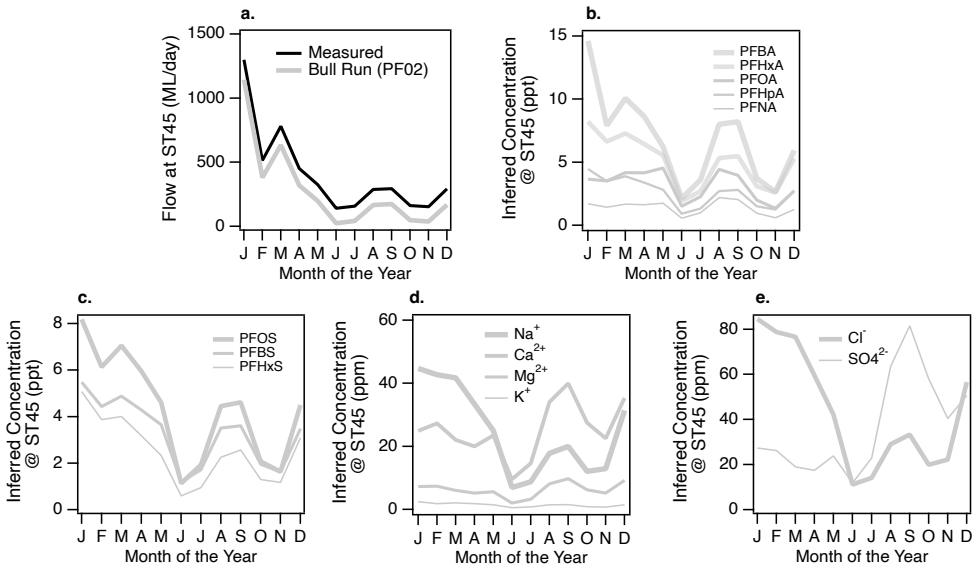
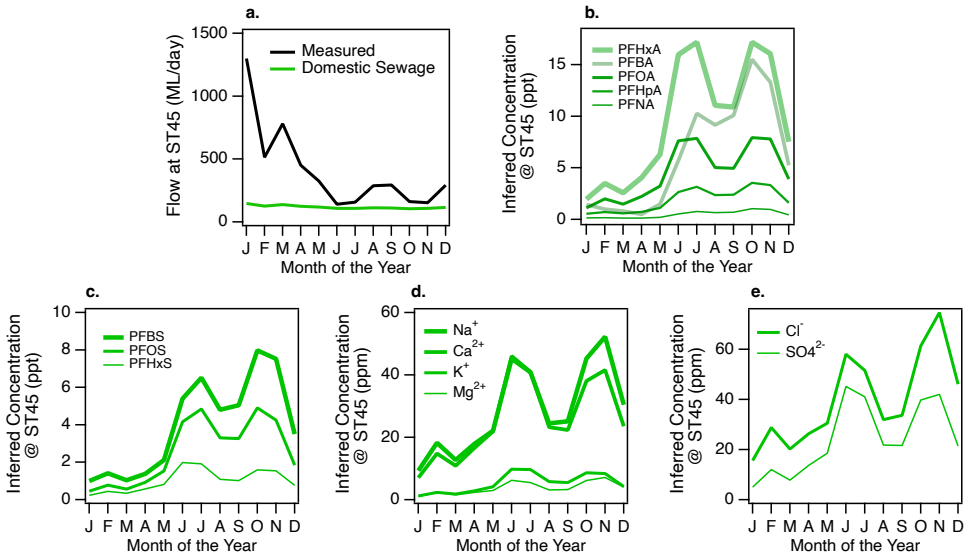
Supplementary Information for, "Mass balance and a system-scale experiment reveal PFAS sources in a One Water system"

This file includes:

