Supplementary Material:

A new ODE based Julia implementation of the Anaerobic Digestion Model No. 1 greatly outperforms existing DAE based Java and Python implementations

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1 Julia Code and Data

The Julia code and all associated data can be found in a GitHub repository at:
`https://github.com/CourtA96/ADM1jl`

2 Analysis of high weighted averages and low methane concentrations

High weighted averages do not occur for the same parameter values as low methane concentrations, that is, if the weighted average is high, the methane concentration is not near zero, and vice versa. This indicates that the two phenomena are not likely related. To determine which parameter values might be causing these phenomena, a t-test was used to compare the means of the parameter values corresponding to the outlier cases, with those corresponding to the typical cases. Table 1 lists the parameters where the t-test returned a significant difference between the mean values.

Table 1: Parameter values where the mean value corresponding to the outlier cases is significantly different to that of the typical cases. The names of the parameters are given in Section 3.

	Parameter	Typical Mean	Outlier Mean	T-test P value
Small CO_2	C_ch	0.031	0.028	$7.32 \cdot 10^{-4}$
	C_pr	0.030	0.026	$1.38 \cdot 10^{-6}$
	f_ac_aa	0.40	0.43	$2.45 \cdot 10^{-3}$
	k_dec_X_aa	0.020	0.021	0.04
	pH_UL_h2	5.99	5.67	0.04
	V_gas	297.71	321.46	$3.39 \cdot 10^{-3}$
Small CO_2 (constant pressure)	C_ch	0.031	0.028	0.01
	C_pr	0.030	0.026	$2.46 \cdot 10^{-5}$
	f_ac_aa	0.40	0.43	$7.09 \cdot 10^{-3}$
	k_dec_X_aa	0.020	0.021	0.04
	pH_LL_aa	4.43	4.07	0.04
	pH_LL_h2	5.25	4.83	0.03
	pH_UL_h2	6.00	5.57	0.02
	V_gas	297.99	320.96	0.01
Large Weighted Average	f_bu_aa	0.26	0.25	0.02
	k_m_pro	13.07	12.47	0.02
	N_aa	0.0071	0.0066	$2.63 \cdot 10^{-3}$
	pH_LL_ac	6.22	7.23	$6.54 \cdot 10^{-10}$
	pH_LL_h2	5.19	5.57	$1.79 \cdot 10^{-3}$
	pH_UL_ac	6.69	7.91	$4.68 \cdot 10^{-10}$
	pH_UL_h2	5.97	6.27	$7.36 \cdot 10^{-3}$
	Y_ac	0.05	0.047	0.04
Large Weighted Average (constant pressure)	f_bu_aa	0.26	0.25	0.01
	k_m_c4	20.29	18.87	0.02
	N_aa	0.0071	0.0067	0.02
	pH_LL_ac	6.22	7.14	$2.10 \cdot 10^{-10}$
	pH_LL_h2	5.19	5.57	$9.53.79 \cdot 10^{-4}$
	pH_UL_ac	6.95	7.89	$8.5 \cdot 10^{-11}$
	pH_UL_h2	5.96	6.18	$6.43 \cdot 10^{-3}$
	Y_ac	0.05	0.047	0.03

3 Paramter Names

Table 2: Table of parameter names and the amount they were varied.

Parameter	Name	Varied by
R	Gas law constant	Constant
T_base	Base reactor temperature	Constant
P_atm	Atmospheric pressure	±5%
T_op	Reactor Operating Temperature	±0.15%
f_sI_xc	Yield (catabolism only) of soluble inerts on composite material	±15%
f_xI_xc	Yield (catabolism only) of particulate inerts on composite material	±15%
f_ch_xc	Yield (catabolism only) of carbohydrates on composite material	±15%
f_pr_xc	Yield (catabolism only) of proteins on composite material	±15%
f_li_xc	Yield (catabolism only) of lipids on composite material	±15%
N_xc	Nitrogen content of composite material	±15%
N_I	Nitrogen content of inerts	±15%
N_aa	Nitrogen content of amino acids	±15%
C_xc	Carbon content of composite material	±15%
C_sI	Carbon content of soluble inerts	±15%
C_ch	Carbon content of carbohydrates	±15%
C_pr	Carbon content of proteins	±15%
C_li	Carbon content of lipids	±15%
C_xI	Carbon content of particulate inerts	±15%
C_su	Carbon content of monosaccharides	±15%
C_aa	Carbon content of amino acids	±15%
f_fa_li	Yield (catabolism only) of long chain fatty acids on composite material	Constant
C_fa	Carbon content of long chain fatty acids	Constant
f_h2_su	Yield (catabolism only) of hydrogen on monosaccharides	±15%
f_bu_su	Yield (catabolism only) of butyrate on monosaccharides	±15%
f_pro_su	Yield (catabolism only) of propionate on monosaccharides	±15%
f_ac_su	Yield (catabolism only) of acetate on monosaccharides	±15%
N_bac	Nitrogen content of bacteria	Constant
C_bu	Carbon content of butyrate	Constant
C_pro	Carbon content of propionate	Constant
C_ac	Carbon content of acetate	Constant
C_bac	Carbon content of bacteria	Constant
Y_su	Yield of biomass on monosaccharides	±15%
f_h2_aa	Yield (catabolism only) of hydrogen on amino acids	±15%
f_va_aa	Yield (catabolism only) of valerate on amino acids	±15%
f_bu_aa	Yield (catabolism only) of butyrate on amino acids	±15%
f_pro_aa	Yield (catabolism only) of propionate on amino acids	±15%
f_ac_aa	Yield (catabolism only) of acetate on amino acids	±15%
C_va	Carbon content of valerate	Constant
Y_aa	Yield of biomass on amino acids	±15%
Y_fa	Yield of biomass long chain fatty acids	±15%
Y_c4	Yield of biomass methane	±15%
Y_pro	Yield of biomass propionate	±15%
C_ch4	Carbon content of methane	Constant
Y_ac	Yield of biomass on acetate	±15%
Y_h2	Yield of biomass on hydrogen	±15%
k_dis	First prder parameter for disintegration	±15%
k_hyd_ch	First order parameter for hydrolysis on carbohydrates	±15%
k_hyd_pr	First order parameter for hydrolysis on proteins	±15%
k_hyd_li	First order parameter for hydrolysis on lipids	±15%
K_S_IN	Half saturation value of inorganic carbon	±15%
k_m_su	Monod maximum specific uptake rate of monosaccharides	±15%

