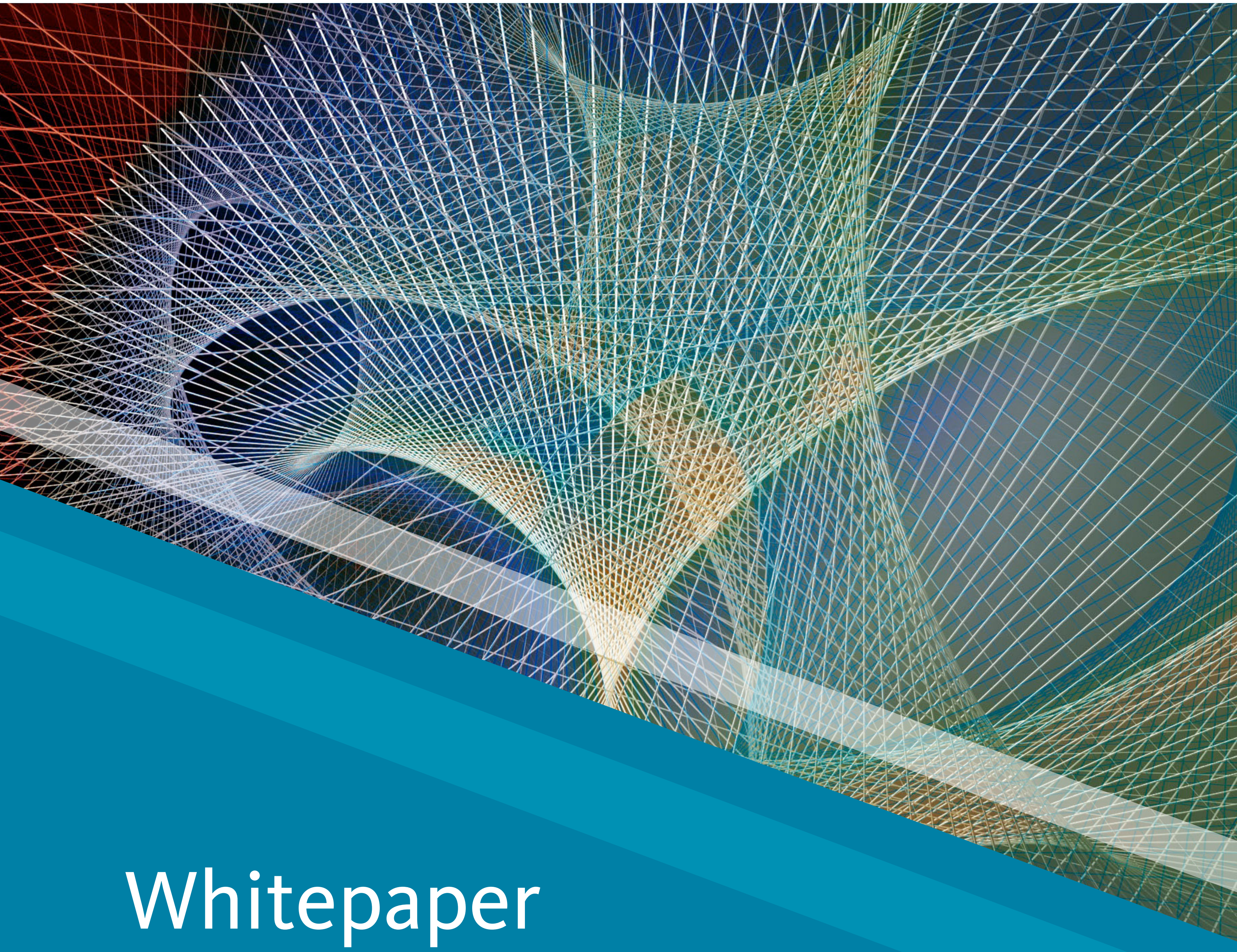
MODELA



Whitepaper Modeling and Simulation

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EXECUTIVE SUMMARY

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A team of engineers with multidisciplinary support and extensive experience in the field takes part in Modela, ProCycla's modeling and simulation spinoff. The team is oriented on addressing the current challenges that industries present, especially considering aspects of environmental sustainability and circular economy in its industrial process chain.

To this end, Modela applies mathematical and computational tools that enable the creation of digital twins of the systems to be studied for virtual prototyping. Mainly, we focus on optimizing energy and sustainable processes that will help the transition to a circular economy.

We guide and advise companies in their R+D+i research lines and processes regarding the design and optimization of prototypes. Also, we help them implement mathematical models according to the needs and requirements of each client.

This document summarizes some of the fundamentals and solutions that Modela employs and can offer to the industry, including bioprocess modeling, biological water treatment, or desalination process.

EDITORIAL

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“The industry needs to embrace and take advantage of all the benefits that applying modeling as a conventional control and monitoring tool brings. Plenty of the current challenges they face can be tackled by mathematical modeling with the consequent reduction in their emissions, risk, and economic resources”.

— Andrés Donoso Bravo

“There exist many operational and design challenges in the industry that could be better addressed by modeling tools, however, there is often no time nor human resources devoted to this task. Bridging this gap requires bringing together process engineering and modeling understanding. If that is achieved, virtual prototyping will contribute to finding efficient and sustainable solutions”.

