Whitepaper Modeling and Simulation

Editorial

A lot has happened in 2.5 years in the realm of modeling, particularly with the rise of IA that is inundating every aspect of our professional and personal life. People unfamiliar with this may feel overwhelmed by all the information related to blue collar jobs extinction and the big replacement of traditional skills. It is our role, as people close to data, models and their benefit to keep the expectations realistic.

As of mid-2025, **AI is everywhere**. New tools are being developed and released almost daily. Is this a bubble (btw, we can model that too) I think it's still too early to say, but we are likely at the **peak of inflated expectations,** according to the Gartner Hype Cycle. A period of disillusionment and reduced expectations will likely follow, but eventually, we will reach a **productivity plateau,** where the most relevant AI tools and applications become an integral part of everyday life for the foreseeable future.

As of mid-2025, AI permeates all aspects of process engineering, yet the peak of inflated expectations underscores the need to maintain realistic outlooks. Updated projections indicate the global biogas market, valued at approximately $65 billion in 2022, is expected to reach $95 billion by 2032, with a compound annual growth rate CAGR of 4-6.4%, reaching $68-129B by 2030-2034, with upgrading subsector at 11-15% CAGR driven by Europe with a 40% market share. Mechanistic modeling, such as CFD and ODE, provides essential interpretability to optimize these markets, distinguishing itself from black-box AI approaches and enabling verified ROI in applications like hydrogen green blending. In the UK/Chile context, opportunities like Innovate UK grants for biogas and CORFO for green hydrogen highlight the integration of renewable energy in modeling.

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Executive Summary

The profitability of critical industrial processes, such as biogas and water treatment, is under threat from volatile energy costs, the risk of costly operational failures, and growing regulatory and market pressure for sustainability. "Black-box" AI solutions lack the trust required for high-stakes process control, while traditional models fall short of capturing real-world dynamic complexity.

This Whitepaper demonstrates how hybrid modeling—an industrially-validated synergy of process physics and AI—resolves this gap. We create "digital copilots" that not only optimize operations but do so transparently, enabling ROI to be quantified prior to CAPEX investment.

The value is demonstrable: double-digit energy OPEX reductions, risk mitigation by preventing costly oversizing, and a verifiable improvement in carbon footprint and resource circularity. Modela is the strategic partner that deciphers this complexity, converting operational uncertainty into verifiable ROI and a resilient competitive advantage.

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THE CURRENT UBIQUITOUS ROLE OF MODELING

The irruption of artificial intelligence—particularly marked by the release of ChatGPT at the end of 2022—will be remembered as one of the major breakthroughs of the past century. This tool, built on a foundation of advanced models, is capable of processing, generating, and predicting outcomes based on user input (commonly referred to as a prompt in this field), supported by rigorous training and testing procedures that must be updated periodically.

Suddenly, commonly used and often overlapping terms such as machine learning (the title of a subsection in our previous white paper), data-driven, empirical, and phenomenological, among others, seemed outdated or overshadowed by the ubiquitous presence of artificial intelligence.

One major drawback of artificial intelligence is that the results of certain simulations are often difficult—or impossible—to interpret. A key advance in 2025 lies in the ability of mechanistic models to quantify ROI interpretably, for instance, mitigating failure rates in anaerobic digestion exceeding 50-80% in historical agricultural plants, resulting in 50% revenue losses for six months or more. ODE and ML hybrids enable predictive validation, ensuring profitability from startup and distinguishing from opaque AI simulations.

In contrast, theory-based models can replicate specific processes with transparency, allowing a complete understanding of the model's behavior and, consequently, of the real-world process being modeled. It is hoped that future developments in AI will bridge this gap between prediction and interpretability. Advances in XAI such as SHAP and LIME enable integration with mechanistic models, but the fundamental basis remains transparency for regulated processes, distinguishing from purely black-box approaches. Hybrid models, combining mechanistic first-principles with ML, address plant-model mismatches, enabling up to10-30% efficiency gains in nonlinear processes like biogas production. While these tools help narrow the gap between prediction and interpretability, ongoing developments are needed to address their limitations in engineering contexts.

1.1. MODELING DEFINITION AND APPROACHES

Modeling involves implementing a mathematical representation of a certain reality or more specifically of a process in engineering, whereas simulating consists of taking these models, solving them, and postprocessing and visualizing the results in a particular software and computer system, in other words, making a use of the model. Thus, modeling and simulation aim at describing the essential aspects of behavior over time and/or space of a process or system of interest allowing us to understand how it works. The use of modeling and computational simulation allows us to strengthen and speed up the decision-making process related to a particular process or system performance. This way, companies can make decisions faster than through experimental procedures, avoiding extra costs simultaneously. In addition, it reduces the risk to operators and the environmental impact. Nowadays, the exercise of modeling and simulation is also related to creating a digital twin or a virtual replica of a specific process or system.

1.2. MODELS USEFULNESS

Models can be used for a wide range of reasons but if we want to sum this up is to give answers to a question that otherwise will be difficult to answer and that is **prediction.** Regardless of whether it is about knowing how temperature will rise due to climate change, how the weather will be tomorrow or if by increasing the rotation speed of my impeller will improve the efficiency of my process, knowing how my system will behave in the future will always be something useful to find through models.

One may want to predict how a system of interest will behave due to several factors:

Operation conditions: It refers to the set of circumstances or factors under which a system, process, or piece of equipment is intended to function effectively and safely. This includes various parameters like temperature, pressure, flow rate, change of feedstock, variations of the inlet flows, presence of unexpected compounds and other relevant variables, that determine how well a device or system performs its intended functions. Proper operating conditions are crucial for ensuring efficiency, safety, and reliability of any operation.

Environmental conditions: it corresponds to the environmental factors surrounding a process or object that can affect its operation or performance. These conditions include outside temperature, humidity, air pressure, light, noise, vibration, marine current behavior, salinity, etc. In essence, it's the overall environment that influences how a process runs and how materials behave within that environment

Retrofitting: System retrofitting is the process of upgrading or modifying existing systems, buildings, or equipment with new technologies or features aiming to improve their performance, efficiency, or safety. This involves integrating new components or functionalities into legacy systems without complete replacement, though some redesign may be required. Before executing any retrofitting, it may be wise to see virtually how these actions will impact the system performance with minimal disturbance on the actual physical system, therefore minimizing the possible impact on the current process throughput.

Detailed engineering: During the execution of an feasibility engineering project, particularly after the early stages of basic or conceptual engineering—where fundamental principles are applied to generate a preliminary estimation of system performance—detailed process engineering takes a deeper dive into the intricacies of these processes. It provides comprehensive specifications and documentation necessary for precise execution. Traditional empirical equations or correlations can now be complemented or even fully replaced by the complete resolution of the governing equations of the system. Today, critical phenomena such as pressure, turbulence, heat transfer, erosion, and corrosion can be accurately modeled through mechanistic simulations, creating a virtual replica of the process.

Regardless of the reason for using modelling, you can basically carry out countless experiments under different conditions and extract where those best results you were looking for are obtained.

Along with prediction, a collateral or complementary use of modeling could be for **explanatory** purposes. Once you have an accurate predictive model of a system, you may want to understand the reasons behind specific behaviors. For example, in a wastewater treatment plant where only a handful of parameters are measured periodically and a biological process is represented with a mechanistic model, you can infer the current biological diversity of the bioreactor or detect the potential accumulation of undesired intermediates beyond certain thresholds. This insight allows you to anticipate possible future behaviors and take corrective action.

Similarly, in a process unit where mixing is achieved through liquid recirculation, if a pipe cracks and requires shutdown and repair, you may need to determine the root cause to prevent recurrence. By modelling the mixing process, you can analyse the pressure exerted on the pipe walls to determine whether the mixing intensity was the culprit.

