

Kinetic modeling in biofuel production: A critical review and roadmap for model selection

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Kinetic modeling plays a central role in interpreting experimental behaviour and supporting reactor design in biofuel production systems. Commonly applied models range from empirical curve-fitting equations to mechanistically derived growth models, each constructed upon distinct theoretical assumptions. However, inappropriate model selection can compromise interpretability and predictive reliability beyond the experimental domain. Thus, kinetic model selection should be guided by scientific suitability rather than conventional or statistical convenience. This review provides a critical and comparative evaluation of kinetic models applied in biofuel production systems by comparing their mechanistic basis, parameter identifiability, data requirements, and extrapolation capability. Empirical models such as First-order, Logistic and Gompertz-type models are assessed for their descriptive accuracy but limited mechanistic insight. Growth-based models like Monod model capable of representing substrate consumptions, evaluated for their ability to represent biological and biochemical constraints, while highlighting persistent challenges related to data availability, parameter identifiability, and validation. More structured and hybrid approaches, such as Luedeking-Piret type model examined for their ability to couple microbial growth and product formation under data-rich conditions. Systematic comparison shows that model suitability is governed primarily by research objective, system complexity, and experimental resolution rather than by conventional usage. On this basis, a decision-oriented framework is developed to guide context-specific kinetic model selection to enhance methodological rigor in biofuel process analysis.

Keywords: Biofuel, Empirical and mechanistic models, Kinetic models, Model selection, Parameter identifiability

Introduction

Kinetic modeling has become an indispensable tool in biofuel research for interpreting experimental data, predicting process behaviour, and supporting reactor design and scale-up¹. Over the past decades, modeling approaches have evolved from simple empirical correlations to increasingly sophisticated mechanistic representations applied to systems producing biohydrogen, biomethane, biohythane, bioethanol, and biodiesel. Despite this evolution, the practical application of kinetic models remains methodologically inconsistent, with models frequently employed without adequate consideration of their underlying assumptions and domains of validity²⁻⁴. In some studies, empirical and curve-fitting models are adopted based on precedent or ease of implementation rather than scientific justification. As a result, statistical goodness-of-fit is often indirectly treated as

evidence of mechanistic validity, even though these criteria address fundamentally different aspects of kinetic analysis. This concern has become more pronounced as biofuel production systems themselves have grown more complex, involving multi-substrate feedstocks, microbial interactions, inhibitory effects, and dynamically varying operating conditions⁵. The application of overly simplified kinetic descriptions to such systems can lead to misleading interpretations, particularly when models are extrapolated for process optimisation, cross-study comparison, or scale-up. Consequently, the expanding body of kinetic modeling studies has not always yielded proportional gains in process understanding or industrial relevance⁶. The critical issue is therefore not the usefulness of kinetic modeling itself, but the appropriateness of model selection relative to system characteristics, data quality, and research objectives.

Although substantial effort has been devoted to proposing new kinetic formulations or modifying existing ones, comparatively little attention has been paid to clearly defining their applicability limits and conditions of valid use in specific biofuel contexts⁷⁻⁹.

The primary objective of the review is to address the need by providing a critical evaluation and comparative synthesis of kinetic models used in biofuel production, with a specific focus on guiding context-aware model selection. Instead of providing a comprehensive derivation of the kinetic equations theoretically, the present study is more focused on the applicability, limitations, data requirements and interpretability of the popular models in use. It is decision-oriented and shifts the focus from model inventory to scientifically defensible model choice. Specifically, the present review classifies kinetic models conceptually, then critically evaluates their strengths, limitations, and common modes of appropriate application, and finally proposes a practical roadmap for kinetic model selection based on biofuel type, experimental scale, data availability, and research objectives.

Classification of Kinetic Models in Biofuel Systems

Kinetic models used in biofuel research differ not only in their mathematical form but, more

fundamentally, in the assumptions they make about microbial activity, substrate transformation, and product formation. For this reason, models reported in the literature are more meaningfully classified according to their conceptual basis, data requirements, and intended analytical function rather than by increasing mathematical complexity¹⁰. Broadly, kinetic models used in biofuel systems can be divided into two categories: (i) empirical formulations that describe observed process behaviour, and (ii) semi-mechanistic, mechanistic and structured approaches that attempt to represent underlying biological and physicochemical mechanisms^{1,11}. Empirical models are primarily data-driven and describe observed system behaviour without explicitly representing underlying biological or physicochemical mechanisms. In contrast, mechanistic models are based on fundamental principles and aim to represent microbial growth, substrate utilisation, and process interactions through biologically interpretable parameters. Semi-mechanistic models occupy an intermediate position, combining simplified mechanistic concepts with empirical relationships, thereby allowing partial representation of biological processes while maintaining relatively low data requirements^{12,13}. Table 1 summarises representative formulations from these categories to explain their differing analytical roles.

Table 1 — Mathematical expressions and conceptual attributes of commonly used kinetic models in biofuel research

Kinetic model	Equations	Key assumptions	Reference
First-order kinetic model	$P(t) = P_{max}(1 - e^{-kt})$	Degradation rate proportional to remaining biodegradable substrate; lumped substrate representation; no explicit biomass growth, inhibition, or multi-step reaction pathways	14
Modified Gompertz Model	$P(t) = P_{max} \cdot \exp \left\{ -\exp \left[\frac{R_{max} \cdot e}{P_{max}} (\lambda - t) + 1 \right] \right\}$	Phenomenological sigmoidal description of cumulative production; parameters depend on operating conditions and do not represent intrinsic mechanistic constants	26
Modified Logistic model	$P(t) = \frac{P_{max}}{1 + \exp \left[\frac{4R_{max}}{P_{max}} (\lambda - t) + 2 \right]}$	Symmetric sigmoidal production profile; does not explicitly account for substrate limitation, inhibition, or mechanistic microbial dynamics	27, 28
Monod Model	$\mu = \mu_{max} \frac{S}{K_s + S}$	Microbial growth controlled by a single limiting substrate; homogeneous population assumed;	29, 30
Cone model	$P(t) = \frac{P_{max}}{1 + (kt)^{-n}}$	Empirical cumulative degradation model; flexible shape parameter captures overall degradation pattern; lacks explicit microbial or physicochemical mechanisms	5
Luedeking-Piret model	$\frac{dP}{dt} = \alpha \frac{dX}{dt} + \beta X$	Product formation linked to biomass growth via growth-associated and non-growth-associated terms; coefficients assumed constant under given conditions	20

Empirical kinetic models

Empirical models represent the most widely applied class of kinetic tools in biofuel research, particularly in laboratory-scale and batch investigations. These types of models explain observable changes across time in the production of biofuels without necessarily modeling the inherent biological or biochemical processes that occur⁵. Common examples include first-order kinetics and sigmoidal expressions such as the Gompertz, Logistic, and Cone models¹⁴⁻¹⁸. Their widespread use arises from modest data requirements, computational simplicity, and their ability to reproduce cumulative production profiles under controlled experimental conditions¹⁹. Conceptually, empirical models are descriptive rather than mechanistic. Their fitted parameters characterise system behaviour under a specific set of experimental conditions instead of representing intrinsic kinetic constants. As a result, parameter values are strongly influenced by factors such as substrate composition, reactor configuration, and data robustness¹⁰. These models are therefore most appropriately applied for trend analysis, preliminary evaluation, or comparison within individual studies, rather than for mechanistic interpretation or extrapolative prediction.