— María Constanza Sadino Riquelme

“Many companies in the industry do not exploit the potential of the data they generate. Both mechanistic and data-driven prediction models require real data to be effectively applied in the industry and provide essential information for making decisions”.

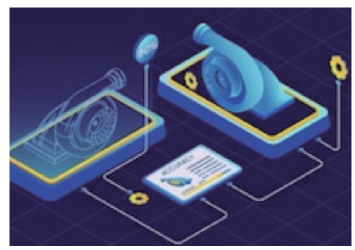
— Fernando Zorrilla Medrano

Every modeling project is supported by a multidisciplinary team of bio/chemists, programmers, environmental engineers and management personal that help in defining the global context of challenge, the development strategy and tool’s deployment to ensure a successful execution of the project.

3

WHAT IS MODELING?

Modeling involves implementing a mathematical representation of a certain reality whereas simulating consists of taking these models, solving them, and postprocessing and visualizing the results in a particular software and computer system. Thus, modeling and simulation aim at describing the essential aspects of the behavior over time and/or space of a process or system of interest allowing us to understand how it works.

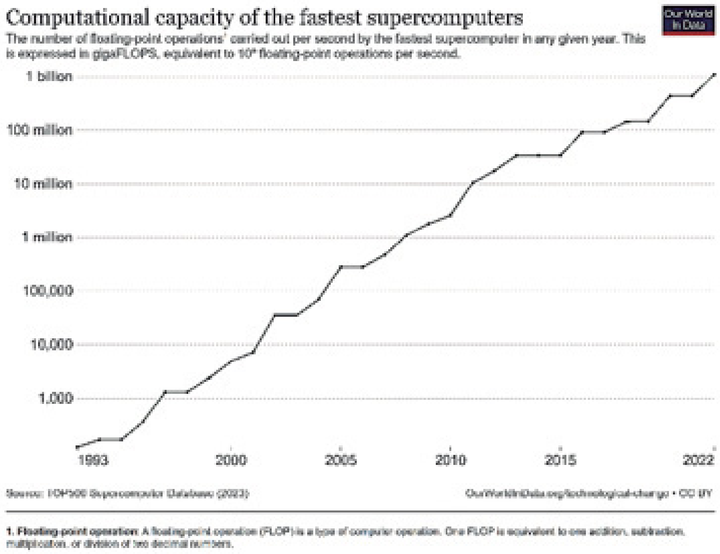


The use of modeling and computational simulation allows us to strengthen and speed up the decision-making process related to a particular process or system performance. This way, companies can make decisions faster than through experimental procedures, avoiding extra costs simultaneously. In addition, 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 of a specific process or system .

Basically, models are composed of equations, sometimes lots of them, some of which have been known for decades or even centuries. So, what has changed now that the industry should start making use of mathematical modeling? Besides there are new and up-to-date numerical methods to solve the system of equations, the main factor that is pushing the modeling work is the growth that computing, and software power has experienced. Despite this, it is worth noting that it is still very expensive to replicate complex systems, and for that purpose, supercomputers are usually required. For example, with an 8-16 CPU for high-performance computing, a 3D system can be simulated in a few days.

Overall, modeling can be divided into two main categories: mechanistic and data-driven modeling. The first one tries to represent the fundamental principles that govern a process, whereas the second one looks for correlations between inputs-outputs data without considering the underlying phenomena that are taking place. There is also a combination of both approaches, called hybrid modeling, that is also gaining attention.

Computing power is the computer's capability to process data information to get an output. So far, computing power doubles about every two years, as predicted by Intel co-founder Gordon Moore in 1975. Consequently, computers become faster and cheaper. Certain research fields have significantly high requirements for computing power, such as scientific computing, engineering computing, and intelligent computing. In those areas, about 49-94% of the performance improvements can be explained by the growth of computing power (Thompson et al., 2022)[1].



1 Thompson, N. C., Ge, S., & Manso, G. F. (2022). The importance of (exponentially more) computing power. arXiv preprint arXiv:2206.14007.

3.1 ODE-BASED MODELS

With the use of ordinary differential equations (ODEs), a mechanistic kinetics model describes the biochemical mechanisms for biomass growth, substrate consumption, and product generation. Therefore, this kind of model has been used to analyze the effect of bio- and physicochemical factors on the bioprocess yield and productivity, among other performance parameters. A kinetic model normally assumes that the species' concentration changes with time but not with space. Thus, the system is modeled as homogeneous regardless of the mixing configuration and the fluid properties.

