

Modeling seasonal redox dynamics and the corresponding fate of the pharmaceutical residue phenazone during artificial recharge of groundwater

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This part of the Online Supporting Information contains 8 pages (8 Figures)

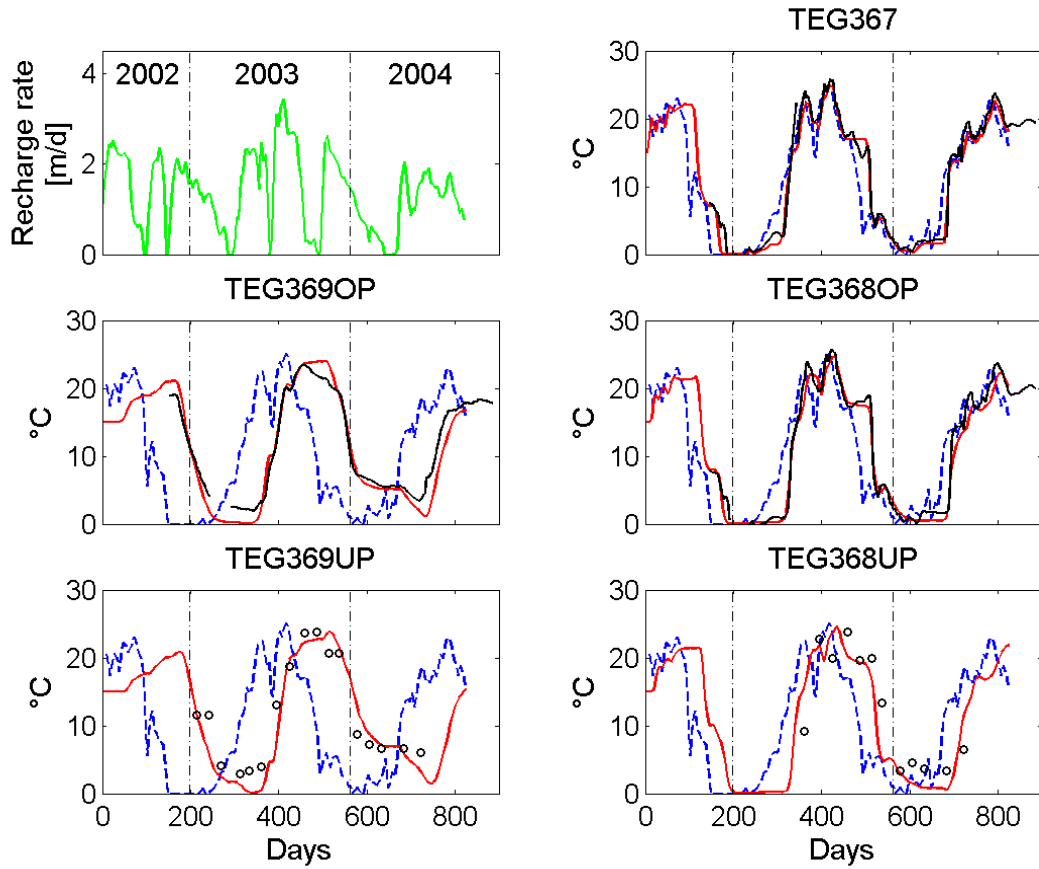


Figure S11. Times series of recharge rate for Pond 3 (green line, data kindly provided by BWB) and calibration results of the non-reactive transport model for the monitoring wells TEG367, TEG368OP/UP and TEG369OP/UP. Dashed blue lines represent the measured pond water temperature. Thin black lines and circles represent the observed temperature with data loggers and (monthly) manual measurements, respectively. Thick red lines indicate the simulated temperature. Note that the monitoring wells TEG365 and TEG366 were not considered for the calibration of the nonreactive model because the measured temperatures were not clearly distinguishable from the pond water temperatures due to the short travel times to those wells.

