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Integrating Rheology into ADM1: A Viscosity-Driven Model (ADM1_Visc) for Dry Anaerobic Digestion

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Abstract

Dry anaerobic digestion (DAD) is gaining industrial relevance as a sustainable technology for converting solid biomass and organic waste into renewable energy. Unlike wet anaerobic digestion, where the Anaerobic Digestion Model No. 1 (ADM1) successfully represents biochemical processes, there is no validated model capable of accurately predicting DAD performance. High total solids (TS > 15%) induce rheological constraints that limit mass transfer and substrate accessibility, which are not considered in existing ADM1 extensions. This study proposes a new model, ADM1_visc, incorporating a viscosity dependent correction factor (Kηi) into the combined hydrolysis-acidogenesis kinetic term (KmXi) of ADM1_Bollon. The model was calibrated and validated against batch DAD data at 37˚C and 55˚C using crushed potato residues (TS 18% - 35%). ADM1_visc reproduced the dynamics of pH, VFAs, biogas, and CH_4 with Nash-Sutcliffe Efficiency > 0.6 for all cases. Comparative analysis showed ADM1_visc outperforms ADM1 and ADM1_Bollon under high-viscosity conditions. Viscosity is therefore a key driver of DAD performance, and ADM1_visc offers a robust predictive tool for optimizing DAD and improving biomethane yield.

Keywords

Dry Anaerobic Digestion, ADM1, Viscosity, Kinetic Modelling, Biogas, Mass Transfer Limitation

1. Introduction

Dry anaerobic digestion (DAD) is a promising technology for renewable energy recovery from solid organic wastes [1]-[9]. Compared with wet digestion (TS <

15%), DAD operates at high total solids (18% - 35%), reducing reactor volume, water demand, and investment cost [10]. Yet, increasing TS causes strong rheological effects, elevated viscosity and yield stress that hinder mass transfer between substrates and microorganisms [11] [12]. These constraints alter hydrolysis and acidogenesis kinetics, leading to VFA accumulation and potential process instability [13].

Despite these limitations being well-recognized, the underlying mechanisms remain insufficiently characterized, and DAD performance is still difficult to predict [14]. The ADM1 model of Batstone *et al.* [6] is the international benchmark for wet anaerobic digestion; several adaptations have been proposed to extend it to DAD [6] [15]-[17]. Among them, ADM1_Bollon simplified microbial pathways and lumped kinetic terms to better reflect dry digestion practice [16]. However, ADM1_Bollon does not consider viscosity-driven mass-transfer limitations, even though viscosity increases exponentially with TS [16]-[19].

Recent works have emphasized that rheological parameters significantly affect substrate accessibility, diffusion, and microbial activity [20] [21]. These studies underline the need to couple physical and biochemical processes for reliable DAD modelling.

In this context, the present work introduces ADM1_visc, a modified ADM1_Bollon version integrating a viscosity-dependent correction factor (Kηi) in the combined hydrolysis–acidogenesis kinetic term. The objectives are to: 1) represent the influence of viscosity on reaction rates, 2) validate the model with experimental data across 18% - 35% TS at 37˚C and 55˚C, and 3) compare its predictive performance with ADM1 and ADM1_Bollon. This study aims to mechanistically link viscosity effects to ADM1 kinetics to improve model fidelity under high total solids.

2. Material and Methods

2.1. Reference ADM1 Structure

The Anaerobic Digestion Model No. 1 (ADM1) describes 19 biochemical reactions involving 32 state variables across solid, liquid, and gas phases [3] [22]. Hydrolysis and disintegration are modelled as extracellular first-order kinetics, while acidogenesis, acetogenesis, and methanogenesis use Monod-type kinetics. ADM1 is validated for wet digestion (TS < 15%) but fails to simulate high-solids systems where rheology affects diffusion [23].

2.2. ADM1_Bollon Adaptation

ADM1_Bollon simplifies ADM1 by lumping hydrolysis and acidogenesis into a single step (DHA), reducing substrates from 14 to 6 fractions, and using a composite kinetic term KmXi. It improves numerical robustness but neglects viscosity effects. While these simplifications improved numerical robustness [16] [17], viscosity induced mass-transfer limitations were still neglected, leading to errors under high TS conditions [18].