Semi-mechanistic, mechanistic, and structured kinetic models

In contrast to empirical formulations, semi-mechanistic and mechanistic models seek to represent biofuel production processes through explicit relationships between microbial growth, substrate consumption, and product formation²⁰. These models attempt to capture governing biological interactions rather than merely reproducing observed trends. Growth-based expressions, particularly Monod-type kinetics, are widely applied to describe substrate-limited microbial activity in fermentation and anaerobic digestion systems^{21,22}. Their parameters are therefore interpreted in relation to physiological behaviour, such as substrate affinity and maximum growth capacity, rather than as purely statistical descriptors.

Product-linked models, such as the Luedeking-Piret model, extend this framework by distinguishing between growth-associated and non-growth-associated product formation, thereby enabling analysis of the coupling between biomass development and biofuel generation. In the Luedeking-Piret model, the parameter α represents growth-associated product formation, while β represents non-growth-associated product formation. When $\alpha \neq 0$ and $\beta = 0$, product formation is purely

growth-associated; when $\alpha = 0$ and $\beta \neq 0$ it is non-growth-associated, and when both parameters are non-zero, product formation is mixed²³.

While these approaches introduce a degree of biological interpretability, they generally remain simplified and do not explicitly resolve intracellular metabolic pathways²⁰. Structured and hybrid models build upon mechanistic concepts by incorporating multiple biological processes, inhibitory effects, and system-level interactions. Examples include structured anaerobic digestion model no. 1 (ADM1) and hybrid approaches that combine mechanistic rate expressions with data-driven components^{24,25}. Such models are typically employed for dynamic simulation, process analysis, predictive evaluation and consequently require more detailed datasets and experimental validation than empirical formulations. The conceptual relationship between these modeling approaches and the major biological stages involved in biofuel production is illustrated schematically in Fig. 1.

Kinetic Models: Strengths and Limitations

Building on the classification presented in the above section, the practical usefulness of kinetic models depends not only on their mathematical form but also on the extent to which their assumptions represent the biological system, data quality, and intended application. In many cases, models that provide excellent statistical fits do not necessarily offer meaningful insight into process behaviour, highlighting the need to distinguish descriptive adequacy from scientific validity³¹. Empirical formulations, including first-order and sigmoidal models, remain widely used because of their modest data requirements and ease of implementation³². First-order kinetics provides a simplified approximation of overall substrate degradation. However, the assumption of a single rate-limiting step inherently limits the applicability of such models to relatively homogeneous substrates under stable conditions; consequently, their application to multi-component feedstocks or inhibition-dominated environments may oversimplify complex system behaviour and significantly reduce predictive reliability³³.

Sigmoidal models such as the Gompertz and logistic equations are commonly used to describe cumulative biofuel production, particularly in batch biohydrogen and biogas studies^{34,36}. The modified Gompertz and modified logistic models are empirical adaptations of their classical forms that incorporate lag phase and maximum production rate to better describe cumulative biofuel production. These models

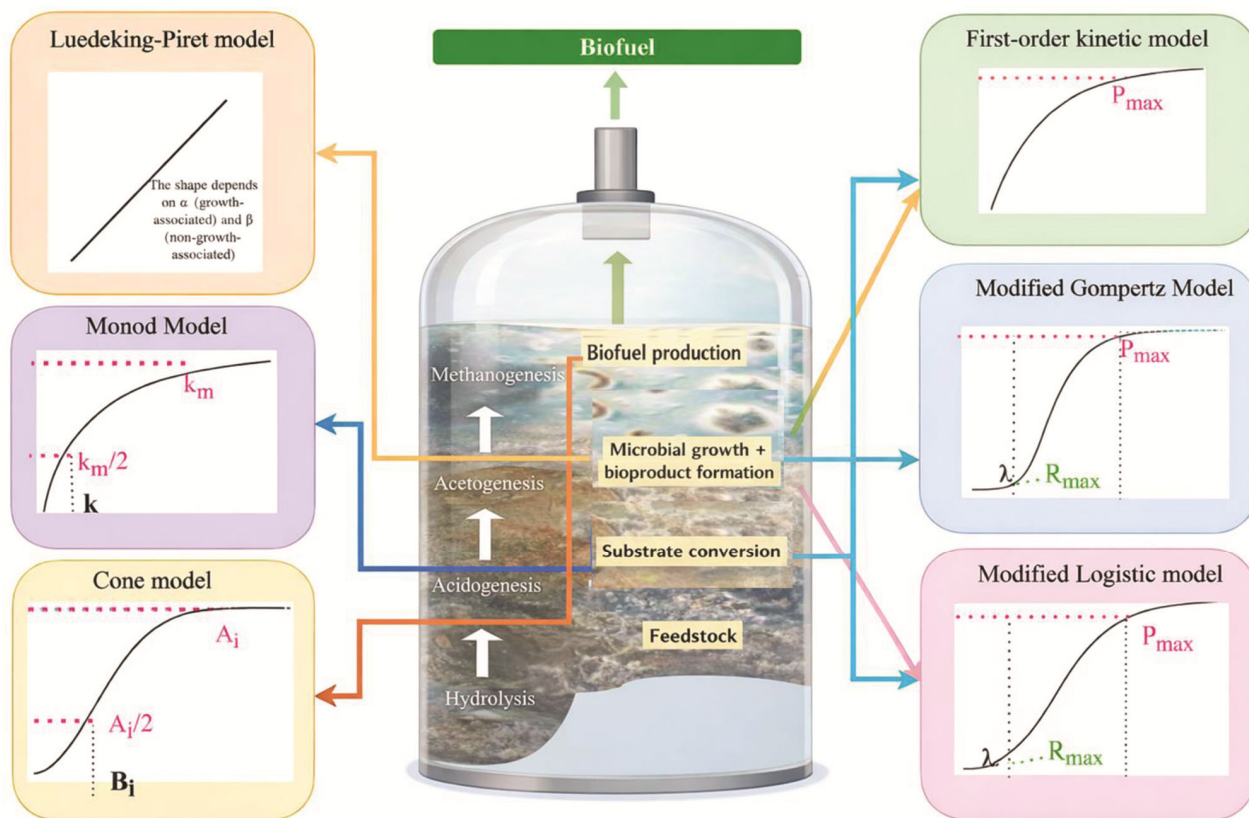


Fig. 1 — Process-oriented mapping of kinetic models to biological stages in biofuel production

