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## **Modelling Anaerobic Digesters in Three Dimensions**

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**ABSTRACT** Anaerobic digesters are an environmental technology that treats waste products while simultaneously producing renewable energy in the form of biogas. Modelling this process is challenging as it involves dozens of interrelated biochemical processes driven by hundreds of species of microorganisms whose populations are constantly in flux. The current state-of-the-art model is the Anaerobic Digestion Model No. 1 (ADM1), published by the International Water Association [1]. ADM1 is a bulk model with no spatial resolution, useful for lab-scale digesters, but problematic for full-scale digesters. The purpose of this research is to improve on this model by adding three-dimensional spatial resolution, as well as a fully realized Computational Fluid Dynamics (CFD) flow model. The resulting model, Anaerobic Digestion Model with Multi-Dimensional Architecture (ADM-MDA), is presented.

**Keywords:** anaerobic digesters, ADM1, CFD, biogas

**INTRODUCTION** Anaerobic digestion, a process that breaks down biomass in a low-oxygen environment, has been used reliably by animals even before humans walked the Earth. Today, the process is well suited to waste-management and energy production, as it reduces complex biological wastes to simpler constitutive components, while simultaneously producing an energy-rich biogas. Despite the prevalence of anaerobic digestion in nature, attempting to harness this process industrially has proven to be challenging as it can be unreliable, difficult to control, and relatively costly. As such, the current state of anaerobic digester technology can be likened to the

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early automotive industry: a driver also had to be a mechanic because the car would likely breakdown before arriving at the destination. That is, to operate an anaerobic digester, skilled professionals and trained personnel are required, particularly during the start-up phase.

Classical scaling issues could explain their low reliability whereby lab-scale digesters do not behave the same as full-scale digesters. Biochemical computer models for anaerobic digesters have seen some success when validated against lab-scale experimental data; however, validation against data from full-scale digesters has been more difficult to achieve. Batstone et al. (2005) validated an anaerobic digester model against two different size reactors and found entirely different physical dynamics occurring in each. Anaerobic digestion models are almost exclusively bulk models, with properties assumed uniform throughout the reactor. Furthermore, anaerobic digesters are modelled almost exclusively from a biochemical perspective, with the dynamics of fluid flow largely being ignored. These are valid assumptions for a beaker in a lab environment, but perhaps not for full-scale thousand to million litre digesters where significant stagnation regions, and various concentration, shear stress and temperature gradients can develop. A conventional anaerobic digestion model cannot capture these phenomena; however, a spatially resolved model with an integrated fluid flow package would. Anaerobic Digestion Model with Multi-Dimensional Architecture (ADM-MDA) is this model, using Anaerobic Digestion Model No. 1 (ADM1) (Batstone et al., 2002) for the biochemistry and computational fluid dynamics (CFD) for the fluid flow.

**LITERATURE REVIEW** Literature covering numerical models of anaerobic digesters can be divided into three broad categories: models with fluid flow, models with biochemistry, and models with both fluid flow and biochemistry.

**Models with Fluid Flow** Numerical studies of digester fluid flow generally ignore the biochemical reactions, and focus only on the fluid motion. Rudniak et al. (2004) performed a CFD and experimental investigation into a lab-scale impeller-stirred reactor, with a focus on the thermodynamics of exothermal chemical reactions. Vesvikar et al. (2005) studied a gas-mixed mock digester with Newtonian fluids. The authors used both CFD and radioactive particle tracking, and found good agreement between the two, with the exception of velocity data. Wu et al. (2008) performed a CFD study into flow in lab-scale and pilot-scale digesters, focusing on the effect of using a non-Newtonian fluid model. Meroney et al. (2009) studied the effect of draft tube mixing on pilot-scale and full-scale anaerobic digesters using CFD and tracer injection experimental data. Terashima et al. (2009) performed a CFD investigation into mixing in full-scale anaerobic digesters. The authors incorporated rheological properties of the biomass into the simulation using a pseudo-plastic viscosity model. They compared the results against a dye tracer experiment, and found the results to be in good agreement. The authors also created a non-dimensional parameter, “uniformity index” that proved useful in interpreting the data. Yu et al. (2011) performed an experimental and CFD study into the use of a helical impeller for mixing digesters with high %TS. The authors address the trade-off between improving mixing and increasing shear rate, which can be detrimental for biological components.

