Supplementary Material for

QSDsan: An Integrated Platform for Quantitative Sustainable Design of Sanitation and Resource Recovery Systems

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**S1. Additional Morris Analysis Results of the Bwaise System**

### Figure S1

Complete figure of the Morris analysis results (refer to Figure 3 in the main text for the full legend). Parameters in red fonts were one of the five parameters with the largest normalized $\mu^*$ values for a given metric of the corresponding system, but the normalized $\mu^*$ values were smaller than 0.1 and not considered as “key parameters”. Raw data (including full list of the parameters and their $\mu^*$ and $\sigma$ values) can be found in the *bwaise* module (the cached_results_figures folder) of the EXPOsan repository online ([https://github.com/QSD-Group/EXPOsan/tree/main/exposan/bwaise](https://github.com/QSD-Group/EXPOsan/tree/main/exposan/bwaise)).
Figure S2. Alternative figure presenting the Morris analysis results (refer to Figure S1 for the name and unit of the parameters, parameters were listed in the same order as in the legend table in Figure S1). Raw data (including full list of the parameters and their $\mu^*$ and $\sigma$ values) can be found in the *bwaise* module (the cached_results_figures folder) of the EXPOsan repository [online](https://github.com/QSD-Group/EXPOsan/tree/main/exposan/bwaise).
S2. BSM1 Simulation Settings

S2a. BSM1 system settings

Table S1. BSM1 system settings in baseline dynamic simulation and in uncertainty analysis. All uncertainty ranges were obtained from Sin et al.¹

| Variable      | Description                                      | Unit           | Baseline       | Uncertainty Analysis | Minimum | Maximum | Distribution |
|---------------|--------------------------------------------------|----------------|----------------|----------------------|---------|---------|--------------|
| **Influent**  |                                                  |                |                |                      |         |         |              |
| $Q_{in}$      | Volumetric flowrate                              | m³·d⁻¹         | 18,446         | -                    | -       | -       |              |
| $T_{water}$   | Water temperature                                | K              | 293.15         | -                    | -       | -       |              |
| $DO_{sat}$    | Saturation DO at field condition                 | mg-O₂·L⁻¹      | 8.0            | 7.2                  | 8.8     | Uniform |
| $S_s$         | Soluble organic substrate                        | mg-COD·L⁻¹     | 69.5           | -                    | -       | -       |              |
| $X_{RH}$      | Active heterotrophic biomass                     | mg-COD·L⁻¹     | 28.17          | -                    | -       | -       |              |
| $X_s$         | Particulate organic substrate                    | mg-COD·L⁻¹     | 202.32         | -                    | -       | -       |              |
| $X_i$         | Particulate inert organic matter                 | mg-COD·L⁻¹     | 51.2           | -                    | -       | -       |              |
| $S_{NH}$      | Ammonium nitrogen                                | mg-N·L⁻¹       | 31.56          | -                    | -       | -       |              |
| $S_l$         | Soluble inert organic matter                     | mg-COD·L⁻¹     | 30             | -                    | -       | -       |              |
| $S_{ND}$      | Soluble biodegradable organic nitrogen           | mg-N·L⁻¹       | 6.95           | -                    | -       | -       |              |
| $X_{ND}$      | Particulate biodegradable organic N              | mg-N·L⁻¹       | 10.59          | -                    | -       | -       |              |
| $S_{ALK}$     | Alkalinity, assumed to be bicarbonate            | mmol·L⁻¹       | 7              | -                    | -       | -       |              |
| **Environment**|                                                |                |                |                      |         |         |              |
| $T_{air}$     | Air temperature                                  | K              | 293.15         | -                    | -       | -       |              |
| $P$           | Atmospheric pressure                             | Pa             | 101,325        | -                    | -       | -       |              |
| **Reactors**  |                                                  |                |                |                      |         |         |              |
| $V_a$         | Anoxic CSTR volume                               | m³             | 1,000          | 900                  | 1,000   | Uniform |
| $V_o$         | Aerobic CSTR volume                              | m³             | 1,333          | 1,200                | 1,333   | Uniform |
| $K_i\alpha_1$| Oxygen mass transfer coefficient at field condition for O1 and O2 reactors | d⁻¹ | 240       | 180                  | 360     | Uniform |
| $K_i\alpha_2$| Oxygen mass transfer coefficient at field condition for O3 reactor | d⁻¹ | 84       | 75.6                 | 92.4     | Uniform |
| $H$           | Clarifier height                                 | m              | 4              | -                    | -       | -       |              |
| $A$           | Clarifier surface area                           | m²             | 1,500          | -                    | -       | -       |              |
| $Q_{RAS}$     | RAS flowrate                                     | m³·d⁻¹         | $1 \times Q_{in}$ | $0.75 \times Q_{in}$ | $1 \times Q_{in}$ | Uniform |
| $Q_{WAS}$     | WAS flowrate                                     | m³·d⁻¹         | 385            | 346.5                | 423.5  | Uniform |
| $Q_{intr}$    | Internal recirculation flowrate                  | m³·d⁻¹         | $3 \times Q_{in}$ | $2.25 \times Q_{in}$ | $3.75 \times Q_{in}$ | Uniform |
### S2b. ASM1 parameters