effectively capture lag phases and production saturation, making them useful for trend description and comparative evaluation^{26,27}. However, their parameters are often misinterpreted as intrinsic kinetic constants, whereas they are phenomenological descriptors influenced by inoculum characteristics, substrate properties, and experimental conditions. Parameter identifiability refers to the ability to uniquely estimate model parameters; poor identifiability can lead to multiple parameter sets fitting the same data, reducing model reliability. Consequently, comparisons of these parameters across studies have limited mechanistic significance despite strong statistical goodness-of-fit¹⁷. The Cone model represents another flexible empirical approach that has gained attention for modeling production from heterogeneous substrates such as lignocellulosic residues, manures, and co-digestion mixtures³⁷. The inclusion of adjustable parameters within this kinetic framework enables the representation of diverse degradation behaviours and often yields strong statistical agreement, even when applied to relatively sparse datasets³⁸. Nevertheless, the absence of mechanistic representation restricts interpretability,

and unconstrained fitting or extrapolation beyond measured data remains a common source of misuse^{39,40}. Beyond the limitations of individual models, the way kinetic analyses are implemented and reported also affects their reliability. A survey of representative studies, summarised in Table 2, shows that model selection is frequently based primarily on goodness-of-fit indicators such as R^2 , RMSE, or MAPE, sometimes without independent validation, uncertainty analysis, or explicit discussion of model assumptions. In addition, validation approaches such as residual analysis and parameter sensitivity analysis can provide further insight into model robustness by identifying systematic deviations and assessing the influence of model parameters on predicted outcomes^{41,42}. Variability in reported parameters often reflects differences in experimental design, reactor configuration, feedstock characteristics, and temporal resolution of measurements rather than intrinsic differences in model capability.

Mechanistic and semi-mechanistic models attempt to relate substrate utilisation and microbial activity through biologically interpretable relationships, most commonly using Monod-type growth expressions^{43,44}.

Table 2 — Reported goodness-of-fit metrics for kinetic models used in biofuel production studies

Reactor	Substrate	Kinetic models	Biofuel	R ²	RMSE	Reference
CSTR	Food waste	First-order kinetic model	Biogas	0.88	3.972	48
CSTR	Food waste	Modified Gompertz model	Biogas	0.99	0.62	48
CSTR	Food waste	Logistic function model	Biogas	0.99	0.85	48
CSTR	Glucose	Monod model	Biohydrogen	0.96	-	49
AnAS-RBC reactor	Molasses wastewater	Luedeking-Piret model	Biohydrogen	0.97	-	46
Fed batch reactor	RhodobacterCapsulatus-Vernon Growth Medium	Luedeking-Piret model	Biohydrogen	0.99	-	20
Batch reactor	OFMSW	First-order kinetic model	Biogas	0.92	51.63	50
Batch reactor	OFMSW	Cone model	Biogas	0.99	6.9	50
Batch reactor	Organic waste	Luedeking-Piret model	Biohydrogen	0.96	-	51
Batch reactor	Organic wastes	Cone model	Biogas	0.98	-	39
Batch reactor	Food waste	First-order kinetic model	Biomethane and Biohydrogen	0.95	-	5
Batch reactor	Food waste	Cone model	Biomethane and Biohydrogen	0.99	-	5
Batch reactor	Food waste	Logistic model	Biomethane and Biohydrogen	0.98	-	5
Batch reactor	Food waste	Modified Gompertz model	Biogas	0.98	-	52
Batch reactor	Microalgae	Modified Gompertz model	Biohydrogen	0.99	-	53
Batch reactor	Macroalgae	Modified Gompertz Model	Biohydrogen	0.99	-	54
Batch reactor	Macroalgae	Logistic function model	Biohydrogen	0.99	-	54
Batch reactor	Corncob powder	Modified Gompertz model	Biohydrogen	0.99	-	55
Batch reactor	Dairy waste	Monod model	Biohydrogen	0.99	-	56
Batch reactor	Dairy waste	Luedeking-Piret model	Biohydrogen	0.95	-	56
Batch reactor	Dairy waste	Logistic function model	Biohydrogen	0.99	-	57
Batch reactor	Tofu wastewater	Cone model	Biogas	0.99	2.562	58
Batch reactor	Animal manure and wastewater	Monod model	Biogas	0.98	-	59
Batch reactor	Animal manure and lignocellulosic wastes	Cone model	Biogas	0.99	-	60
Batch reactor	Lignocellulosic wastes	Modified Gompertz model	Biohydrogen	0.98	-	61
Batch reactor	Lignocellulosic wastes	Logistic function model	Biogas	0.97	27.24	62
Batch reactor	Lignocellulosic wastes	Cone model	Biogas	0.99	8.03	62
Batch reactor	Lignocellulosic wastes	Monod model	Biogas	0.99	17.52	62
Batch reactor	Lignocellulosic wastes	Cone model	Biogas	0.96	-	38
Batch reactor	Lignocellulosic wastes	Cone model	Biogas	0.98	18.60	63
Batch reactor	Water hyacinth	Logistic function model	Biogas	0.99	0.042 (MAPE)	28

These mechanistic approaches are particularly useful for interpreting process behaviour and for making limited, biologically consistent predictions when supported by sufficiently detailed experimental data. However, the classical Monod formulation assumes a single limiting substrate and does not inherently account for inhibition, microbial decay, or metabolic shifts, thereby limiting its applicability in complex biofuel systems. Without suitable extensions incorporating inhibition or multi-substrate interactions, such models may yield misleading parameter interpretations⁴⁵. The Luedeking-Piret model provides an intermediate representation by

linking product formation to microbial growth through growth-associated and non-growth-associated terms. This allows quantitative assessment of the coupling between biomass development and biofuel generation in anaerobic systems. Nevertheless, its use of constant coefficients limits its applicability under strongly dynamic conditions or in systems influenced by inhibition, maintenance metabolism, or changing environmental constraints^{46,47}.