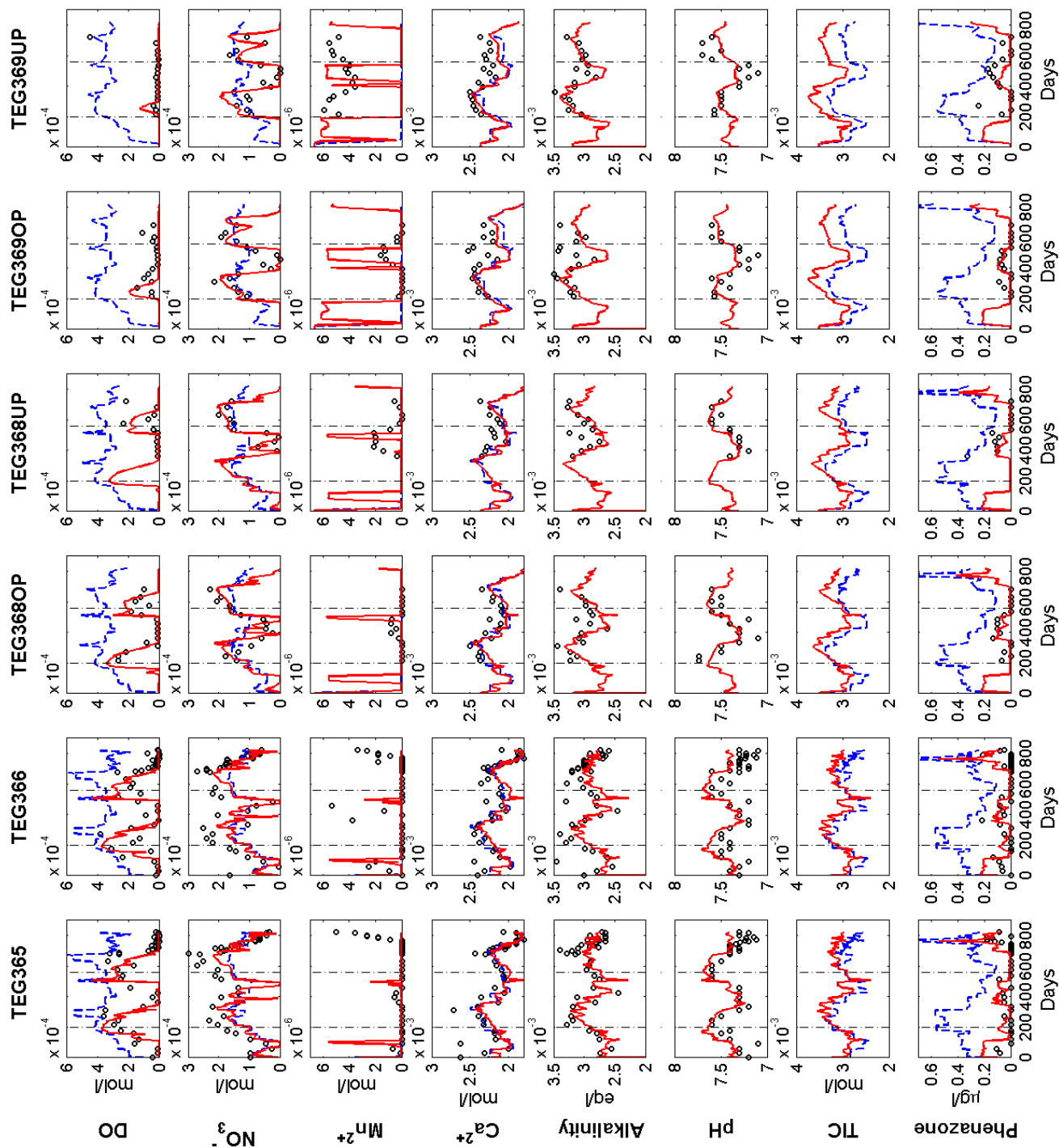


Figure SI2. Simulation results for dissolved oxygen (DO), nitrate, Mn^{2+} , calcium, alkalinity, pH, TIC and phenazone at the monitoring wells TEG365, TEG355, TEG368OP/UP and TEG369OP/UP. Black circles represent the observed data and red lines represent the final calibrated reactive transport simulation. The dashed blue lines represent the nonreactive simulation, in which all biogeochemical reactions were excluded. Note that observed phenazone concentrations $<0.05 \mu\text{g L}^{-1}$ (LOQ) were set to 0.