Figure 1 shows a schematic view of a systematic modeling practice procedure. First, it is of course very important to define the purpose of the modeling exercise. Therefore, the level of detail of the description has to be selected with care, depending on the targeted application of the model, whether its goal is related to a physical/chemical/biological investigation, process design, dynamic simulation, optimization, control, or supervision. Once an

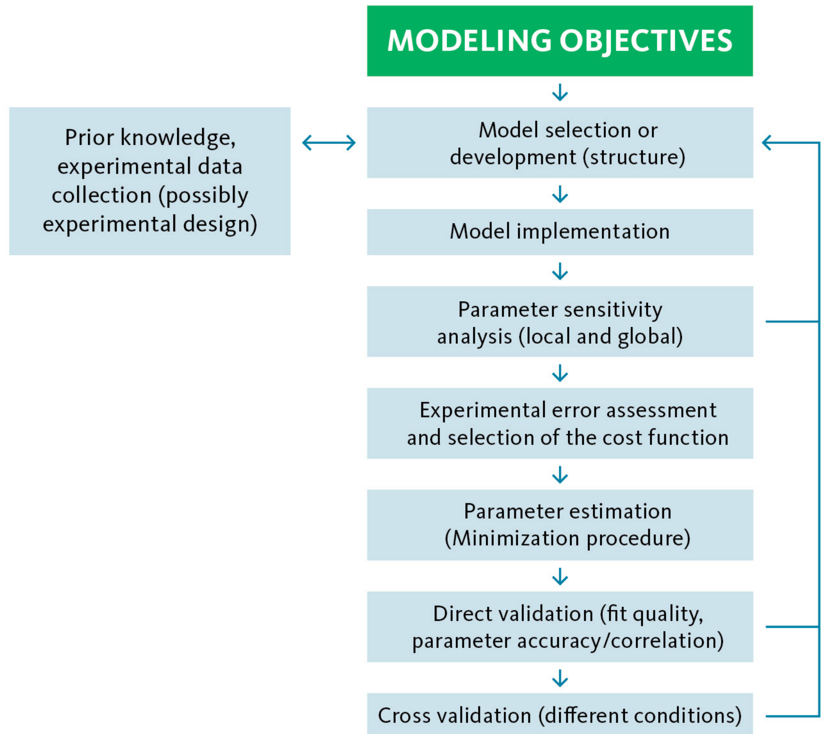


Figure 1. Flow diagram of a typical modeling practice procedure.

appropriate model structure has been selected (usually a system of non-linear differential equations including a number of unknown or uncertain parameters), a simulator can be implemented using a platform of choice (Matlab® or Python are popular options). Local and global parametric sensitivity analysis can then be used to assess, on the one hand, the most influential parameters and, on the other hand, the parameters with weaker influences on the measured outputs (at least in the scenario under consideration), possibly involved in correlation with other parameters. This first analysis can lead to a model reformulation or simplification, eliminating correlated parameters, and it can also lead to the reformulation of a new experimental design and data collection methods in order to have more informative data concerning the parameters to be estimated. Next, the experimental data must be examined in terms of potential errors (outliers, missing data, etc) and the deviation between the model prediction and the measured outputs. In this last part, special attention has to be paid to the selected cost function. Finally, the model must be evaluated with regard to the experimental data used so far (direct validation), as well as fresh data (unseen in the identification process, ie. cross-validation). These last two steps, if unsuccessful, can lead back to model reformulation and/or experiment design and data collection.

3.2 CFD-BASED MODELS

With the use of partial differential equations (PDEs), a fluid dynamics model describes the fluid flow motion based on the transport phenomena con-

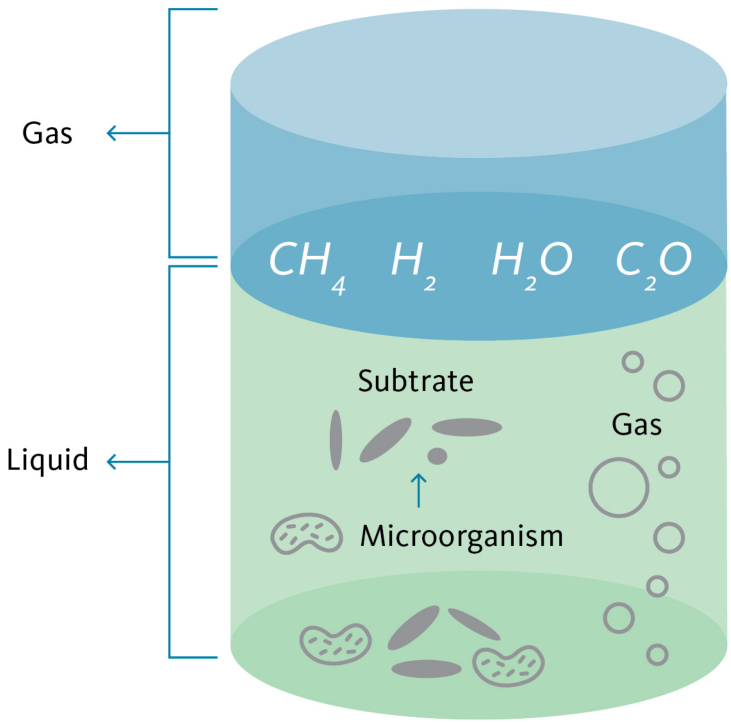


Figure 2. Anaerobic digestion's main components.

In the WWT field, the more extensively applied kinetics models are the Anaerobic Digestion Model No.1 (ADM1) and the Activated Sludge Models (ASM) for describing the AD and AS processes, respectively[2].