**Models with Biochemistry** Early biochemistry models for anaerobic digesters were simple and steady-state, most of which applied only to CSTR digesters (Tramšek et al., 2007); however as anaerobic digester technology became more complex, the models also needed to be more complex (Parker, 2005). Up until 2002 anaerobic digester modelling focused on model fundamentals (Batstone et al., 2006a), and the field was populated with a diversity of multispecies models with differing assumptions and configurations (Parker, 2005), leading to confusion as to which models could or could not be compared (Kleerebezem, 2006). In an attempt to create a universal framework for anaerobic digestion models, and building on earlier success with activated sludge models (Parker, 2005), the International Water Association (IWA) published Anaerobic Digestion Model No. 1 (ADM1) (Batstone et al., 2002). Based on the subsequent dearth of papers featuring

non-ADM1 models of anaerobic digesters, some of the original ADM1 authors make the assertion that it has, therefore, been successful (Batstone, et al. 2006a). There have been non-ADM1 models employed since this time (Siegrist et al., 2002; Keshtkar et al., 2003; Paquin et al., 2006; Biswas et al., 2007; Rodríguez et al., 2008; Jones et al., 2008; von der Schulenburg et al., 2009; and Valle-Guadarrama et al. 2011); however this may be partly attributed to the complexity of ADM1, and the need for a simplified model for specific applications. There have been considerably more ADM1-related publications.

Depending on the specific implementation, ADM1 has approximately one hundred coefficients, each of which affects the model behaviour. One of the chief criticisms of ADM1 is that some of these coefficients are difficult, or impossible to determine experimentally (Kleerebezem, 2006). A large cross-section of ADM1 studies focuses on determining these coefficients (Jeong et al., 2004; Picioreanu et al., 2005; de Gracia et al., 2006; Batstone et al., 2006b; Tramšek et al., 2007; Page et al., 2008; Mu et al., 2008; Tartakovsky et al., 2008; Lee et al., 2009; and Batstone et al., 2009). Some studies also perform a sensitivity analysis (Jeong et al., 2004; Tartakovsky et al., 2008; and Lee et al., 2009) in which coefficients are varied individually and their relative impact is evaluated.

Since its publication, there have been many studies in which ADM1 modifications are introduced and validated. This suggests that the anaerobic digestion community has accepted ADM1 as the standard model foundation. Some of these modifications are presented here. Blumensaat et al. (2005) modified ADM1 for two-stage anaerobic digestion, and validated it against a pilot-scale reactor. Parker et al. (2006) modified ADM1 to include odorous emissions modelling; however the parameters for the model had large uncertainty. Rodríguez et al. (2006) modified the carbohydrate fermentation model, but found no significant effect compared to the original model. Huete et al. (2006) created a modified version of ADM1 that characterizes all components in terms of elemental mass fractions, and is therefore mass-conserving. The authors also provided an example of its implementation. This model is further extended by de Gracia et al. (2006), de Gracia et al. (2007) and Galí et al. (2009). Kauder et al. (2007) combined ADM1 with the IWA's Activated Sludge Model (ASM) for a sequencing batch reactor. Lübken et al. (2007) modified the disintegration model and other parameters to better capture inlet conditions, and performed an energy balance of the digestion process. Jeppsson et al. (2007) reports on a larger project undertaken to evaluate control schemes for wastewater treatment plants. The project successfully incorporates ADM1 into a wider simulation system. Brdjanovic et al. (2007) combined ADM1 with ASM to improve process control at a wastewater treatment plant in India. Nielsen et al. (2008) modified the ion model in ADM1 and validated the changes against a series of lab-scale experiments.