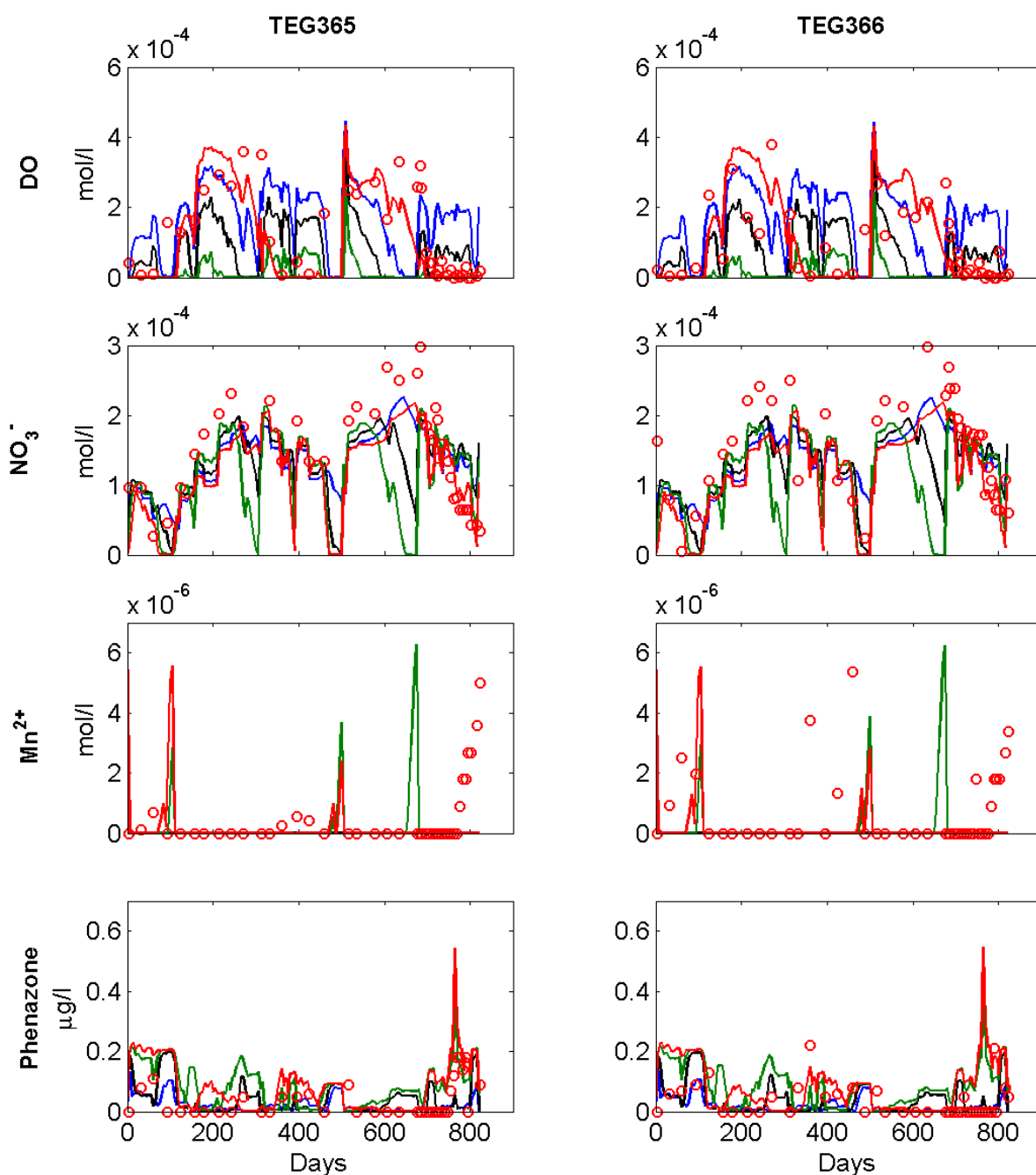


Figure SI3. Temperature dependence of dissolved oxygen (DO), nitrate, Mn^{2+} and phenazone at the monitoring wells TEG365, TEG366. The blue, black and green lines represent simulations with constant temperatures of 5°C, 10°C and 15°C, respectively. The red lines represent the final calibrated reactive transport simulation (variable temperature). Red circles represent the observed data. Note, measured phenazone concentrations $<0.05 \mu\text{g L}^{-1}$ (LOQ) were set to 0.

