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The IWA Anaerobic Digestion Model No 1 (ADM1)

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Abstract The IWA Anaerobic Digestion Modelling Task Group was established in 1997 at the 8th World Congress on Anaerobic Digestion (Sendai, Japan) with the goal of developing a generalised anaerobic digestion model. The structured model includes multiple steps describing biochemical as well as physico-chemical processes. The biochemical steps include disintegration from homogeneous particulates to carbohydrates, proteins and lipids; extracellular hydrolysis of these particulate substrates to sugars, amino acids, and long chain fatty acids (LCFA), respectively; acidogenesis from sugars and amino acids to volatile fatty acids (VFAs) and hydrogen; acetogenesis of LCFA and VFAs to acetate; and separate methanogenesis steps from acetate and hydrogen/CO₂. The physico-chemical equations describe ion association and dissociation, and gas-liquid transfer. Implemented as a differential and algebraic equation (DAE) set, there are 26 dynamic state concentration variables, and 8 implicit algebraic variables per reactor vessel or element. Implemented as differential equations (DE) only, there are 32 dynamic concentration state variables.

Keywords Acetogenesis; acidogenesis; ADM1; anaerobic digestion; hydrolysis; kinetics; methanogenesis; model; VFA

Introduction

High organic loading rates and low sludge production are among the many advantages anaerobic processes exhibit over other biological unit operations. But the one feature emerging as a major driver for the increased application of anaerobic processes is the energy production. Not only does this technology have a positive net energy production but the biogas produced can also replace fossil fuel sources and therefore has a direct positive effect on greenhouse gas reduction. This will most certainly ensure the ongoing, and likely drastically increased, popularity of anaerobic digestion processes for waste treatment in the future. But why is there a need for a generic model? Several benefits are expected from the development of this first generic model of anaerobic digestion:

- increased model application for full-scale plant design, operation and optimization;
- further development work on process optimization and control, aimed at direct implementation in full-scale plants;
- common basis for further model development and validation studies to make outcomes more comparable and compatible;
- assisting technology transfer from research to industry.

Many of the above points relate to practical, industrial applications. Indeed, this is one of the areas where most benefits from the application of a generalised process model can be gained. While many different anaerobic models have been devised over the years (and indeed form the basis of the ADM1), their use by engineers, process technology providers and operators has been very limited. Two of the limiting factors have likely been the wide variety of models available and often their very specific nature. We hope that this model will help to achieve widespread utilisation of the large body of knowledge of anaerobic processes available from research studies and operational experience. Ultimately the model will support the increased application of anaerobic technology as a

sustainable waste treatment option and a viable alternative to other energy generating processes.

In this paper, the model structure, kinetic rate equations (Appendix) as well as implementation in a simple fixed volume CSTR are presented. An IWA Scientific and Technical Report (STR) was published in early 2002 (Batstone *et al.*, 2002), and contains a more complete discussion of the included processes, a review of parameter values, and a suggested base parameter set. Specific limitations of the model, the influence of these limitations on outcomes, and a conceptual approach to correcting for them are also discussed in the form of inserts.

Reaction system

The reaction system in an anaerobic digester is complex with a number of sequential and parallel steps. These reactions can be divided into two main types.

- (a) *Biochemical reactions*. These are normally catalysed by intra or extracellular enzymes and act on the pool of biologically *available* organic material. Disintegration of composites (such as dead biomass) to particulate constituents and the subsequent enzymatic hydrolysis of these to their soluble monomers are extracellular. Degradation of soluble materials are mediated by organisms intracellularly, resulting in biomass growth and subsequent decay.
- (b) *Physico-chemical reactions*. These are not biologically mediated and encompass ion association/dissociation, and gas-liquid transfer. An additional reaction, not included in the ADM1 is precipitation.

Biochemical processes

Distinguishing between available degradable (substrate) and total input COD is very important, as a considerable fraction of the input COD may be anaerobically not biodegradable (Gossett and Belser, 1982). In general, we use the term “substrate” to indicate degradable COD. Biochemical equations are the core of any model and it is possible to represent an anaerobic system using only these equations. However, to describe the effect on biochemical reactions of the physico-chemical state (such as pH and gas concentrations), physico-chemical conversions must be included as well. Most recent anaerobic models include intermediate products and the Task Group agreed on a structured model because of a number of scientific and application advantages. The philosophy of process and component inclusion was to maximise applicability while maintaining a reasonably simple model structure. The model includes the three overall biological (cellular) steps, (i.e. acidogenesis or fermentation, acetogenesis, or anaerobic oxidation of both VFAs and LCFAs and methanogenesis) as well as an extracellular (partly non-biological) disintegration step and an extracellular hydrolysis step (Figure 1).