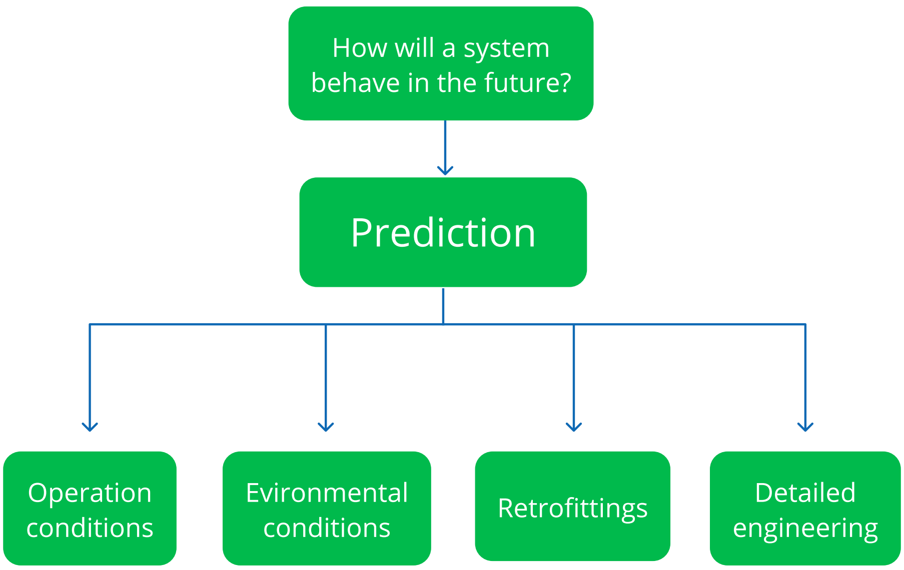


Figure 1. General diagram of the main application of modelling for prediction purposes in processengineering.

1.3. MECHANISTIC (Theory-based) VS IA

The broader perception of AI as a **black box** still holds — we often don't know how these models truly work, and in many cases, **not even their creators fully understand** their internal mechanisms. In contrast, **mechanistic models** aim to represent the **fundamental principles** behind specific processes. These are sometimes referred to as **"white-box"** or **"transparent-box"** models[1]. However, even mechanistic models are **never fully physics-based**, because it's impossible to capture every underlying process — from macroscopic to microscopic — that takes place in a real system. There is always some part of the system that is left out, either knowingly or unknowingly.

In the following we will describe the main characteristics that nowadays differentiate IA and mechanistic modelling.

1.3.1. The issue of interpretability

AI models are not inherently interpretable, though current research aims to enhance their explainability. In this regard, mechanistic modeling far surpasses AI tools in explanatory power.

At present, the primary use of AI prioritizes predictive capability over interpretability. For instance, when using **ChatGPT** to draft an email response or generate a database from photos of shelved books, the focus is on output quality—not the underlying process. Some neural networks and similar models may be composed of more than a million (hyper) parameters, making it extremely difficult to trace what actually produced the results[2].

However, in **process engineering**, understanding how and why certain results are achieved is often critical when leveraging a model. Mechanistic models allow engineers to trace outcomes back to specific parameters—such as reaction rates or stoichiometric conversions—providing clear insights into the causal relationships behind the results.

1.3.2. The issue of data

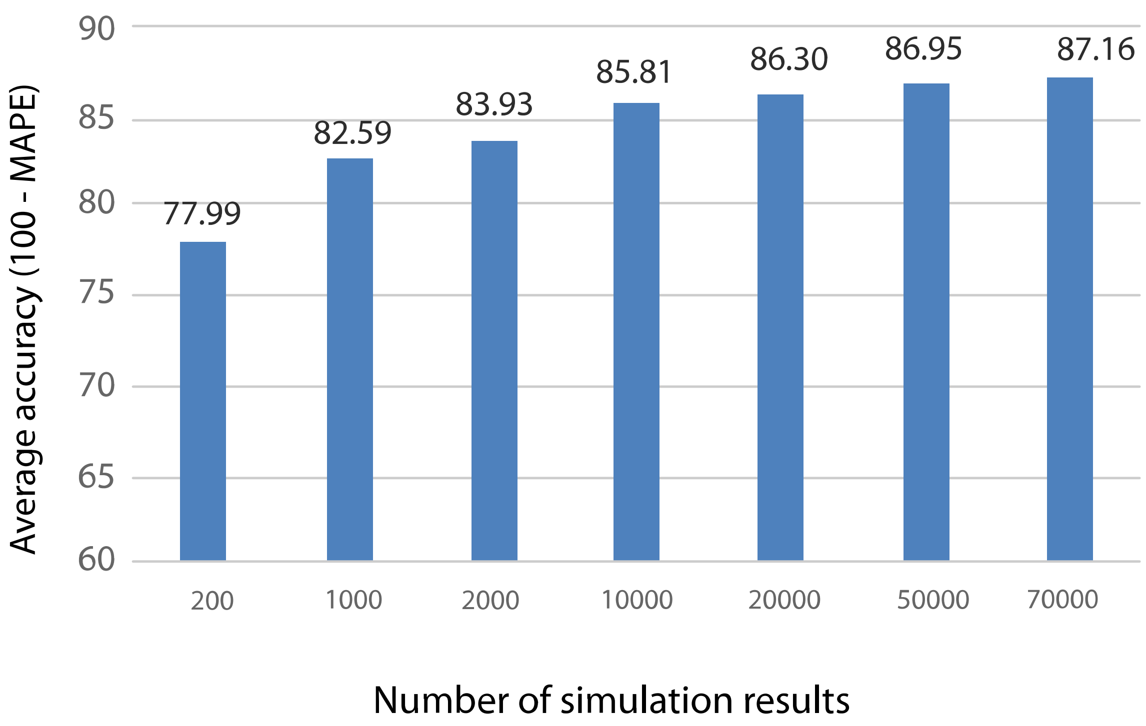
Real data is always necessary to calibrate and validate models, regardless of their nature. However, when it comes to **AI models,** which are data-driven by definition, the amount of data required to produce a useful and robust model can be substantial. This requirement presents a challenge in **process engineering,** where collecting large and informative datasets is often expensive and time-consuming.

In contrast, for some modeling goals, **real data may not be strictly necessary** when using **mechanistic models.** These models aim to represent the underlying physics or biology of a process and can be useful even in the absence of complete datasets — for example, when evaluating new technologies or understanding **mass balances** within a system.

[1] Mathew, D.E., Ebem, D.U., Ikegwu, A.C. et al. Recent Emerging Techniques in Explainable Artificial Intelligence to Enhance the Interpretable and Understanding of AI Models for Human. Neural Process Lett 57, 16 (2025). https://doi.org/10.1007/s11063-025-11732-2

[2] https://www.nytimes.com/2024/05/21/technology/ai-language-models-anthropic.html?searchResultPosition=54

The efficiency of AI models is highly dependent on the data. To assess this, several predictive models based on decision trees were generated and evaluated.



These models were applied to databases containing different volumes of simulations. By averaging the prediction accuracy and plotting it as a function of the number of data points. The Figure shows how the average accuracy of the generated models increases asymptotically with the number of data points. The improvement in accuracy from 50,000 to 70,000 data points was only 0.29%.

Identifying the point at which the results become independent of the number of training data is crucial to increasing confidence in the final outcomes, as it allows this potential source of variability to be ruled out. Running these 70,000 simulations on a high-performance computer with 8 cores takes approximately 5 days. Model accuracy reaches asymptotic convergence with approximately 70,000 data points, but in wastewater treatment (WWTP), aeration accounts for 45-55% of total OPEX, generating annual costs exceeding $80,000 in large plants. Digital twins based on ODE and ML can enable up to 10-30% reductions in energy OPEX, with ROI under six months, highlighting the superiority of interpretable hybrid approaches.

1.3.3. The issue of time

One variable plays a crucial role in mechanistic modeling—whether using ODE- or PDE-based models—when the system is not in steady state: time. In such models, the current value of a variable always depends on its previous state. This temporal dependency requires us to define initial conditions at the start of the simulation.

One of the main challenges will be evaluating the performance of models trained on stationary data when applied to real-world data, where a truly steady state is rarely achieved. In AI models, this time dependency is not always straightforward, as the training and testing datasets are often based on near-steady-state conditions. Many AI models (especially feedforward neural networks or regressors) are trained on static input–output pairs. If trained only on steady-state or snapshot data, they may perform poorly on transient conditions unless time-dependent patterns are incorporated.