2.3. Experimental Data and Rheological Measurements

Batch DAD experiments were performed in duplicate 12 L Plexiglas reactors at 37˚C (mesophilic) and 55˚C (thermophilic). Crushed potato residues (TS 18%, 20%, 22%, 25%, 30%, 35%) served as substrate. Substrate composition and biodegradability were characterized according to Beugré and Gnagne [24].

Rheological properties were measured using a TA Instruments AR 2000 rheometer with vane geometry, suitable for non-Newtonian slurries [19]. Shear-rate ramps (0 - 200 s^{-1}) were applied; apparent viscosities and yield stresses were determined and fitted to the Herschel–Bulkley model [20] [25].

Biogas production was monitored volumetrically and standardized to STP (0˚C, 101 kPa). Gas composition (CH_4, CO_2) was analyzed via micro-GC (Agilent 490). VFAs, alkalinity, and pH were determined by standard methods [26] [27]. These data were used for model calibration and validation.

2.4. Development of ADM1_Visc

The novelty of this work lies in coupling the apparent viscosity (η) of the digestion medium with the first-order disintegration-hydrolysis-acidogenesis (DHA) kinetic term of the ADM1_Bollon framework.

In dry anaerobic digestion (DAD), elevated total solids (TS) content significantly increases viscosity, which in turn limits mass transfer and reduces effective contact between microorganisms and substrates.

To capture this physical limitation, the substrate degradation rate for each reaction i is expressed as inversely proportional to the medium viscosity:

$$\rho_i = K_{\eta_i} \cdot \left(K_{m,i} X_i \right)$$

where ρ_i is the degradation rate (kg COD·m^{-3}·d^{-1}), $K_{m,i}$ is the composite kinetic constant for reaction i (d^{-1}), X_i is the biodegradable substrate concentration (kg COD·m^{-3}), and K_{η_i} is a viscosity dependent correction factor that accounts for the reduction in diffusion and biomass substrate accessibility.

When viscosity increases, K_{η_i} decreases, thereby reducing the overall degradation rate, which reflects the experimentally observed kinetic slowdown at high TS.

In this work, the empirical coefficients α and β were obtained through a two-step procedure.

First, raw rheological measurements (η vs. shear rate) for each TS level were fitted to the Herschel–Bulkley model to obtain apparent viscosity values at representative shear conditions.

Second, α and β were calibrated within the global model optimization by minimizing the error between measured and simulated VFA, pH, biogas, and methane production.

This combined procedure ensured that the correction factor K_{η_i} reflected both the intrinsic rheology of the feedstock and its effective influence on biochemical kinetics.

The viscosity correction factor is defined as:

$$K_{\eta_i} = \frac{1}{1+\alpha\left(\eta/\eta_0\right)^{\beta}}$$

where η is the apparent viscosity of the digestate (Pa·s), η_0 is a reference viscosity (that of water at 25˚C, ≈0.001 Pa·s), and α and β are empirical coefficients determined experimentally for each TS level.

This formulation enables the model to dynamically link rheological properties to reaction kinetics, providing a mechanistic description of viscosity induced mass-transfer limitations in DAD.

The complete ADM1_visc model structure was implemented in MATLAB/Simulink using the stiff solver *ode15s*, following the original ADM1 formulation proposed by Batstone *et al.* [3]. All state variables, stoichiometric relationships, and biochemical conversions were retained from ADM1_Bollon, except for the modified kinetic term incorporating the viscosity correction factor K_{η_i}.

2.5. Initialization and Parameter Estimation

Initial state variables were obtained from experimental measurements of COD fractions, soluble compounds, VFAs, ammonium, and bicarbonate at t = 0. COD partitioning among carbohydrates, proteins, lipids, and inert fractions used known COD equivalence factors [17] [26].

Stoichiometric coefficients and kinetic parameters were calibrated by manual + automated optimization (−50% to +200% of nominal values) using least-squares minimization [27]. Model performance was quantified by the Nash–Sutcliffe Efficiency (NSE) [28], where NSE > 0.6 indicates satisfactory simulation accuracy.

3. Results

3.1. Volatile Fatty Acid (VFA) Dynamics

At both 37˚C and 55˚C (**Figure 1** and **Figure 2**), acetate accumulated rapidly during the first 10 - 12 days, reaching about 0.45 kg COD·m^{-3} at 37˚C and 0.47 kg COD·m^{-3} at 55˚C before decreasing to a stable plateau near 0.20 - 0.25 kg COD·m^{-3}. Propionate accumulated gradually, reaching 0.38 kg COD·m^{-3} (37˚C) and 0.62 kg COD·m^{-3} (55˚C). Butyrate and valerate were consumed faster, vanishing after 17 days at 37˚C and 30 days at 55˚C.