Even as recently as 2005, little experience existed in the use of ADM1 (Blumensaat et al., 2005). Since then, several validations have been published for ADM1. These are papers that compare model results with experimental results. Most of the studies focusing on modifications or parameters also included validations (Blumensaat et al., 2005; Lübken et al., 2007; Page et al., 2008; and Galí et al., 2009). Additionally, Shang et al. (2005) validated ADM1 against two full-scale wastewater treatment plants under steady-state conditions, and found most values within 10%, although there were few data points. Lee et al. (2009) performed a sensitivity analysis, parameter calibration, and validation for a lab-scale temperature-phased anaerobic digester, and found good agreement between model and experiment. Ozkan-Yucel et al. (2010) calibrated and validated ADM1 against a full-scale wastewater treatment plant under dynamic conditions. The model results are in good agreement with the experimental data.

***Models with both Fluid Flow and Biochemistry*** A general anaerobic digester model requires not only the inclusion of CFD, it also requires a fully spatially resolved ADM1 model. Some studies have accomplished some aspects of this undertaking. In a PhD thesis, Fleming (2002) presented an anaerobic digestion model that incorporates both a biochemistry model as well as a CFD flow model for anaerobic digesters. As such, this model achieves some of the objectives of ADM-MDA;

however, it is specific only to covered lagoon psychrophilic digesters, whereas ADM-MDA aims to be a general anaerobic digestion model. Furthermore, Fleming's model employs a biochemistry model from 1988. Its application-specific nature, coupled with the fact that ADM1 was published in the same year may have limited its subsequent use. Keshtkar et al. (2003) simulated non-ideal mixing conditions in an anaerobic digester by breaking the fluid into two bulk regions: a flow-through region, and a retention region. By varying the interface between the two regions, non-ideal flow conditions were approximated. The authors used a non-ADM1 biochemical model. Batstone et al. (2005) employed two strategies to simulate plug-flow conditions. The first was Aquasim 2.1d, a proprietary implementation of ADM1 for plug-flow reactors that involves one spatial dimension of discretization. The second was to link multiple ADM1 simulations in series to produce an approximation of one dimensional discretization. The authors compared a lab-scale reactor with a pilot-scale reactor and found that the lab-scale reactor behaved like a plug-flow digester; whereas the pilot-scale reactor behaved like a CSTR digester. Mu et al. (2008) and Tartakovsky et al. (2008) developed a model for anaerobic digesters that has one dimension of spatial resolution; however, the spatial variation is achieved using an empirical relation, not discretization.

Anaerobic digesters with fixed-film microbial growth, known as a biofilm, have obvious spatial variations, exhibiting strong concentration gradients at the interface between the biofilm and the fluid. Numerous studies have focused on spatial resolution inside these reactors (Picioreanu et al., 2004; Picioreanu et al., 2005; Laspidou et al., 2005; Batstone et al., 2006b; and von der Schulenburg et al., 2009). Most of these focus only on the spatial distribution of the biofilm itself, employing ADM1 only at the interface between the biofilm and the fluid, and applying a bulk model to the fluid region (Picioreanu et al., 2004; and Picioreanu et al., 2005), or ignoring the bulk fluid entirely (Batstone et al., 2006b). von der Schulenburg et al. (2009) resolves fluid flow within porous media, but again, the biochemical model is only applied close to the biomass where advection is assumed to be zero. Laspidou et al. (2005) employs the mathematical concepts of cellular automata to modelling biofilm growth, an entirely different construct than the other models. Cellular automata are strictly Cartesian in space, and simulations with these produce grid-related artefacts. The model employs a simple biochemistry model, and does not have a CFD flow model.

**THEORY** ADM1 models an anaerobic digester as two volumes: a liquid volume representing the bulk fluid, and a gas volume representing the head space above the reactor. Most reactions occur within a bulk liquid volume where the mass balance equation for an arbitrary species, *var*, is:

$$V_{liq} \frac{dS_{var}}{dt} = \frac{V_{liq}}{Q_{liq}} (S_{var,in} - S_{var}) + R_{var}. \quad (1)$$

The equations for the gas volume vary depending on the specific implementation, but they are similar in form to this equation.

