

Electronic Supplementary Material

Table S1 Characteristics of the original and simplified models (Weinrich & Nelles, 2021)

Model	ADM1	ADM1-R1	ADM1-R2	ADM1-R3	ADM1-R4
Simplification	-	Hydrogenotrophic methanogenesis	Acidogenesis	Acetogenesis	Acetoclastic methanogenesis
Unit	COD ^{a)}	Mass	Mass	Mass	Mass
No. processes	19	17	12	6	4
No. components	34	31	26	17	10
No. parameters	52	44	38	24	11
Kinetics		Monod and 1 st order			1 st order
No. inhibitors	4	3	3	3	0

Notes: a) Chemical oxygen demand (COD).

Table S2 Model inputs for process simulation.

		Data set A		Data set B	
		Grass silage	Cattle slurry	Grass silage	Cattle slurry
ADM1					
$X_{ch}^{a)}$	[kg/m ³]	106.34	28.4	139.2	30.79
$X_{pr}^{a)}$	[kg/m ³]	32.48	7.05	36.12	8.74
$X_{li}^{a)}$	[kg/m ³]	6.35	3.29	7.2	3.65
$S_{ac}^{a),b)}$	[kg/m ³]	17.02	4.96	30.23	4.57
$S_{pro}^{a)}$	[kg/m ³]	0.12	1.34	0.42	1.34
$S_{bu}^{a)}$	[kg/m ³]	0.362	0.61	0.096	0.552
$S_{va}^{a)}$	[kg/m ³]	0	0.21	0	0.207
$S_{h2o}^{a)}$	[kg/m ³]	799	933	733	925
$S_{IN}^{a)}$	[kg/m ³]	5.1	4.35	4.24	5.95
$S_{cat^+}^{c)}$	[mol/L]	0.2	0.2	0.27	0.27
$S_{an^-}^{c)}$	[mol/L]	0.015	0.015	0.01	0.01
ADM1-R3					
$X_{ch}^{a)}$	[kg/m ³]	106.34	28.4	139.2	30.79
$X_{pr}^{a)}$	[kg/m ³]	32.48	7.05	36.12	8.74
$X_{li}^{a)}$	[kg/m ³]	6.35	3.29	7.2	3.65
$S_{ac}^{a),b)}$	[kg/m ³]	22.98	6.57	30.15	6.16
$S_{h2o}^{a)}$	[kg/m ³]	799	933	733	925
$S_{IN}^{a)}$	[kg/m ³]	5.1	4.35	4.24	5.95
$S_{cat^+}^{c)}$	[mmol/m ³]	0.2	0.2	0.27	0.27
$S_{an^-}^{c)}$	[mmol/m ³]	0.015	0.015	0.01	0.01

Notes: a) Average values. b) Included lactic acid. c) Manually adjusted.

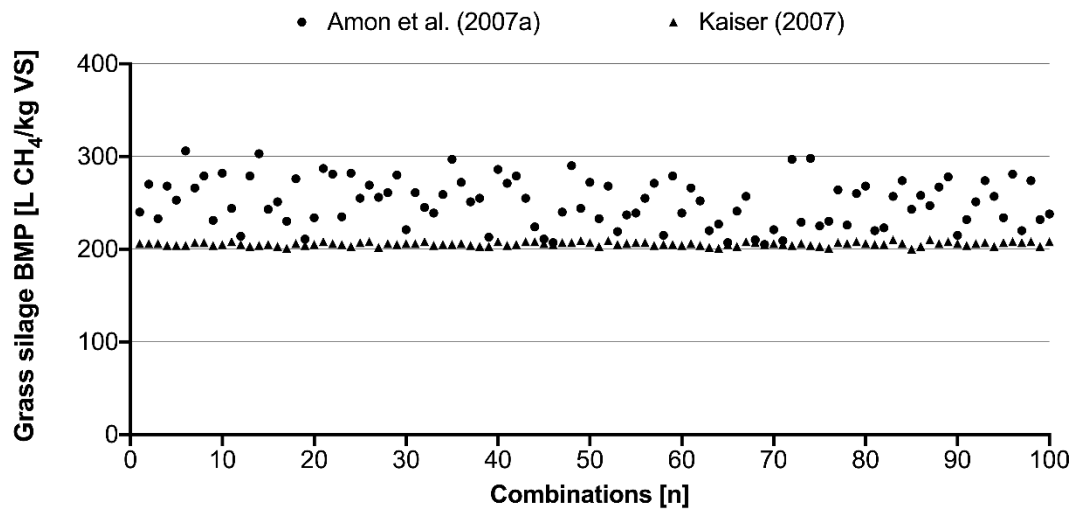


Fig. S1 Results of grass silage Biochemical Methane Potential (BMP) estimated by Amon et al. (2007) and Kaiser (2007) from the different crude protein and crude lipids combinations used in this study.

