Supporting Information

Analysis of the Bromate-Sulfite-Ferrocyanide pH Oscillator Using the Particle Filter

-Toward the Automated Modeling of Complex Chemical Systems-

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Table S1. Optimized rate constants in the extended RKH model.[a]

| Fitting method	$k_3 / M^{-1}s^{-1}$	$k_4 / M^{-1}s^{-1}$	k_5 / Ms^{-1}	k'_5 / M
Single-curve fitting[b]	9.8×10^{-2}	22	2.9×10^{-5}	8.0×10^{-4}
Two-curve fitting[c]	1.0×10^{-1}	20	2.7×10^{-5}	7.3×10^{-4}

[a] Fixed parameters: $[BrO_3^-]_0$ =75 mM, $[Fe(CN)_6^{4-}]_0$ = 15 mM, $[H^+]_0$ = 15 mM and temperature = 40.0°C.

[b] Control parameters of the reference data: $[SO_3^{2-}]_0$ = 90 mM and k_0 = 0.05 min^{-1}.

[c] Control parameters of the reference data: $[SO_3^{2-}]_0$ = 90 mM and k_0 = 0.05 min^{-1}, and $[SO_3^{2-}]_0$ = 80 mM and k_0 = 0.1 min^{-1}, respectively.
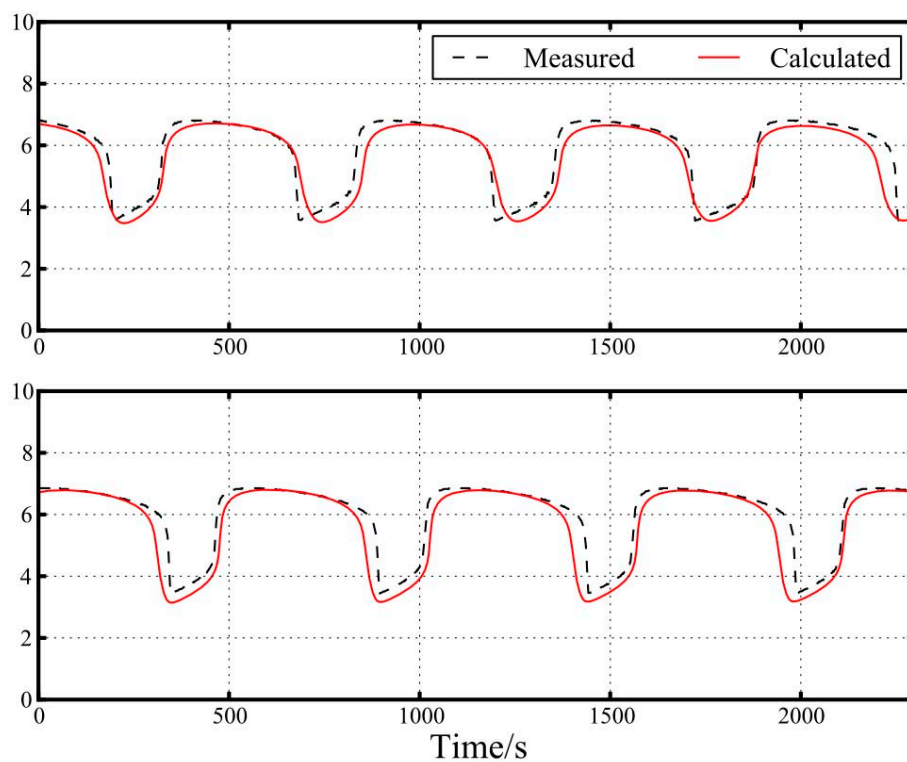
Figure S1. Best-fit oscillatory pH curves in the extended RKH model (red solid lines) obtained by the simultaneous curve fitting of the two experimental data (black dashed lines). See Table S1 for the optimized rate constants. Fixed parameters: $[BrO_3^-]_0 =75$ mM, $[Fe(CN)_6^{4-}]_0 = 15$ mM, $[H^+]_0 = 15$ mM and temperature $= 40.0°C$. Control parameters: (a) $[SO_3^{2-}]_0 = 90$ mM and $k_0 = 0.05$ min^{-1}, (b) $[SO_3^{2-}]_0 = 80$ mM and $k_0 = 0.1$ min^{-1}.
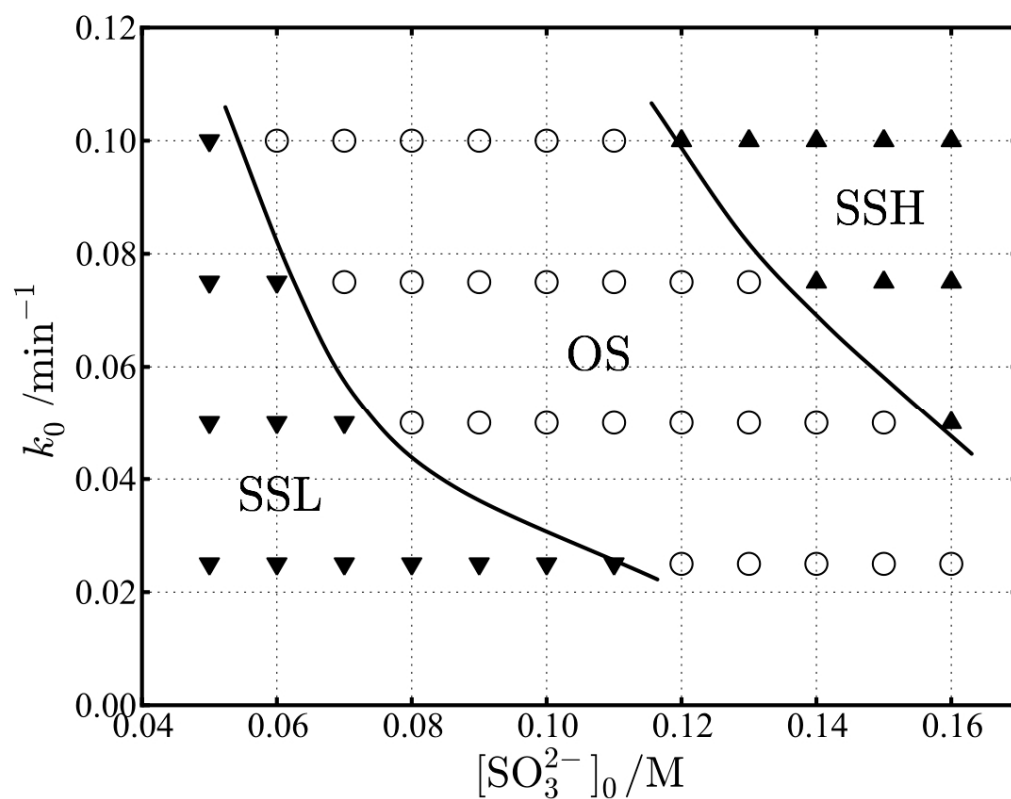
Figure S2. State diagram in the extended RKH model calculated with the rate constants obtained by the two-curve fitting method (Table S1). Fixed parameters: $[BrO_3^-]_0 = 75$ mM, $[Fe(CN)_6^{4-}]_0 = 15$ mM, $[H^+]_0 = 15$ mM and temperature $= 40.0°C$. Steady state with high/low pH (SSH/SSL) and oscillatory state (OS) are indicated by closed triangle up/down and open circle, respectively.