**Reaction Kinetics** The last term in Equation (1),  $R_{var}$ , is the mass produced or lost in biochemical reactions. This reaction term is what ties together the mass balance equations for all the species in the model. Researchers often use a Peterson matrix to express this term in an easily readable form. Table 1 is a sample Peterson matrix, representing the reactions shown in Figure 1 below it. Each row in the matrix represents a single process, showing the relative changes in mass, and the rate at which this reaction takes place. The terms in the centre of the matrix are yields, and the rightmost column is the reaction rate. The reaction term is calculated by summing the mass contribution to that species from each row. Table 1 is a simplified Peterson matrix; the full Peterson matrix has more than 30 variables and more than 20 reactions, although many variations exist.

**Inhibition** Several types of inhibition are included in ADM1, such as pH inhibition, hydrogen inhibition, and competitive uptake inhibition. The exact inhibitions depend on the implementation. Inhibition is most often modelled as a reduction in the reaction rate, although yield reductions, and increased decay rates are also possible.

Table 1. Peterson matrix for disintegration and hydrolysis

	Component →	i	0	1	2	3	4	5	6	7	8	Rate
j	Process ↓		$S_{su}$	$S_{aa}$	$S_{fa}$	$S_l$	$X_c$	$X_{ch}$	$X_{pr}$	$X_{li}$	$X_l$	$\rho_j$
0	Disintegration					$f_{sl,xc}$	-1	$f_{ch,xc}$	$f_{pr,xc}$	$f_{li,xc}$	$f_{xl,xc}$	$k_{dis}X_c$
1	Hydrolysis of Carbohydrates	1						-1				$k_{hyd,ch}X_{ch}$
2	Hydrolysis of Proteins			1					-1			$k_{hyd,pr}X_{pr}$
3	Hydrolysis of Lipids	$1-f_{fa,li}$			$f_{fa,li}$					-1		$k_{hyd,li}X_{li}$

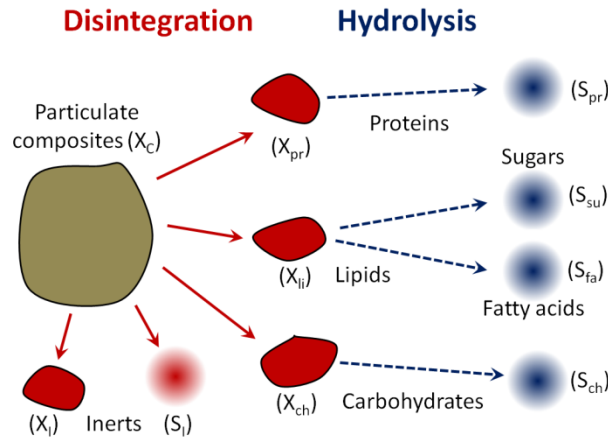


Figure 1. Disintegration and hydrolysis stages

**Numerical Methods** Solving ADM1 as a pure ODE set is not feasible, as its timestep and numerical precision requirements are impractical. To solve this problem, researchers remove several variables from the ODE set and solve them independently, based on equilibrium conditions. These solution methods are custom written.

**ADM-MDA Theory** When spatial variation is introduced into ADM1, the set of ODEs becomes a set of partial differential equations (PDE). Analogous to Equation (1), the mass balance equation for an arbitrary species,  $var$ , is:

$$\frac{\partial S_{var}}{\partial t} + \frac{\partial U_x S_{var}}{\partial x} + \frac{\partial U_y S_{var}}{\partial y} + \frac{\partial U_z S_{var}}{\partial z} = \frac{1}{\rho} \left[ \frac{\partial}{\partial x} \left( \Gamma \frac{\partial S_{var}}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma \frac{\partial S_{var}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \Gamma \frac{\partial S_{var}}{\partial z} \right) \right] + R_{var}. \quad (2)$$

In a typical ADM-MDA simulation, there are thirty to forty manifestations of Equation (2).

**SOLVER DEVELOPMENT** Challenges that must be overcome include:

- handling the reaction term;
- accommodating ADM1 modifications; and
- time and length scale differences.

**Handling the Reaction Term** Most of the terms in Equation (2) come from convective and diffusive transport. These terms are handled regularly in the field of CFD; however, the reaction term,  $R_{var}$ , is not. Conventional CFD handles equations of this kind one at a time, but the presence of  $R_{var}$  makes this undesirable, given the stiff nature of the equation set. Consequently, a method must be found that solves these simultaneously. There are two types of solution methods that can achieve this: using an ODE reaction solver, or using a coupled PDE solver. Both of these methods are implemented in ADM-MDA.

