Supplementary Material

Optimizing ADM1 calibration and input characterization for effective co-digestion modelling

Arianna Catenacci[1]*, Matteo Grana[1], Francesca Malpei[1], Elena Ficara[1]

[1] Politecnico di Milano, *Dipartimento di Ingegneria Civile e Ambientale, Piazza Leonardo da Vinci 32, 20133 Milano, Italy*;
* Correspondence: arianna.catenacci@polimi.it; Tel.: 02.2399 6241

Table S1. Kinetic parameters estimated at each iterative step of the calibration process.

Parameter	Unit	Initial	1st	2nd	3rd	4th	5th	6th
k_{dis}	d^{-1}	0.4	1.2	2	1.5	1.5	1.5	1.5
$k_{hyd,ch}$	d^{-1}	0.25	0.75	0.75	0.3	0.3	0.3	0.3
$k_{hyd,pr}$	d^{-1}	0.2	0.6	0.6	0.2	0.2	0.2	0.5
$k_{hyd,li}$	d^{-1}	0.1	0.3	0.8	0.45	0.5	0.5	0.5
$k_{m,su}$	d^{-1}	30	30	38	38	8	8	8
$k_{m,aa}$	d^{-1}	50	50	8	8	8	8	8
$k_{m,ac}$	d^{-1}	8	8	6	6	8	8	8
$K_{S,su}$	$kg_{COD}\cdot m^{-3}$	0.5	0.5	0.4	0.3	0.3	0.3	0.3
$K_{S,aa}$	$kg_{COD}\cdot m^{-3}$	0.3	0.3	0.2	0.2	0.2	0.2	0.2
$K_{S,ac}$	$kg_{COD}\cdot m^{-3}$	0.15	0.15	0.3	0.01	0.01	0.01	0.01
$K_{S,pro}$	$kg_{COD}\cdot m^{-3}$	0.3	0.3	0.3	0.3	0.3	0.2	0.2

Table S2. Model performance criteria (TIC and MARE) evaluated at varying of the iterative step for selected batch activity tests and BMP tests.

Testing substrate (Phase - Date)	Model fitting criteria	1st Iteration	5th Iteration	6th Iteration
Acetate	TIC	0.157	0.102	0.102
(Phase I - 26.11.2020)	MARE	0.080	0.056	0.056
Glucose	TIC	0.093	0.038	0.038
(Phase I - 19.11.2020)	MARE	0.060	0.023	0.023
BSA	TIC	0.194	0.075	0.075
(Phase I - 26.11.2020)	MARE	0.185	0.058	0.058
BMP – Sludge	TIC	0.042	0.015	0.032
(Phase I - 19.11.2020)	MARE	0.039	0.016	0.031
BMP – Sludge	TIC	0.104	0.055	0.094
(Phase II - 25.02.2021)	MARE	0.131	0.080	0.126
BMP – Yogurt	TIC	0.028	0.060	0.034
(Phase I - 30.12.2020)	MARE	0.020	0.040	0.025
BMP – Yogurt	TIC	0.038	0.049	0.038
(Phase II - 25.02.2021)	MARE	0.026	0.036	0.026
BMP – Co-digestion	TIC	0.013	0.047	0.009
(Phase I - 30.12.2020)	MARE	0.012	0.037	0.009
BMP – Co-digestion	TIC	0.014	0.053	0.011
(Phase II - 25.02.2020)	MARE	0.011	0.038	0.011

Table S3. Model performance criteria **(**TIC and MARE) evaluated at the varying of the iterative step for the seven output variables monitored during the operation of the pilot plant. A distinction is made between the mono-digestion period (Phase I and Phase III) the co-digestion period (Phase II).

Fitting parameter	Pilot plant operation mode	1st iteration		5th iteration		6th iteration		Tentative iteration	
		MARE	TIC	MARE	TIC	MARE	TIC	MARE	TIC
Q_{CH4}	Total	0.162	0.070	0.274	0.112	0.274	0.112	0.274	0.112
Alkalinity	Total	0.100	0.066	0.151	0.107	0.139	0.095	0.089	0.054
	Mono-digestion	0.080	0.049	0.110	0.075	0.110	0.075	0.099	0.064
	Co-digestion	0.145	0.088	0.243	0.147	0.203	0.122	0.065	0.035
TVFA	Total	2.002	0.475	0.443	0.194	0.472	0.199	0.507	0.207
	Mono-digestion	1.342	0.446	0.188	0.162	0.191	0.162	0.190	0.162
	Co-digestion	3.542	0.632	1.038	0.338	1.127	0.356	1.246	0.379
pH	Total	0.018	0.011	0.023	0.014	0.022	0.013	0.017	0.011
	Mono-digestion	0.019	0.011	0.024	0.014	0.024	0.013	0.019	0.011
	Co-digestion	0.015	0.012	0.021	0.014	0.018	0.013	0.011	0.009
NH_4^+	Total	0.150	0.080	0.118	0.070	0.099	0.055	0.099	0.055
	Mono-digestion	0.198	0.103	0.107	0.060	0.107	0.059	0.107	0.059
	Co-digestion	0.043	0.026	0.143	0.083	0.082	0.050	0.082	0.050
VS	Total	0.339	0.220	0.233	0.151	0.238	0.156	0.238	0.156
	Mono-digestion	0.353	0.230	0.255	0.167	0.256	0.167	0.256	0.167
	Co-digestion	0.307	0.196	0.181	0.111	0.196	0.127	0.196	0.127
COD	Total	0.198	0.097	0.147	0.067	0.156	0.070	0.156	0.070
	Mono-digestion	0.213	0.099	0.200	0.084	0.200	0.084	0.200	0.084
	Co-digestion	0.169	0.095	0.041	0.024	0.069	0.041	0.069	0.041