

Supplementary Material - Bayesian Uncertainty Quantification for Anaerobic Digestion models

Table 1: Computation time for calibration and UQ routines in hours

	SA	Calib.	FIM	Beale	Bootstrap	Bayes init.	VarBUQ
AM2 LN	n.a.	0.50	0.00 (0.50)	0.95 (0.45)	50.10 (50.60)	n.a.	1.70
AM2 HN	n.a.	0.43	0.00 (0.43)	0.95 (1.38)	56.25 (56.68)	n.a.	1.68
AM2 LF	n.a.	0.47	0.00 (0.47)	0.6 (1.07)	46.14 (46.65)	n.a.	1.50
AM2 HF	n.a.	0.43	0.00 (0.43)	0.92 (1.35)	47.14 (47.62)	n.a.	1.55
ADM1 LN	0.33	2.32	0.02 (2.67)	1.63 (4.29)	n.a.	0.59	4.82 (5.40)
ADM1 HN	0.32	3.15	0.02 (3.49)	1.92 (5.39)	n.a.	0.59	4.80 (5.39)
ADM1 LF	0.32	2.29	0.02 (2.62)	2.22 (4.82)	n.a.	0.75	4.77 (5.52)
ADM1 HF	0.33	5.32	0.02 (5.67)	1.43 (6.42)	n.a.	0.72	6.02 (6.74)

SA: Sensitivity analysis, Calib.: Calibration, Bayes init.: initialisation of the posterior. For each UQ routine, the total time, including optimisation, is indicated in bold.

Table 2: Default parameter values, uncertainty and calibration results for AM2

	Block	θ_0	$\sigma_{\log(\theta)}$	θ_N^*	$\hat{\theta}_{LN}$	$\hat{\pi}_{LN}$	$\hat{\theta}_{HN}$	$\hat{\pi}_{HN}$	θ_F^*	$\hat{\theta}_{LF}$	$\hat{\pi}_{LF}$	$\hat{\theta}_{HF}$	$\hat{\pi}_{HF}$
$\mu_{1\max}$ (Day ⁻¹)	1	1.2	0.20	1.23	0.55	1.17	0.91	1.18	0.99	0.86	1.02	0.91	0.86
$\mu_{2\max}$ (Day ⁻¹)	2	0.74	0.48	1.05	0.99	0.74	0.90	0.78	1.32	2.00	0.95	1.21	1.16
K_{S1} (kgCOD m ⁻³)	1	7.1	0.32	7.51	5.76	7.34	6.25	7.20	15.98	15.38	15.98	15.13	14.40
K_{S2} (mole m ⁻³)	2	9.28	0.48	11.0	11.0	9.84	10.1	9.09	4.97	5.36	4.5	4.85	4.68
K_{I2} (mole m ⁻³)	2	256	0.40	196.0	135	256	259	259	345	328	252	290	260

Block indicates groups of parameters which can be correlated in the posterior distribution. θ_0 contains the means of the prior distribution, $\sigma_{\log(\theta)}$ the standard deviation for the prior distribution (in log space). θ^* is the set of parameters used to generate the data. $\hat{\theta}$ is the result of the non bayesian calibration. $\hat{\pi}[\theta]$ is the means of the posterior distribution (i.e. the result of the bayesian calibration).