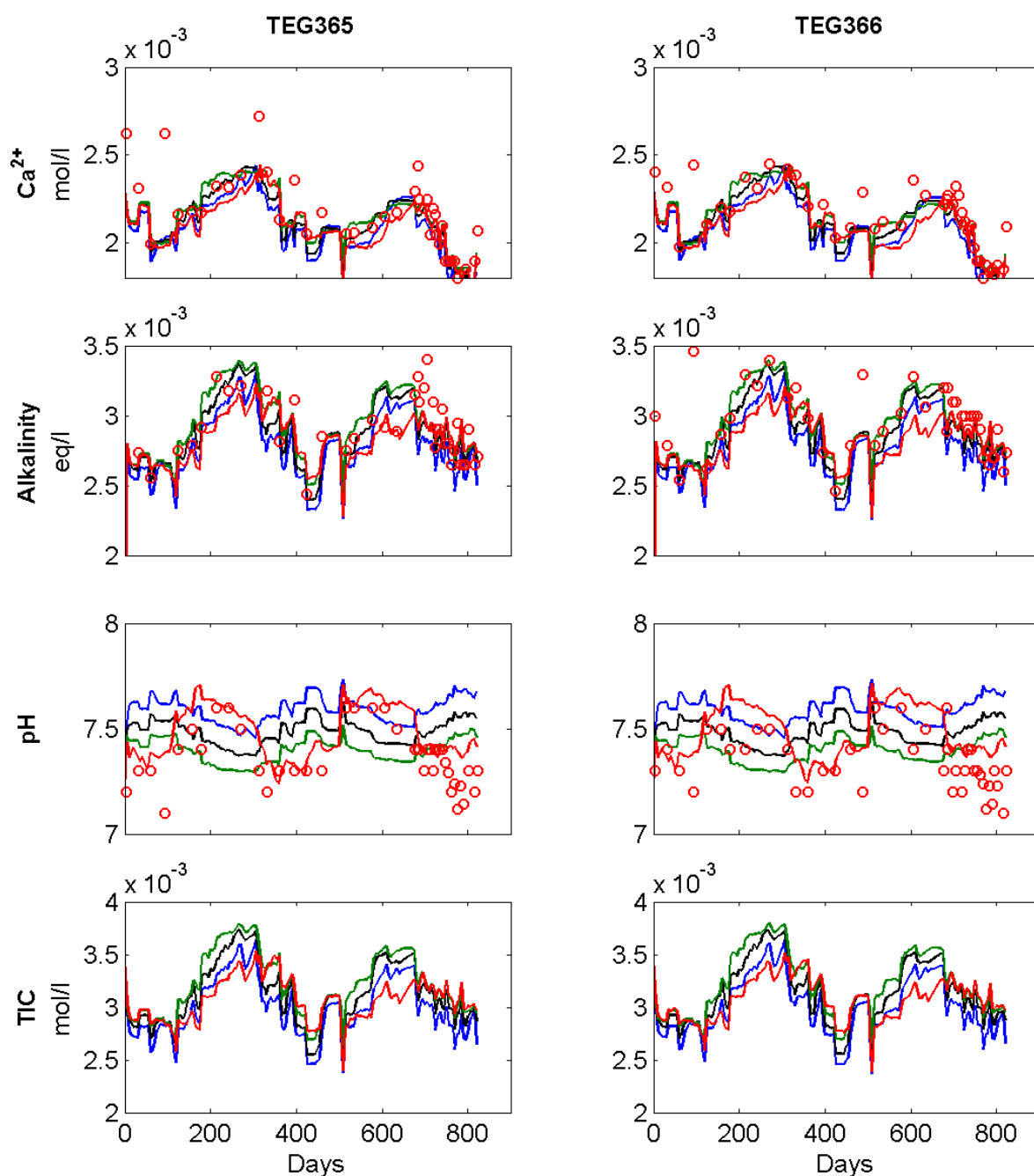


Figure SI4. Temperature dependence of calcium, alkalinity, pH and TIC at the monitoring wells TEG365, TEG366. The blue, black and green lines represent simulations with constant temperatures of 5°C, 10°C and 15°C, respectively. The red lines represent the final calibrated reactive transport simulation (variable temperature). Red circles represent the observed data.