ADM1_visc reproduced the accumulation and degradation patterns accurately, outperforming ADM1 and ADM1_Bollon [16] [17].

3.2. pH Evolution

pH increased from 5.6 ± 0.1 initially to 7.1 - 7.2 by day 19, stabilizing thereafter. Simulated values matched experimental profiles ($R^2 > 0.9$). The correct timing of pH recovery demonstrates that the viscosity coupled kinetics properly capture intermediate conversion and buffering [11] [20] (**Figure 3**).

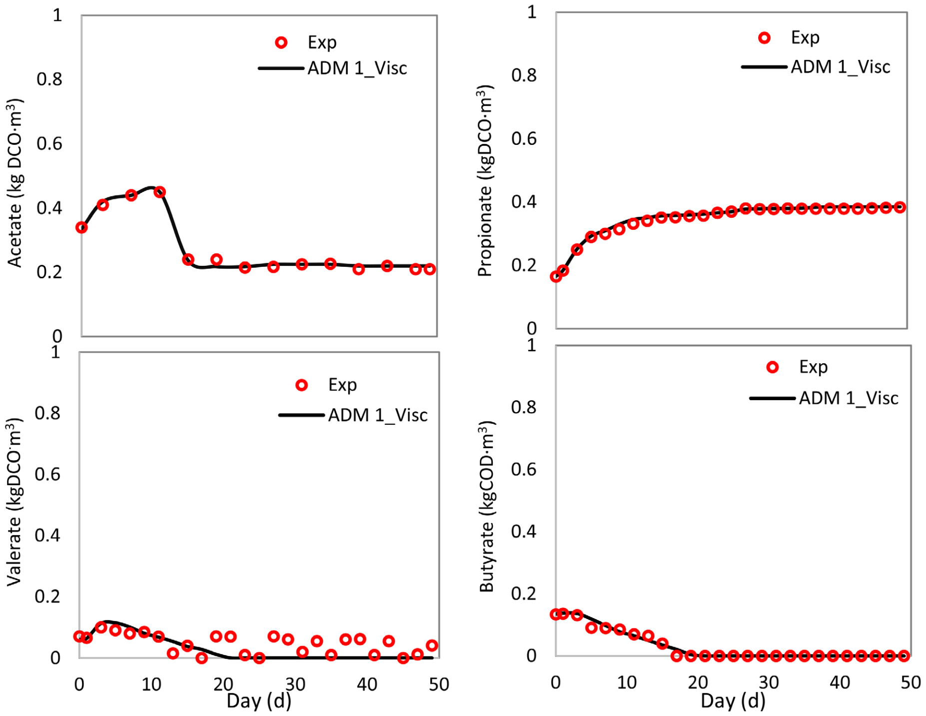

Figure 1. Experimental and simulated VFA concentrations (acetate, propionate, butyrate, valerate) during DAD of potato residues at 35% TS and 37˚C using ADM1_visc.