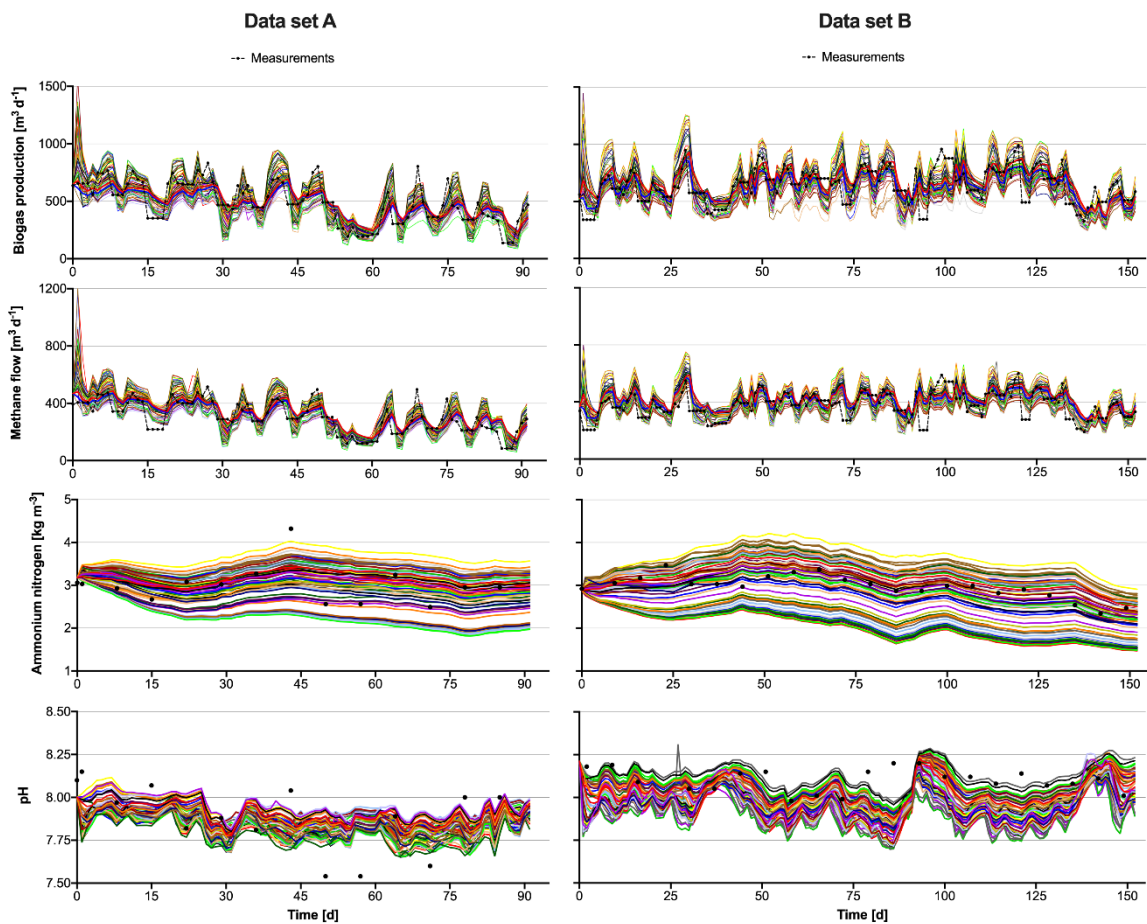


Fig. S2 Measurements and simulation results of biogas production, methane flow, ammonium nitrogen and pH from varying crude carbohydrates, proteins and lipids content of each data set and parameter estimates in each input combination.

Table S3 Weekly Nash-Sutcliffe efficiency (NSE) of each model output for the nutrient concentration scenario with their corresponding parameter estimates from fmincon results. A different initial parameter value (x0) was implemented in each input combination.

Model output	Data set A	Data set B
Nutrient concentration scenario with different parameter estimates ^{a)}		
Biogas production	0.63 (-0.23)	0.19 (-0.35)
Methane flow	0.60 (-0.22)	0.21 (-0.29)
Ammonium nitrogen	-1.05 (-1.09)	-4.99 (-4.93)
pH	-0.78 (-1.04)	-6.52 (-2.89)

Notes: a) Values in brackets indicate differences with the default nutrient concentration scenario (with default parameter set).