Complex particulate waste first disintegrates to carbohydrate, protein and lipid particulate substrate, as well as particulate and soluble inert material. This step was mainly included to facilitate modelling of activated sludge digestion, as a disintegration step is thought to precede more complex hydrolytic steps (Pavlostathis and Gossett, 1986). The complex particulate waste pool is also used as a pre-lysis repository of decayed (inactive) biomass. Therefore the disintegration step could include an array of processes such as lysis, non-enzymatic decay, phase separation, and physical breakdown (e.g. shearing). All biochemical extracellular steps were assumed to be first order, which is a simplification based on empiricism, reflecting the cumulative effect of a multi-step process (Eastman and Ferguson, 1981).

Two separate groups of acidogens degrade monosaccharide and amino acids to mixed organic acids, hydrogen and carbon dioxide. The organic acids are subsequently converted

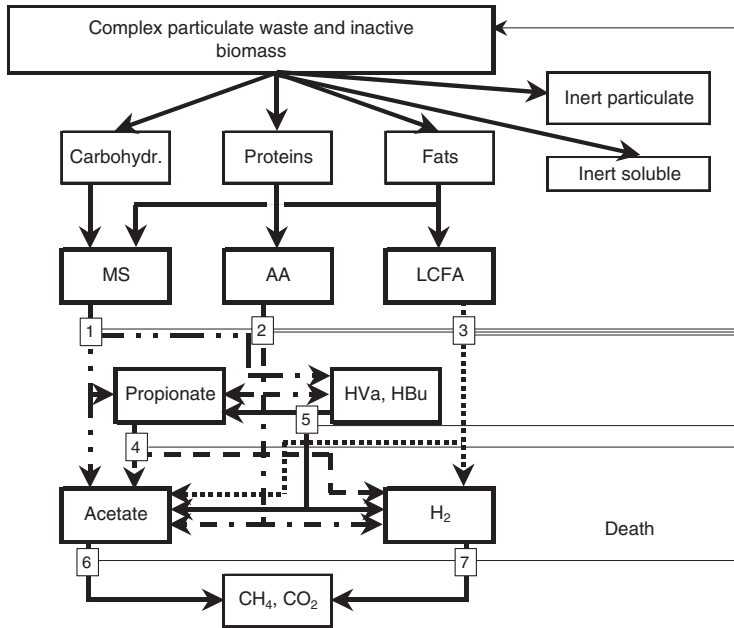


Figure 1 The anaerobic model as implemented including biochemical processes: (1) acidogenesis from sugars, (2) acidogenesis from amino acids, (3) acetogenesis from LCFA, (4) acetogenesis from propionate, (5) acetogenesis from butyrate and valerate, (6) acetoclastic methanogenesis, and (7) hydrogenotrophic methanogenesis

to acetate, hydrogen and carbon dioxide by acetogenic groups that utilise LCFA, butyrate and valerate (one group for the two substrates), and propionate. The hydrogen produced by these organisms is consumed by a hydrogen-utilising methanogenic group, and the acetate by an acetoclastic methanogenic group. Substrate uptake Monod-type kinetics (slightly different from ASM Monod growth kinetics) are used as the basis for all intracellular biochemical reactions. Biomass growth is implicit in substrate uptake. Death of biomass is represented by first order kinetics, and dead biomass is maintained in the system as composite particulate material. Inhibition functions include pH (all groups), hydrogen (acetogenic groups) and free ammonia (acetoclastic methanogens). pH inhibition is implemented as one of two empirical equations, while hydrogen and free ammonia inhibition are represented by non-competitive functions. The other uptake-regulating functions are secondary Monod kinetics for inorganic nitrogen (ammonia and ammonium), to prevent growth when nitrogen is limited, and competitive uptake of butyrate and valerate by the single group that utilises these two organic acids.

The biological kinetic rate expressions and coefficients are shown in Peterson matrix form in the Appendix (Tables A3 and A4) and follow the format of Henze *et al.* (1986). COD balancing is implicit in these equations. In many cases, inorganic carbon (i.e. CO₂ family) is the carbon source for or a product of catabolism, (i.e. uptake of sugars, amino acids, propionate, acetate and hydrogen; $j = 5, 6, 10, 11, 12$), and in these cases, the inorganic carbon rate coefficient ($v_{10,5,6,10,11,12}$) can be expressed as a carbon balance (see entries in Tables A3 and A4).