**Table S2.** ASM1 parameters in baseline dynamic simulation and in uncertainty analysis. All uncertainty ranges were obtained from Sin et al.\(^1\)

| Variable | Description | Unit | Baseline | Uncertainty Analysis | Distribution |
|----------|-------------|------|----------|----------------------|--------------|
|         |             |      | Minimum  | Maximum              |              |
| \(Y_H\) | Heterotrophic biomass yield on soluble substrate | g-COD\-(g-COD)\(^{-1}\) | 0.67 | 0.64 | 0.70 | Triangular |
| \(Y_A\) | Autotrophic biomass yield on ammonium N | g-COD\-(g-N)\(^{-1}\) | 0.24 | 0.23 | 0.25 | Triangular |
| \(F_{Pobs}\) | Observed fraction of inert particulate generated during biomass decay | unitless | 0.21 | 0.16 | 0.26 | Triangular |
| \(i_{XB}\) | Active biomass N content | g-N\-(g-COD)\(^{-1}\) | 0.08 | 0.04 | 0.12 | Triangular |
| \(i_{XP}\) | Cell product and inert particulate N content | g-N\-(g-COD)\(^{-1}\) | 0.06 | 0.057 | 0.063 | Triangular |
| \(f_{SS,COD}\) | mass-to-COD ratio of particulates | g\-(g-COD)\(^{-1}\) | 0.75 | 0.7 | 0.95 | Triangular |
| \(\mu_H\) | Heterotrophic maximum specific growth rate | d\(^{-1}\) | 4 | 3 | 5 | Triangular |
| \(K_S\) | Readily biodegradable substrate half saturation coefficient | g-COD\-m\(^{-3}\) | 10 | 5 | 15 | Triangular |
| \(K_{OH}\) | Oxygen half saturation coefficient for heterotrophic growth | g-O\(_2\)-m\(^{-3}\) | 0.2 | 0.1 | 0.3 | Triangular |
| \(K_NO\) | Nitrate half saturation coefficient | g-N\-m\(^{-3}\) | 0.5 | 0.25 | 0.75 | Triangular |
| \(b_H\) | Heterotrophic biomass decay rate constant | d\(^{-1}\) | 0.3 | 0.285 | 0.315 | Triangular |
| \(\mu_A\) | Autotrophic maximum specific growth rate | d\(^{-1}\) | 0.5 | 0.475 | 0.525 | Triangular |
| \(K_{NH}\) | Ammonium (nutrient) half saturation coefficient | g-N\-m\(^{-3}\) | 1 | 0.5 | 1.5 | Triangular |
| \(K_{OA}\) | Oxygen half saturation coefficient for autotrophic growth | g-O\(_2\)-m\(^{-3}\) | 0.4 | 0.3 | 0.5 | Triangular |
| \(b_A\) | Autotrophic biomass decay rate constant | d\(^{-1}\) | 0.05 | 0.04 | 0.06 | Triangular |
| \(\eta_g\) | Reduction factor for anoxic growth of heterotrophs | unitless | 0.8 | 0.6 | 1.0 | Triangular |
| \(k_a\) | Ammonification rate constant | m\(^3\)-(g-COD)\(^{-1}\)-d\(^{-1}\) | 0.05 | 0.03 | 0.08 | Triangular |
| \(k_h\) | Hydrolysis rate constant | d\(^{-1}\) | 3 | 2.25 | 3.75 | Triangular |
| \(K_X\) | Slowly biodegradable substrate half saturation coefficient for hydrolysis | g-COD\-(g-COD)\(^{-1}\) | 0.1 | 0.075 | 0.125 | Triangular |
| \(\eta_h\) | Reduction factor for anoxic hydrolysis | unitless | 0.8 | 0.6 | 1.0 | Triangular |
S2c. Initial conditions