They are both made of a set of ordinary differential equations combined with algebraic equations that are described in a Petersen Matrix. The equations take a form similar to the one here presented:

$$\frac{dx}{dt} = \frac{F}{V}(x_{in} - x) \pm k \cdot r_x \pm gas_{transfer}$$

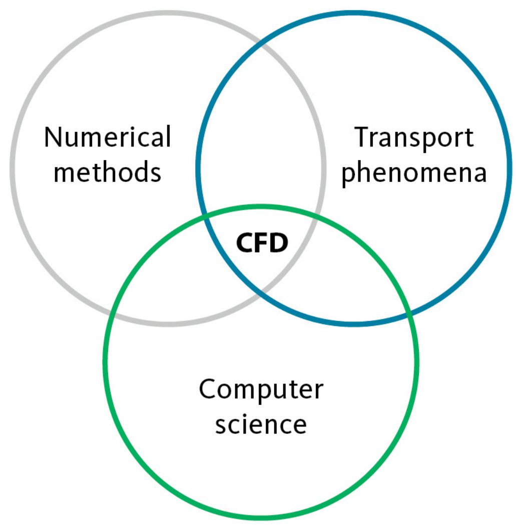
where,
x: state variable (substrate, biomass, or product concentration)
x_in: x in the inlet
F: inlet flow
V: reactor volume
k·r: rate of consumption or production
gas_transfer: rate of gas-liquid mass transfer

2 V. Alcaraz-Gonzalez, Modelling and Control of Wastewater Treatment Processes: An Overview and Recent Trends, in: A. Bahadir Müfit and Haarstrick (Ed.), Water and Wastewater Management: Global Problems and Measures, Springer International Publishing, Cham, 2022: pp. 143–150. https://doi.org/10.1007/978-3-030-95288-4_12.

servation laws for mass, momentum, and energy. Due to the complexity of the resulting model, its resolution requires the application of computational fluid dynamics (CFD) that brings together numerical methods and computer science to solve the system of equations. This mechanistic modeling approach has been used to analyze the effect of mixing systems, operating conditions, and broth fluid properties on the mixing times, the appearance of dead zones, and energy consumption, among other fluid dynamics variables of interest in different kinds of processes.

For the implementation of a CFD model, Modela uses an iterative workflow that comprises four stages: pre-processing, solution, post-processing, and verification and validation.

Figure 3. Scientific fields engaged in CFD.



Unlike the ODE-based models, CFD can be used to characterize tridimensional and transient heterogeneous systems, achieving a highly accurate representation of the process of interest.

For example, the Navier-Stokes equation models how the momentum is transferred between fluid layers via friction. Its solution allows us to analyze the velocity fields within the system.

$$\rho\left[\frac{\partial\vec{v}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{v}\right] = -\vec{\nabla}p + \mu\nabla^2\vec{v} + \left(\kappa + \frac{\mu}{3}\right)\vec{\nabla}(\vec{\nabla}\cdot\vec{v}) + \vec{b}$$

where:

ρ: fluid density
μ: fluid shear viscosity
κ: fluid dilatational viscosity
p: pressure
$\vec{b}$: body forces
$\vec{v}$: velocity field

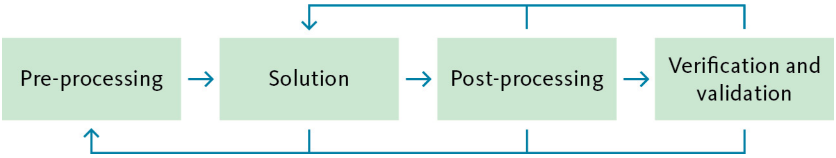


Figure 4. Workflow for preparing a CFD-based model.

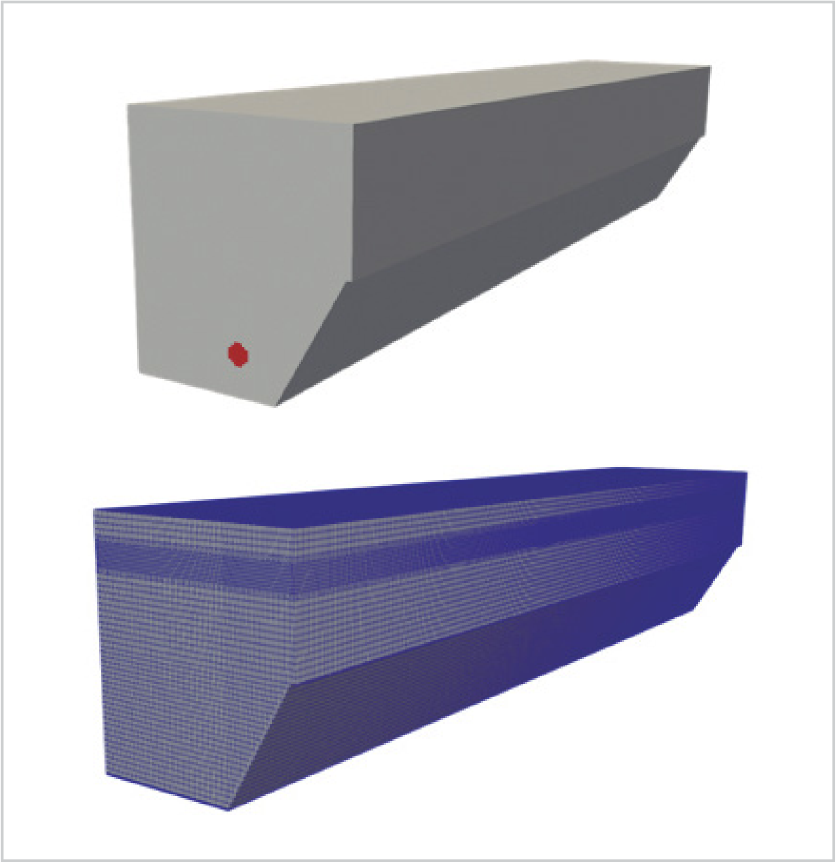


Figure 5. Domain and mesh of a reactor.