A comparative overview of the principal characteristics, strengths, and typical domains of applicability of these model classes is presented in Table 3. The comparison reinforces that no single

Table 3 — Comparative summary of commonly used kinetic models in biofuel production

Models	Model type	Key strengths	Major limitations	Typical misapplication	Reference
First-order model	Empirical	Simple representation with minimal data	Oversimplifies degradation as a single-rate process	Used for heterogeneous substrates without validating rate assumption	78, 79
Gompertz / Modified Gompertz model	Empirical sigmoidal	Effectively describes lag and production phases	Descriptive model lacking direct biological meaning	Treating fitted parameters as intrinsic kinetics	80, 81
Logistic model	Empirical sigmoidal	Stable mathematical form for cumulative trends	Imposes symmetric growth behaviour not always biologically realistic	Selected solely based on goodness-of-fit	81, 82
Monod model	Mechanistic (growth-based)	Links substrate availability to microbial growth	Classical form assumes single limitation and steady physiology	Applied without inhibition or multi-substrate extensions	45, 49
Cone model	Empirical sigmoidal	Flexible shape captures multi-phase trends	High flexibility may mask underlying mechanisms	Overfitting sparse datasets or extrapolating final yield	83
Luedeking-Piret model	Semi-mechanistic	Separates growth and non-growth product formation	Assumes constant growth-product coupling	Used under dynamic conditions without validating coefficient stability	23, 84

kinetic model can be universally applied across biofuel production systems. Empirical models are well-suited for rapid descriptive analysis and preliminary screening in controlled environments, but become less reliable when used for mechanistic interpretation or prediction. Mechanistic and semi-mechanistic approaches offer greater biological insight but require sufficiently resolved datasets and careful validation to avoid parameter estimation uncertainty⁵. Hybrid and data-assisted models may address intermediate levels of system complexity, although their effectiveness remains contingent on data quality, validation strategy, and transparent model formulation. Taken together, these observations indicate that model effectiveness arises from context-sensitive selection rather than mathematical form alone, providing the basis for the decision-oriented guidance discussed in the following section.

Roadmap for Kinetic Model Selection in Biofuel Production Systems

The comparative evaluation presented in the preceding sections indicates that the effectiveness of a kinetic model in biofuel production is more closely contingent upon alignment with system characteristics, data availability, and clearly defined research objectives^{8,64}. Misinterpretation and limited predictive reliability in the literature often arise not from the use of simple models, but from the selection of models that are inconsistent with the intended application⁶⁵. In response, a context-based roadmap for kinetic model selection is proposed, schematically represented in Fig. 2, to assist

researchers in making application-specific and scientifically defensible modeling decisions.

Model selection based on research objective

such as the Luedeking-Piret model provide a useful intermediate framework, allowing quantitative assessment of growth-associated and non-growth-associated product formation⁶⁸. For system-level analysis, dynamic simulation, or control-oriented applications, structured frameworks or hybrid approaches may be considered, provided that the additional complexity is justified by the intended analytical objective rather than by convention alone. The first and most critical step in kinetic model selection is the clear definition of the modeling objective. When the primary goal is descriptive analysis, such as comparing cumulative gas yields or identifying overall production trends, empirical or sigmoidal models such as Gompertz, logistic, or Cone kinetic model are generally appropriate⁶⁶. These models efficiently summarise experimental behaviour and facilitate intra-study comparisons, provided that their fitted parameters are not interpreted as intrinsic kinetic constants. When the objective is to obtain mechanistic insight into substrate utilisation, identify rate-limiting steps, or analyse growth dynamics, models based on Monod-type kinetics or suitable inhibition-based extensions are more appropriate⁶⁷. In cases where the relationship between microbial growth and product formation is of specific interest, semi-mechanistic formulations

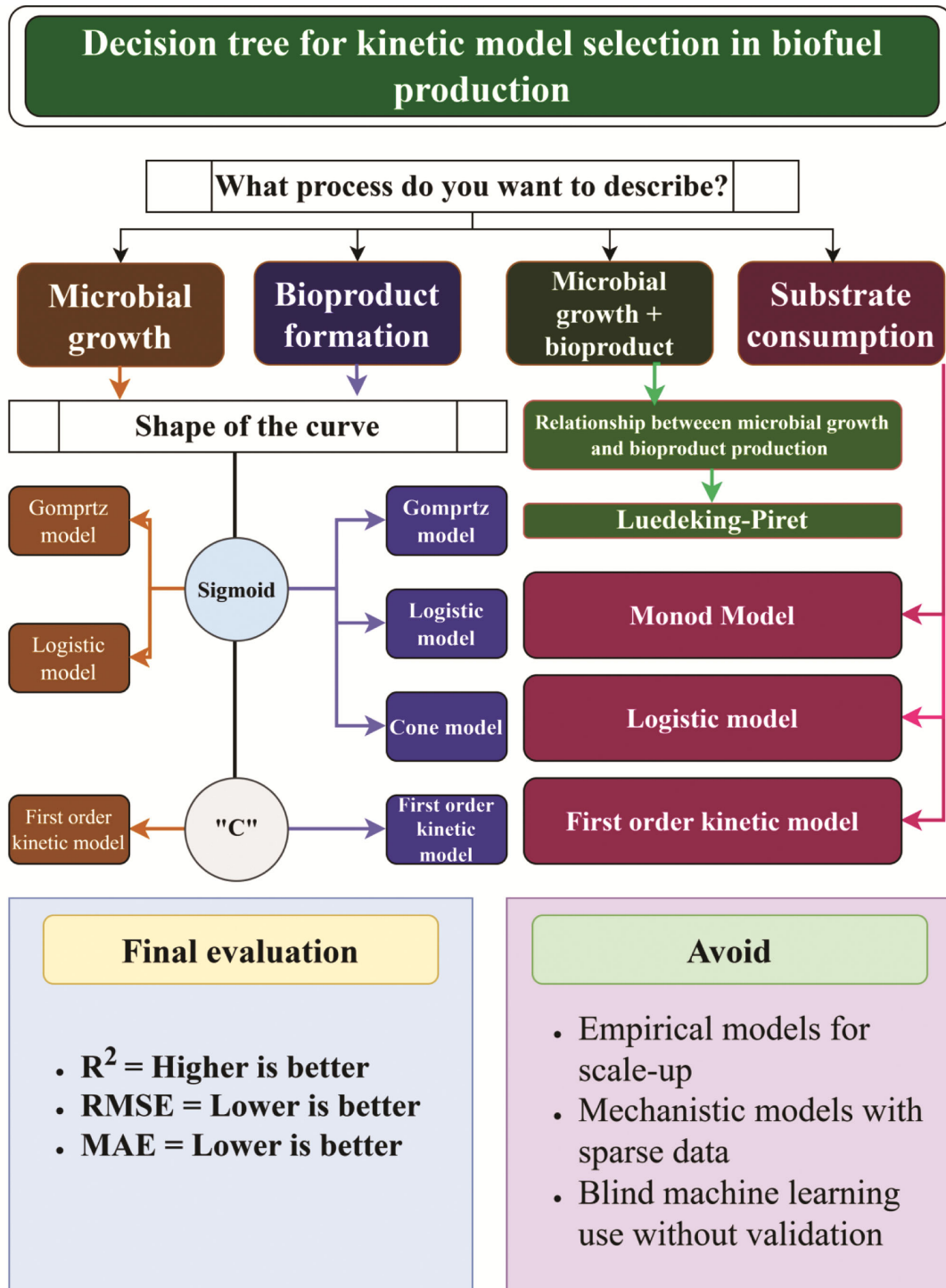


Fig. 2 — Decision-oriented framework for kinetic model selection in biofuel production

Model selection based on data availability and quality

Data availability plays a fundamental constraint on model complexity. In data-limited sceneries, such as short-duration batch studies with sparse temporal resolution, empirical models such as Gompertz, logistic, and Cone formulations often provide the

most reliable representation because they minimise parameter uncertainty and reduce the risk of overfitting^{69,70}. Applying mechanistic or highly parameterised models under such conditions can lead to poorly identifiable parameters and unjustified confidence in predictions⁷¹. When moderate-

resolution datasets are available, including time-resolved measurements of substrate concentration and product formation, mechanistic or inhibition-based models become more feasible. However, increases in model complexity should be introduced gradually, and additional parameters must be supported by independent experimental evidence^{72,73}. Highly structured models, such as ADM1-based formulations or machine-learning-assisted approaches, are generally defensible only in systems supported by extensive datasets, such as long-term pilot-scale operations or continuously monitored processes^{25,74}.