The ODE reaction solver uses CFD to transport the species, and then employs a conventional ODE solver for the reactions. Currently this algorithm is limited by the relation:

$$\frac{U\Delta t}{\Delta x} \leq 1, \quad (3)$$

where  $\Delta t$  is the timestep and  $\Delta x$  is the grid spacing.

The coupled PDE solver simultaneously solves the species transport and reaction terms by incorporating these relations directly into the solution matrix. At present, a point-implicit coupled solver is employed, which cannot be easily paralleled; however a full field block-coupled solver is currently being implemented.

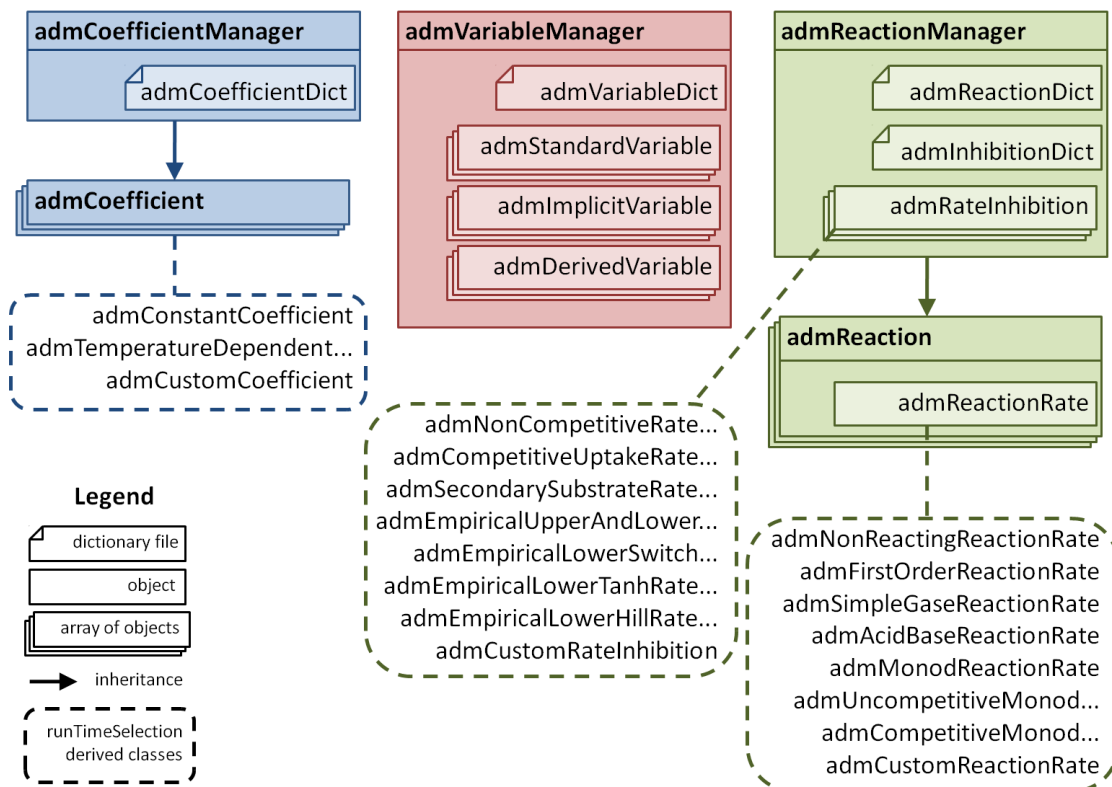


Figure 2. ADM-MDA model framework

**Accommodating ADM1 Modifications** As discussed in the literature review, ADM1 researchers frequently make modifications to the model. Furthermore, variables are often pulled out of the ODE set and solved using custom-written routines. To accommodate modifications, ADM-MDA is given a flexible design where nothing is hard-coded. The Peterson matrix is read from text files; custom reaction rates, inhibition models, and coefficient dependencies can be designed and input in text files. To accommodate the custom-written routines, ADM-MDA allows *user-defined functions* can be created. These are called by the solver at various positions in the algorithm using *function hooks*.