If the models show insufficient performance under these conditions, we will consider adopting less interpretable but more suitable approaches for predicting transient processes, such as long short-term memory (LSTM) recurrent neural networks.

1.3.4. The environmental burden

Modeling can significantly enhance the sustainability of processes by reducing emissions associated with costly and labor-intensive physical and field testing. In this regard, mechanistic models can be solved within a reasonable time using the power of a standard personal computer. For example, I ran the ADM1 model—solving 40 ODEs simultaneously—on a 5-year-old Core i7 with 1 CPU laptop in under a minute.

In contrast, training and running AI models (which uses GPU) typically requires the continuous processing of massive datasets, which takes place in large data centers being built worldwide to meet the growing demand for AI capabilities. This raises two major sustainability concerns: **the high energy consumption** required to operate these facilities, and the **significant water use** for cooling. Numerous recent studies have quantified the energy, and water demands of data centers[3]. Fortunately, the expansion of **renewable energy,** particularly solar, has accelerated in recent years, reducing concerns about short-term energy scarcity. Additionally, advances in **water treatment** technologies and **thermal energy recovery** from hot water are helping to mitigate the environmental impact of data center operations.

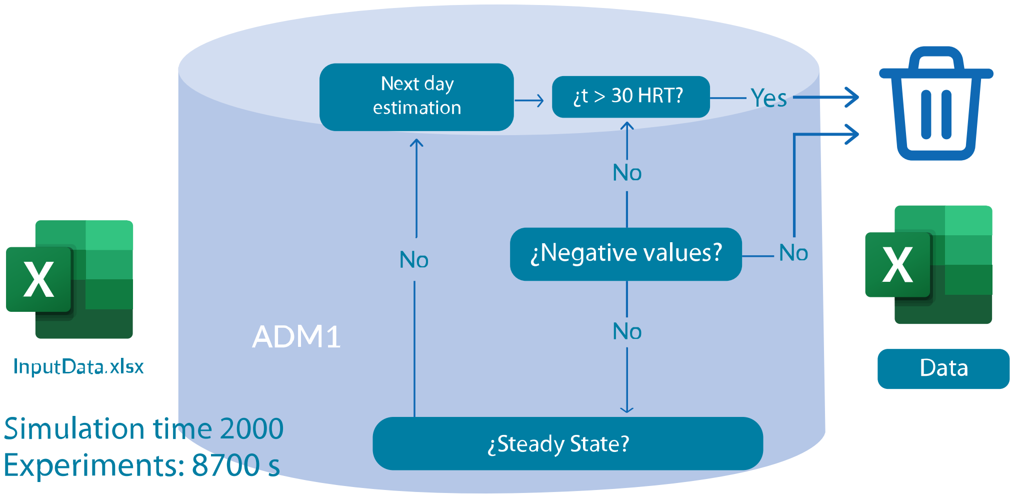
1.3.5. Mechanistic with IA. Exploiting the synergy

Thus far, we have compared mechanistic and AI models in general terms. However, these approaches can be **combined** to leverage the strengths of both.

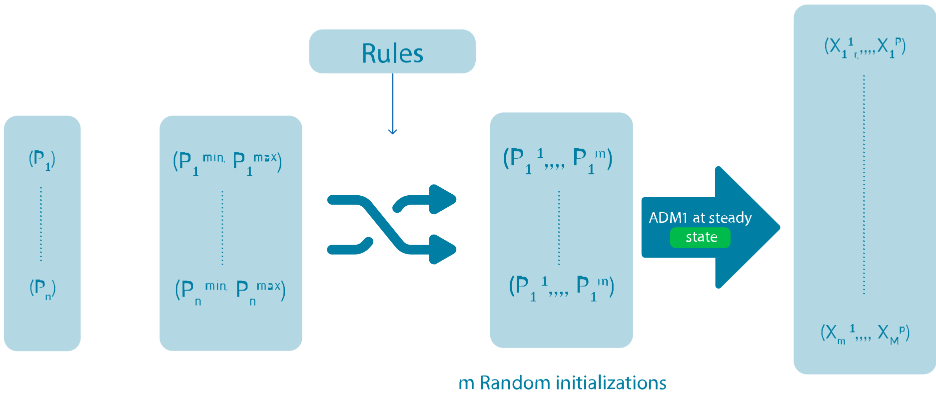
One straightforward application—and something we frequently implement at **Modela**—is using a mechanistic model to create a **virtual replica (digital twin)** of a process. This allows us to generate the **large datasets required to train AI models.**

In this **hybrid approach**, the mechanistic model (typically more time-consuming and computationally expensive) is used to develop a **data-driven surrogate model.** This surrogate can then be executed and utilized in **real-time applications**, offering both accuracy and efficiency.

[3] James O'Donnell and Casey Crownhart. 2025. We did the math on AI's energy footprint. Here's the story you haven't heard. MIT Technology Review. https://www.technologyreview.com/2025/05/20/1116327/ai-energy-usage-climate-footprint-big-tech/



In our research project, **MAAPDA**, we recognized the challenges of obtaining sufficient real-world data to test AI models effectively. To address this, we implemented the **ADM1** (Anaerobic Digestion Model No. 1), a theory-based model of the anaerobic digestion process, in its original form as well as an extended version. The extended model incorporates additional critical processes, such as **H_2S** generation and **digestate quality component prediction.**



We then developed an **automated algorithm** to run the virtual AD process simulations repeatedly based on a predefined set of inputs and their permissible variation ranges. For example, in one of our setups, we successfully executed **2,000 virtual experiments in just 2.5 hours.** All generated data underwent **data science analysis** and was subsequently used for **AI model training and calibration.**

1.4 Hybrid Modeling Trends (2025–26)

The convergence of mechanistic modeling and artificial intelligence (AI) has advanced significantly over the past five years, giving rise to hybrid modeling frameworks that combine first-principles knowledge with data-driven learning. These approaches address two limitations of conventional methods: (i) the lack of robustness of purely statistical models when facing extrapolation, and (ii) the rigidity of deterministic models in capturing nonlinear and context - dependent dynamics. By 2025, hybrid modeling is emerging as a cross-sector standard for high-stakes industrial processes where reliability, explainability, and efficiency converge. Its trajectory suggests a paradigm in which hybrid digital twins not only augment real-time operations but also become essential tools for regulatory compliance, risk management, and sustainable performance.

Teams typically start from first-principles models (mass/energy balances, ADM1/ASM, membrane transport) and add machine learning where parameters are uncertain or data are rich. This preserves explainability and keeps decisions within safety limits and operating objectives. Methodological progress integrates physics-informed neural networks (PINNs), Koopman theory paired with Model Predictive Control (MPC), and causal AI for root-cause analysis; reinforcement learning (RL) is considered only with hard constraints and human oversight. Adoption is projected to grow at ~10–15% CAGR in chemical engineering (Internal estimate, Modela 2025 based on market trends). In wastewater, hybrid prediction plus MPC is associated with measurable aeration-energy reductions[4] (illustrative: US$80,000–120,000/year in medium-scale plants assuming electricity at US$0.12/kWh). In Seawater Reverse Osmosis SWRO, supervisory MPC reduces specific energy by ~0.3–0.8 kWh/m^3 (illustrative: ~US$50,000/year in large plants assuming 30,000 m^3/d)]. In aquaculture, hybrid forecasting reduces exposure to algal blooms ($5-7B annually, illustrative: ~10-20% risk mitigation).

[4] M. Salomé Duarte, Gilberto Martins, Pedro Oliveira, Bruno Fernandes, Eugénio C. Ferreira, M. Madalena Alves, Frederico Lopes, M. Alcina Pereira, and Paulo Novais. A Review of Computational Modeling in Wastewater Treatment Processes. ACS ES&T Water 2024 4 (3), 784-804 DOI: 10.1021/acsestwater.3c00117

2

GAS APPLICATIONS

KEY FOR PROCESS EFFICIENCY AND DEFOSSILIZATION

Gas compounds play a fundamental role across a wide range of engineering and sustainable processes. They can serve as essential feedstocks, intermediate supplies, valuable products, or, in some cases, undesired by-products or emissions. Their presence and behavior are often critical to the efficiency, safety, and environmental impact of a process. For instance, gases may be injected intentionally to initiate or sustain a reaction, generated as part of a transformation, or released into the atmosphere as part of the system's output.