Model selection based on system complexity

The structural complexity of the biofuel system represents a key determinant in selecting an appropriate kinetic model. Systems characterised by relatively simple substrates, stable operating conditions, and limited inhibitory interactions can often be described adequately using empirical formulations or basic growth-based models⁷⁵. In such cases, additional model complexity rarely improves interpretive value and may instead introduce unnecessary parameter uncertainty. As system complexity increases, such as in mixed-feedstock digestion, multi-stage biochemical conversion, or environments influenced by inhibition, syntrophic interactions, or fluctuating loading conditions, models that incorporate mechanistic relationships become more appropriate. Monod-type formulations with suitable extensions, or semi-mechanistic approaches such as the Luedeking-Piret model, allow representation of coupled biological processes that cannot be explicitly represented by purely empirical expressions⁷⁴.

Decision logic, reporting, and validation principles for kinetic model selection

Based on the evidence synthesised in this review, kinetic model selection may be guided by the following general principles:

- When the objective is descriptive trend analysis and data availability is limited, empirical or sigmoidal models (including Gompertz, logistic, or Cone formulations) are generally appropriate.
- When a mechanistic understanding of microbial growth or substrate utilisation is required and adequately resolved datasets are available, Monod-type or inhibition-based models may be employed.
- When the analytical focus is on the quantitative relationship between microbial growth and product formation, semi-mechanistic models such as the Luedeking-Piret formulation may provide an

appropriate balance between interpretability and simplicity.

- When system-level analysis, process control, or long-term prediction is the primary goal and extensive datasets exist, structured mechanistic models such as ADM1 or hybrid models may be justified.
- When predictive performance is prioritised over mechanistic interpretability and sufficiently high-quality data are available, data-driven approaches may be considered cautiously, with explicit acknowledgement of their assumptions and limitations.

Empirical models are generally unsuitable for independent scale-up or optimisation analysis; mechanistic models should not be applied without sufficient data support; and advanced data-driven approaches should not be treated as substitutes for process understanding. In addition to appropriate model selection, transparent reporting and validation practices are essential to ensure scientific rigor and reproducibility. Modeling studies should clearly state model assumptions, parameter estimation procedures, and validation strategies. Kinetic parameters should be accompanied by uncertainty estimates, such as confidence intervals or sensitivity analyses, and model performance should be evaluated using both statistical criteria and consistency with underlying biological mechanisms. Wherever feasible, independent datasets should be used for validation, particularly when models are intended for predictive, comparative, or decision-support applications. Common validation approaches in biofuel kinetic modeling include validating model predictions against independent experimental datasets, testing model performance under different operating conditions such as varying substrate concentrations or temperatures, and comparing predicted cumulative gas production profiles with measured data^{76,77}. comparative analysis presented in the preceding sections clearly demonstrates that the effectiveness of a kinetic model in biofuel production is governed not by its mathematical sophistication, but by its alignment with system characteristics, data availability, and clearly defined research objectives^{8,64}. Instead of a simple model, it is rather an inappropriate model choice that is the overriding cause of misinterpretation and low predictive power of existing literature⁶⁵. Based on this, the following section suggests that a context-based roadmap to kinetic model selection, schematically shown in Fig. 2, would be useful in helping researchers make

defensible, application-compromised modeling decisions.

Future Scope

Several methodological directions emerge from the present analysis of kinetic modeling practices in biofuel production systems. Future research should focus on strengthening the integration between experimental design and model development, particularly by generating datasets that support parameter identifiability, inhibition verification, and mechanistic validation. Improved treatment of parameter uncertainty remains an important area for advancement. The systematic incorporation of uncertainty quantification, sensitivity analysis, and independent validation strategies would enhance the reliability and comparability of kinetic studies. The development of standardized reporting guidelines specific to biofuel kinetic modeling may further improve reproducibility across the literature. Emerging hybrid and data-assisted approaches also warrant careful methodological development. Rather than replacing mechanistic formulations, data-driven techniques may serve complementary roles in pattern recognition and parameter estimation. Future work should emphasise interpretability, validation under varying operational conditions, and transparency of assumptions to ensure that predictive improvements remain scientifically meaningful.

Conclusion

This review underscores that kinetic modeling in biofuel production cannot be reduced to the selection of mathematically convenient equations. No single model is universally applicable; rather, the suitability of a kinetic formulation depends on the alignment between model assumptions, system complexity, data resolution, and analytical objectives. A comparative assessment of empirical, semi-mechanistic, and mechanistic approaches demonstrates that each model class serves distinct purposes but may yield misleading interpretations when applied beyond its domain of validity. This comparative perspective highlights clear differences in model applicability, data requirements, and interpretability across model classes. The analysis further indicates that widespread reliance on statistical goodness-of-fit, without sufficient attention to parameter identifiability and mechanistic consistency, limits the interpretive and predictive strength of many published studies. The decision-oriented framework developed in this work provides a structured basis for selecting models

according to objective, data quality, and system characteristics, thereby promoting more transparent and scientifically defensible modeling practices. Advancing kinetic analysis in biofuel research will depend not primarily on increasing mathematical complexity, but on disciplined alignment between model structure, experimental design, and intended application.

Nomenclature

RMSE	Root mean square error
MAPE	Mean absolute percentage error
CSTR	Continuous stirred-tank reactor
AnAS-RBC	Anaerobic activated sludge-rotating biological contactor
OFMSW	Organic fraction of municipal organic waste
$P(t)$	Cumulative gas production at time (t)
P_{MAX}	Maximum gas yield
R_{MAX}	Maximum gas production rate
t	Retention time
k	Rate constant
λ	Lag phase duration
e	Euler's number (≈ 2.71828)
μ	Specific microbial growth rate
μ_{MAX}	Maximum specific growth rate
S	Substrate concentration
K_s	Half-saturation constant
X	Microbial biomass concentration
α	Growth-associated product formation coefficient
β	Non-growth-associated product formation coefficient

Conflict of Interest

The authors declare no conflict of interest.