Table 3: Default parameter values, uncertainty and calibration results for ADM1

	Block	θ_0	$\sigma_{\log(\theta)}$	θ_N	$\hat{\theta}_{LN}$	$\hat{\pi}_{LN}$	$\hat{\theta}_{HN}$	$\hat{\pi}_{HN}$	θ_F	$\hat{\theta}_{LF}$	$\hat{\pi}_{LF}$	$\hat{\theta}_{HF}$	$\hat{\pi}_{HF}$
k_{dis} (Day ⁻¹)	1	0.5	0.24	0.36	0.50	0.58	0.50	0.601	0.23	0.50	0.44	0.50	0.49
k_{hyd_CH} (Day ⁻¹)	1	10	0.12	10	10	11	10	9.9	5.2	10	9.7	10	9.3
k_{hyd_PR} (Day ⁻¹)	1	10	0.12	8.7	10	9.1	10	10	12	10	9.9	10	8.8
k_{hyd_LI} (Day ⁻¹)	1	10	0.24	23	10	9.5	10	10.3	2.40	10.0	10	10	9.4
k_{m_su} (Day ⁻¹)	2	30	0.12	38	30	32	2.4	30	48	30	32	107	28
k_{m_aa} (Day ⁻¹)	3	50	0.12	45	50	48	50	56	49	50	51	2.2	51
k_{m_fa} (Day ⁻¹)	4	6	0.24	5.2	6.0	5.4	6.0	6.5	4.5	6.0	7.1	6.0	5.5
k_{m_c4+} (Day ⁻¹)	5	20	0.12	21	90	18	12	19	18	37	17	44	16
k_{m_pro} (Day ⁻¹)	6	13	0.12	13	93	12	26	13	9.9	49	14	9.4	15
k_{m_ac} (Day ⁻¹)	7	8	0.12	11	80	10	21	11	10	53	8.4	9.3	9.8
k_{m_h2} (Day ⁻¹)	8	35	0.12	28	35	33	35	33	29	35	37	35	35
K_{S_su} (kgCOD m ⁻³)	2	0.5	0.12	0.43	0.50	0.50	0.50	0.54	0.29	0.50	0.47	0.50	0.47
K_{S_aa} (kgCOD m ⁻³)	3	0.3	0.046	0.31	0.30	0.31	0.30	0.31	0.29	0.30	0.30	0.30	0.30
K_{S_fa} (kgCOD m ⁻³)	4	0.4	0.24	0.39	0.40	0.44	0.40	0.40	0.58	0.40	0.42	0.40	0.43
K_{S_c4+} (kgCOD m ⁻³)	5	0.2	0.24	0.30	1.2	0.24	2.0	0.26	0.40	0.90	0.37	0.94	0.35
K_{S_pro} (kgCOD m ⁻³)	6	0.1	0.12	0.16	0.86	0.100	0.30	0.12	6.5e-2	0.38	9.4e-2	5.1e-2	0.10
K_{S_ac} (kgCOD m ⁻³)	7	0.15	0.12	0.15	1.2	0.13	0.21	0.13	0.24	1.5	0.15	0.23	0.19
K_{S_h2} (kgCOD m ⁻³)	8	7e-6	0.12	6.7e-6	7.0e-6	7.6e-6	7.0e-6	6.1e-6	6.1e-6	7.0e-6	7.5e-6	7.0e-6	7.3e-6
$K_{I_H2_fa}$ (kgCOD m ⁻³)	4	5e-6	0.046	5.0e-6	5.0e-6	4.9e-6	5.0e-6	5.1e-6	5.6e-6	5.0e-6	5.2e-6	5.0e-6	5.0e-6
$K_{I_H2_c4+}$ (kgCOD m ⁻³)	5	1e-5	0.046	1.1e-5	1.e-5	1.e-5	1.0e-5	1.0e-5	1.1e-5	1.0e-5	1.0e-5	1.0e-5	9.9e-6
$K_{I_H2_pro}$ (kgCOD m ⁻³)	6	3.5e-6	0.046	3.2e-6	3.5e-6	3.5e-6	3.5e-6	3.6e-6	3.4e-6	3.5e-6	3.7e-6	3.5e-6	3.6e-6
K_{I_NH3} (kMole m ⁻³)	9	1.8e-3	0.046	1.9e-3	1.8e-3	1.9e-3	7.9e-4	1.8e-3	2.1e-3	1.8e-3	1.8e-3	2.9e-3	2.1e-3
$pH_{UL_LL_aa}$	10	1.5	0.12	1.2	1.1	1.6	1.3	1.3	1.4	0.31	1.5	1.4	1.5
pH_{LL_aa}	10	4	0.12	5.1	5.2	3.6	6.0	3.5	4.4	2.6	3.8	5.2	3.6
$pH_{UL_LL_ac}$	9	1	0.046	1.0	1.0	1.0	0.83	0.99	1.0	1.0	1.0	1.0	1.0
pH_{LL_ac}	9	5	0.046	4.5	5.0	5.0	5.3	4.9	4.8	5.0	5.0	3.8	4.9
$pH_{UL_LL_h2}$	11	1	0.12	0.52	1.0	1.0	1.0	1.1	1.6	1.0	0.94	1.0	1.0
pH_{LL_h2}	11	5	0.046	5.5	5.0	5.0	5.0	5.0	6.1	5.0	4.9	5.0	4.8
k_{dec} (Day ⁻¹)	12	0.02	0.12	1.6e-2	2.0e-2	1.8e-2	6.2e-3	1.7e-2	1.5e-2	1.2e-2	1.7e-2	2.8e-2	2.1e-2
K_{S_IN} (kMole m ⁻³)	13	1e-4	0.046	9.3e-5	1.0e-4	1.0e-4	1.0e-4	9.9e-5	9.5e-5	1.0e-4	1.0e-4	1.0e-4	9.9e-5

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Table 4: Overview of UQ routines

	Bootstrap	FIM	Beale	VarBUQ
Confidence region shape	Any	Ellipse	Any*	User chosen**
Output	Samples	Covariance	Samples	Distribution
Prerequisite	None	Statistical Model	Mean squared error calibration	Prior
Theory	None	Cramer-Rao	Beale	PAC-Bayes
Error hypothesis	None	Gaussian***	Gaussian	Bounded
Model hypothesis	None	Linear***	Linear	None

A detailed description of the methods can be found in the documentation section of <https://github.com/BayesianUncertaintyQuantifAnaeroDig/AnaeroDigUQ>

* The algorithm approximating Beale's confidence regions assumes they are connex.

** Through probability distribution class.

*** While Cramer-Rao's result holds for any statistical model, it only provides an equality for Gaussian noise and linear model.

Table 5: Parameter selection through Morris sensitivity analysis for ADM1.

	LN	HN	LF	HF
k_{m_su}		✓		✓
k_{m_aa}		✓		✓
k_{m_c4+}	✓	✓	✓	✓
k_{m_pro}	✓	✓	✓	✓
k_{m_ac}	✓	✓	✓	✓
k_{dec}	✓	✓	✓	✓
K_{S_c4+}	✓	✓	✓	✓
K_{S_pro}	✓	✓	✓	✓
K_{S_ac}	✓	✓	✓	✓
$K_{I,NH3}$		✓		✓
$pH_{LL\ aa}$	✓	✓	✓	✓
$pH_{UL:LL\ aa}$	✓	✓	✓	✓
$pH_{LL\ ac}$		✓		✓
$pH_{UL:LL\ ac}$		✓		