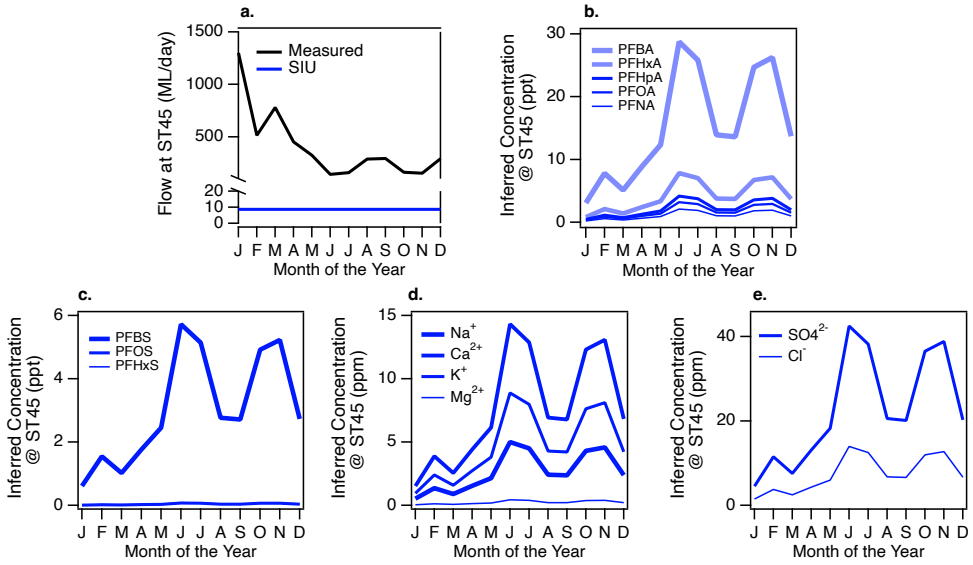
Supplementary Figures



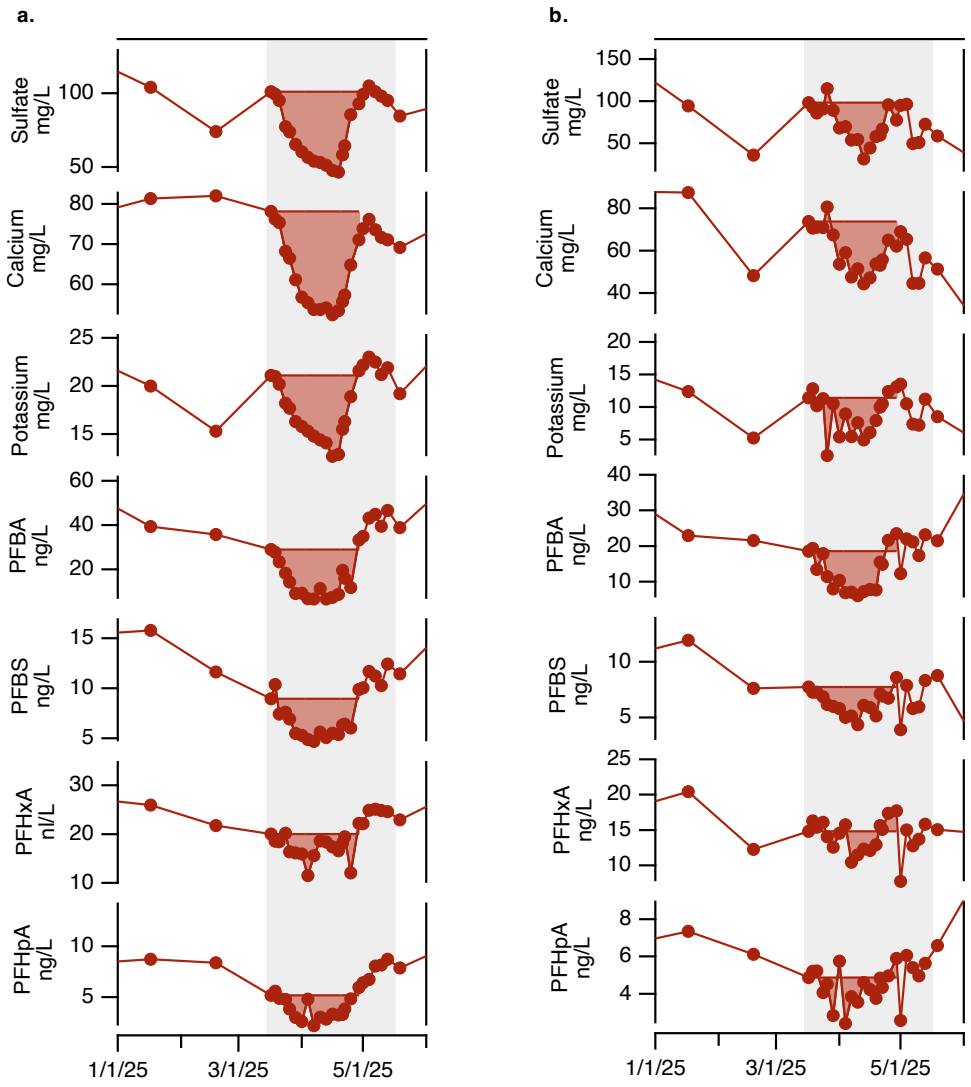
Supplementary Fig. 1 Seasonal flow and water quality contributions from the Bull Run watershed (PF02) to ST45. a, Monthly-average discharge at ST45 (black) and the corresponding contribution from Bull Run inflow (gray). textbfb-c, Inferred Bull Run contributions to concentrations of carboxylated PFAS (PFBA, PFHxA, PFOA, PFHpA, PFNA) and sulfonated PFAS (PFOS, PFBS, PFHxS) at ST45. textbfd-e, Inferred Bull Run contributions to major-ion concentrations (Na^+, Ca^{2+}, Mg^{2+}, K^+, Cl^-, SO_4^{2-}). Across analytes, Bull Run contributions exhibit a pronounced bimodal seasonal structure with dominant winter maxima and secondary late-summer peaks, broadly tracking seasonal variation in watershed inflow and indicating hydrologically mediated mobilization of PFAS and major ions.