Modeling and simulation provide powerful tools for understanding and predicting the behavior of gases within these processes. Whether analyzing gas blending in energy systems, CO_2 emissions in bioprocesses, or hydrogen dynamics in sustainable fuel technologies, computational models can offer insight into mass transfer, reaction kinetics, and environmental dispersion. These tools enable engineers and decision-makers to optimize performance, ensure compliance with regulatory standards, and support the transition to greener technologies

In renewable gas applications, CFD optimizes mixing and hydrogen blending, reducing biogas upgrading costs. With Europe capturing 40% of the global biogas market, these mechanistic simulations can extend equipment lifespan by mitigating H2S corrosion ensuring regulatory compliance in UK and Chile grids.

2.1. MAKING THE GRID GREENER AND SAFER

One of the key challenges in the energy sector is transforming the existing gas grid into a greener, more sustainable system by increasing the share of renewable gases in the overall mix. These renewable gases include biogas, biomethane, green hydrogen, and others that offer low-carbon or carbon-neutral alternatives to conventional fossil fuels. Alongside this transition, ensuring the safe handling, distribution, and integration of these gases is essential to protect infrastructure, the environment, and public health.

2.1.1. Renewables gas mix

The natural gas distribution network is a well-developed infrastructure globally, consisting of pipelines that transport gas from extraction to consumption points. However, it contributes significantly to greenhouse gas emissions through combustion and leaks. As part of the energy transition, there is a growing need to replace traditional hydrocarbons with cleaner alternatives, such as hydrogen. Yet, this shift presents several challenges[5]. The use of CFD simulation can help study in detail the mixing of these gases within the natural gas distribution network. The information provided by these simulations can be used to make decisions regarding the suitability of gas replacement, as well as to study the effect of different operational parameters on the performance of the transportation network. Several geometries of gas blending units can be represented in CFD as it is shown in Figure 2. And the results obtained through the modeling application are well validated with other studies.

[5] Topolski, Reznicek, E. P., Erdener, B. C., San Marchi, C. W., Ronevich, J. A., Fring, L., ... & Chung, M. (2022). Hydrogen blending into natural gas pipeline infrastructure: review of the State of technology.

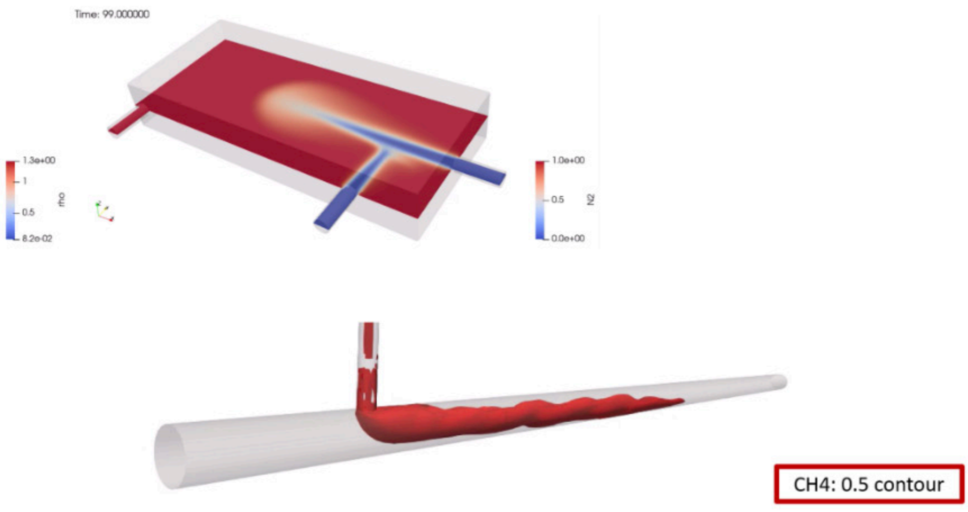
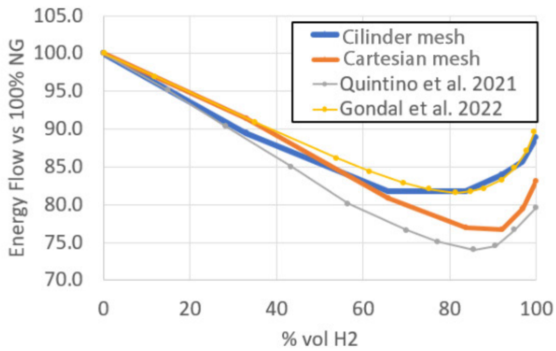


Figure 2. Virtual replica and simulation of two gas blending configurations systems.

NG (%) Frac. Vol.	H2 (%) Frac. Vol.	Energy Flow Cartesian (J/s)	Energy Flow Cylinder (J/s)
100	0	1.11E+07	1.08E+07
67.02	32.98	1.01E+07	9.65E+06
34.16	65.83	8.86E+06	8.83E+06
16.29	83.70	8.53E+06	8.83E+06
7.96	92.03	8.49E+06	9.07E+06
3.14	96.85	8.88E+06	9.26E+06
0	100	9.19E+06	9.60E+06



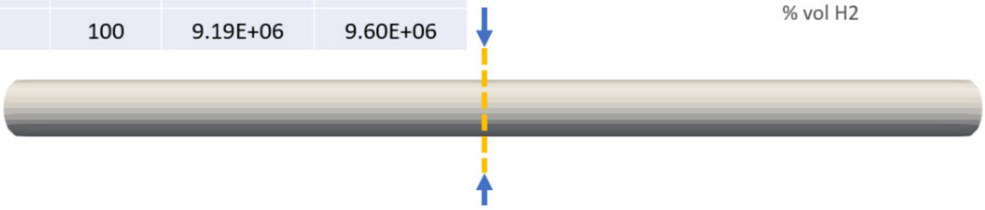


Figure 3. Gas blending simulation results with reported values from literature.

As shown in Figure 3, the transported energy is initially zero since the system starts at rest. Over time, the pressure drop accelerates the flow until it reaches a steady state. By simulating the same scenario with different gas compositions, the results of Gondal et al[6]. can be replicated, as shown in Figure 3.

[6] Gondal, I. A., & Sahir, M. H. (2012). Prospects of natural gas pipeline infrastructure in hydrogen transportation. International Journal of Energy Research, 36(15), 1338-1345.

2.1.2. Hazardous gas release

H_2S (hydrogen sulfide) is a highly toxic and corrosive compound that can cause death within seconds, even at very low concentrations. Unfortunately, it is commonly produced under anaerobic biological conditions in waste treatment processes, as well as during crude oil refining. Since we cannot completely eliminate its presence, it is essential to design systems and define operating conditions that minimize the impact of H_2S on the environment surrounding the emission point. One effective approach is to simulate the dispersion plume of an H_2S-rich gas stream to evaluate exposure zones and ensure regulatory compliance. The shape and reach of the plume depend on several factors. As illustrated in the Figure 4, both the outlet mass flow rate and outlet velocity significantly influence the plume's behavior. This model was implemented in OpenFOAM, considering a turbulent flow regime, thermodynamic and transport models, and using Cantera[7] to obtain accurate parameter values.

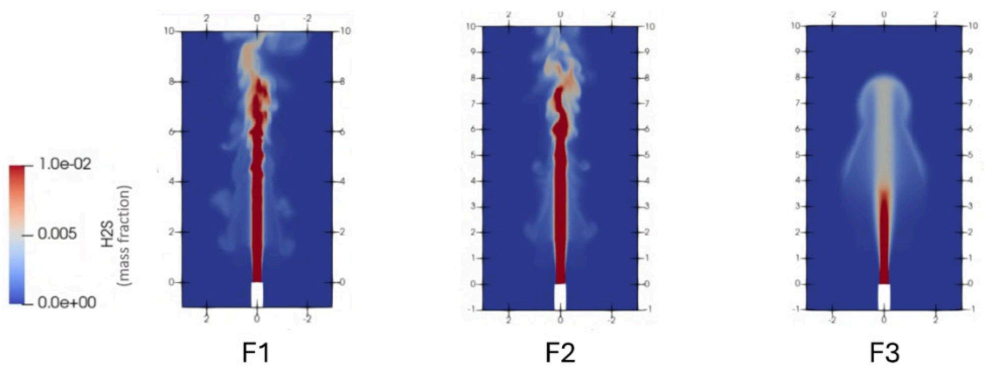


Figure4. Simulation of the H_2S-rich gas stream under various operating conditions.