The baseline initial conditions were used in both benchmarking dynamic simulation and the Monte Carlo simulations for uncertainty analysis. In steady-state convergence test, the five CSTRs shared identical initial conditions in each simulation, and the clarifier’s initial soluble concentrations were set to equal its influent’s concentrations at t=0. The clarifier’s initial TSS in each layer, if not specified, were assumed proportional to influent TSS by fixed factors, which can be found in the Clarifier class of QSDsan. Per the assumption of the 1D 10-layer settling model,2,3 the compositions of particulates in clarifier influent are propagated immediately to its effluents.

Table S3. Initial conditions used in dynamic simulations and varied to test convergence of steady states.

| Variable | Description                                      | Unit             | Baseline CSTRs | Clarifier | Steady-State Convergence Test Minimum | Maximum | Distribution |
|----------|--------------------------------------------------|------------------|----------------|-----------|---------------------------------------|---------|--------------|
| $S_5$    | Soluble organic substrate                        | mg-COD L$^{-1}$  | 5              | 5         | 2.5                                   | 7.5     | Uniform      |
| $S_1$    | Soluble inert organic matter                     | mg-COD L$^{-1}$  | 0              | 0         | -                                     | -       | -            |
| $X_i$    | Particulate inert organic matter                 | mg-COD L$^{-1}$  | 1,000          | -         | 500                                   | 1,500   | Uniform      |
| $X_s$    | Particulate organic substrate                    | mg-COD L$^{-1}$  | 100            | -         | 50                                    | 150     | Uniform      |
| $X_{RH}$ | Active heterotrophic biomass                     | mg-COD L$^{-1}$  | 500            | -         | 250                                   | 750     | Uniform      |
| $X_{RA}$ | Active autotrophic biomass                       | mg-COD L$^{-1}$  | 100            | -         | 50                                    | 150     | Uniform      |
| $X_p$    | Particulate product from biomass decay           | mg-COD L$^{-1}$  | 100            | -         | 50                                    | 150     | Uniform      |
| $S_O$    | Dissolved oxygen                                 | mg-O$_2$ L$^{-1}$| 2              | 2         | 1                                     | 3       | Uniform      |
| $S_{NO}$ | Nitrate and nitrite nitrogen                     | mg-N L$^{-1}$    | 20             | 20        | 10                                    | 30      | Uniform      |
| $S_{NH}$ | Ammonium nitrogen                                | mg-N L$^{-1}$    | 2              | 2         | 1                                     | 3       | Uniform      |
| $S_{ND}$ | Soluble biodegradable organic nitrogen           | mg-N L$^{-1}$    | 1              | 1         | 0.5                                   | 1.5     | Uniform      |
| $X_{ND}$ | Particulate biodegradable organic N              | mg-N L$^{-1}$    | 1              | -         | 0.5                                   | 1.5     | Uniform      |
| $S_{ALK}$| Alkalinity, assumed to be bicarbonate            | mmol L$^{-1}$    | 7              | 7         | 3.5                                   | 10.5    | Uniform      |
| $TSS_1$  | Total suspended solids in layer 1 (top)          | mg L$^{-1}$      | -              | 10        | -                                     | -       | -            |
| $TSS_2$  | Total suspended solids in layer 2                | mg L$^{-1}$      | -              | 20        | -                                     | -       | -            |
| $TSS_3$  | Total suspended solids in layer 3                | mg L$^{-1}$      | -              | 40        | -                                     | -       | -            |
| $TSS_4$  | Total suspended solids in layer 4                | mg L$^{-1}$      | -              | 70        | -                                     | -       | -            |
| $TSS_5$  | Total suspended solids in layer 5                | mg L$^{-1}$      | -              | 200       | -                                     | -       | -            |
| $TSS_6$  | Total suspended solids in layer 6                | mg L$^{-1}$      | -              | 300       | -                                     | -       | -            |
| $TSS_7$  | Total suspended solids in layer 7                | mg L$^{-1}$      | -              | 350       | -                                     | -       | -            |
| $TSS_8$  | Total suspended solids in layer 8                | mg L$^{-1}$      | -              | 350       | -                                     | -       | -            |
| $TSS_9$  | Total suspended solids in layer 9                | mg L$^{-1}$      | -              | 2000      | -                                     | -       | -            |
| $TSS_{10}$| Total suspended solids in layer 10 (bottom)       | mg L$^{-1}$      | -              | 4000      | -                                     | -       | -            |
S3.  Additional Uncertainty Analysis Results of BSM1

