A general three-dimensional extension to ADM1: the importance of an integrated fluid flow model

David L. F. Gaden[1] and Eric L. Bibeau[2]

[1]Department of Mechanical & Manufacturing Engineering, University of Manitoba, R3T 2N2, Winnipeg, Canada (Email: *david_gaden@umanitoba.ca*)
[2]Department of Mechanical & Manufacturing Engineering, University of Manitoba, R3T 2N2, Winnipeg, Canada (Email: *Eric.Bibeau@ad.umanitoba.ca*)

Abstract
The current state-of-the-art model for anaerobic digesters is Anaerobic Digestion Model No. 1 (ADM1). It is a bulk model with a framework that ignores spatial variations, leading to several inherent limitations. Anaerobic Digestion Model with Multi-Dimensional Architecture (ADM-MDA) is an extension to ADM1 that incorporates spatial discretization and computational fluid dynamics (CFD). A comparison between ADM1 and ADM-MDA shows that under some conditions, spatial variation alone can make the difference between a healthy digester and digester failure. These findings underscore the importance of CFD in digester simulations. This paper presents the results of this four-year numerical model development project.

Keywords
3D; ADM1; CFD; modelling; OpenFOAM; spatial resolution

INTRODUCTION

Anaerobic digestion modelling has traditionally been more focused on the biochemistry of digestion, and less focused on the fluid flow and reactor geometry. Anaerobic Digestion Model No. 1 (ADM1) (Batstone, Keller et al., 2002) is such a model, with a solid biochemical foundation, but little, if any, consideration of fluid flow. Intuitively this makes sense, as the biochemistry of anaerobic digesters is considerably more complicated than the fluid flow, particularly considering the fluid velocities can be near zero. However, fluid flow and thermal gradients may impact the model more significantly than this line of thinking suggests. Therefore, this project implements Anaerobic Digestion Model with Multi-Dimensional Architecture (ADM-MDA) (Gaden, 2013), a three-dimensional implementation of ADM1 with an integrated flow model.

MODEL DEVELOPMENT

Extending the governing equations of ADM1 from a bulk model to three dimensions is achieved by including spatial variables in the derivation. For instance, the mass balance for a species changes from:

$$\frac{dS_{var}}{dt} - \frac{V_l}{Q_l}\left(S_{var,in} - S_{var}\right) = r_{var},$$

to:

$$\frac{\partial S_{var}}{\partial t} + \boldsymbol{\nabla} \bullet \left(\mathbf{U} S_{var}\right) - \boldsymbol{\nabla} \bullet \Gamma_{var} \boldsymbol{\nabla} S_{var} = r_{var}.$$

However, solving the new equation set is non-trivial as the introduction of spatial resolution changes a differential-algebraic equation set (DAE) to a partial differential algebraic equation set (PDAE), and few suitable solvers exist.

This project develops Coupled-Reaction-Advection-Flow Transient Solver (CRAFTS) to handle the new numerical framework. CRAFTS is a general reaction solver for single-phase, incompressible fluid flows. It allows users to define their own variables, reactions, inhibitions, coefficients and control logic without requiring any programming. CRAFTS also has a framework for User-Defined Functions (UDFs) that allows for custom algebraic algorithms, such as ADM1's Newton-Raphson ion model. CRAFTS is a novel PDAE solver that also employs a novel programmable logic controller (PLC) emulator. CRAFTS is built using OpenFOAM®, a free and open source CFD suite.

CASE SETUP

The case involves a 100 m^3 rectangular digester. Fluid injection events of occur daily for two minutes at a velocity of 0.05 ms^{-1}, giving a hydraulic retention time of only 8.33 days. Fluid mixing events occur for ten minutes every hour.

RESULTS

ADM1 and ADM-MDA simulations were performed identically for these conditions. Most variables show little differences between the two models, however, the continuum assumption of ADM1 leads to subtle differences in mass exchanged during each fluid injection event. These differences can amplify quickly with highly sensitive dynamic systems, such as ADM1. Figure 1a shows the two models have a significant disagreement with the total acetate concentration, S_{ac}. ADM1 suggests a stable digester, whereas ADM-MDA indicates an unhealthy digester. This disagreement can be explained by the fact that acetate degraders can be seen washing out only in ADM-MDA, Figure 1b.