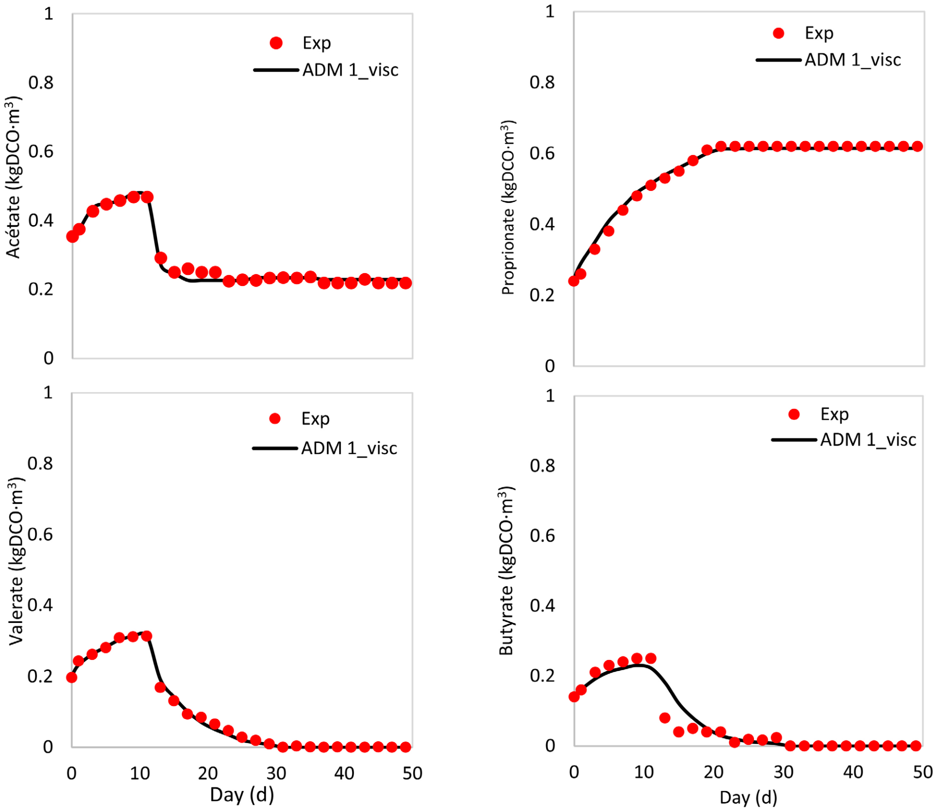

Figure 2. Experimental and simulated VFA concentrations (acetate, propionate, butyrate, valerate) during DAD of potato residues at 35% TS and 55˚C using ADM1_visc.

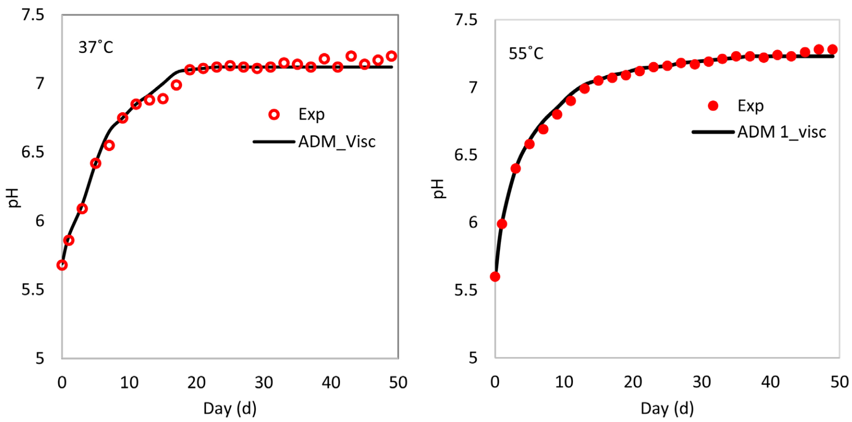

Figure 3. Experimental and simulated pH evolution at 37˚C and 55˚C (35% TS substrate).

3.3. Cumulative Biogas Production

Cumulative biogas reached 3627 kg COD·m^{-3} at 37˚C and 3812 kg COD·m^{-3} at 55˚C. No lag phase was observed. ADM1_visc reproduced exponential growth and plateau phases precisely, confirming its ability to describe substrate hydrolysis under mass-transfer limitation [29] (**Figure 4**).

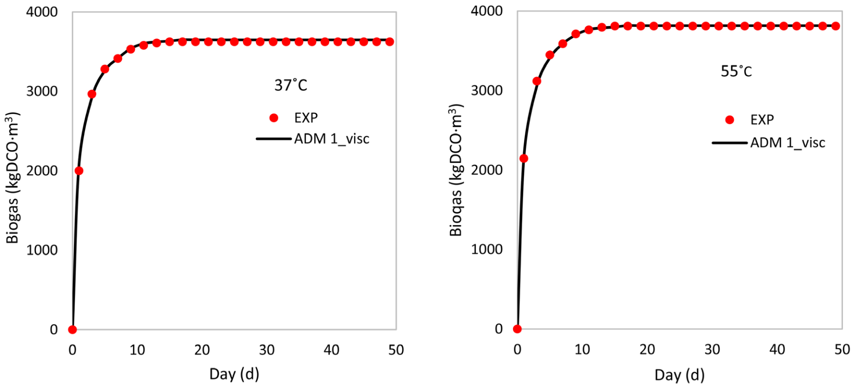

Figure 4. Experimental vs. ADM1_visc cumulative biogas production at 37˚C and 55˚C (35% TS).