References

- 1 Pendse D S, Deshmukh M & Pande A, Different pre-treatments and kinetic models for bioethanol production from lignocellulosic biomass: A review, *Heliyon*, 9 (2023) e16604.
- 2 Asvad M, Hajinezhad A, Jafari A & Moosavian S F, Multiscale kinetic modeling for biohydrogen production: A study on membrane bioreactors, *Int J Hydrogen Energy*, 48 (2023) 29641.
- 3 Yang H, Wang M, Bai X, Dai Z, Zhao Y, Hu Y & Li J, Advancing bioethanol production with a new kinetic model based on structure-oriented lumping for cellulose conversion, *Fuel*, 373 (2024) 132302.
- 4 Olatunji K O, Olugbemide A D, Akerejola R F & Madyira D M, Kinetic modelling of the biomethane production potential of acidic pretreated groundnut shells, *Biomass Convers Biorefin*, 15 (2025) 17139.
- 5 Yahya M, Herrmann C, Ismaili S, Jost C, Truppel I & Ghorbal A, Kinetic studies for hydrogen and methane co-

- production from food wastes using multiple models, *Biomass Bioenergy*, 161 (2022) 106449.
- 6 Javed M A & Hassan A A, A kinetic modeling and energy conversion evaluation of biohydrogen production using a co-culture of green microalgae and wastewater activated sludge, *Int J Hydrog Energy*, 57 (2024) 148.
 - 7 Borisov M, Dimitrova N & Simeonov I, Mathematical modeling and stability analysis of a two-phase biosystem, *Processes*, 8 (2020) 1.
 - 8 Abilmazhinov Y, Shakerkhan K, Meshechkin V, Shayakhmetov Y, Nurgaliyev N & Suychinov A, Mathematical modeling for evaluating the sustainability of biogas generation through anaerobic digestion of livestock waste, *Sustain*, 15 (2023) 5707.
 - 9 Chorukova E & Simeonov I, Mathematical modeling of the anaerobic digestion in two-stage system with production of hydrogen and methane including three intermediate products, *Int J Hydrog Energy*, 45 (2020) 11550.
 - 10 Guo X & Wang J, The Gompertz model for biohydrogen production kinetics: Origin, application and solving methods, *Int J Hydrogen Energy*, 88 (2024) 242.
 - 11 Tai T H & A Noymer, Models for estimating empirical Gompertz mortality: With an application to evolution of the Gompertzian slope, *Popul Ecol*, 60 (2018) 171.
 - 12 Da-Silva C, Astals S, Peces M, Campos J L & Guerrero L, Biochemical methane potential (BMP) tests: Reducing test time by early parameter estimation, *Waste Manag*, 71 (2018) 19.
 - 13 Kythreotou N, Florides G & Tassou S A, A review of simple to scientific models for anaerobic digestion, *Renew Energy*, 71 (2014) 701.
 - 14 Kumar V K, Mahendiran R, Subramanian P, Karthikeyan S, Surendrakumar A, Kumargouda V, Ravi Y, Choudhary S, Singh R & Verma A K, Optimization of biogas potential using kinetic models, response surface methodology, and instrumental evidence for biodegradation of tannery fleshings during anaerobic digestion, *Open Life Sci*, 18 (2023) 20220721.
 - 15 Wu H, Li J, Liao Q, Fu Q & Liu Z, Enhanced biohydrogen and biomethane production from *Chlorella* sp with hydrothermal treatment, *Energy Convers Manag*, 205 (2019) 112373.
 - 16 Silva F M S, Mahler C F, Oliveira L B & Bassin J P, Hydrogen and methane production in a two-stage anaerobic digestion system by co-digestion of food waste, sewage sludge and glycerol, *Waste Manag*, 76 (2018) 339.
 - 17 Zhang H, An D, Cao Y, Tian Y & He J, Modeling the methane production kinetics of anaerobic co-digestion of agricultural wastes using sigmoidal functions, *Energies*, 14 (2021) 258.
 - 18 Groot J C J, Cone J W, Williams B A, Debersaques F M A & Lantinga E A, Multiphasic analysis of gas production kinetics for in vitro fermentation of ruminant feeds, *Anim Feed Sci Technol*, 64 (1996) 77.
 - 19 Pererva Y, Miller C D & Sims R C, existing empirical kinetic models in biochemical methane potential (BMP) testing, their selection and numerical solution, *Water*, 12 (2020) 1831.
 - 20 Deseure J, Obeid J, Willison J C & Magnin J P, Reliable determination of the growth and hydrogen production parameters of the photosynthetic bacterium *rhodobacter capsulatus* in fed batch culture using a combination of the gompertz function and the ludedeking-piret model, *Heliyon*, 7 (2021) e07394.
 - 21 Lee E, Cumberbatch J, Wang M & Zhang Q, Kinetic parameter estimation model for anaerobic co-digestion of waste activated sludge and microalgae, *Bioresour Technol*, 228 (2017) 9.
 - 22 Jamaludin N F M, Abdullah L C, Idrus S, Engliman N S, Tan J P & Jamali N S, Nickel-iron doped on granular activated carbon for efficient immobilization in biohydrogen production, *Bioresour Technol*, 391 (2024) 129933.
 - 23 R Luedeking and E L Piret, "A kinetic study of the lactic acid fermentation Batch process at controlled pH," *J Biochem Microbiol Technol Eng*, vol 1, no 4, pp 393–412, Dec 1959, doi: 101002/jbmte390010406
 - 24 Ding D & Benson D A, Simulating biodegradation under mixing-limited conditions using michaelis-menten (Monod) kinetic expressions in a particle tracking model, *Adv Water Resour*, 76 (2015) 109.
 - 25 Donoso-Bravo A, Sadino-Riquelme M C, Valdebenito-Rolack E, Paulet D, Gómez D & Hansen F, Comprehensive ADM1 extensions to tackle some operational and metabolic aspects in anaerobic digestion, *Microorganisms*, 10 (2022) 948.
 - 26 Ding L, Cheng J, Qiao D, Li H & Zhang Z, Continuous co-generation of biohydrogen and biomethane through two-stage anaerobic digestion of hydrothermally pretreated food waste, *Energy Convers Manag*, 268 (2022) 116000.
 - 27 Bouchareb E M, Derbal K, Bedri R, Slimani K, Menas S, Lazreg H, Maaref F, Ouabdelkader S, Saheb A, Bouaita R, Bouchareb R & Dizge N, Improving biohydrogen production by dark fermentation of milk processing wastewater by physicochemical and enzymatic pretreatments, *Appl Biochem Biotechnol*, 196 (2024) 2741.
 - 28 Omondi E A, Ndiba P K, Chepkoech G K & Kegode A A, Modeling anaerobic co-digestion of water hyacinth with ruminal slaughterhouse waste for first order, modified gompertz and logistic kinetic models, *Int J Renew Energy Dev*, 12 (2023) 627.
 - 29 Akhbari A, Zinatizadeh A A, Vafaeifard M, Mohammadi P, Zainal B S & Ibrahim S, Effect of operational variables on biological hydrogen production from palm oil mill effluent by dark fermentation using response surface methodology, *Desalin Water Treat*, 137 (2019) 101.
 - 30 Sinharoy A, Baskaran D & Pakshirajan K, Sustainable biohydrogen production by dark fermentation using carbon monoxide as the sole carbon and energy source, *Int J Hydrogen Energy*, 44 (2019) 13114.
 - 31 Chhabra P, Mosbach S, Karimi I A & Kraft M, Practically useful models for kinetics of biodiesel production, *ACS Sustain Chem Eng*, 7 (2019) 4983.
 - 32 Soares B S, Borges A C, de Matos A T, Barbosa R B G & e Silva F F, Exploring the removal of organic matter in constructed wetlands using first order kinetic models, *Water*, 14 (2022) 472.
 - 33 Bekins B A, Warren E & Godsy E M, A comparison of zero-order, first-order, and monod biotransformation models, *Groundwater*, 36 (1998) 261.
 - 34 Abdelwahab T A M, Pan J, Ni J Q, Yang C, Mohanty M K, Darwish E A, Desoky S H M, Yang H & Fodah A E M, Nanoparticles for improving biogas production and effluent biofertilizer, *Sci Rep*, 15 (2025) 19233.