Figure S3. Kernel density plots of BSM1 system performance metrics at steady state. Black dashed lines indicate the assumed discharge limits of corresponding composite variables. The plots were created with the stats module in QSDsan.
### S4. Sensitivity Analysis (Monte Carlo Filtering) Results of BSM1

Table S4. Monte Carlo filtering results generated with simulation data from uncertainty analysis. A *p* value less than 0.05 means the sample distributions of a variable significantly differ between the group with the metric values above the threshold (i.e., discharge limit) and the group below the threshold. The *D* value indicates the “distance” between the variable’s two sample distributions (**p < 0.01; *p < 0.05).**

| Variable | Effluent TN | Effluent TKN |
|----------|-------------|--------------|
| Metric   | *D* | *p* | *D* | *p* |
| ASM1 parameters | | | | |
| **Y**_H | 0.077 | 0.568 | 0.042 | 0.746 |
| **Y**_A | 0.086 | 0.422 | 0.058 | 0.358 |
| **f**_Pobs | 0.073 | 0.622 | 0.102* | 0.011 |
| **t**_XB | 0.062 | 0.806 | 0.050 | 0.545 |
| **t**_XP | 0.140* | 0.035 | 0.055 | 0.420 |
| **f**_SS,CO | 0.056 | 0.896 | 0.034 | 0.924 |
| **μ**_H | 0.113 | 0.140 | 0.080 | 0.081 |
| **k**_G | 0.070 | 0.683 | 0.048 | 0.611 |
| **K**_OH | 0.246*** | 0.000 | 0.090* | 0.034 |
| **K**_NO | 0.117 | 0.117 | 0.083 | 0.063 |
| **b**_H | 0.126 | 0.074 | 0.051 | 0.517 |
| **μ**_A | 0.173** | 0.004 | 0.145*** | 0.000 |
| **K**_NH | 0.146* | 0.025 | 0.161*** | 0.000 |
| **K**_OA | 0.168** | 0.006 | 0.114** | 0.003 |
| **b**_A | 0.125 | 0.080 | 0.110** | 0.005 |
| **η**_A | 0.142* | 0.032 | 0.081 | 0.073 |
| **k**_A | 0.135* | 0.045 | 0.082 | 0.070 |
| **k**_G | 0.155* | 0.015 | 0.058 | 0.358 |
| **K**_X | 0.064 | 0.778 | 0.041 | 0.793 |
| **η**_H | 0.081 | 0.492 | 0.057 | 0.380 |
| Decision variables | | | | |
| **V**_A | 0.092 | 0.335 | 0.054 | 0.443 |
| **V**_B | 0.251*** | 0.000 | 0.229*** | 0.000 |
| **K**_1a | 0.512*** | 0.000 | 0.503*** | 0.000 |
| **K**_2a | 0.066 | 0.752 | 0.085 | 0.054 |
| **Q**_RAS | 0.108 | 0.178 | 0.167*** | 0.000 |
| **Q**_MWS | 0.130 | 0.063 | 0.185*** | 0.000 |
| **Q**_WAT | 0.068 | 0.714 | 0.055 | 0.437 |
| Contextual parameters | | | | |
| **DO**_sat | 0.263*** | 0.000 | 0.269*** | 0.000 |
References

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3 K. V. Gernaey, U. Jeppsson, P. A. Vanrolleghem and J. B. Copp, *Benchmarking of Control Strategies for Wastewater Treatment Plants*, IWA Publishing, 2014.