[7] https://cantera.org/2.6/sphinx/html/cython/thermo.html

2.2. OXIGEN SUPPLY AND MIXING

Air or oxygen injection plays a critical role in various industrial processes, primarily in two key aspects: maintaining aerobic conditions necessary for biological or chemical reactions and promoting effective mixing within the system. Depending on the application, this injection can take several forms, including jet injection, gas bubbling, and surface aeration, among others. Each method has different implications for mass transfer, energy efficiency, and process control.

2.2.1. Gas bubbling

Aeration typically occurs through the injection of bubbles, usually from the bottom of a process unit. These bubbles can vary in shape and size depending on operational conditions and the diffuser's design. Their physical characteristics directly influence oxygen transfer efficiency, mixing dynamics, and the overall effectiveness of the aeration process.

Traditional modeling approaches often cannot represent individual bubbles explicitly and instead treat the gas as a continuous secondary phase—an approximation that may introduce limitations. Simulating bubble injection systems using fully resolved Euler–Euler models is highly computationally demanding. In contrast, hybrid Euler–Lagrange approaches offer a substantial reduction in computational cost while maintaining accuracy. Figure 5 illustrates the development and impact of a bubble-type air injection system within a process unit. These models have been validated in the literature against both high-fidelity simulations and experimental data. Building capabilities around these methods allows for faster, more scalable simulations of real-world systems, enabling better design and operational optimization.

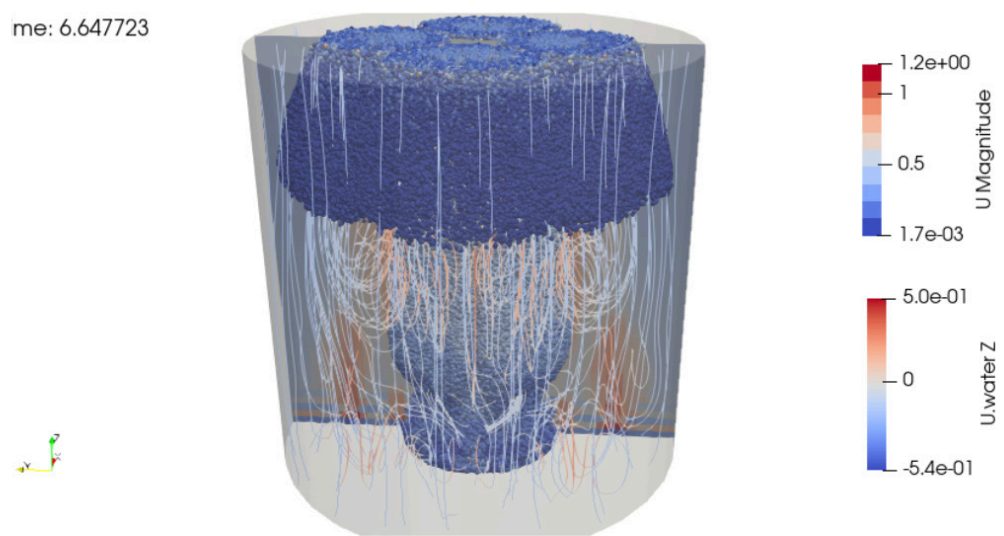


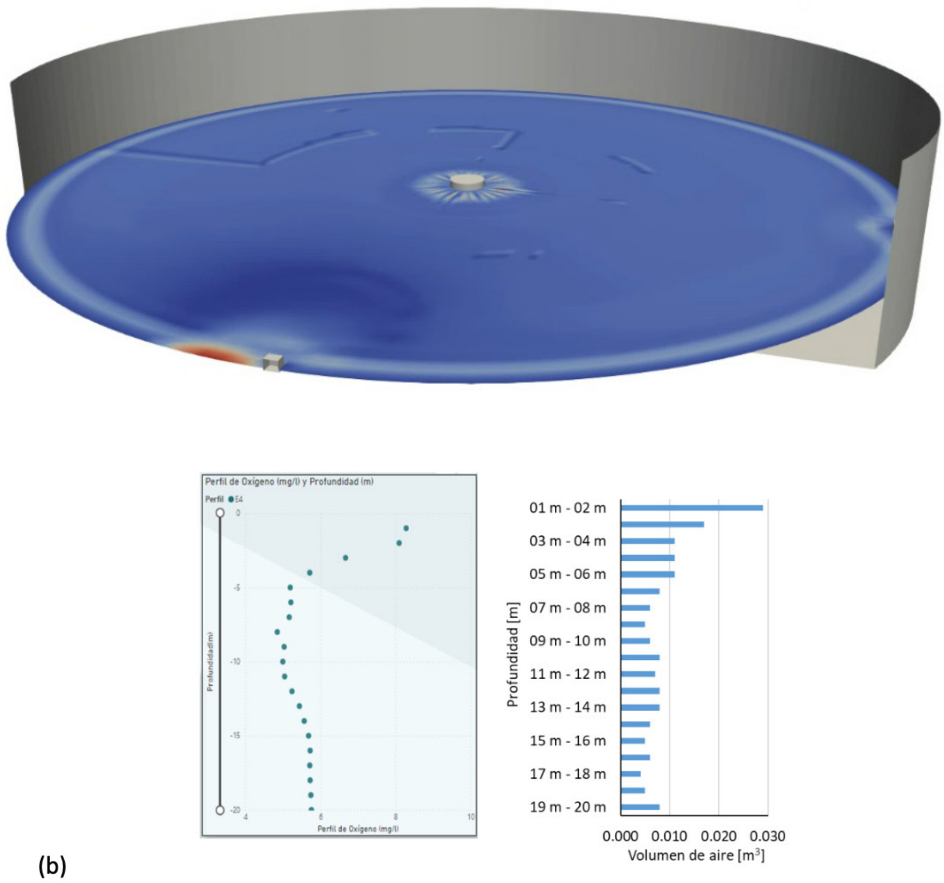
Figure 5. Simulation of the injection of air using a bubbling system.

2.2.2. Oxygen concentration

The transfer of oxygen from the gas phase to the liquid phase is key to ensuring that the oxygen concentration is appropriate for the process to take place. An oxygen concentration below the desired threshold may limit the (bio) reaction, reducing product growth (e.g., from fish, bacteria, yeast, etc.) or product generation. Conversely, a concentration above the set point can lead to excessive energy consumption for air injection and, consequently, unnecessary economic costs.

Various technologies have been developed to ensure that the required oxygen concentration is achieved in the process unit. In Figure 6, we show a CFD modeling application capable of representing oxygen transfer between phases and predicting whether the levels required by the process are met. Such simulations can be leveraged across the air injection technology development industry to optimize performance and efficiency.

(a)



(b)

Figure 6. Validation of CFD model for (a) optimal oxygen homogenization in tank for a recirculating unit in Aquaculture and (b) comparison of predicted OD values versus experimental ones.

3

ADVANCED BIOLOGICAL PROCESS

ENHANCING RESILIENCE THOUGH DIGITAL COPILOTING

Biological processes—or bioprocesses—are expected to play a pivotal role in the transition toward a circular economy and in advancing the environmental sustainability of industrial systems. These processes harness the power of microorganisms or enzymes to convert waste into valuable resources, reduce emissions, and promote the efficient use of materials and energy.

Modeling these bioprocesses provides a powerful way to understand, predict, and optimize their behavior. When integrated into operations, a well-developed model can function as a real-time digital copilot—running in parallel with the physical system to offer continuous insights, simulate alternative scenarios, and support informed decision-making. This added layer of information helps reduce uncertainty, improve process reliability, and ultimately enhance the overall performance and resilience of sustainable technologies.