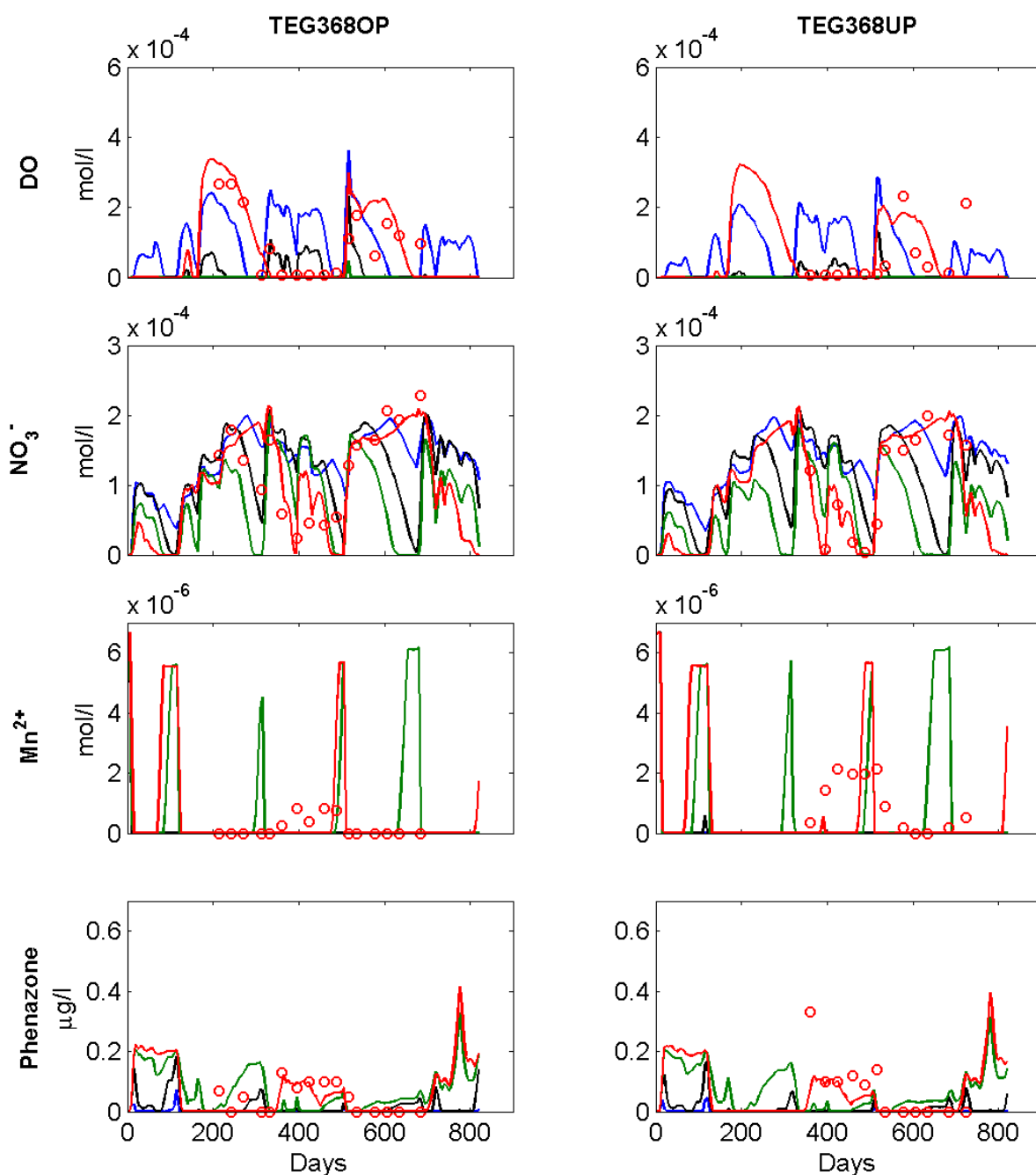


Figure SI5. Temperature dependence of dissolved oxygen (DO), nitrate, Mn^{2+} and phenazone at the monitoring wells TEG368OP and TEG368UP. The blue, black and green lines represent simulations with constant temperatures of 5°C, 10°C and 15°C, respectively. The red lines represent the final calibrated reactive transport simulation (variable temperature). Red circles represent the observed data. Note, measured phenazone concentrations $<0.05 \mu\text{g L}^{-1}$ (LOQ) were set to 0.