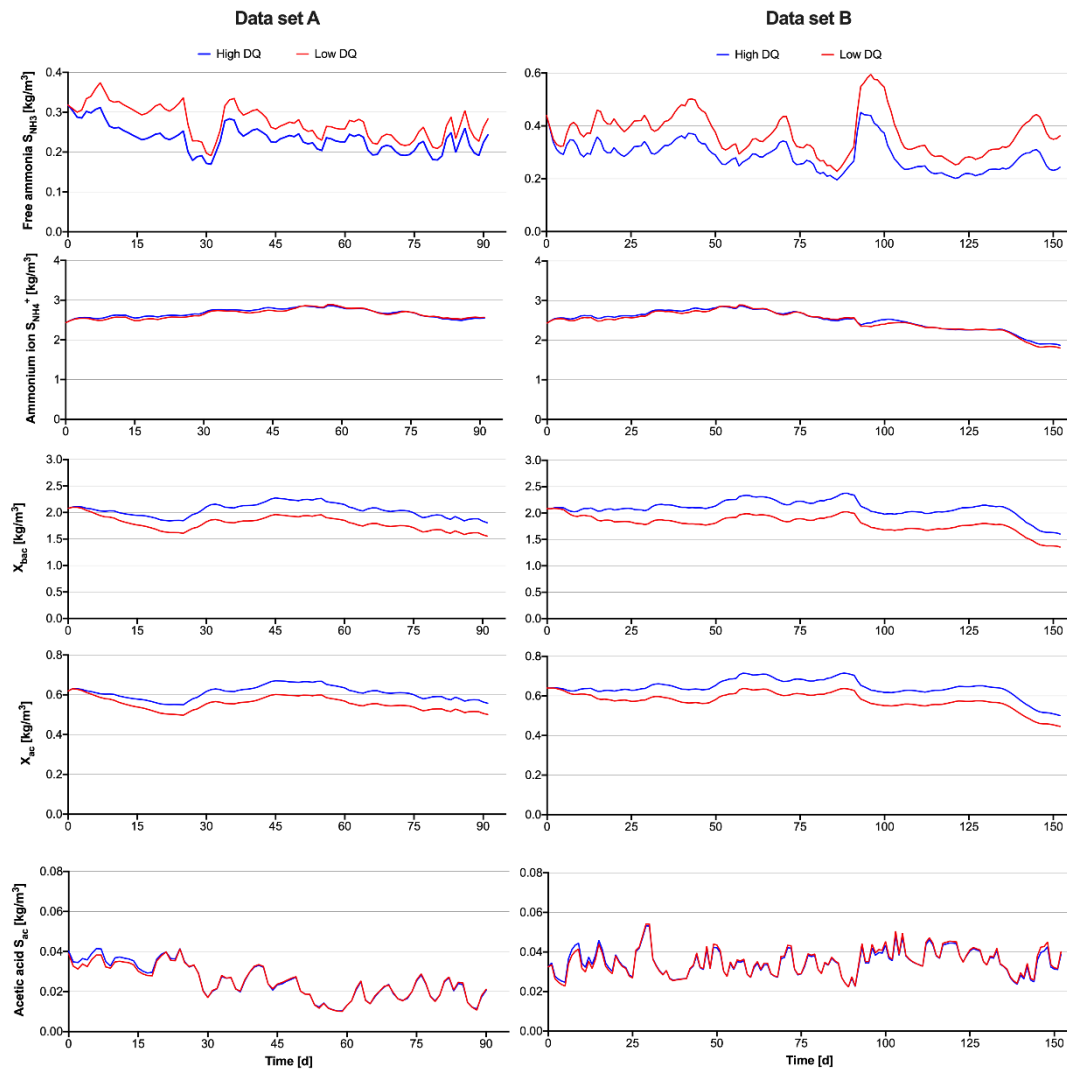


Fig. S3 Results of free ammonia (S_{NH_3}), ammonium ion ($S_{NH_4^+}$), X_{bac} , X_{ac} and acetic acid (S_{ac}) concentrations from the degradability (DQ) scenarios, for both data sets.