Physico-chemical processes

Physico-chemical reactions are defined here as those not mediated by micro-organisms, and which commonly occur in anaerobic digesters such as:

1. Liquid-liquid reactions (i.e. ion association/dissociation: rapid).

2. Gas–liquid exchanges (i.e. gas transfer: rapid-medium).
3. Liquid–solid transformations (i.e. precipitation and solubilisation of ions: medium–slow).

Only the first two process types have been commonly addressed in anaerobic digestion models, probably because of the difficulties in implementation of liquid–solid transformations. However, liquid–solid reactions are very important in systems with high levels of cations; especially those that readily form carbonate precipitates such as Mg^{2+} and Ca^{2+} . Because modelling precipitation is complicated, and because models that include precipitation reactions are recent (van Langerak *et al.*, 1997), the Task Group decided not to include precipitation in the ADM1.

The physico-chemical system is very important when modelling anaerobic systems because:

- a number of biological inhibition factors can be expressed such as pH, free acids and bases, and dissolved gas concentrations;
- major performance variables such as gas flow and carbonate alkalinity are dependent on correct estimation of physico-chemical transformations;
- often, pH control with a strong acid or base is the major operating cost. In this case the control setpoint (pH) is calculated from the physico-chemical state.

The most important acid-base pairs in anaerobic systems are: NH_4^+/NH_3 ($pK_a = 9.25$), CO_2/HCO_3^- ($pK_a = 6.35$), and VFA/VFA^- ($pK_a \sim 4.8$), as well as the $H_2O/OH^-/H^+$ system ($pK_w = 14.00$) (all pK_a values for 298 K (Lide, 2001)). Because dissociation/association processes are very rapid compared to other reactions (especially biochemical), they are often referred to as equilibrium processes, and can be described by algebraic (rather than differential) equations. The three main process gas components are: CO_2 (medium solubility), CH_4 (low solubility) and H_2 (low solubility), as well as water vapour. Equations describing physico-chemical reactions are not shown in the Appendix, but details on the implementation methodology are given below.

Implementation

An anaerobic digestion system normally consists of a reactor with a liquid volume, and a sealed gas headspace at atmospheric pressure with the gas removed to downstream utilisation. The system to be demonstrated here is a completely stirred reactor with a single input and output stream, and constant liquid volume ($q_{out} = q_{in}$, Figure 2).

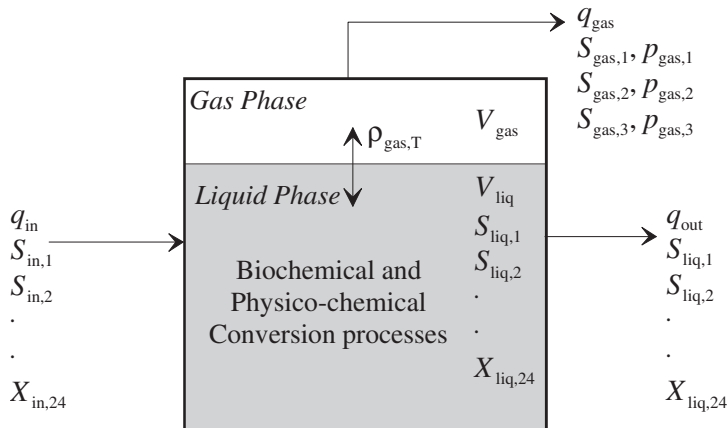


Figure 2 Schematic of a typical single-tank digester (q = flow, $m^3 \cdot d^{-1}$; V = volume, m^3 ; $S_{stream,i}$ = concentration of liquid components; $X_{stream,i}$ = concentration of particulate components; all in $kg \text{ COD} \cdot m^{-3}$; i is the component index).

Implementation depends on whether the liquid phase physico-chemical processes are implemented as algebraic or kinetic rate equations. In the first case, a differential and (implicit) algebraic equation (DAE) solver is required. In the second case, there is a larger number of differential equations, the model is stiffer, and some errors may be introduced. The mass balance for each state component in the liquid phase is as shown in Equation 1:

$$\frac{dS_{\text{liq},i}}{dt} = \frac{q_{\text{in}}S_{\text{in},i}}{V_{\text{liq}}} - \frac{S_{\text{liq},i}q_{\text{out}}}{V_{\text{liq}}} + \sum_{j=1-19} \rho_j v_{i,j} \quad (1)$$

where the term $\sum_{j=1-19} \rho_j v_{i,j}$ is the sum of the kinetic rates for process j multiplied by $v_{i,j}$ (see Appendix).