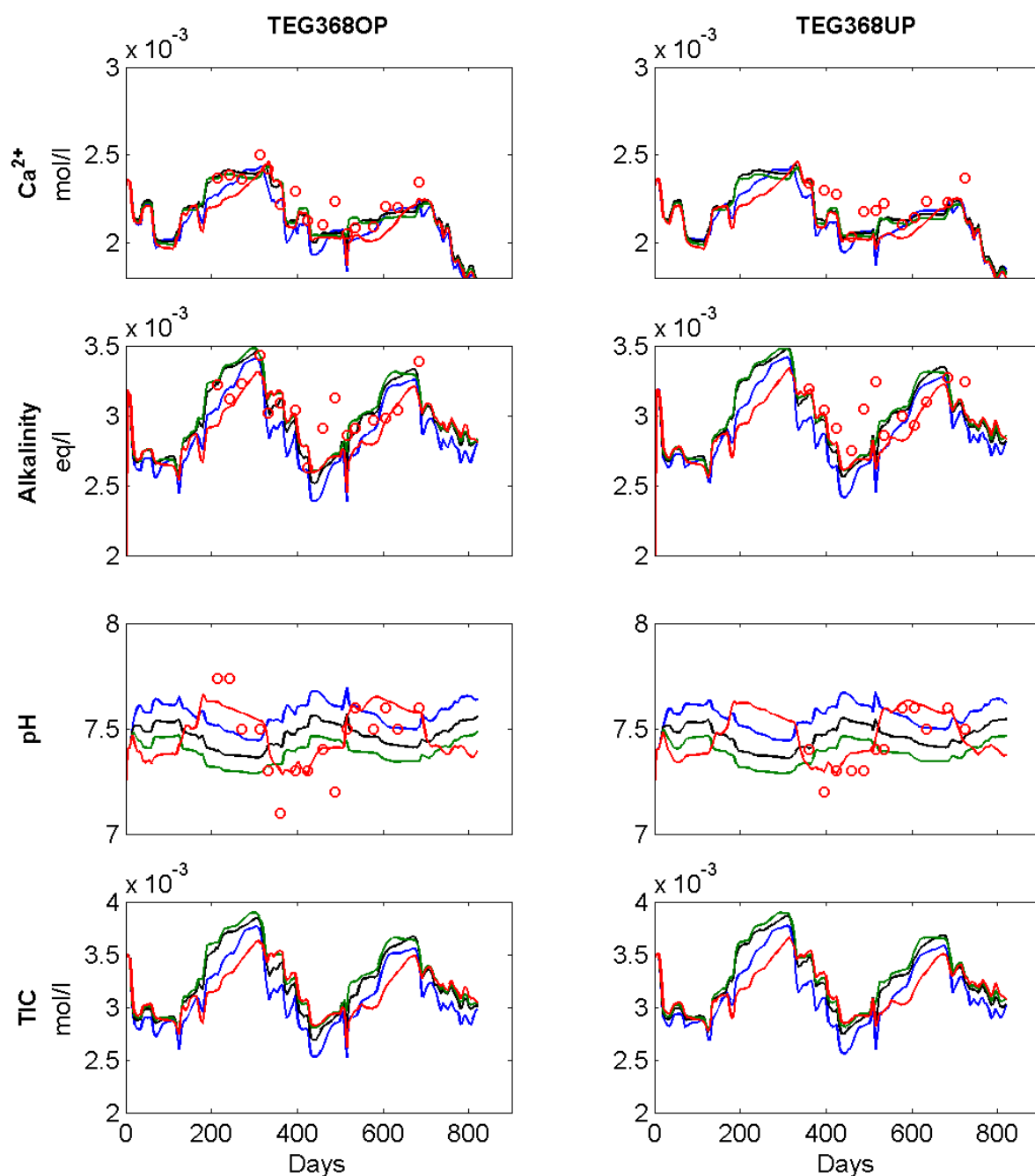


Figure SI6. Temperature dependence of calcium, alkalinity, pH and TIC at the monitoring wells TEG368OP and TEG368UP. The blue, black and green lines represent simulations with constant temperatures of 5°C, 10°C and 15°C, respectively. The red lines represent the final calibrated reactive transport simulation (variable temperature). Red circles represent the observed data.

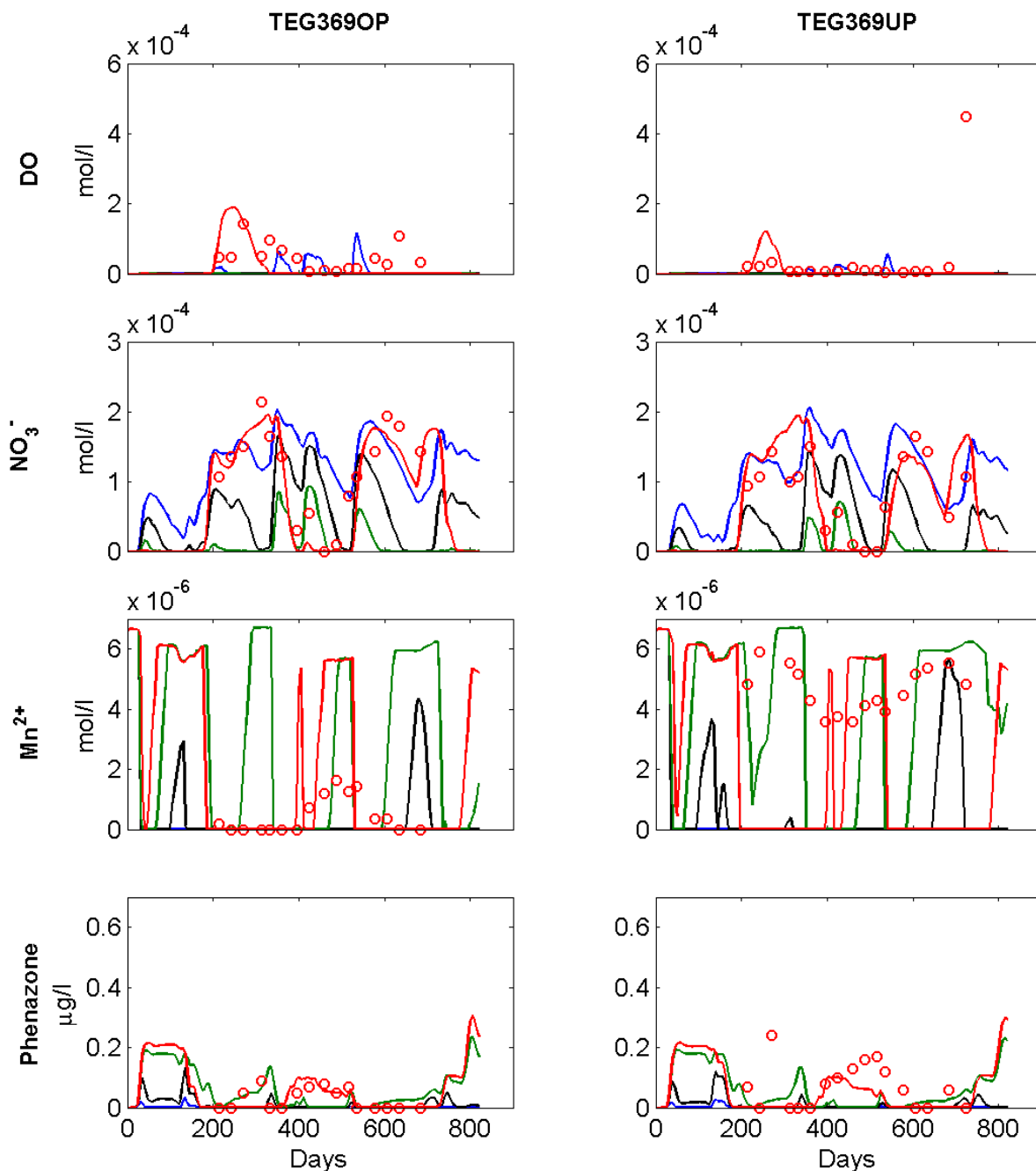


Figure SI7. Temperature dependence of dissolved oxygen (DO), nitrate, Mn^{2+} and phenazone at the monitoring wells TEG369OP and TEG369UP. The blue, black and green lines represent simulations with constant temperatures of 5°C, 10°C and 15°C, respectively. The red lines represent the final calibrated reactive transport simulation (variable temperature). Red circles represent the observed data. Note, measured phenazone concentrations $<0.05 \mu\text{g L}^{-1}$ (LOQ) were set to 0.