- 35 Usevičiūtė L, Januševičius T, Danila V, Mažeikienė A, Zagorskis A, Pranskevičius M & Marčiulaitienė E, Performance and kinetics of anaerobic digestion of sewage sludge amended with zero-valent iron nanoparticles, analyzed using sigmoidal models, *Energies*, 18 (2025) 1425.
- 36 Sohale A P, Janardanan S, Yadav D, Dash B & Yadav M D, Dark fermentative biohydrogen production: recent advances and challenges, *Ind Eng Chem Res*, 62 (2023) 14755.
- 37 Abubakar A M, Umdagas L B, Waziri A Y & Itamah E I, Estimation of biogas potential of liquid manure from kinetic models at different temperature, *Int J Sci Res Comput Sci Eng*, 10 (2022) 46.
- 38 Syaichurrozi I, Biogas production from co-digestion *Salvinia molesta* and rice straw and kinetics, *Renew Energy*, 115 (2018) 76.
- 39 Nguyen D D, Jeon B H, Jeung J H, Rene E R, Banu J R, Ravindran B, Vu C M, Ngo H H, Guo W & Chang S W, Thermophilic anaerobic digestion of model organic wastes: Evaluation of biomethane production and multiple kinetic models analysis, *Bioresour Technol*, 280 (2019) 269.
- 40 Leite V D, Ramos R O, Lopes W S, de Araújo M C U, de Almeida V E, da Silva Oliveira N M & Viriato C L, Kinetic modeling of anaerobic Co-digestion of plant solid waste with sewage sludge: Synergistic influences of total solids and substrate particle size in biogas generation, *Bioenergy Res*, 17 (2024) 744.
- 41 Martin J, De-Adana D D R & Asuero A G, Fitting models to data: Residual analysis, a primer, *Uncertain Quantif Model calibration*, 133 (2017).
- 42 Sámano V, Tirado A, Félix G & Ancheyta J, Revisiting the importance of appropriate parameter estimation based on sensitivity analysis for developing kinetic models, *Fuel*, 267 (2020) 117113.
- 43 Kumar J L G & Zhao Y Q, A review on numerous modeling approaches for effective, economical and ecological treatment wetlands, *J Environ Manag*, 92 (2011) 400.
- 44 Ahlamine I, Alla A & El-Khattabi N, Mathematical analysis of an anaerobic digestion model for biogas production from solid waste, *Sci Rep*, 14 (2024) 1.
- 45 Monod J, The growth of bacterial cultures, *Annu Rev Microbiol*, 3 (1949) 371.
- 46 Mohammadi M & Mohammadi P, Developing single-substrate steady-state model for biohydrogen production in continuous anaerobic activated sludge-rotating biological contactor system: Novel insights on the process, *Int J Energy Res*, 46 (2022) 2041.
- 47 Rao R & Basak N, Sequential dark-photo batch fermentation and kinetic modelling for biohydrogen production using cheese whey as a feedstock, *Appl Biochem Biotechnol*, 194 (2022) 3930.
- 48 Pramanik S K, Suja F B, Porhemmat M & Pramanik B K, Performance and kinetic model of a single-stage anaerobic digestion system operated at different successive operating stages for the treatment of food waste, *Processes*, 7 (2019) 600.
- 49 Park J H, Sim Y B, Kumar G, Anburajan P, Park J H, Park J H & Kim S H, Kinetic modeling and microbial community analysis for high-rate biohydrogen production using a dynamic membrane, *Bioresour Technol*, 262 (2018) 59.
- 50 Achinas S & Euverink G J W, Effect of combined inoculation on biogas production from hardly degradable material, *Energies*, 12 (2019) 217.
- 51 Mahata C, Dhar S, Ray S & Das D, Effect of thermal pretreated organic wastes on the dark fermentative hydrogen production using mixed microbial consortia, *Fuel*, 284 (2021) 119062.
- 52 Moharir S, Bondre A, Vaidya S, Patankar P, Kanaskar Y & Karne H, Comparative analysis of the amount of biogas produced by different cultures using the modified gompertz model and logistic model, *Eur J Sustain Dev Res*, 4 (2020) e0141.
- 53 Jacob A, Alaswad A, Ashok B, Praveen V & Jino L, An innovative dual-phase platform for biohydrogen production: *Chlorella* -based nutrient removal and *E aerogenes* fermentation with PEMFC power generation evaluation, *Chem Eng Sci*, 326 (2026) 123491.
- 54 Taşkan B, Köroğlu E O & Taşkan E, *Cladophora* sp as a sustainable feedstock for dark fermentative biohydrogen production, *Int J Hydrogen Energy*, 47 (2022) 15410.
- 55 Duan Z, Yang J, Yu H, Mou H & Zhang J, Enhanced biohydrogen production by Fe-based metal-organic framework/hydrothermal carbon composite, *Int J Hydrogen Energy*, 199 (2026) 152885.
- 56 Rao R & Basak N, Process optimization and mathematical modelling of photo-fermentative hydrogen production from dark fermentative cheese whey effluent by *Rhodobacter sphaeroides* OU001 in 2-L cylindrical bioreactor, *Biomass Convers Biorefinery*, 13 (2023) 3929.
- 57 Santos G A, Bortoli L D, Santos D A, Lobato F S, Cardoso V L & Batista F R X, Insights of light spectra on biohydrogen production by photo-fermentation, *Int J Hydrogen Energy*, 149 (2025) 150088.
- 58 Syaichurrozi I, Rusdi R, Hidayat T & Bustomi A, Kinetics studies impact of initial pH and addition of yeast *Saccharomyces cerevisiae* on biogas production from tofu wastewater in Indonesia, *Int J Eng Trans B Appl*, 29 (2016) 1037.
- 59 Jijai S & Siripatana C, Kinetic Model of biogas production from co-digestion of thai rice noodle wastewater (Khanomjeen) with chicken manure, *Energy Procedia*, 138 (2017) 386.
- 60 Parralejo A I, Royano L, González J & González J F, Small scale biogas production with animal excrement and agricultural residues, *Ind Crops Prod*, 131 (2019) 307.
- 61 Campos-Flores R C, Suárez-Vázquez S I, Trably E, Bernet N & Cruz-López A, White-rot fungi as a sustainable pretreatment approach to improve lignocellulosic biomass conversion for biohydrogen production, *Biomass Bioenergy*, 210 (2026) 109040.
- 62 Akbay H E G, Anaerobic mono and co-digestion of agro-industrial waste and municipal sewage sludge: Biogas production potential, kinetic modelling, and digestate characteristics, *Fuel*, 355 (2024) 129468.
- 63 Syaichurrozi I, Suhirman S & Hidayat T, Effect of initial pH on anaerobic co-digestion of *Salvinia molesta* and rice straw for biogas production and kinetics, *Biocatal Agric Biotechnol*, 16 (2018) 594.
- 64 Mogilicharla A & Reddy P S, Kinetic modeling and development of optimal trajectories for biodiesel production using multi-objective optimization, *Environ Technol Innov*, 20 (2020) 101111.