In addition to the rates in the Appendix, a rate term for transfer of gas components to the gas headspace should be added. Because the rate of gas transfer is comparable to that of biological processes, a dynamic equation should be used. As an example, transfer of CO_2 is shown in Equation 2.

$$\rho_{10,T} = k_L a_{\text{CO}_2} (S_{\text{CO}_2,\text{liq}} - K_{\text{H,CO}_2} p_{\text{CO}_2,\text{gas}}) \quad (2)$$

where $\rho_{10,T}$ is the additional rate term, $k_L a$ is the dynamic gas–liquid transfer coefficient (d^{-1}), $K_{\text{H,CO}_2}$ is the Henry's law equilibrium constant ($\text{M}\cdot\text{bar}^{-1}$), p_{CO_2} is the CO_2 gas phase partial pressure (bar) and $S_{\text{CO}_2,\text{liq}}$ is the liquid CO_2 concentration (M).

If the liquid phase physico-chemical equations are implemented as algebraic equations, the acid/base pairs are normally lumped as a combined dynamic state variable. The concentrations of individual acids and bases are calculated from acid-base equilibria, and a charge balance is used to complete the implicit set of equations (in S_{H^+}). Therefore, implemented as a DAE system, carbon dioxide (S_{CO_2}) and bicarbonate ($S_{\text{HCO}_3^-}$) are lumped as a single dynamic state variable in inorganic carbon ($S_{\text{IC}} \equiv S_{10}$). However, if the liquid phase physico-chemical equations are implemented as dynamic equations, S_{CO_2} and $S_{\text{HCO}_3^-}$ are implemented as dynamic state variables, S_{IC} is redundant, and an additional dynamic rate equation is used for acid-base transfer (Eq. 3). The biological production rates in the Appendix can be either in the acid state equations or the base state equations (but not both), though we recommend having the equations in the free form (i.e. CO_2 , HAc , etc).

$$\rho_{\text{A/BCO}_2} = -\rho_{\text{A/BHCO}_3} = k_{\text{A/B CO}_2} (S_{\text{HCO}_3^-} \cdot S_{\text{H}^+} - K_{\text{a,CO}_2} \cdot S_{\text{CO}_2}) \quad (3)$$

where $\rho_{\text{A/BCO}_2}$ is the production rate of CO_2 from HCO_3^- , $k_{\text{A/BCO}_2}$ is the dynamic constant (nominally set to only one order of magnitude higher than the highest biological rate constant to reduce model stiffness) and $K_{\text{a,CO}_2}$ is the $\text{CO}_2/\text{HCO}_3^-$ equilibrium coefficient. S_{H^+} is the only algebraic variable in this set of equations, and it is calculated from the charge balance (with hydroxide, S_{OH^-} either substituted for using the equilibrium expression, or eliminated from the charge balance). Therefore the algebraic equation set is explicit. When implemented as either DAE or DE sets, cations and anions can also be included (S_{cat} , S_{an} , respectively), to simulate the influence of strong bases or acids, respectively, in feed streams. These are included in the charge balance according to their nominal valency, but are otherwise inert dynamic state components.

Gas phase mass balance equations are as for Eq. 2, except that there is no production rate term except for gas transfer to liquid, no input stream, and the output flow is generally set equal to the total transfer rate, or calculated from headspace pressure and restricted flow through an orifice (the outlet pipe and downstream units). It is important to correct the headspace pressure or flow for the water vapour partial pressure at the reactor temperature.

Because of space limitations, parameters are not presented here. However, the STR contains a review of parameters, as well as a suggested parameter set. Alternatively, the review paper by Pavlostathis and Giraldo-Gomez (1991) is recommended.