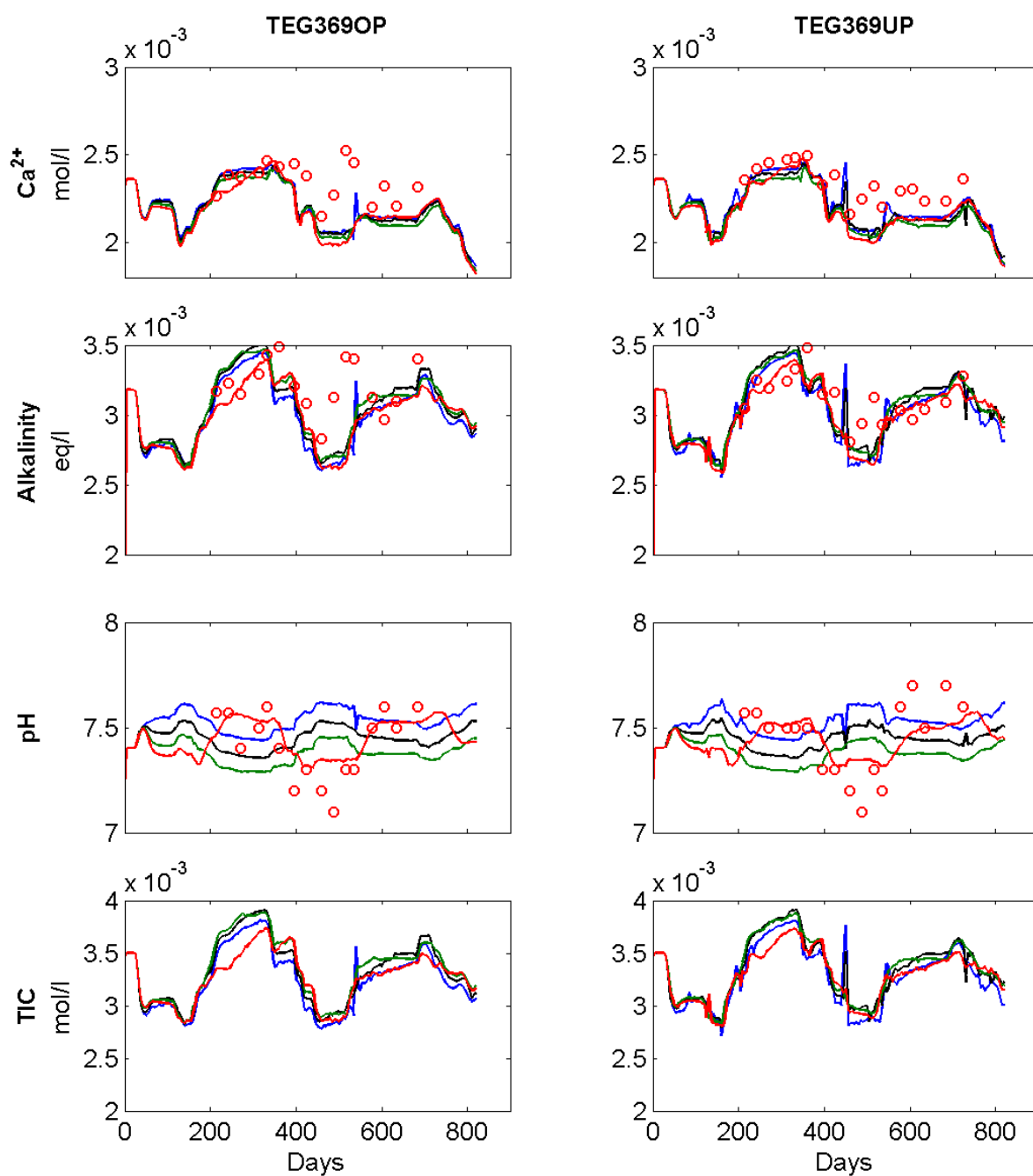


Figure SI8. Temperature dependence of calcium, alkalinity, pH and TIC at the monitoring wells TEG369OP and TEG369UP. The blue, black and green lines represent simulations with constant temperatures of 5°C, 10°C and 15°C, respectively. The red lines represent the final calibrated reactive transport simulation (variable temperature). Red circles represent the observed data.