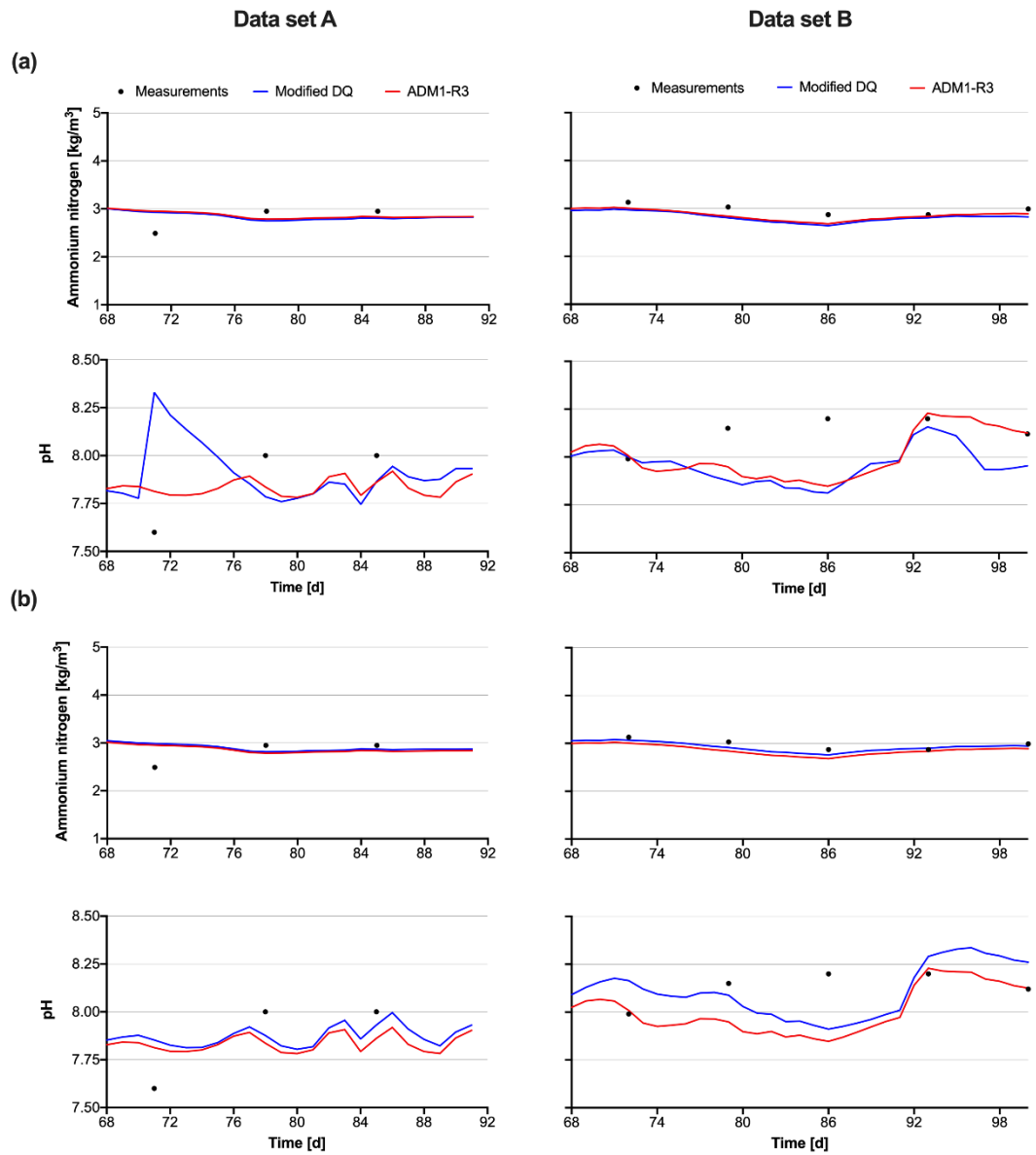


Fig. S4 Measurements and simulation results of ammonium nitrogen and pH after modifying the degradability quotient (DQ) of carbohydrates on days 68-90 and 68-99 of Data set A and B, respectively, for (a) high hydrolysis constant of carbohydrates ($k_{ch} = 0.8$) and (b) low hydrolysis constant of carbohydrates ($k_{ch} = 0.1$).