3.4. Cumulative Methane Production

Methane yield rose sharply during the first 15 days, attaining 1950 kg COD·m^{-3} (37˚C) and 2310 kg COD·m^{-3} (55˚C). ADM1_visc predictions aligned closely with experiments, with minor deviation on day 20 under mesophilic conditions (**Figure 5**).

3.5. Predictive Performance Using Nash-Sutcliffe Efficiency

Model performance across all TS levels (18% - 35%) and both operating temperatures is summarized in **Table 1**. All NSE values exceeded 0.6, confirming satisfactory to excellent prediction capability for VFA, pH, biogas, and methane. ADM1_visc demonstrated robust predictive accuracy across a wide range of TS levels and operational conditions.

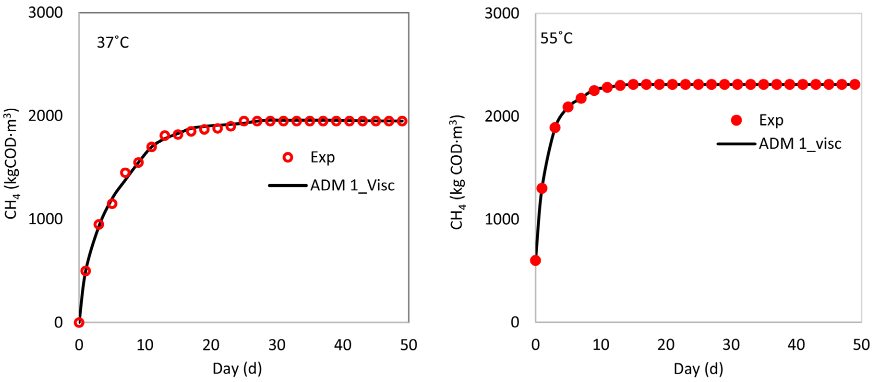

Figure 5. Experimental vs. ADM1_visc cumulative methane production under identical conditions.

Table 1. NSE values of experimental parameters simulated by ADM1_visc.

	MS (%)	18	20	22	25	30	35
pH	NSE 37˚C	0.90	0.90	0.91	0.89	0.92	0.88
	NSE 55˚C	0.89	0.88	0.91	0.90	0.92	0.89
VFA	NSE 37˚C	0.78	0.80	0.85	0.82	0.90	0.79
	NSE 55˚C	0.78	0.81	0.86	0.82	0.89	0.88
Biogas	NSE 37˚C	0.90	0.92	0.90	0.90	0.94	0.91
	NSE 55˚C	0.90	0.94	0.91	0.91	0.94	0.93
CH_4	NSE 37˚C	0.90	0.89	0.90	0.91	0.89	0.88
	NSE 55˚C	0.90	0.89	0.91	0.91	0.87	0.88

3.6. Comparative Evaluation of Models

The standard ADM1 systematically underpredicted hydrolysis because it assumes ideal mixing and low-viscosity conditions, implicitly treating mass transfer as non-limiting. Under high TS conditions, this results in unrealistic substrate accessibility, leading to excessive VFA accumulation and delayed conversion.

ADM1_Bollon improved numerical robustness and stability by simplifying the DHA pathway but still relied on the assumption of perfect mixing and did not include any viscosity-dependent mass-transfer limitation. As a result, it failed to reproduce both the timing and magnitude of VFA consumption, particularly at 55˚C where faster solubilization amplifies diffusion limitations.

By explicitly integrating viscosity into the kinetic term, ADM1_visc corrects this structural limitation.

It reduces the effective reaction rate when viscosity increases, thereby capturing the time delays, peak magnitudes, and conversion dynamics observed experimentally. This mechanistic enhancement explains why ADM1_visc consistently achieved NSE > 0.85, outperforming ADM1 and ADM1_Bollon across all conditions [16] [17] [30].

This confirms that apparent viscosity must be explicitly accounted for to simulate dry anaerobic digestion reliably (**Figure 6** and **Figure 7**).