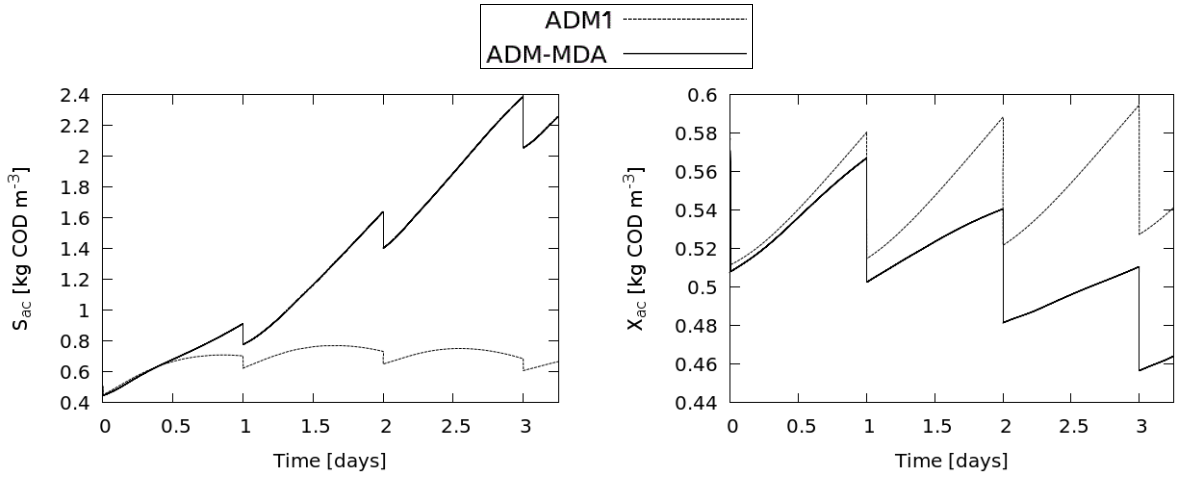

Figure 1a. Total acetate concentration, S_{ac}

Figure 1b. Acetate degraders, X_{ac}

The spatial data that ADM-MDA provides can also be useful for design purposes. For instance, the model showed dissolved methane building up at the centre of the reactor, Figure 2a. This suggests a change in mixing strategy might improve gas transfer rate. By way of contrast, ADM1 does not include spatial data, Figure 2b.

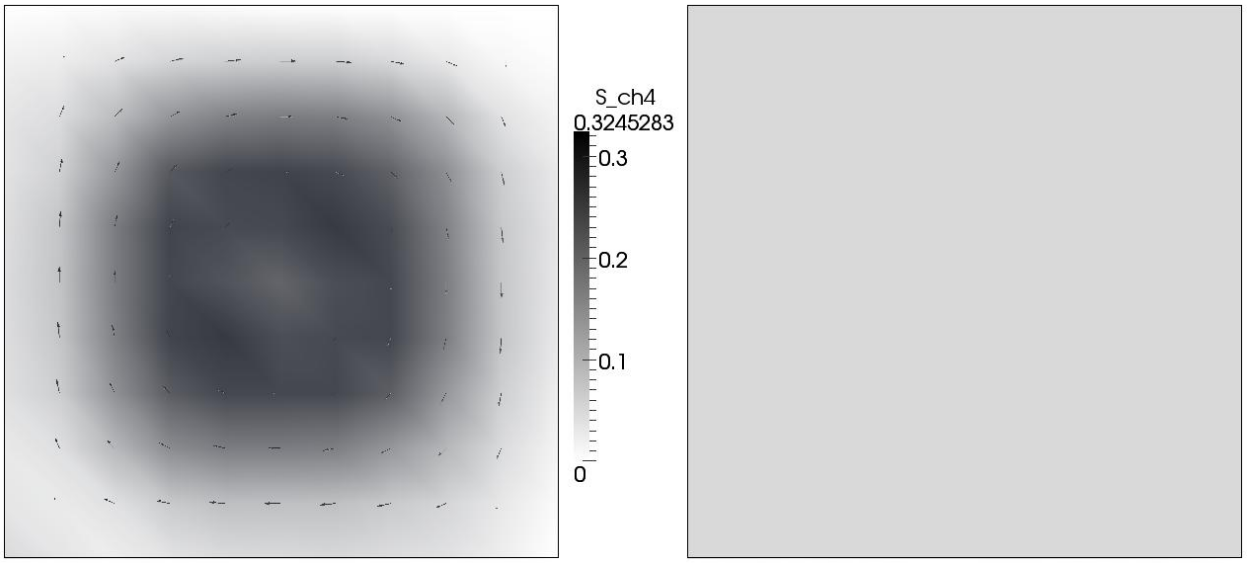

Figure 2a. ADM-MDA Figure 2b. ADM1

Dissolved methane concentration, S_{ch4}, spatial distribution at t = 56,651 s (15h 44m 11s).

FUTURE DEVELOPMENT

This research project has produced a strong foundation for a spatially-resolved implementation of ADM1; however, the second-order accuracy inherent in CRAFTS' finite volume method can conflict with the numerical stiffness of ADM1. This may limit the practicality of the model, such as reduce the maximum mesh size. There are several promising areas for model improvement, including the gas model and the transport model. Source code from this research endeavour is being released as free and open source software to the ADM1 modelling community to facilitate further model developments.

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