3.1 MOVING LIMITS/ BREAKING BOUNDARIES

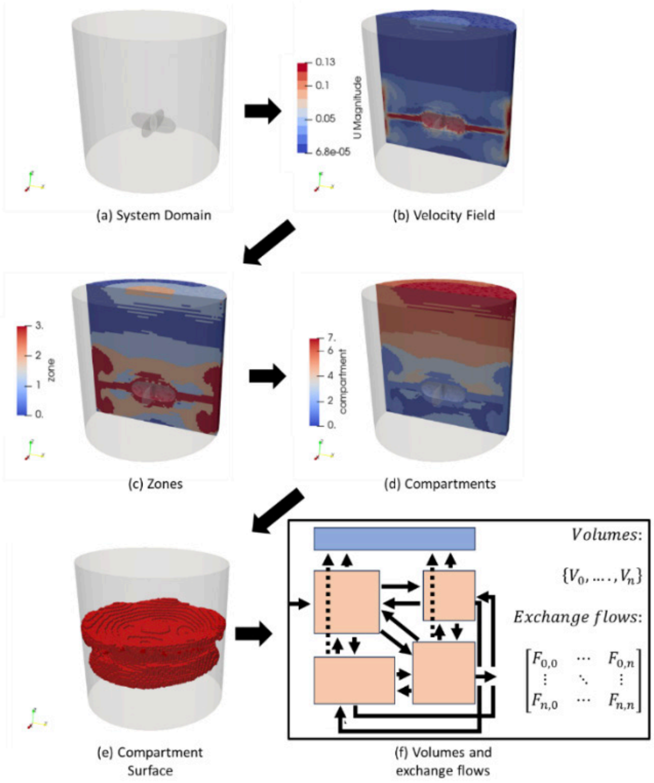
Exploring modeling tools allows us to move beyond the traditional constraints and boundaries imposed by the physical domain. We should continuously seek new approaches and think beyond conventional methods. This mindset of forward-looking and out-of-the-box thinking enables us to test innovative ideas, challenge the status quo, and develop new tools that can scale up the benefits of using modeling.

3.1.1 A methodology for fluid dynamic and kinetic integration

So far, there is no fully automated methodology available to integrate fluid dynamic models—typically solved through CFD—with the kinetics of a process in a seamless and efficient way. While several methodologies attempting to bridge this gap have been reported in the literature—including in a review we published couple years ago[8] —these approaches still rely heavily on manual procedures and subjective decisions. As a result, the overall workflow becomes time-consuming and highly dependent on the individual modeler's expertise and judgment.

This lack of standardization not only limits scalability and reproducibility but also introduces significant variability in results, making it difficult to consistently evaluate or compare outcomes across different systems or modeling teams. Developing a robust, automated framework that can couple CFD with kinetic models in a transparent and repeatable manner remains a critical challenge—and a major opportunity—for the modeling and simulation community.

[8] M.C. Sadino-Riquelme, A. Donoso-Bravo, F. Zorrilla, E. Valdebenito-Rolack, D. Gómez, F. Hansen, Computational fluid dynamics (CFD) modeling applied to biological wastewater treatment systems: An overview of strategies for the kinetics integration, Chemical Engineering Journal, 466, 2023, 143180, https://doi.org/10.1016/j.cej.2023.143180.



The developed compartmentalization procedure is fully automated with a self-developed tool utilizing OpenFOAM and C++. OpenFOAM which facilitates direct access to the mesh's data and the corresponding fields from the CFD simulation.

The tool first takes a user-defined scalar field from a CFD simulation and a specified number of zones. It calculates threshold values to divide the domain into equal-volume zones, assigning each mesh cell accordingly (Figure a–c). Connected cells are grouped into compartments, and those below a minimum volume are merged with neighbors based on the highest exchange flow (Figure d). The tool then identifies boundary faces between compartments (Figure e) and sums the flow through them to compute an **N** × **N** exchange flow matrix (Figure f). Compartments can also be refined manually using primitive shapes.

The described approach simplifies the system's stationary flow field and the geometric details of the CFD simulation into a reduced set of compartments and their exchange flows. The more compartments there are, the more details from the original flow field prevail. Therefore, increasing the number of compartments reduces information loss. Actually, a CFD model is a compartmentalized system itself, where each mesh cell is a perfectly mixed compartment. Using the developed tool, compartmentalization can be performed based on any field defined in the CFD simulation. To ensure reliability, the total liquid volume is verified to match the sum of all compartment volumes. Additionally, an algorithm checks the mass balance for every compartment and iteratively corrects its exchange flows until the balance is fulfilled under a defined tolerance.

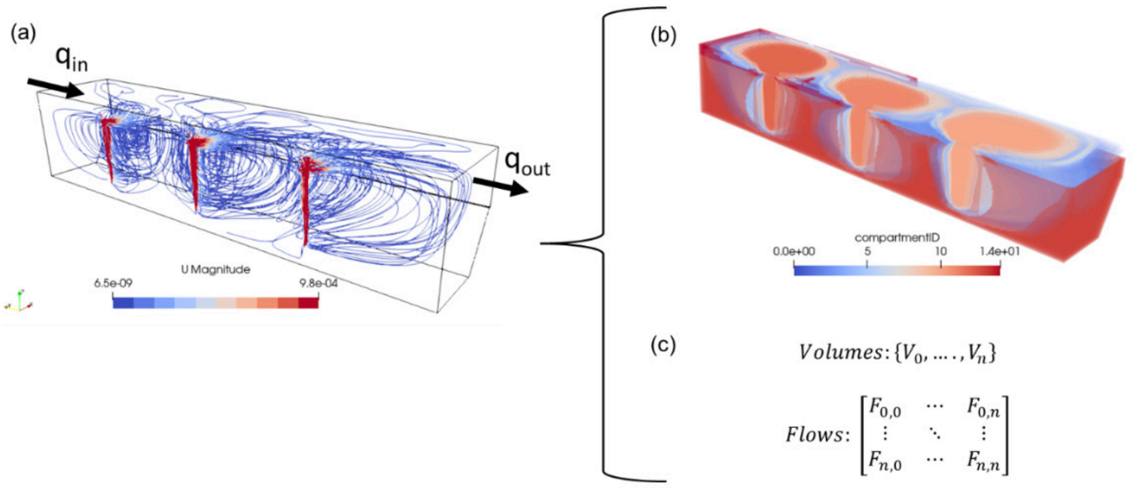


Figure 7. Compartmentalization of C1. (a) Streamlines of the velocity field, (b) compartments visualization, and (c) vector of volumes and exchange flow matrix.

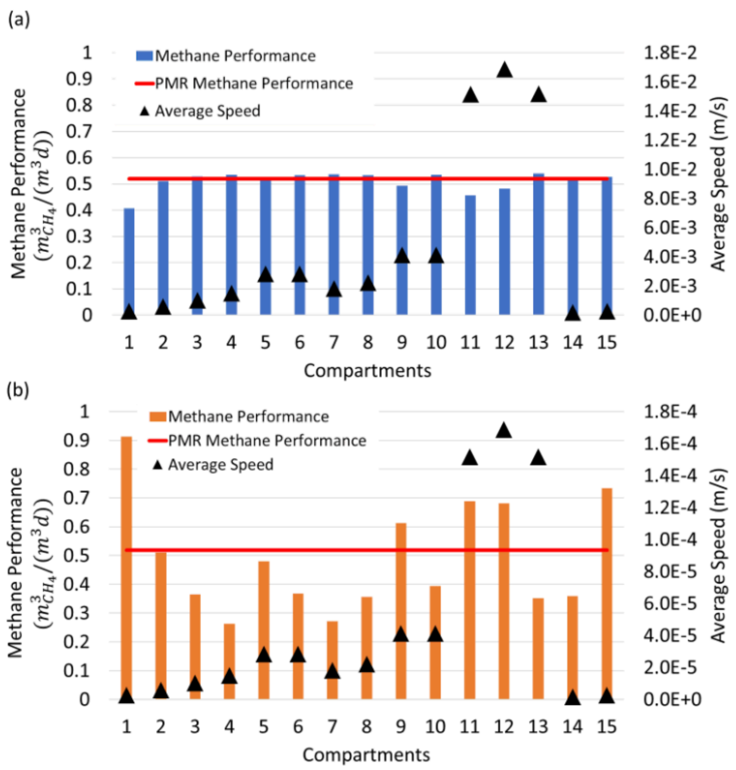


Figure 8. Compartmental methane performance and average speed for (a) C1 and (b) C2.