Supplementary Fig. 2 Seasonal flow and water quality contributions from domestic sewage to ST45. a, Monthly-average discharge at ST45 (black) and the corresponding contribution from domestic sewage (green). **b–c,** Inferred domestic sewage contributions to concentrations of carboxylated PFAS (PFHxA, PFBA, PFOA, PFHpA, PFNA) and sulfonated PFAS (PFBS, PFOS, PFHxS) at ST45. **d–e,** Inferred domestic sewage contributions to major-ion concentrations (Na^+, Ca^{2+}, K^+, Mg^{2+}, Cl^-, SO_4^{2-}). Across analytes, domestic sewage contributions exhibit a bimodal seasonal structure that is broadly out of phase with Bull Run inflow (see Fig. S1), with minimal wintertime influence and pronounced maxima in early summer and late fall, consistent with seasonal variation in dilution and the fractional contribution of reclaimed water to total inflow.



Supplementary Fig. 3 Seasonal flow and water quality contributions from the significant industrial user (SIU) to ST45. a, Monthly-average discharge at ST45 (black) and the corresponding contribution from SIU effluent (blue). **b–c,** Inferred SIU contributions to concentrations of carboxylated PFAS (PFBA, PFHxA, PFHpA, PFOA, PFNA) and sulfonated PFAS (PFBS, PFOS, PFHxS) at ST45. **d–e,** Inferred SIU contributions to major-ion concentrations (Na^+, Ca^{2+}, K^+, Mg^{2+}, SO_4^{2-}, Cl^-). Across analytes, SIU contributions exhibit low wintertime influence followed by pronounced early-summer and late-fall maxima, reflecting approximately constant SIU discharge combined with seasonal variation in dilution at ST45. Short-chain carboxylated PFAS—most notably PFBA—dominate the SIU signal and reach substantially higher concentrations than contributions from other sources during peak periods.



Supplementary Fig. 4 Concentration measurements at the reclaimed water stream (PF01, panel a) and downstream of the confluence (ST45, panel b) for PFAS and major ions that load significantly on principal component 1 (see red arrows in Fig. 5a, main text).