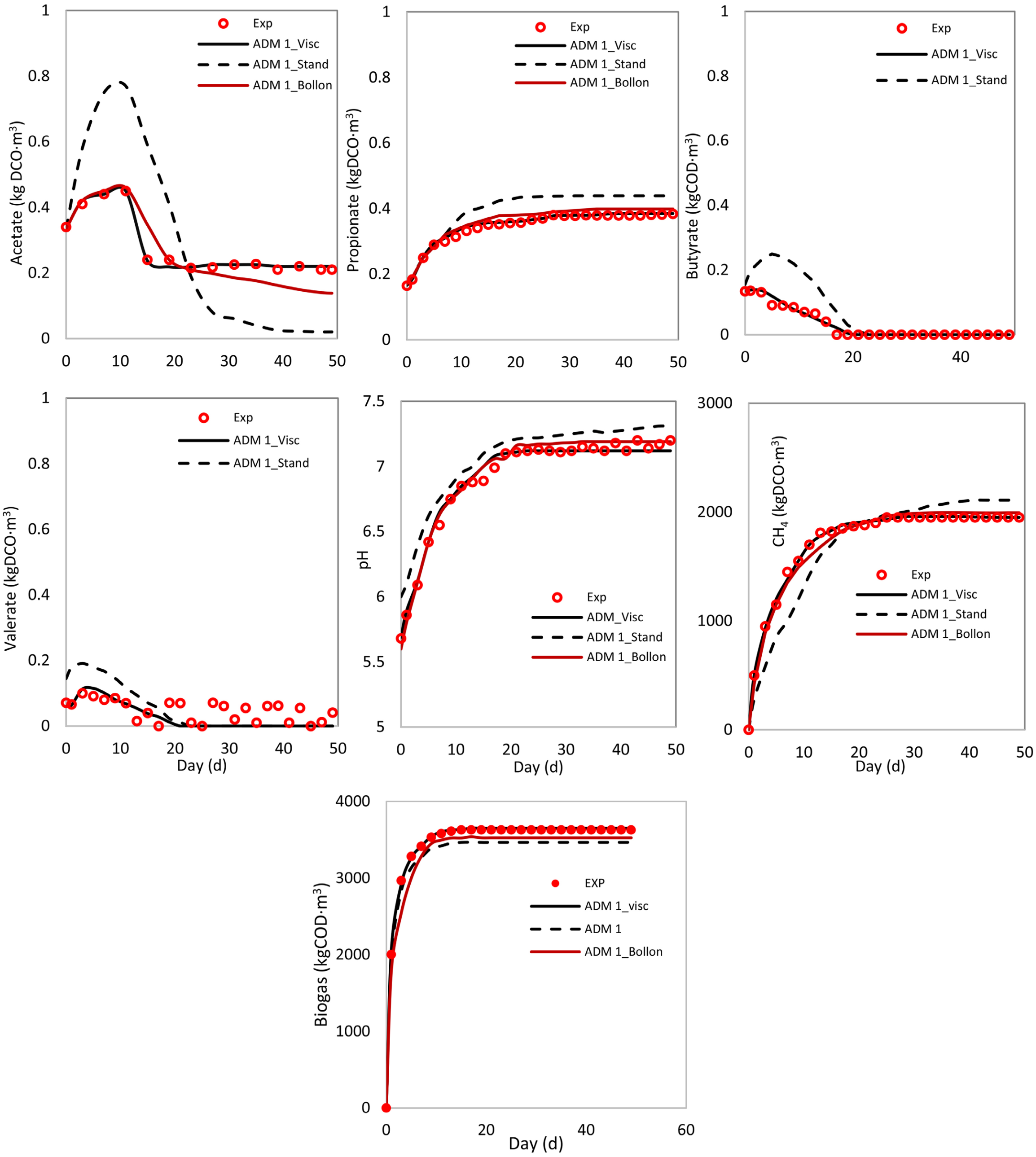

Figure 6. Comparison of simulated and experimental results using ADM1, ADM1_Bollon, and ADM1_visc at 37˚C and 35% TS.