3.1.2 An improved approach to evaluate dead zones in bioprocesses

Dead zones are commonly used as indicators of mixing efficiency within a biorreactor. An effective mixing system ensures a well-homogenized volume, resulting in biogas production comparable to that of a Perfectly Mixed Reactor (PMR). In this context, a dead zone refers to a region where biorreactor performance is reduced, often due to nutrient deficiencies that impair microbial activity and survival. Traditional definitions of dead zones rely on absolute or relative velocity thresholds. We used the above desribed procudre to study detah zone definition in anaerobic digestion.

When simulating the AD process alongside the flow field (Figure 7), it becomes evident that methane production depends on multiple factors beyond flow velocity alone. In C2, the compartments with the highest methane performances do not always correspond to those with the highest average speeds; a pattern also observed in C1. This indicates that velocity thresholds alone are insufficient for evaluating dead zones (Figure 8). Other factors, such as connectivity to the inflow location and substrate characteristics, may significantly impact AD performance locally. Moreover, classifying reactor volumes solely as dead or active may overlook nuances in performance. The full integration of the compartmentalization approach with the ADM1 model enables the calculation of this performance metric. These findings have direct and severe financial implications for project design and profitability. For instance, case C1 exhibits a methane yield of 98.1% relative to a PMR, even though conventional criteria would classify up to 99.7% of its volume as a dead zone. An engineer or investor relying on that flawed metric would be induced to specify a more powerful and expensive mixing system (increasing CAPEX) with higher lifetime energy consumption (increasing OPEX). This decision would permanently damage the project's ROI without delivering any proportional benefit in methane yield.

3.2 BIOFERTILIZER PRODUCTION

Transitioning to a circular economy also involves moving away from fossil fuel-based chemical fertilizers toward renewable, sustainable sources of nutrients that support long-term soil health. One promising pathway is the use of anaerobic digestion—a biological process in which organic matter is broken down by microorganisms in the absence of oxygen, producing biogas as a renewable energy source. In addition to energy production, this process generates a nutrient-rich byproduct known as digestate, which can serve as a valuable biofertilizer.

Digestate contains essential nutrients and minerals such as nitrogen, phosphorus, potassium, and trace elements that are beneficial for agricultural applications. However, the effective handling, treatment, and valorization of digestate are critical to ensuring both the economic viability and environmental sustainability of anaerobic digestion systems. If not properly managed, digestate can become a waste stream rather than a valuable resource.

To fully unlock its potential, digestate must be treated not merely as a residual output, but as a co-product with quantifiable value. Therefore, accurate modelling of the anaerobic digestion process should include a detailed representation of the composition and dynamics of digestate. This includes tracking the presence and transformation of key components that directly influence its agronomic value, marketability, and environmental impact. Such a comprehensive modelling approach can support better decision-making, optimize system performance, and promote the integration of anaerobic digestion into broader circular economy strategies.

3.2.1 Phosphorus presence in digestate

The original ADM1 model does not include certain elements in its equations, such as sulfur, phosphorus, or iron, due to the limited research available on these topics at the time the model was developed. As a result, the model is unable to describe mechanisms that occur in processes involving, for example, phosphorus-rich wastewater. For this reason, several extensions to the original model have been developed to capture these dynamics. One such extension focuses on phosphorus and considers the release of phosphate from the substrate into the liquid phase of digestion, followed by its precipitation in the form of struvite or k-struvite[9]. Capturing these mechanisms is particularly relevant for phosphate-rich influents, and it also enables modelling of phosphate concentration in the digestate and its potential use as a higher-quality fertilizer. We developed an extended version of the ADM1 called ADM1-FB that considers the phosphorus cycle as well as the H2S presence in the biogas. A general diagram of this extended version of the model as well the result of simulation using the model, depicting the dynamic of the nutrients in the digestate and the struvite buildup, are shown in Figure 9. The environmental impact transforms digestate from waste to a valuable co-product, with markets in sustainable agriculture showing growing value in 2025.

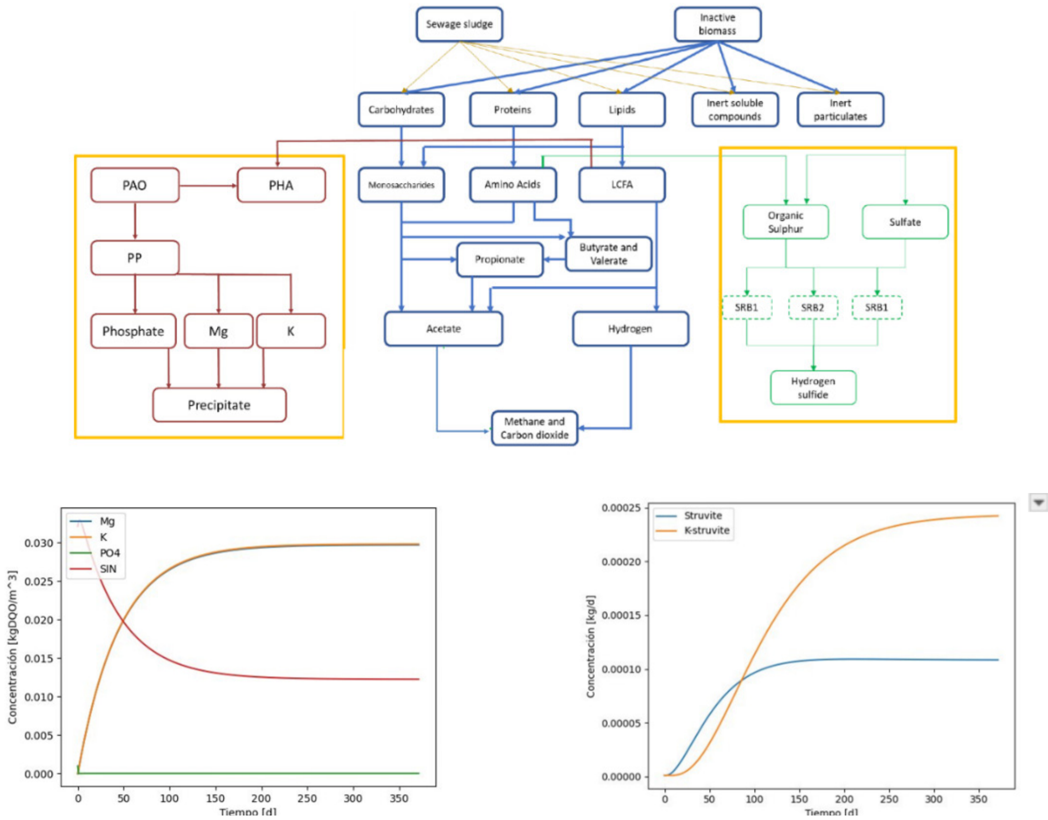


Figure 9. General diagram of the new processes included (yellow squares) in the extended version of the ADM1 model called ADM1-FB.

[9] Ruyi Wang, Yongmei Li, Wenling Chen, Jinte Zou, Yinguang Chen, Phosphate release involving PAOs activity during anaerobic fermentation of EBPR sludge and the extension of ADM1, Chemical Engineering Journal, Volume 287, 2016, Pages 436-447. https://doi.org/10.1016/j.cej.2015.10.110.

3.2.2 Nutrient removal

The sister company Aroma has conceptually developed the **Nitrogen Removal Process (PEN).** This innovative solution aims to reduce the nitrogen content in the digestate through a biological process. PEN uses the action of **three bacterial strains,** which, through their metabolism, transform nitrogen compounds into gaseous nitrogen. This enables a natural reduction of nitrogen content, allowing for more balanced and environmentally friendly management in agricultural settings. **Figure 10** shows a general diagram of this solution and its main components. The performance of PEN depends critically on several operating parameters. Therefore, with modeling, an **advanced exploitation code** has been developed to analyze the effect of each of these parameters on system performance. This code allows the generation of a large number of operational scenarios. Subsequently, using data analysis algorithms, these scenarios are examined to identify correlations and extract conclusions. All the information can be used to support the piloting of the PEN system. Figure 10 present the comprehensive modelling application to understand and optimize the operation of this bioreactor.

