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SUPECA kinetics for scaling redox reactions in networks of mixed substrates and consumers and an example application to aerobic soil respiration

Jin-Yun Tang and William J. Riley

Correspondence to: Jin-Yun Tang (jinyuntang@lbl.gov)

Below we provide auxiliary information for the numerical benchmark of the SUPECA kinetics.

The equations for fixed-point iteration are

$$\left[S_1\right]_{new} = \left[S_1\right]_T \left(1 + \frac{\left[M\right]_{old}}{K_{MS1}} + \frac{k_{BS1}\left[B\right]_{old}}{k_{BS2}\left[S_2\right]_{old}} + \frac{k_{BS2}}{k_2^+}\left[B\right]_{old}\frac{\left[S_2\right]_{old}}{\left[S_1\right]_{old}} + \frac{k_{BS1}}{k_2^+}\left[B\right]_{old} \right)^{-1} \tag{S-1}$$

$$\left[S_2\right]_{new} = \left[S_2\right]_T \left(1 + \frac{k_{BS2}\left[B\right]_{old}}{k_{BS1}\left[S_1\right]_{old}} + \frac{k_{BS2}}{k_2^+}\left[B\right]_{old} + \frac{k_{BS1}}{k_2^+}\left[B\right]_{old}\frac{\left[S_1\right]_{old}}{\left[S_2\right]_{old}} \right)^{-1} \tag{S-2}$$

$$\left[B\right]_{new} = \left[B\right]_T \left(1 + \frac{k_{BS1}\left[S_1\right]_{old}}{k_{BS2}\left[S_2\right]_{old}} + \frac{k_{BS2}\left[S_2\right]_{old}}{k_{BS1}\left[S_1\right]_{old}} + \frac{k_{BS2}}{k_2^+}\left[S_2\right]_{old} + \frac{k_{BS1}}{k_2^+}\left[S_1\right]_{old} \right)^{-1} \tag{S-3}$$

$$\left[M\right]_{new} = \left[M\right]_T \left(1 + \frac{\left[S_1\right]_{old}}{K_{MS1}} \right)^{-1} \tag{S-4}$$

The iteration starts with initial condition $\left[S_1\right]_{old} = \left[S_1\right]_T$, $\left[S_2\right]_{old} = \left[S_2\right]_T$, $\left[B\right]_{old} = \left[B\right]_T$, and $\left[M\right]_{old} = \left[M\right]_T$. The iteration stops when the relative change between two consecutive iterations is smaller than 10^{-4}.