Pre-processing requires the characterization of the system's geometrical design, operating conditions, and fluid properties. The geometry is discretized into a mesh able to capture the features that are relevant to the process's fluid flow evolution.

Solution requires the selection of the numerical methods suitable for the resolution of the model, which will determine the level of accuracy and stability of the simulation.

Post-processing involves the treatment of the simulation's data for the calculation of suitable parameters and visualization of graphs to analyze information of interest.

Verification and validation consist of the evaluation of the simulation's results from a numerical and modeling point of view. Does the model accurately represent the system and phenomena of interest?

Several softwares are available for the implementation, execution, and analysis of CFD models. Modela offers the use of open-source softwares (Blender, OpenFoam, and Paraview) or commercial software (Ansys). Overall, both types of software can be used to simulate a wide range of fluid dynamic systems.

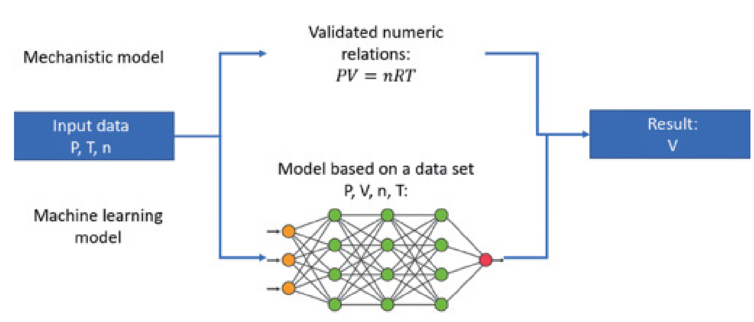
3.3 MACHINE LEARNING MODELING

When facing the challenge of modeling a system lacking a mechanistic model, a data-driven machine learning (ML) method can do the work. These are algorithms that combine linear and non-linear algebraic functions with logical sentences to transform input values into outputs. These models are trained on data and are built in order to predict key variables or to recognize patterns in that data.

Once the model is trained, it can be used with further samples of data to obtain information. Although building a machine learning model doesn't need the fundamental mathematical relationships between the variables involved, a big amount of quality data is required for it to work properly.

Bioprocesses modeling is challenging due to the complex interactions among a big number of variables. As a result, many bioprocesses are lacking a mechanistic model to describe them. On top of that, the application of bioprocess models can be challenging since they require the calibration of many parameters to work properly. In this context, ML models can offer an alternative that shortcuts the problems of a poor mechanistic model. Since the model is constructed only on the data, it does not require the mathematical description of the problem and it does not need to calibrate any parameter.

Figure 6. Mechanistic and ML models can relate the same input and output data.

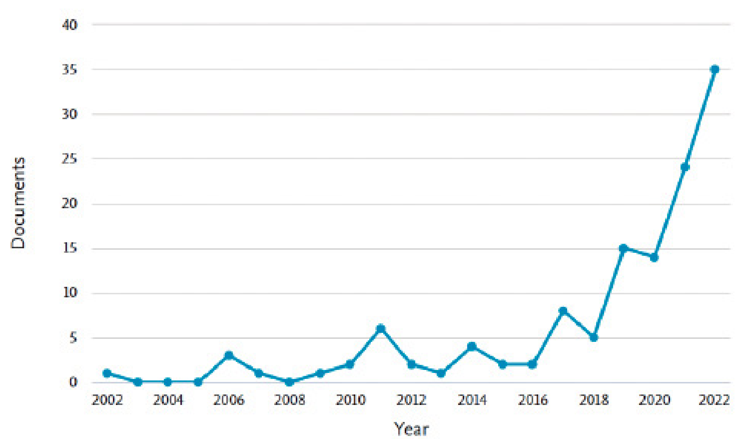


"In contrast to mechanistic modeling, ML models do not need a mathematical formulation and are built on data".

There is a wide variety of ML algorithms, from simple linear regression models to decision tree methods or complex deep-learning neural[3]. However, the choice of the algorithm that best suits a given problem is not trivial and has to be carefully analyzed. ML learning models can also work together with the mechanistic description of a system to create a hybrid model.

This type of model combines the use of a partial or total mathematical description of the modeled process with the use of data to create a more robust model. This wide variety of algorithms can be used to generate models for the prediction of key variables, classification of input data, surrogated models, or digital twins for industry applications. Even though there exist commercial packages for the implementation of those models, the programming language Python has a wide variety of open-source libraries to develop in-house solutions.

However, the use of ML algorithms has its drawbacks. The success of a ML model is highly dependent on the data into which it is built. This data needs to have a notable size and good quality for the model to successfully work. Also, the lack of a mathematical formulation for these models makes the results untraceable and difficult to interpret. They constitute what is known as a black box model.