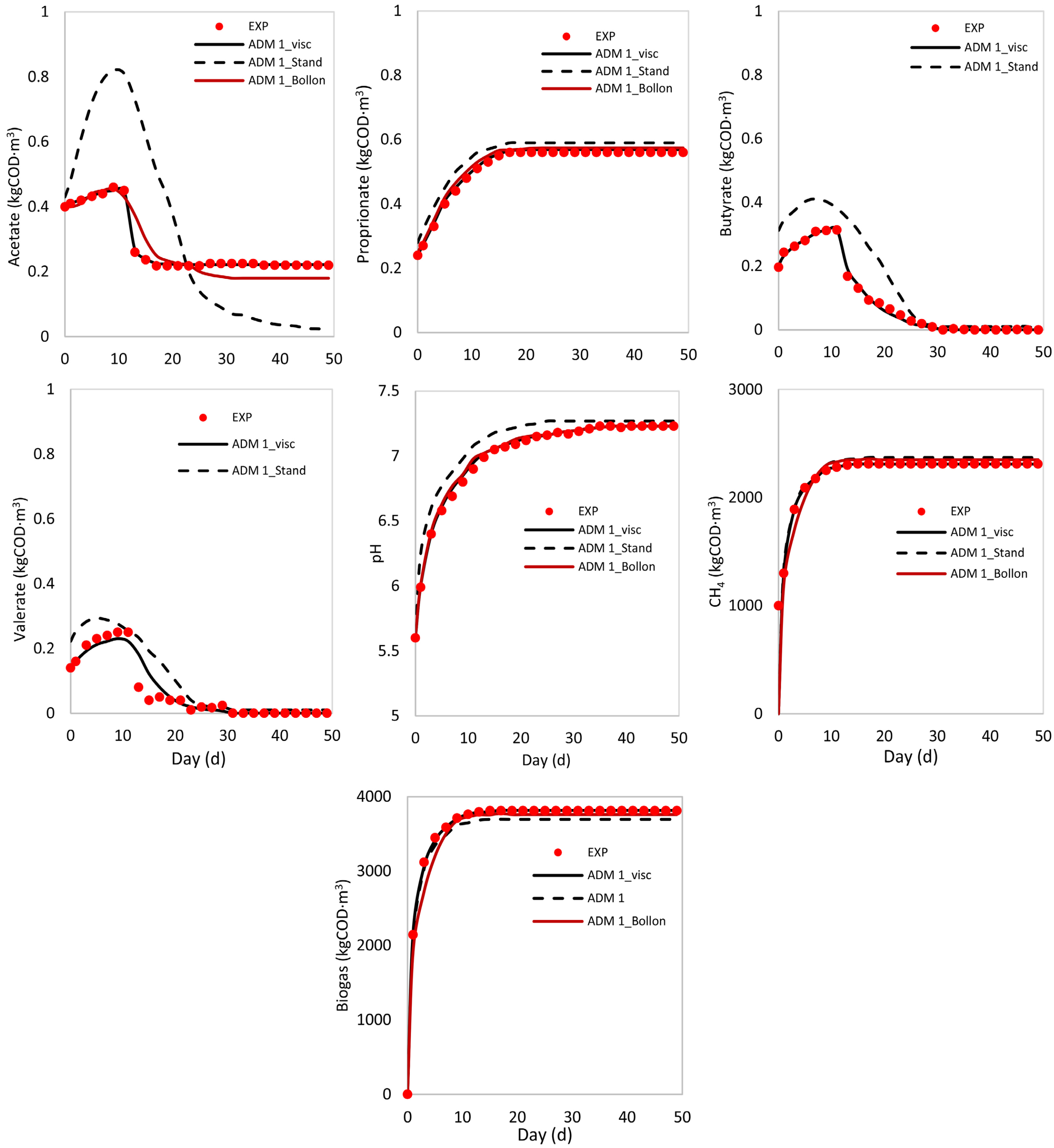

Figure 7. Comparison of simulated and experimental results using ADM1, ADM1_Bollon, and ADM1_visc at 55˚C and 35% TS.

4. Discussion

4.1. Influence of Viscosity on Hydrolysis and Acidogenesis

The accumulation of acetate and propionate during the first 10 - 20 days of digestion highlights that hydrolysis and acidogenesis remain rate limiting steps under dry conditions. Apparent viscosity increases exponentially with TS, restricting interfacial contact between enzymes, bacteria, and particulate substrates [12] [31]

[32].

These mass-transfer limitations delay substrate conversion, resulting in higher VFA peaks at 55˚C due to faster solubilization combined with kinetically constrained conversion, particularly of propionate a well-known indicator of metabolic imbalance under high VFA fluxes.

The ability of ADM1_visc to reproduce these dynamics confirms that viscosity must be explicitly included in kinetic expressions to capture early-stage process behavior.

