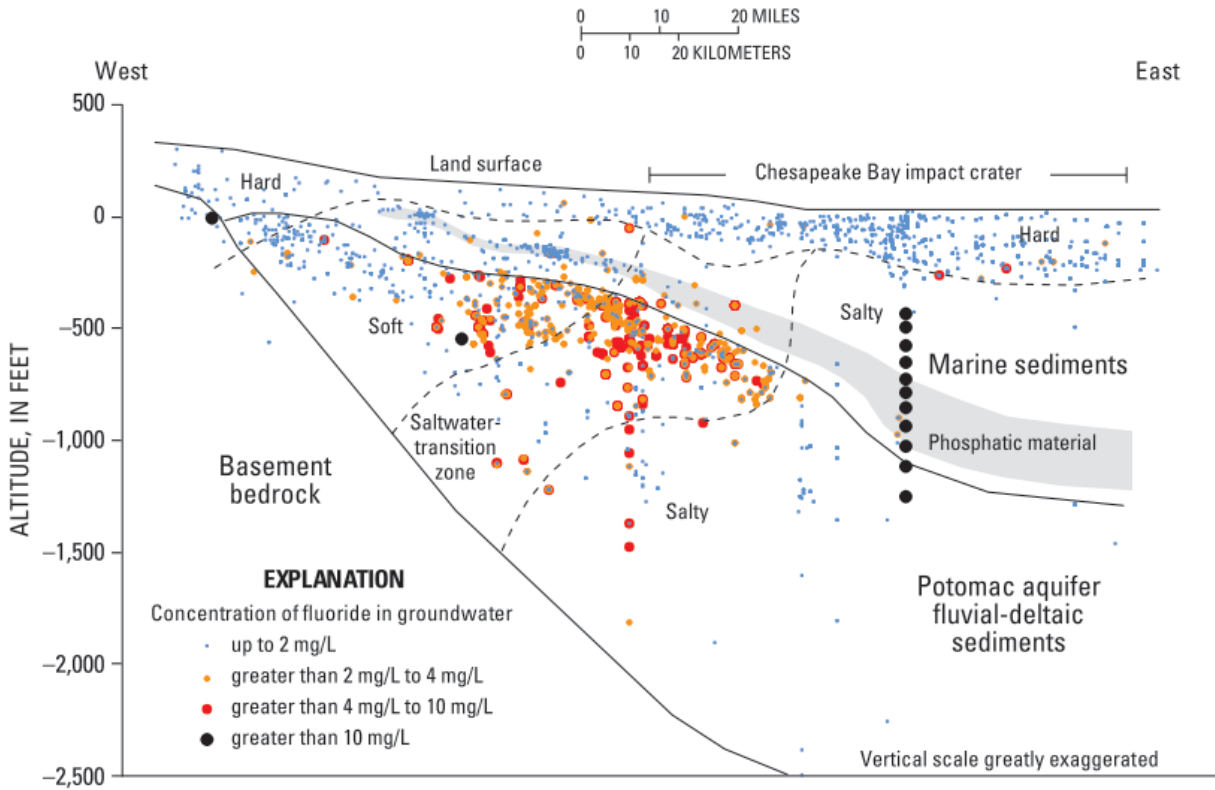


Fig. S17. Generalized fluoride distribution in the Virginia Coastal Plain (McFarland 2010).

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