"Academic publications about machine learning in bioprocesses are experiencing an exponential growth. It is expected that those newly found applications will be transferred from academia to industry in the coming years".

3 Marsland, S. (2015). Machine learning: an algorithmic perspective. CRC press.

Figure 7. Number of publications on machine learning in bioprocesses in the academic literature.

4

WHY USE MODELING?

Modeling and simulation can be exploited for the following purposes: control, monitoring, prediction, and system improvement. Control requires a rapid model response to count with a real-time tool whereas system improvement does not require an instant response and it can work by asynchronously delivering batches of information.

4.1 CONTROL AND SUPERVISION – pseudo real-time

With a properly defined and calibrated model, we can add another layer of supervision to have more robust control of the process.

The model can be mechanistic, i.e., made of a set of ordinary differential or algebraic equations, with the advantage of representing the process and its variables so the simulation results can be explanatory about the system and its behavior.

The model can be data-driven or based on Machine Learning, formed by sets of correlations (usually polynomial) with no physical meaning but, depending on the data used to train and test the model, with a high predicting power.

In general, these models can be running in parallel to the actual operation. If we know the system's inputs, this virtual representation can yield pseudo real-time information on the process's performance (nothing can be considered real-time). We can run a model with over 50 ODEs and get a solution in seconds.

4.2 DESIGN AND SYSTEM IMPROVEMENT – Asynchronous

The design and optimization of industrial processes is a complex task. Their scale-up commonly results in the onset or increase of heterogeneities or other undesired features. Besides, many times their experimental characterization is not technically feasible or is too expensive. For those situations, Modela recommends the use of CFD models as virtual pilots.

For this purpose, the use of partial differential equations (PDEs) in the model is required which dramatically increases the computer power needed to solve the system's mathematical representation. Therefore, we cannot give the model's response in pseudo-real-time, and it must be exploited for asynchronous purposes.

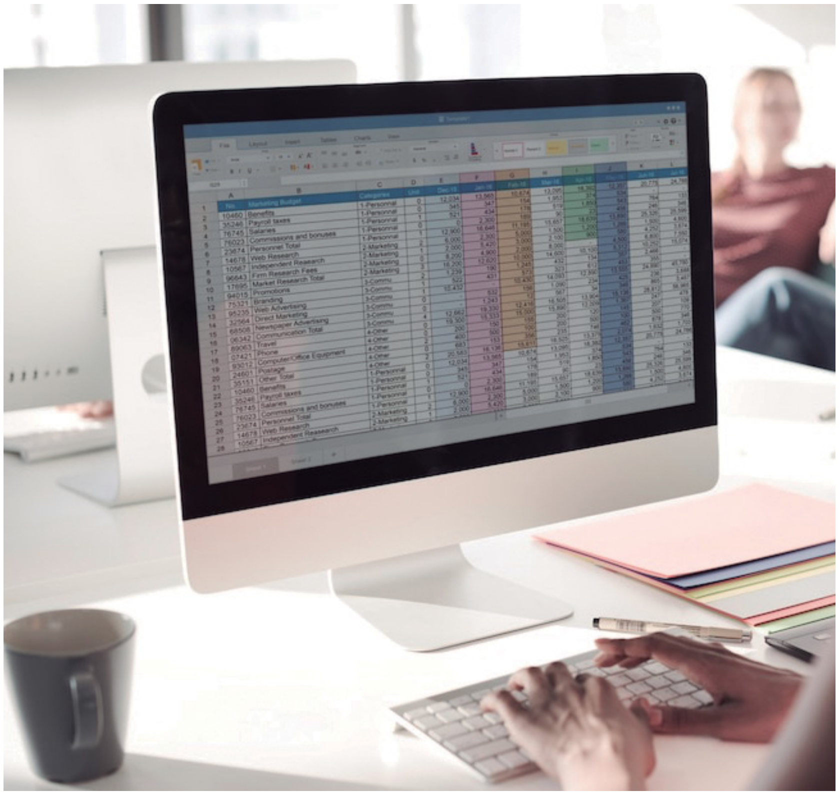
CFD allows us to simulate the system in two or three dimensions. Hence, it can be applied to test the impact of making physical changes in the system configuration or structure, such as inlet ports, vessel shape, and mixing system, on key aspects of a process fluid dynamics, such as the formation of certain fluid flow patterns, the onset of dead zones, temperature profiles, mixing times, power consumption, etc.

In general, CFD models as systems for virtual prototyping are seen as promising methods for improving the efficiency of industrial-scale processes.

4.3 PREDICTION AND FEASIBILITY ANALYSIS

A model can also be used to predict potential scenarios that can take place during the system's operation. The assessment of undesired input conditions or environmental parameters can be evaluated without the need for physical experiments. In other words, a modeling approach can prepare operators and managers for unforeseen events in a better way.

This model capability can also be used in the early stages of project planning and reduce the uncertainty of a conventional feasibility analysis.



5

BIOPROCESS MODELING Sustainability towards a sustainable future

Any type of bioprocess, from food fermentation to biofuel production or biological treatment/reconversion of waste, will play a key role in the transition toward a circular economy. Bioprocesses harness the capacity of microorganisms or their components to convert different types of feedstocks into added-value products. Bioprocesses basically use the ability of the cycles of nature in an intensive, controlled, and supervised way.