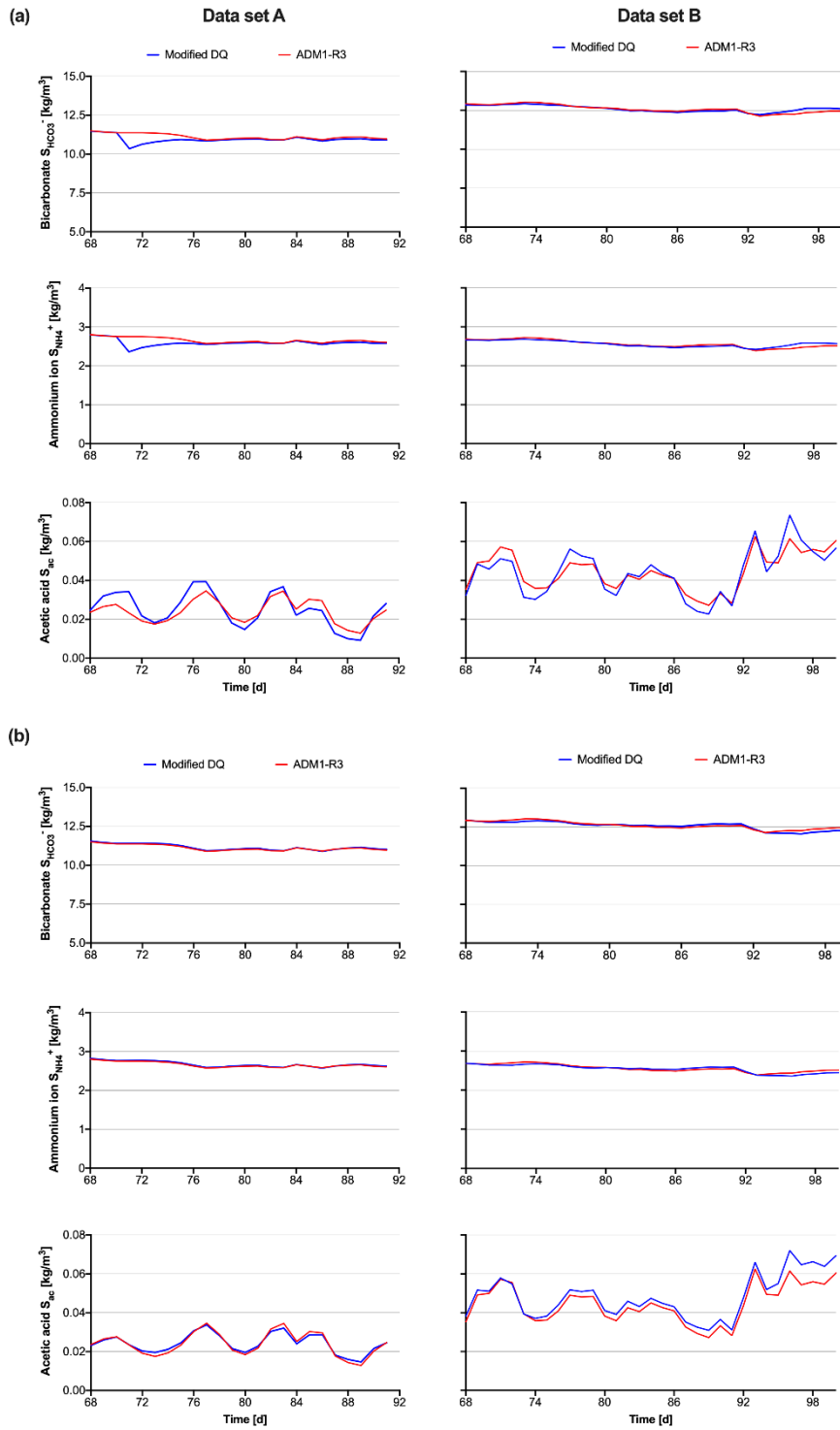


Fig. S5 Simulation results of bicarbonate ($S_{HCO_3^-}$), ammonium ion ($S_{NH_4^+}$) and acetic acid (S_{ac}) after modifying the degradability quotient (DQ) of carbohydrates on days 68-90 and 68-99 of Data set A and B, respectively, for (a) high hydrolysis constant of carbohydrates ($k_{ch} = 0.8$) and (b) low hydrolysis constant of carbohydrates ($k_{ch} = 0.1$).

References

Amon T, Amon B, Kryvoruchko V, Machmüller A, Hopfner-Sixt K, Bódiroza V, Hrbek R, Friedel J, Pötsch E, Wagentristsl H, Schreiner M, Zollitsch W (2007). Methane production through anaerobic digestion of various energy crops grown in sustainable crop rotations. *Bioresource Technology*, 98(17): 3204–3212

Kaiser F L (2007). Einfluss der stofflichen Zusammensetzung auf die Verdaulichkeit nachwachsender Rohstoffe beim anaeroben Abbau in Biogasreaktoren. Dissertation for the Doctoral Degree. München: Technische Universität München

Weinrich S, Nelles M (2021). Systematic simplification of the Anaerobic Digestion Model No. 1 (ADM1) – Model development and stoichiometric analysis. *Bioresource Technology*, 333: 125124