It is important to note that the viscosity parameters α and β were calibrated using crushed potato residues, a substrate with low lignin content and relatively homogeneous particle size.

For substrates with higher structural resistance such as lignocellulosic biomass, manure fibers, or mixed municipal waste different rheological responses may be expected, potentially requiring substrate-specific calibration of α and β.

Therefore, while ADM1_visc captures the general mechanistic effect of viscosity, applying it to highly fibrous or heterogeneous feedstocks may require re-estimating the viscosity correction parameters to account for different mass-transfer regimes.

4.2. Process Stabilization and pH Regulation

As digestion progressed, acetate and butyrate consumption led to pH recovery toward neutrality, improving methanogenic activity. Model accuracy for pH further confirms that the ion balance representation from ADM1_Bollon is valid for DAD, provided that viscosity-driven delays in intermediate reactions are properly accounted for [17].

The fact that simulated pH at 55˚C followed experimental data more closely supports the hypothesis that elevated temperature reduces viscosity, thus mitigating mass-transfer constraints and enhancing microbial resilience. The better accuracy at 55˚C suggests that reduced viscosity at higher temperature enhances buffering and methanogenesis [19].

4.3. Impact on Methanogenesis and Biogas Yield

The higher methane yield obtained at 55˚C indicates that thermophilic conditions enhance both the rate and extent of biodegradation [33] [34], overcoming physical limitations imposed by high TS content.

ADM1_visc correctly simulated the exponential growth phase of methane production, demonstrating that the modified DHA term effectively links physical rheology and biological conversion efficiency.

4.4. Model-Based Evidence of Viscosity as a Critical Operational Factor

Comparisons with ADM1 and ADM1_Bollon provide clear insights into the fundamental role of viscosity in DAD modelling. ADM1 assumes fully mixed, diluted conditions and therefore overestimates substrate accessibility, leading to unrealistic kinetics under high TS conditions [35]. ADM1_Bollon improved stability but still failed to describe the timing and magnitude of VFA turnover.

ADM1_visc, by contrast, consistently achieved NSE values > 0.85, outperforming the other models across all scenarios. This confirms that:

- Rheological properties directly affect biochemical kinetics
- High viscosity reduces biomass-substrate contact efficiency
- Mass transfer, not microbial activity, becomes the controlling step

4.5. Industrial Implications

In practical terms, "rheological thresholds" refer to viscosity levels above which mass-transfer limitations become dominant and significantly slow down hydrolysis and acidogenesis [35].

In this study, a critical apparent viscosity of approximately 4.10×10^4 - 10.3×10^4 Pa·s (measured at a shear rate of 10 s^{-1}) corresponded to the onset of strong kinetic inhibition, as reflected by delayed VFA turnover and reduced methane production.

Maintaining viscosity below such thresholds through TS optimization, controlled mixing, or pre-treatment can therefore prevent kinetic bottlenecks and improve digester stability.

5. Conclusions

Dry anaerobic digestion provides clear advantages for renewable energy recovery from solid wastes but remains constrained by rheological effects. The new ADM1_visc model integrates apparent viscosity into ADM1 kinetics and accurately simulates VFAs, pH, and gas production under high-solids conditions.

Validated at 18% - 35% TS and 37˚C - 55˚C, ADM1_visc outperformed existing ADM1 variants with NSE > 0.6 for all variables. The model offers a robust predictive tool for optimizing solids content, mixing, and operating regimes.

Future work will extend ADM1_visc to TS ≈ 50% and incorporate hydrodynamic descriptors such as local shear rates, mixing power density, energy dissipation distribution, and spatial gradients in velocity fields.

Integrating these CFD-derived quantities with ADM1_visc will enable a fully coupled framework capturing both biochemical kinetics and non-ideal flow behavior in full-scale digesters.

Highlights

1) A viscosity-integrated ADM1 model (ADM1_visc) was developed for dry digestion.

2) The model links rheological behavior with biochemical kinetics.

3) ADM1_visc accurately predicts VFAs, pH, biogas, and methane production under high TS.

4) Viscosity is identified as a key kinetic limitation in dry anaerobic digestion.

5) The approach strengthens mechanistic modeling for future CFD coupling.

Impact Statement

This study introduces a viscosity-integrated ADM1 model that mechanistically links rheological behavior to kinetic performance in high-solids anaerobic digestion, establishing a foundation for future CFD-coupled modeling approaches.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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