Supplementary figure

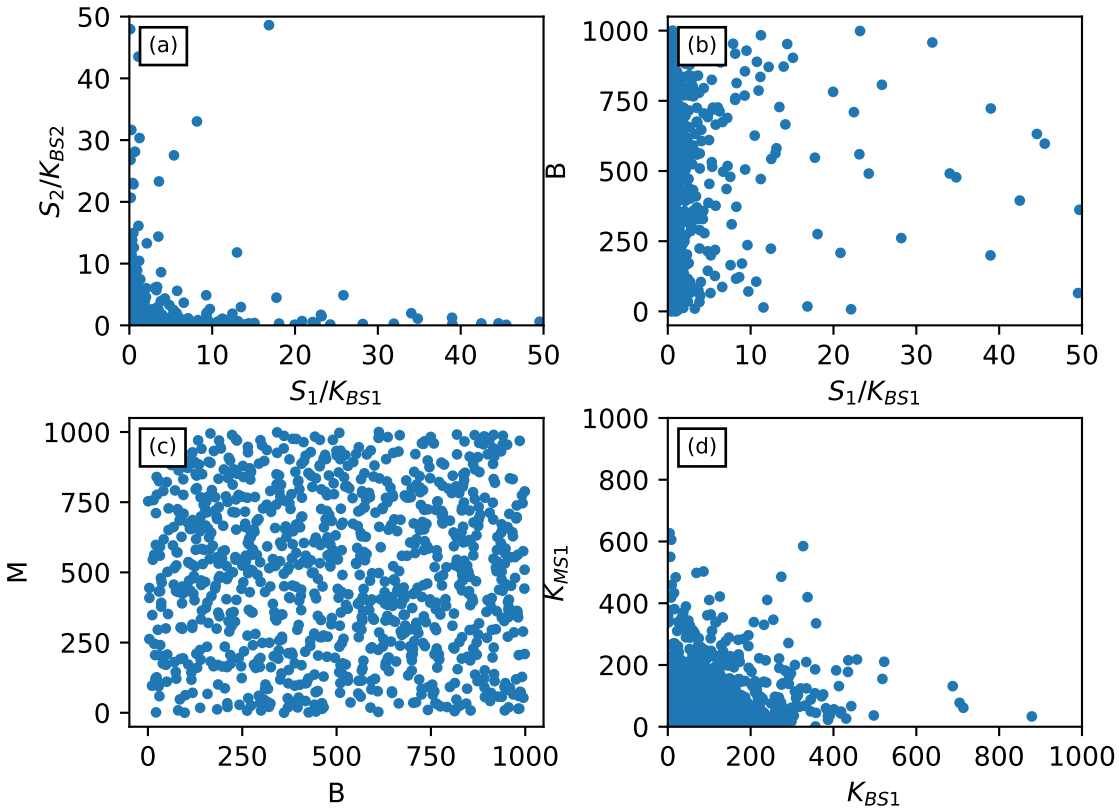

Figure S1. Scatter plots of the parameters used in the numerical benchmark of the SUPECA kinetics (which is Figure 3 in the main text).

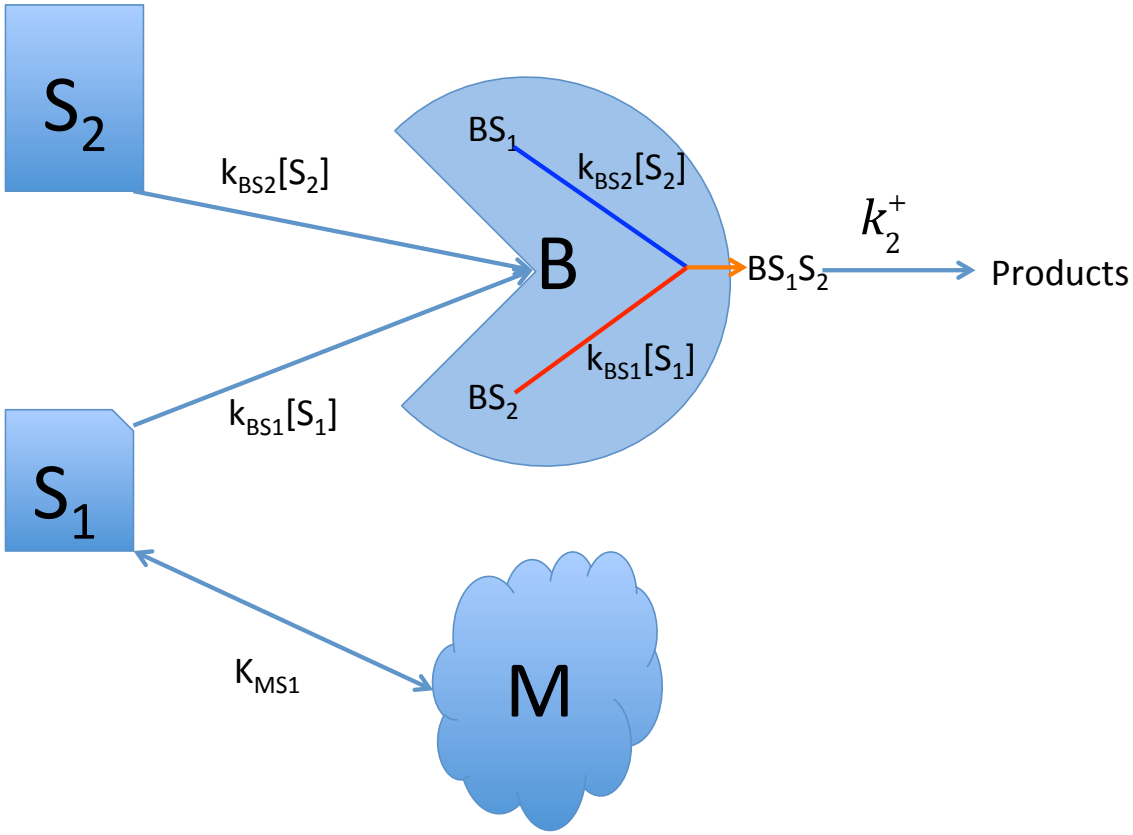

Figure S2. Graphic representation of the reaction network that is used for evaluating the numerical accuracy of SU and SUPECA. The AB-E reaction is of the form $S_1 + S_2 \xrightarrow{B} BS_1S_2 \xrightarrow{k_2^+} B + \text{Products}$, and S_1 also interacts with sorbent M through the reaction $S_1 + M \overset{K_{MS1}}{\leftrightarrow} MS_1$. The equilibrium chemistry formulation of the problem is in Appendix F of the main text.