- 65 Akroum H, Akroum-Amrouche D & Aibeche A, Modeling of conversion kinetics in bioenergy production technologies, *Int J Green Energy*, 21 (2024) 3415
- 66 Alalayah W M, Al-Zahrani A, Edris G & Demirbas A, Kinetics of biological hydrogen production from green microalgae *Chlorella vulgaris* using glucose as initial substrate, *Energy Sources Part A Recover Util Environ Eff*, 39 (2017) 1210.
- 67 Enouy R W, Walton K M, Malton I I, Sra K S, Sihota N N, Daniels E J & Unger A J A, A mechanistic derivation of the Monod bioreaction equation for a limiting nutrient, *J Math Biol*, 84 (2022) 62.
- 68 Alvarez-Ramirez J, Meraz M & Vernon-Carter E J, A theoretical derivation of the monod equation with a kinetics sense, *Biochem Eng J*, 150 (2019) 107305.
- 69 Prabhu S, Kosir N, Kothare M V & Rangarajan S, Derivative-free domain-informed data-driven discovery of sparse kinetic models, *Ind Eng Chem Res*, 64 (2025) 2601.
- 70 Choudhury S, Moret M, Salvy P, Weilandt D, Hatzimanikatis V & Miskovic L, Reconstructing kinetic models for dynamical studies of metabolism using generative adversarial networks, *Nat Mach Intell*, 4, (2022) 710.
- 71 Fedorov A, Perechodjuk A & Linke D, Kinetics-constrained neural ordinary differential equations: Artificial neural network models tailored for small data to boost kinetic model development, *Chem Eng J*, 477 (2023) 146869.
- 72 Baquerizo G, Fiat J, Buffiere P, Girault R & Gillot S, Modelling the dynamic long-term performance of a full-scale digester treating sludge from an urban WRRF using an extended version of ADM1, *Chem Eng J*, 423 (2020) 128870.
- 73 Mo R, Guo W, Batstone, D Makinia J & Li Y, Modifications to the anaerobic digestion model no 1 (ADM1) for enhanced understanding and application of the anaerobic treatment processes-A comprehensive review, *Water Res*, 244 (2023) 120504.
- 74 Ge Y, Tao J, Wang Z, Mu L, Guo W, Cheng Z, Yan B, Shi Y, Su H & Chen G, A hybrid approach of anaerobic digestion model no 1 and machine learning to model and optimize continuous anaerobic digestion processes, *Biomass Bioenergy*, 184 (2024) 07176.
- 75 Rutland H, You J, Liu H, Bull L & Reynolds D, A systematic review of machine-learning solutions in anaerobic digestion, *Bioengineering*, 10 (2023) 1410.
- 76 Donoso-Bravo A, Pérez-Elvira S I & Fdz-Polanco F, Application of simplified models for anaerobic biodegradability tests Evaluation of pre-treatment processes, *Chem Eng J*, 160 (2010) 607.
- 77 Holliger C, Alves M, Andrade D, Angelidaki I, Astals S, Baier U, Bougrier C, Buffière P, Carballa M, de-Wilde Vinnie, Ebertseder F, Fernández B, Ficara E, Fotidis I, Frigon J C, de Lacroix H F, Ghasimi D S M, Hack G, Hartel M, Heerenklage J, Horvath I S, Jenicek P, Koch K, Krautwald J, Lizasoain J, Liu J, Mosberger L, Nistor M, Oechsner H, Oliveira J V, Paterson M, Pauss A, Pommier S, Porqueddu I, Raposo F, Ribeiro T, Pfund F R, Strömberg S, Torrijos M, van Eekert M, van Lier J, Wedwitschka H, Wierinck I, Towards a standardization of biomethane potential tests, *Water Sci Technol*, 74 (2016) 2515.
- 78 Vavilin V A, Fernandez B, Palatsi J & Flotats X, Hydrolysis kinetics in anaerobic degradation of particulate organic material: An overview, *Waste Manag*, 28 (2008) 939.
- 79 Yumnam P & Debnath P, A review on mathematical modeling of different biological methods of hydrogen production, *Hydrogen*, 4 (2023) 881.
- 80 Lay J J, Li Y Y & Noike T, Influences of pH and moisture content on the methane production in high-solids sludge digestion, *Water Res*, 31 (1997) 1518.
- 81 Tinpranee N, Incharoensakdi A & Phunpruch S, Screening cyanobacteria from marine coastal waters of Thailand for biohydrogen production, *J Appl Phycol*, 30 (2018) 3471.
- 82 Zwietering M H, Jongenburger I, Rombouts F M & van 't Riet K, Modeling of the bacterial growth curve, *Appl Environ Microbiol*, 56 (1990) 1875.
- 83 Cone J W, van Gelder A H & Driehuis F, Description of gas production profiles with a three-phasic model, *Anim Feed Sci Technol*, 66 (1997) 31.
- 84 Basak N, Jana A K & Das D, CFD modeling of hydrodynamics and optimization of photofermentative hydrogen production by *Rhodospseudomonas palustris* DSM 123 in annular photobioreactor, *Int J Hydrogen Energy*, 41 (2016) 7301.