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Appendix

The Task Group decided to use a $\text{kgCOD}\cdot\text{m}^{-3}$ (g l^{-1}) basis, with inorganic carbon (HCO_3^- and CO_2) and nitrogen (NH_4^+ and NH_3) in $\text{kmoleC}\cdot\text{m}^{-3}$ and $\text{kmoleN}\cdot\text{m}^{-3}$, respectively ($\text{kmole}\cdot\text{m}^{-3}\equiv\text{mole}\cdot\text{l}^{-1}\equiv\text{M}$). This is not in agreement with the ASM models and waste treatment practice, where mg l^{-1} is generally used. However, upstream and resource utilisation industries (i.e. biogas), and the majority of anaerobic modelling is conducted using $\text{kg}\cdot\text{m}^{-3}$ basis, physico-chemical constants and pH are universally in a molar (M, $\text{mole}\cdot\text{l}^{-1}$ or $\text{kmole}\cdot\text{m}^{-3}$) basis, and this basis is in agreement with the use of SI units. Implementing in $\text{mgCOD}\cdot\text{l}^{-1}$ and mM is relatively simple, as it requires only changes in K_S values, and modification of $\text{p}K_a$ and K_a values, and we encourage the use of $\text{mg}\cdot\text{l}^{-1}$ if required (e.g. in wastewater treatment systems). Integration with the IWA ASM models is specifically addressed in the STR. Nomenclature and units are shown in Table A1.

Table A1 Nomenclature and units used

Symbol	Description	Units
C_i	carbon content of component i	kmoleC·kgCOD ⁻¹
i	component index (see appendix)	
I	inhibition function (various, see Table A2)	
j	process index (see appendix)	
$k_{A/B,i}$	acid-base rate constant for component i	M ⁻¹ ·d ⁻¹
k_{dec}	first order decay rate for biomass death	d ⁻¹
k_{La}	gas-liquid transfer coefficient	d ⁻¹
k_m	specific Monod maximum uptake rate	kgCOD·m ⁻³ _S·kgCOD·m ⁻³ _X·d ⁻¹
K_a	acid-base equilibrium constant	M (kmole·m ⁻³)
K_H	Henry's law coefficient	M·bar ⁻¹
K_I	inhibition constant	nominally kgCOD·m ⁻³
K_S	Monod half saturation constant	kgCOD·m ⁻³
N_i	nitrogen content of component i	kmoleN·kg COD ⁻¹
p_{gas}	pressure of gas	bar
pH	$-\log_{10}[S_{H^+}]$	
pK _a	$-\log_{10}[K_a]$	
q	flow	m ³
S_i	soluble component i (dynamic or algebraic variable)	nominally kgCOD·m ⁻³
S_I	inhibitory component	nominally kgCOD·m ⁻³
t	time	d
T	temperature	K
V	volume	m ³
X_i	particulate component i	kgCOD·m ⁻³
$Y_{substrate}$	yield of biomass on substrate	kgCOD_X·kgCOD_S ⁻¹
$v_{i,j}$	rate coefficients for component i on process j	nominally kgCOD·m ⁻³
$f_{product,substrate}$	yield (catabolism only) of product on substrate	kgCOD·kgCOD ⁻¹
ρ_j	rate for process j	kgCOD·m ⁻³

Table A2 Inhibition expressions

Description	Equation	Used for	ref
Non-competitive inhibition	$I = \frac{1}{1 + S_I / K_I}$	hydrogen inhibition free ammonia inhibition	1
Substrate limitation	$I = \frac{S_I}{S_I + K_I}$	total ammonia limitation	
Empirical	$I = \frac{1 + 2 \times 10^{0.5(pH_{LL} - pH_{UL})}}{1 + 10^{(pH - pH_{UL})} + 10^{(pH_{LL} - pH)}}$	pH inhibition when both high and low pH inhibition occur	2
	$I = \exp\left(-3\left(\frac{pH - pH_{UL}}{pH_{UL} - pH_{LL}}\right)^2\right) \Big _{I=1}$	pH inhibition when only low pH inhibition occurs	3

Note: For the first pH function, pH_{UL} and pH_{LL} are upper and lower limits where the group of organisms is 50% inhibited, respectively. For example, acetate utilising methanogens with a pH_{UL} of 7.5 and a pH_{LL} of 6.5 have an optimum at pH 7. For the second function, pH_{UL} and pH_{LL} are points at which the organisms are not inhibited, and at which inhibition is full respectively. Acetate utilising methanogens with a pH_{UL} of 7 and a pH_{LL} of 6 will be completely inhibited below pH 6 and not inhibited above pH 7.

References: 1. Pavlostathis and Giraldo-Gomez (1991), 2. Angelidaki *et al.* (1993), 3. Ramsay (1997)