Modeling and control of bioprocesses refers to the use of mathematical models and control theory to optimize and manage biological processes. These models consider various factors such as substrate utilization, product formation, and biomass growth to represent the behavior of a bioprocess. Control theory is then used to adjust variables such as temperature, pH, and nutrient levels in real-time to ensure optimal conditions for the desired bioprocess outcome.

The goal of bioprocess modeling is to improve efficiency, increase productivity, and minimize waste in various biological applications such as anaerobic digestion, wastewater treatment, and bioremediation.

5.1 ANAEROBIC DIGESTION

5.1.1 Modeling for process understanding

Anaerobic digestion plants are subjected to different situations that have an impact on the stability of the process and the final biogas output. This variability affects the concentration and prominence of certain microorganisms which will impact the overall digester performance.

For instance, the balance of the methanogenic archaea among the hydrogenotrophic and acetogenic, which have different tolerance to the presence of ammonia and volatile fatty acid, may change. Thus, a proper mathematical representation may detect the population balance shift when a certain deviation of the output variables is detected. When this shift takes place, the system becomes more resistant to other types of substrate which otherwise would not be permitted to be fed into the digester.

An unwanted by-product of the AD is hydrogen sulfide (H_2S) in the biogas since it is a toxic and very corrosive compound that must be removed to

Anaerobic digestion (AD) is a bioprocess that takes place in a mostly free-oxygen environment, called digester. The substrate is inputted into the digester, where anaerobic microorganisms use the organic matter to grow (duplicate), producing biogas as a by-product and digestate, a stabilized organic matter that can be used as a fertilizer.

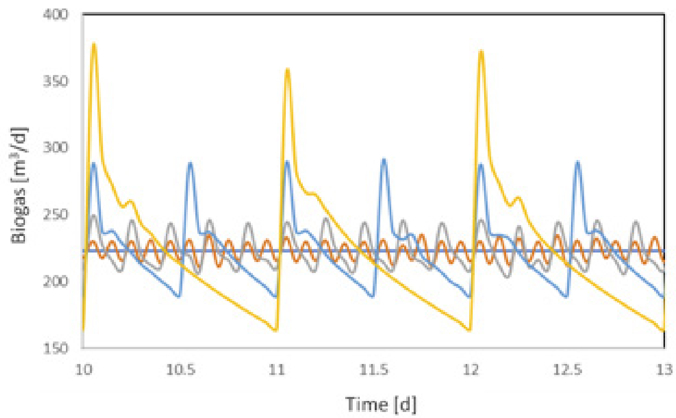
avoid equipment malfunction. This compound is generated when either sulfate or organic sulfur is present in the substrate. Therefore, having a model considering this compound in the main bioreaction paths will allow us to have an extra layer of information regarding the estimation of H_2S concentration in the biogas, the presence of sulfate oxidizing bacteria in the digestate, and the remaining sulfur in the digestate.

5.1.2 Operational issues

Feeding strategy selection: A continuous feeding rate is suggested to avoid process imbalances in digester operations. However, very few of them are fed in a real continuous flow. Instead, they work in a semi-continuous fashion. In other words, a certain amount of substrate, during a specific period, is fed continuously, but no real continuous feeding takes place mainly due to operational limitations such as waste storage and availability, pumping systems requirements, or substrate characteristics. Nevertheless, for any data processing analysis, it is considered that the reactor operates in continuous mode, especially for modeling applications and also for global data analysis. The main reason supporting this assumption is that residence time is so big that the discontinuities will not exert a relevant effect on the bioreactor performance analysis. However, no real assessment of the impact of the feeding mode on the digester performance under a model-based analysis has so far been done. In fact, few studies in literature can be found where this pulse feeding mode has been considered in the model application.

Figure 8. Performance of a digester under different feeding strategies

General balance of the system when is being fed and when is not.

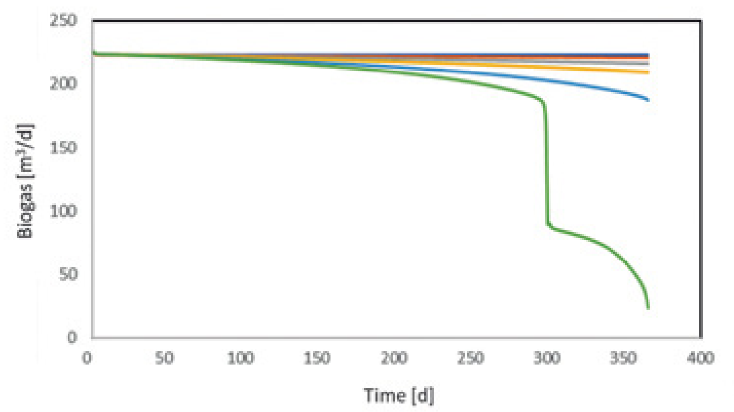


$$\frac{dS}{dt} = \frac{F}{V}(S_{in} - S) \pm \sum r$$

$$\frac{dS}{dt} = \pm \sum r$$

Inert material accumulation: Along with the substrate materials, inert materials such as sand and grit will enter the digester tank and they will accumulate due to sedimentation at the bottom or in dead zones where the agitation system is less effective. This buildup will lead to the need for maintenance and the cleanup of the tank. In the end, the accumulation of material will lead to a reduction of the working volume of the digester or, in other words, an increase in the dead volume. This layer of dirt, which cannot be digested by microorganisms, will cut down on the usable capacity of the digester. This should be somehow monitored to anticipate the moment that the maintenance needs to be carried out. However, to the best of our knowledge, there have been no research studies that attempt to model the reduction of the working volume using conventional ordinary differential equations approaches (ODE) with the ADM1.

