Anaerobic Digestion Model with Multi-Dimensional Architecture (ADM-MDA)

Lunch bag seminar
2011-05-18

Ph.D. Candidacy exam
2011-04-27
David L. F. Gaden
Outline

- Introduction
- Problem
- Proposed solution
- Literature review
- Methodology
- Code development
- Results
- Tasks remaining
What is anaerobic digestion?
- The breaking down of biomass in the absence of oxygen
- Treats waste products while simultaneously producing renewable energy (biogas)

Primary purpose:
- Waste treatment
- Energy production
- Pollution reduction
- Odour mitigation
• Applications
  ◦ Industrial wastewater treatment
  ◦ Municipal wastewater treatment
  ◦ Agricultural wastewater treatment
Stages of anaerobic digestion

1. Disintegration
• Stages of anaerobic digestion

2. Hydrolysis
Introduction

• Stages of anaerobic digestion

3. Acidogenesis

Volatile Fatty Acids
• Stages of anaerobic digestion

4. Acetogenesis

Volatile Fatty Acids \rightarrow \text{Acetate}

\text{Hydrogen}
• Stages of anaerobic digestion

5. Methanogenesis
Introduction

- Types of digesters

Diagram: Plug flow digester with inflow, effluent, and biogas output.
Types of digesters

Influent

Biogas

Effluent

STR digester

Introduction
Introduction

- Types of digesters

- Upflow anaerobic sludge blanket digester

  - Influent
  - Effluent

  Biogas
• Types of digesters

Introduction

Anaerobic clavigester

Influent

Effluent

Biogas
• Reliability issues

Unreliable

Well established
• Modelling anaerobic digesters
  ◦ Current state of the art is ADM1:


- Modelling anaerobic digesters
  - Current state of the art is ADM1:
  - A bulk model

- No spatial variation

\[
\frac{\partial S}{\partial x} = \frac{\partial S}{\partial y} = \frac{\partial S}{\partial z} = 0
\]

- Uniform properties
• Objective: a spatially-resolved ADM1

• ADM-MDA – Anaerobic Digestion Model with Multi-Dimensional Architecture

Proposed solution
Gas volume

\[ S_{\text{gas, var}} \quad (3) \]

Liquid volume

\[ S_{\text{var}} \quad (21) \]
\[ X_{\text{var}} \quad (12) \]
\[
\frac{dm_{\text{var}}}{dt} = m_{\text{var,in}} - m_{\text{var,out}} + m_{\text{var,react}}
\]

\[
V_{\text{liq}} \frac{dS_{\text{var}}}{dt} = Q_{\text{liq}} S_{\text{var,in}} - Q_{\text{liq}} S_{\text{var,out}} + V_{\text{liq}} r_{\text{var}}
\]

\[
\frac{dS_{\text{var}}}{dt} = \frac{V_{\text{liq}}}{Q_{\text{liq}}} (S_{\text{var,in}} - S_{\text{var}}) + r_{\text{var}}
\]
<table>
<thead>
<tr>
<th>Component</th>
<th>j</th>
<th>Process</th>
<th>$S_{su}$</th>
<th>$S_{aa}$</th>
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**Disintegration**
- Particulate composites ($X_c$)
- Inerts ($S_i$)

**Hydrolysis**
- Proteins ($X_{pr}$)
- Sugars ($S_{su}$)
- Lipids ($X_{li}$)
- Fatty acids ($S_{fa}$)
- Carbohydrates ($S_{ch}$)
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\[ r_{S_{su}} = k_{hyd,ch}X_{ch} + (-f_{fa,li}k_{hyd,li}X_{li}) \]

**Methodology – Theory – ADM1**
Methodology – Theory – ADM1
Methodology – Theory – ADM1
• Governing equations:
  ◦ Conservation of mass:
    \[ \nabla \cdot \mathbf{U} = 0 \n\]
  ◦ Conservation of momentum:
    \[ \rho \frac{D\mathbf{U}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{U} - \rho_{ref} \beta (T - T_{ref}) \n\]
  ◦ Conservation of energy:
    \[ \frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{U} T) - \nabla \cdot (\alpha \nabla T) = 0 \n\]
- Two options:
  1. Start with ADM1 and write CFD into it; or
  2. Start with CFD and write ADM1 into it.

- ODE:
  \[
  \frac{dS_{var}}{dt} = \frac{V_{liq}}{Q_{liq}} (\psi_{var,in} - \dot{S}_{var}) + r_{var}
  \]

- PDE:
  \[
  \frac{\partial S_{var}}{\partial t} + \nabla \cdot \nabla S_{var} + \nabla \cdot \Gamma \nabla S_{var} = r_{var}
  \]
Three biochemistry strategies:
1. Source term solver
2. ODE solver
3. Coupled solver
Three biochemistry strategies:

1. Source term solver

\[
\frac{\partial S_{var}}{\partial t} + \nabla \cdot \left( \mathbf{U} S_{var} \right) + \nabla \cdot \mathbf{G} \nabla S_{var} = r_{var}
\]

\[
\frac{dS_{var}}{dt} = \frac{V_{liq}}{Q_{liq}} \left( \xi_{var,in} - S_{var} \right) + r_{var}
\]
- Three biochemistry strategies:
  2. ODE solver
Three biochemistry strategies:

3. Coupled solver

\[ a_p S_p + \sum_i a_i S_i = b_p \]

\[
\begin{bmatrix}
    S_{su} S_{su} & S_{su} S_{aa} & S_{su} S_{fa} \\
    S_{aa} S_{su} & S_{aa} S_{aa} & S_{aa} S_{fa} \\
    S_{fa} S_{su} & S_{fa} S_{aa} & S_{fa} S_{fa}
\end{bmatrix}

\begin{bmatrix}
    S_{su} \\
    S_{aa} \\
    S_{fa}
\end{bmatrix}

+ \sum_i \begin{bmatrix}
    a_i S_{su} & 0 & 0 \\
    0 & a_i S_{aa} & 0 \\
    0 & 0 & a_i S_{fa}
\end{bmatrix}

\begin{bmatrix}
    S_{su,i} \\
    S_{aa,i} \\
    S_{fa,i}
\end{bmatrix} =

\begin{bmatrix}
    b_{su} \\
    b_{aa} \\
    b_{fa}
\end{bmatrix}

\[
\begin{bmatrix}
    a_{p,0} & a_{e,0} & 0 & 0 & 0 \\
    a_{w,1} & a_{p,1} & a_{e,1} & 0 & 0 \\
    0 & a_{w,2} & a_{p,2} & a_{e,2} & 0 \\
    0 & 0 & a_{w,3} & a_{p,3} & a_{e,3} \\
    0 & 0 & 0 & a_{w,4} & a_{p,4}
\end{bmatrix}

\begin{bmatrix}
    S_0 \\
    S_1 \\
    S_2 \\
    S_3 \\
    S_4
\end{bmatrix} =

\begin{bmatrix}
    b_{p,0} \\
    b_{p,1} \\
    b_{p,2} \\
    b_{p,3} \\
    b_{p,4}
\end{bmatrix}

Methodology – Theory – ADM-MDA
• Three biochemistry strategies:
  3. Coupled solver

Methodology – Theory – ADM-MDA
Time scale issue
- ADM1: $dt \approx 15 \text{ min}$
- CFD: $dt \approx 1 \text{ s}$

"multiSolver"
• Length scale issue

ADM1 \rightarrow \text{Prolongation} \rightarrow \text{Restriction} \rightarrow \text{CFD}

“dualGrid”

Methodology – Theory – ADM-MDA
Accessibility

- "equationReader"
- The ability to read equations from a text file
Code development

- **Transient solver**
  - PISO
  - RANS turbulence
  - Temperature
  - Scalar transport
  - Non-Newtonian
  - Buoyancy
  - Particle model
  - Steady state detection

- **Steady state solver**
  - Scalar transport
  - Particle model
  - Gas model

- **Control**
  - multiSolver
  - dualGrid

- **Flow**
  - ODE solver
  - Implicit solver ($S_{h2}$)
  - Implicit solver (ions)

- **Biochemistry**
  - EquationReader
  - Framework
Code development
Code development

Transient solver
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Biochemistry
- ODE solver
- Implicit solver (S_{H2})
- Implicit solver (ions)

Framework
- equationReader

Steady state solver
• Bulk model
  ◦ Written in Excel + Visual Basic macros
• Post processing routines
  ◦ Instantly produce comparisons between bulk model & ADM-MDA
  ◦ Written in Python
Bulk model verification

Results
Results

Boussinesq buoyancy model validation
Two problems with the model:
  ◦ Efficiency
  ◦ Transport deviation
## Results

<table>
<thead>
<tr>
<th>Change</th>
<th>Simulation Time</th>
<th>Real Time</th>
<th>Benchmark Estimate</th>
</tr>
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<tbody>
<tr>
<td>Initial</td>
<td>27 [s]</td>
<td>6 [hr]</td>
<td>&gt;100,000 [yr]</td>
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</table>

(1000 cells, 1000 days)
\[
\dot{S}_{\text{trans}} = \dot{S}_{\text{trans}} \bigg|_{r=0} + \Delta \dot{S}_{\text{trans}} \bigg|_{r \neq 0}
\]
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(1000 cells, 1000 days)
Results

Semi-implicit Bulirsch Stoer

Solve derived
ODE ddt
Implicit $S_{h2}$ solver
Implicit ion solver

"innerLoops"
### Results

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<td>1 [dy] 100 [dy]</td>
<td>12 [min] 5:32[hr:min]</td>
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<td>Static yields</td>
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</table>
float evaluate(float a, float b, string operation) {
    if (operation == "plus") {
        return a + b;
    }
    if (operation == "minus") {
        return a - b;
    }
    if (operation == "times") {
        return a * b;
    }
    if (operation == "divide") {
        return a / b;
    }
}

float plus(float a, float b) {
    return a + b;
}

float minus(float a, float b) {
    return a - b;
}

float times(float a, float b) {
    return a * b;
}

float divide(float a, float b) {
    return a / b;
}
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<td>1[dy] 100 [dy]</td>
<td>58 [s] 7 [min]</td>
<td>3.17 [dy]</td>
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</table>

The solver is now parallelized!
1 day (with flow)

Results
100 days (with flow)
100 days (no flow)
• Quad precision
• Pseudo-coupled solver
• Mini timesteps for transport
• Improve ADM1 numerical stability
• Averaged noisy transport
• Agglomeration
• Judgement day ... (May 21\textsuperscript{st})
• Solve transport error ... (June 1\textsuperscript{st})
• Gas model ... (June 22\textsuperscript{nd})
• Particle model ... (July 15\textsuperscript{th})
• Dual-grid ... (August 1\textsuperscript{st})
• Validate model ... (Octoberuary 15\textsuperscript{th})
• Write thesis ... (November 30\textsuperscript{th})