A potential problem with flexible model design is the loss of efficiency. A flexible model cannot know which calculations are always zero, therefore it must cycle through all possibilities; whereas a hard-coded algorithm can be streamlined, performing only the exact calculations necessary. This is overcome by using an initialization procedure that maps the non-zero functions, thus allowing the flexible model efficiency to approach that of a hard-coded model.

**Time and Length Scale Differences** The time and length scales of the biochemical reactions are greater than that of the fluid flow, possibly several orders of magnitude greater. To account for time scale differences, ADM-MDA distinguishes between *transient* flow and *steady state* flow. When flow conditions are changing, the biochemistry is disabled, and the flow solution is advanced at a small timestep until steady state is achieved. At this point, the flow field is fixed and the biochemistry is solved at a greater timestep. To account for length scale differences, two grids of different densities are used. Algorithms that interpolate between grids, termed *restriction* and *prolongation*, are well established in CFD.

**Model Framework** Three main components to the model are: the coefficients, the variables, and the reactions, as shown in Figure 2, above. The dotted lines group ready-made components specific to ADM1. The last item in each group is a *custom* object that users can use to define virtually any behaviour. Furthermore, should the custom objects be inadequate, the flexible nature of the framework allows users to easily add any other components to these lists without having to change anything else.

**RESULTS** Preliminary results have been acquired. To achieve *verification*, ADM-MDA and ADM1 results are compared under identical conditions, with the volumetric averaging applied to ADM-MDA to enable comparison. All 46 variables show no appreciable deviation after 100 days of simulation time. The dissolved hydrogen gas concentration was chosen as a sample of the dataset and is displayed in Figure 3, below. This is a *verification*, not a *validation*, therefore the results are not tied to any physical experiment; rather, they demonstrate that the algorithm performs correctly.

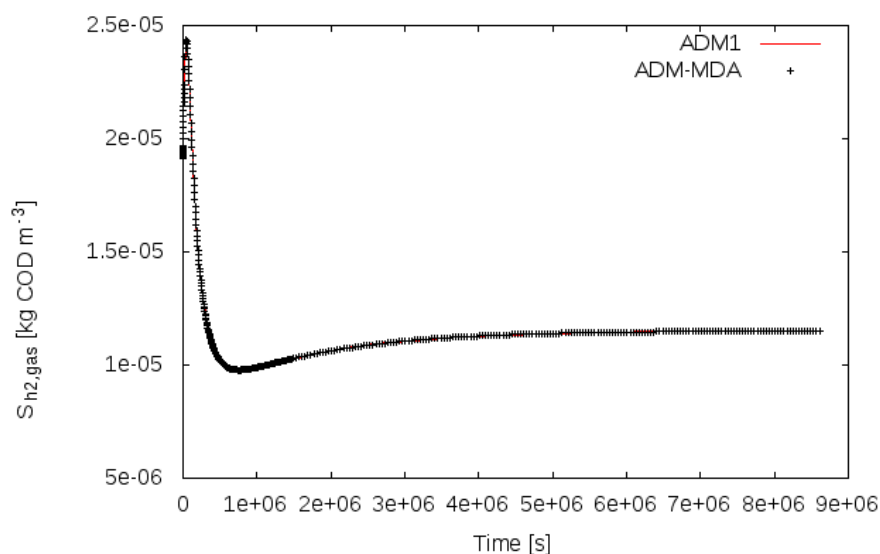


Figure 3. Dissolved hydrogen gas, ADM-MDA and ADM1.

**CONCLUSION** A spatially resolved anaerobic digestion model was developed and has been verified with ADM1. The model is flexible: users can define the variables, reactions, and coefficients to solve; custom reaction rates functions, inhibition models, and coefficient-variable co-dependency can be created using text files alone; and custom implicit routines are possible with user-defined functions and function hooks. Two solver algorithms have been developed: an ODE solver that handles the biochemistry with conventional ODE solution methods, and a coupled PDE solver that uses PDE solution methods to solve biochemistry and transport simultaneously. These solvers have been compared against ADM1 and verification has been achieved.

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