Supporting information

Short-chain fatty acids (SCFAs) production maximization by modeling thermophilic sludge fermentation

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Table S1. Operational conditions of an anaerobic fermentation reactor at 50℃.

Stages	SRT (day)	Fermenting time (day)
Initial fed-batch	-	2
Continuous operation	2	6
	3	9
	4	12

Table S2. Calibrated k and $k_{m,h}$ parameters during the fermentation at 40℃, 50℃ and 60℃. The model simulations for maximum SCFAs yield, CH_4 yield and VSS reduction ratio with the optimal SRT.

Temp (℃)	Parameters		$SRT_{Optimal}$ (day)	SCFAs yield (%)	CH_4 yield (%)	VSS reduction ratio (%)
	k (d^{-1})	$k_{m,h}$ (d^{-1})				
40	2.95±0.50	3.59±0.63	2.8	11	10	38
50	4.03±0.41	6.00±0.47	4.2	18	13	41
60	8.18±1.30	6.12±0.38	3.2	17	13	41

Sensitivity Analysis. A sensitivity analysis was conducted to evaluate the effects of the kinetic parameters on the model outputs. The following absolute–relative sensitivity function is used in this work:

$$\delta\begin{pmatrix} a & r \\ y & p \end{pmatrix} = p\frac{dy}{dp} \quad (1)$$

where y is an arbitrary variable and p is a model parameter represented by a constant variable. The function calculates the absolute change in y for a 100% change in p. The sensitivity analysis evaluates all kinetic parameters in the model. The initial values of these parameters were obtained from the literature.[1] The sensitive analysis showed that k and $k_{m,h}$ were more sensitive to the model output SCOD and S_V than the other parameters, and needed to be calibrated.

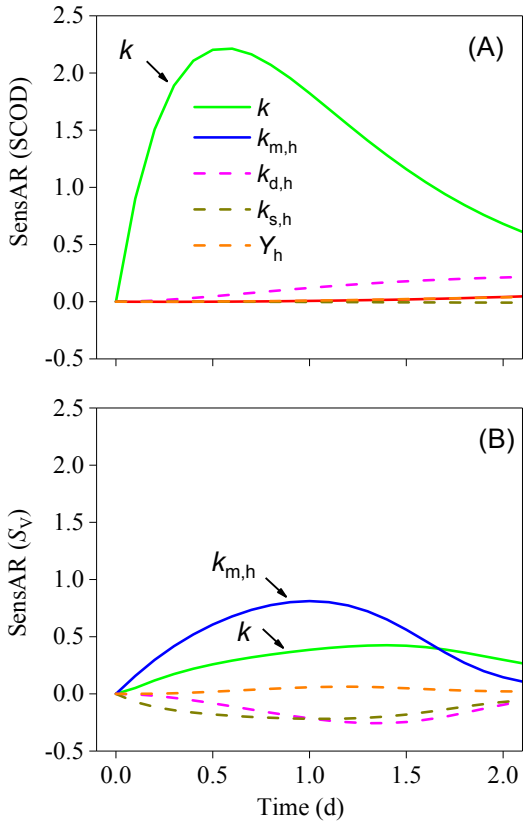

Figure S1. Sensitivity of the model components S_{COD} (A) and S_V (B) to the kinetic parameters.

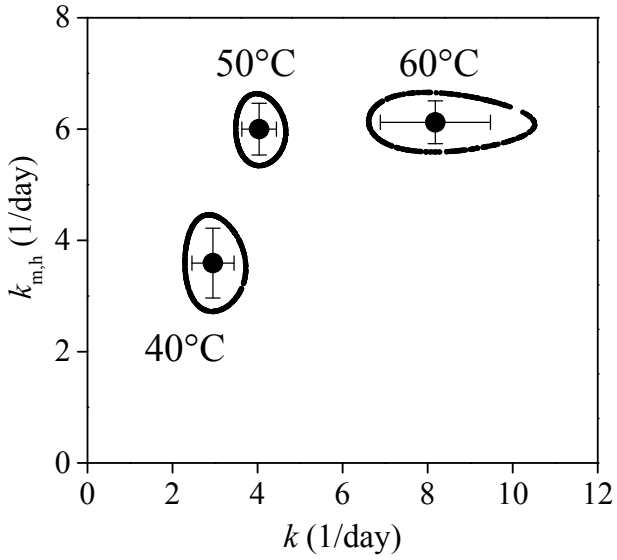

Figure S2. 95% confidence regions for hydrolysis rate k and maximum specific production rate $k_{m,h}$ during sludge fermentation at 40℃, 50℃ and 60℃. The used experimental data is from Xiong *et al.*[2]. Error bars represent standard errors.

Reference

1 P. Zhang, Y. Chen, Q. Zhou, X. Zheng, X. Zhu and Y. Zhao, Understanding Short-Chain Fatty Acids Accumulation Enhanced in Waste Activated Sludge Alkaline Fermentation: Kinetics and Microbiology, *Environ. Sci. Technol.*, 2010, **44**, 9343–9348.

2. H. Xiong, J. Chen, H. Wang and H. Shi, Influences of volatile solid concentration, temperature and solid retention time for the hydrolysis of waste activated sludge to recover volatile fatty acids, Bioresour. Technol., 2012, 119, 285–292.