The advanced exploitation code analyzes operational parameters across multiple scenarios, identifying correlations to optimize PEN system piloting. This could result in up to 10-20% OPEX savings in biological nitrogen reduction, promoting balanced management in agricultural and environmental settings.

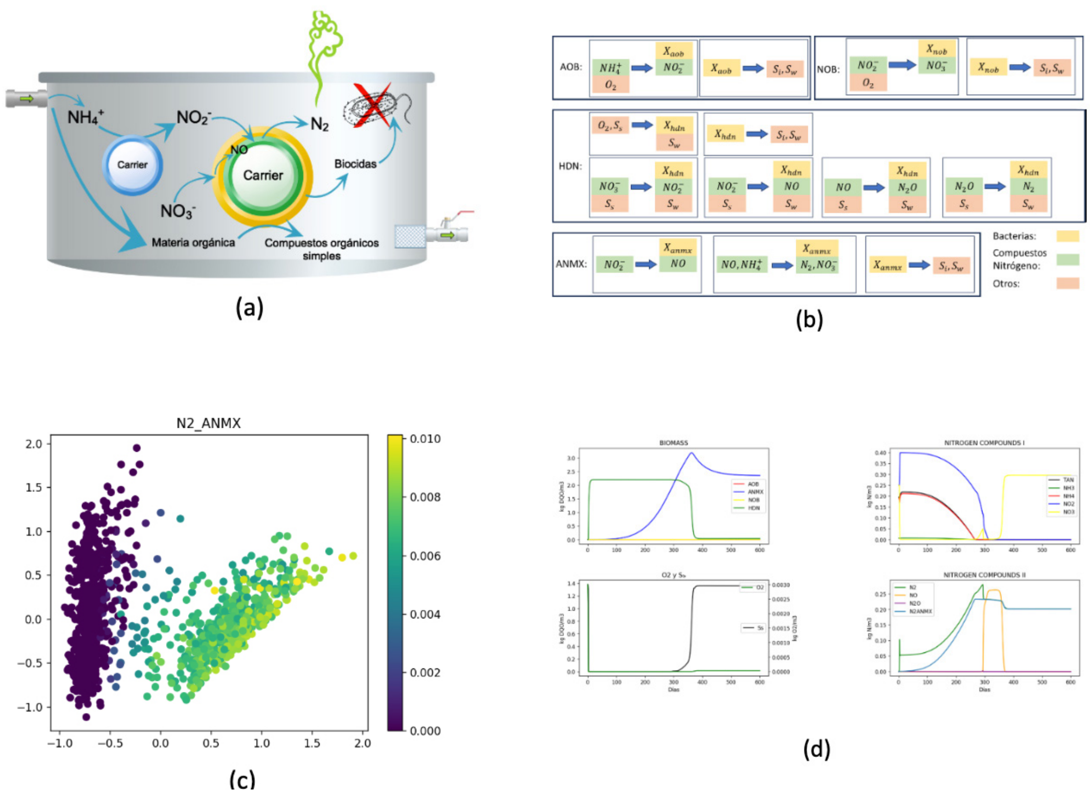
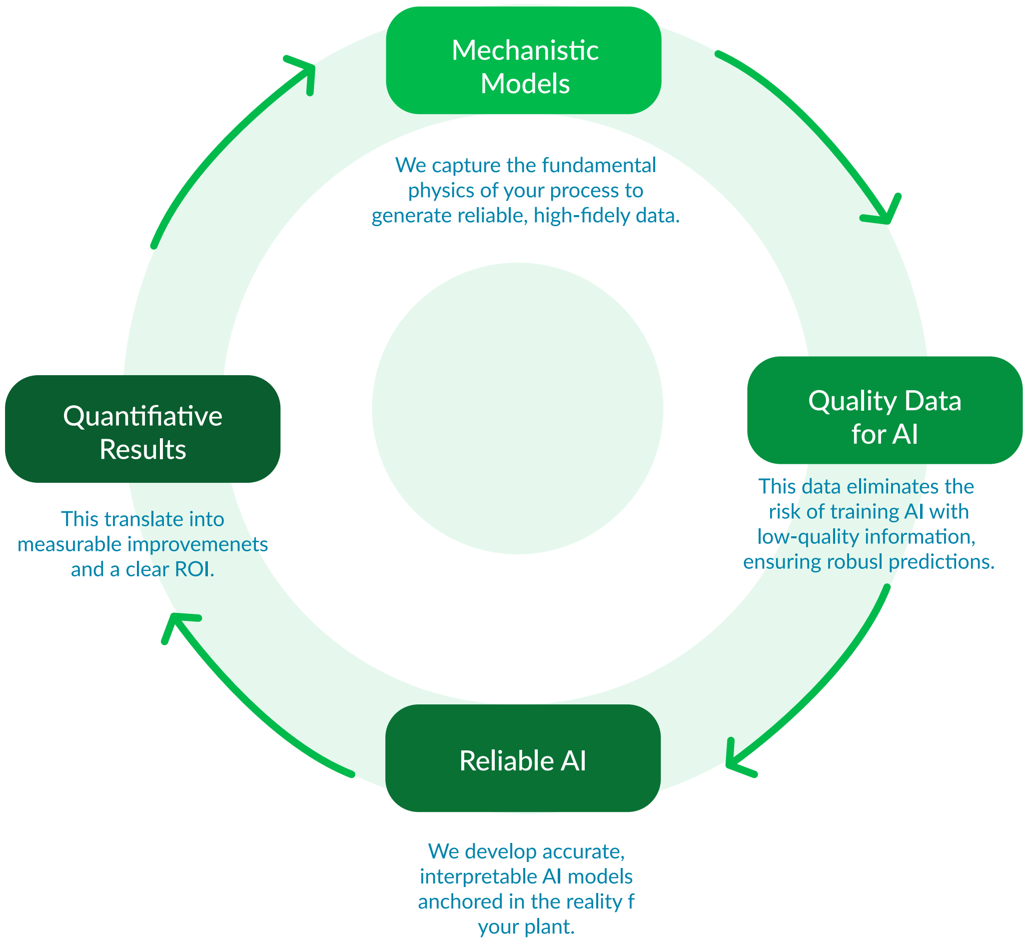


Figure 10. Process modelling of the nutrient removal process (PEN). (a) diagram of the bioreactor (b) bioprocess pathways involved in the system (c) data science application of the model results (d) main variables dynamic of the system in transient model.

The Virtuous Circle of Industrial Modeling



Efficiency

Reduction of OPEX and optimization of CAPEX.

Resilience

Failure anticipation and mitigation of operational risks.

Sustainability

Clear processes aligned with a circular economy.

4 TAKE-HOME MESSAGE

The use of models continues to shape our lives—whether in the recommendations we receive for movies and series or in improving and optimizing the operation of processes to maximize resilience and sustainability indicators. AI will play a key role; however, theory-based models, which capture the fundamentals and the essential processes that govern life on the planet, will remain the backbone of engineering, where understanding what is happening—and the causes of a given behavior—is of paramount importance.

A virtuous cycle may be emerging: AI is hungry for data and new content, and theory-based models can help satisfy that demand by generating large amounts of data at a much lower cost than running equivalent field experiments. For this cycle to work, mechanistic models must be properly implemented—both in terms of their underlying fundamentals and their numerical resolution—so that the generated data is trustworthy and AI applications can build upon it effectively.

Mechanistic models generate reliable data for AI, quantifying ROI in key industries, such as preventing aquaculture mortalities causing global losses of billions annually due to algal blooms and diseases. This integration accelerates the industrial revolution toward resilient and sustainable processes in 2025. By 2025, hybrid modeling will drive efficiency improvement in complex systems, positioning mechanistic foundations as the backbone for AI-driven industrial revolution.

I strongly believe we are at the beginning of an industrial revolution. As with all revolutions, it will bring significant changes to the way work is carried out. We must adapt, embrace, and take full advantage of the benefits that these new tools and capabilities will bring.

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