Table 3: Table of parameter names and the amount they were varied (continued). The lower limits of pH inhibition were calculated by subtracting a random number in the given interval from the upper limit.

Parameter	Name	Varied by
K_S_su	Half saturation value of monosaccharides	±15%
pH_UL_aa	Upper limit where 50% of amino acid particulate is inhibited	±15%
pH_LL_aa	Lower limit where 50% of amino acid particulate is inhibited	pH_UL_aa −rand(0.75, 1.5)
k_m_aa	Monod maximum specific uptake rate of amino acid	±15%
K_S_aa	Half saturation value of amino acid	±15%
k_m_fa	Monod maximum specific uptake rate of long chain fatty acids	±15%
K_S_fa	Half saturation value of long chain fatty acids	±15%
K_I_h2_fa	50% inhibitory concentration of hydrogen on long chain fatty acids	±15%
k_m_c4	Monod maximum specific uptake rate of methane	±15%
K_S_c4	Half saturation value of methane	±15%
K_I_h2_c4	50% inhibitory concentration of hydrogen on methane	±15%
k_m_pro	Monod maximum specific uptake rate of propionate	±15%
K_S_pro	Half saturation value of propionate	±15%
K_I_h2_pro	50% inhibitory concentration of hydrogen on propionate	±15%
k_m_ac	Monod maximum specific uptake rate of acetate	±15%
K_S_ac	Half saturation value of acetate	±15%
K_I_nh3	50% inhibitory concentration of ammonia	±15%
pH_UL_ac	Upper limit where 50% of acetate particulate is inhibited	±15%
pH_LL_ac	Lower limit where 50% of acetate particulate is inhibited	pH_UL_ac −rand(0.5, 1)
k_m_h2	Monod maximum specific uptake rate of hydrogen	±15%
K_S_h2	Half saturation value of hydrogen	±15%
pH_UL_h2	Upper limit where 50% of hydrogen particulate is inhibited	±15%
pH_LL_h2	Lower limit where 50% of hydrogen particulate is inhibited	pH_UL_h2 −rand(0.5, 1)
k_dec_X_su	First order decay rate for monosaccharide particulates	±15%
k_dec_X_aa	First order decay rate for amino acid particulates	±15%
k_dec_X_fa	First order decay rate for long chain fatty acid particulates	±15%
k_dec_X_c4	First order decay rate for methane particulates	±15%
k_dec_X_pro	First order decay rate for propionate particulates	±15%
k_dec_X_ac	First order decay rate for acetate particulates	±15%
k_dec_X_h2	First order decay rate for hydrogen particulates	±15%
T_ad	Temperature of anaerobic digester	Equal to T_op
K_h2o	Acid/base equilibrium coefficient for water	calc. from T_base and T_ad
K_a_va	Acid/base equilibrium coefficient for valerate	Constant
K_a_bu	Acid/base equilibrium coefficient for butyrate	Constant
K_a_pro	Acid/base equilibrium coefficient for propionate	Constant
K_a_ac	Acid/base equilibrium coefficient for acetate	Constant
K_a_co2	Acid/base equilibrium coefficient for carbon dioxide	calc. from T_base and T_ad
K_a_IN	Acid/base equilibrium coefficient for inorganic nitrogen	calc. from T_base and T_ad
k_AB_va	Acid/base kinetic parameter for valerate	rand(0%, 25%)
k_AB_bu	Acid/base kinetic parameter for butyrate	rand(0%, 25%)
k_AB_pro	Acid/base kinetic parameter for propionate	rand(0%, 25%)
k_AB_ac	Acid/base kinetic parameter for acetate	rand(0%, 25%)
k_AB_co2	Acid/base kinetic parameter for carbon dioxide	rand(0%, 25%)
k_AB_IN	Acid/base kinetic parameter for inorganic nitrogen	rand(0%, 25%)
p_gas_h2o	Steady-state gas phase partial pressure of water	calc. from T_base and T_ad
k_p	Gas outlet friction	Constant
k_L_a	Gas-liquid transfer coefficient	Constant
K_H_co2	Henry's law coefficient for carbon dioxide	calc. from T_base and T_ad
K_H_ch4	Henry's law coefficient for methane	calc. from T_base and T_ad
K_H_h2	Henry's law coefficient for hydrogen	calc. from T_base and T_ad
V_liq	Volume of liquid in reactor	±15%
V_gas	Volume of gas in reactor	±15%
Q_ad	Flow rate	±15%