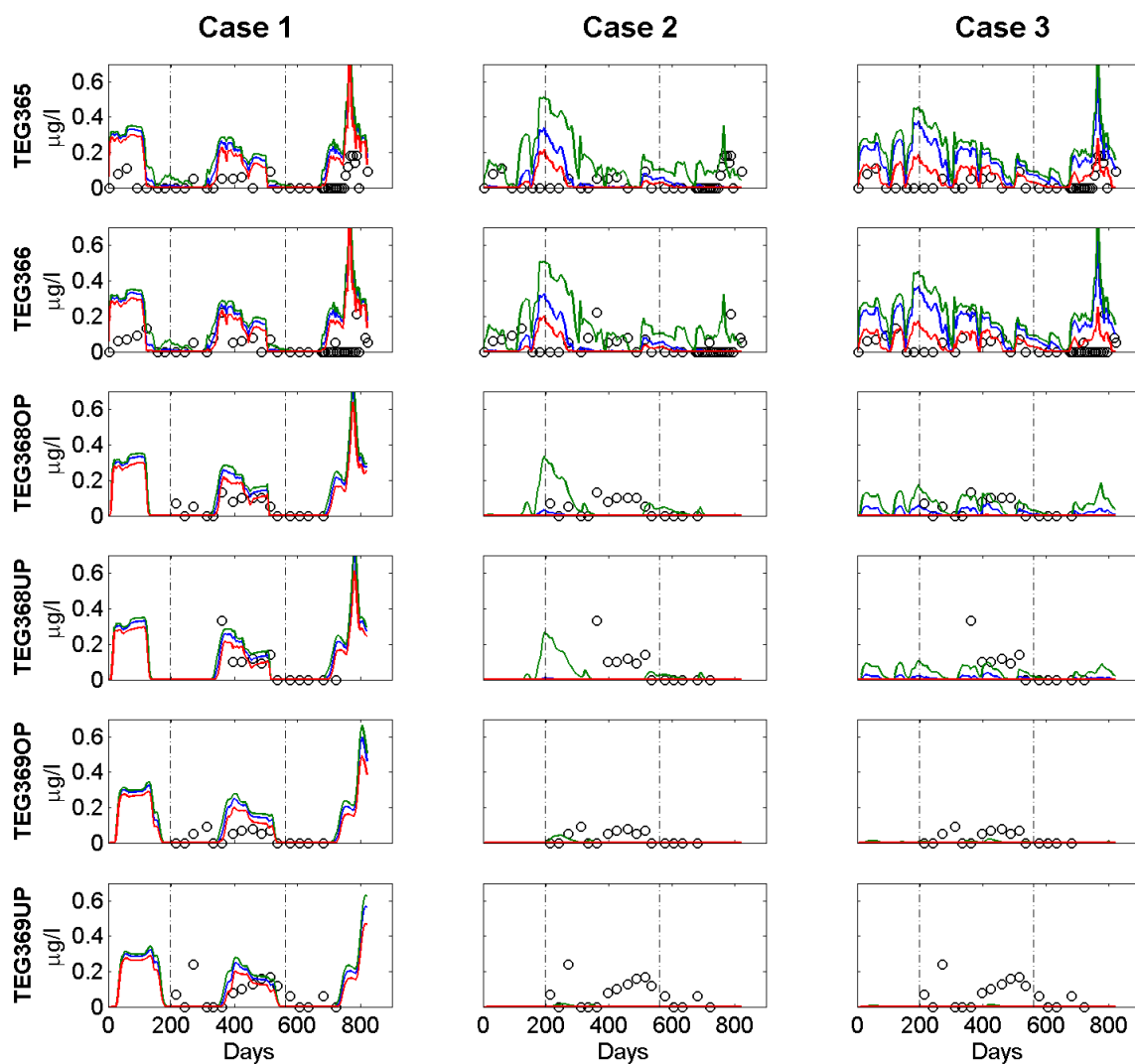


Figure SI9. Simulated phenazone concentrations for temperature decoupled (*Case 1*), redox decoupled (*Case 2*) and using a simple first-order (*Case 3*) degradation rate. Black circles represent the observed data. **Case 1:** red, blue and green lines represent a $r_{\text{phena_max}}$ of 12.0 d^{-1} , 6.0 d^{-1} and 3.0 d^{-1} , respectively; **Case 2:** red, blue and green lines represent a $r_{\text{phena_max}}$ of 3.0 d^{-1} , 1.5 d^{-1} and 0.25 d^{-1} , respectively; **Case 3:** red, blue and green lines represent a $r_{\text{phena_max}}$ of 0.75 d^{-1} , 0.25 d^{-1} and 0.125 d^{-1} , respectively; Note, measured phenazone concentrations $< 0.05 \mu\text{g L}^{-1}$ (LOQ) were set to 0.