Process start-up: Start-up adaptation can be related to a change in the abundance of specific microbial species (selection of a genetically distinct population of microbes), population shift or change in dominance, or a mutation that results from changes in the activity of an enzyme that will provide a selective advantage by allowing growth under new conditions. Particularly in AD, microbial adaptation usually occurs, in time, when the biomass is subjected to a new environmental condition, which can take place during: digester start-up;

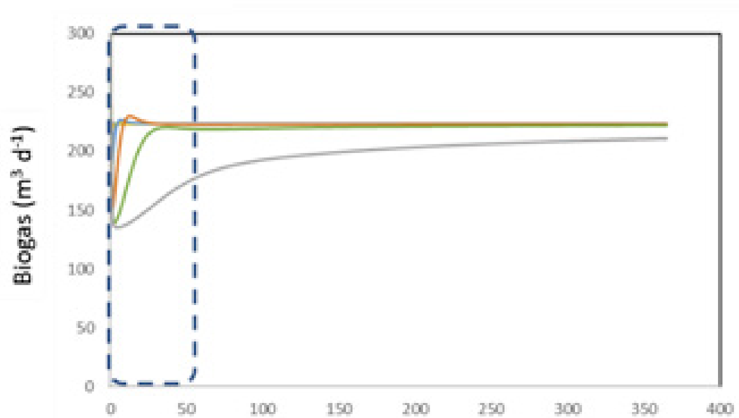


$$\frac{dS}{dt}V = F(S_{in} - S) \pm r \cdot V - \frac{dV}{dt}S$$

$$V = V_0 - \alpha \cdot t$$

Figure 9. General balance of the system with variable working volume and volume as a function of time.

Performance of a digester under different rates (α) of solid material accumulation.



$$k_{H\_CH} = k_{H\_CH\_max} \cdot \frac{(t - t_{change} + 1)}{K_{Ad} + (t - t_{change} + 1)}$$

Figure 10. Performance of a digester during start-up with different inoculum characteristics.

Equation that incorporates the effect of exposure time on the hydrolysis constant.

new substrate incorporation or temperature change; the presence of trace elements or changes in the concentration of compounds such as ammonia.

The application of modeling to represent the adaptation phenomena in AD has been scarcely done. The use of batch tests with different substrate conditions to estimate some kinetic parameters related to biogas production, for instance, at different ammonia concentrations has been a common approach for assessing adaptation.

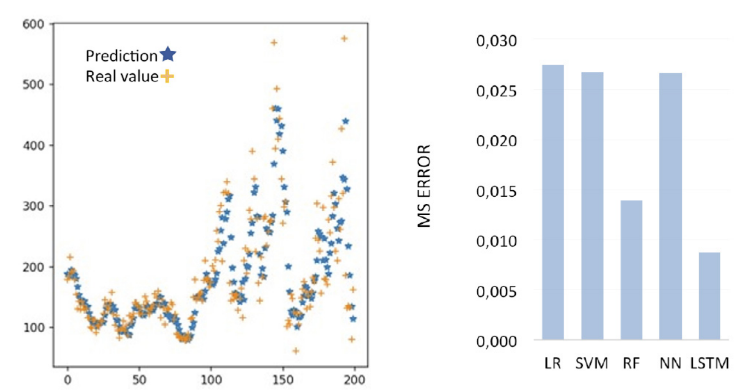
5.2 AEROBIC WATER TREATMENT

Biological water treatment refers to the use of living organisms, such as bacteria, fungi, and algae, to remove pollutants and treat wastewater. This process is typically achieved using biological processes such as aeration, biodegradation, and the action of microorganisms.

In biological water treatment, wastewater is passed through a treatment system that provides conditions for the growth and activity of microorganisms, which consume organic matter and convert it into biomass and carbon dioxide. The treated water is then further processed to remove any residual pollutants and meet specific water quality standards for discharge or reuse. This approach to water treatment is considered environmentally friendly and sustainable, as it relies on natural processes to purify water rather than chemical treatments. Some common examples of biological water treatment include the activated sludge process, aerobic and anaerobic digestion, biofilters, constructed wetlands, bioaugmentation, and composting.

5.2.1 Bulking and Foaming

Figure 8. Prediction of bulking using different ML algorithms.



"Anticipation of bulking through the prediction of future sludge volume index. Recurrent neural networks might outperform other ML models when time-series data can be taken as input".

The appearance of sludge bulking is a phenomenon related to the aeration of poorly sedimented sewage and the growth of filamentous bacteria. Even though sludge bulking affects negatively the performance of a WWTP, there is not a full mathematical formulation of the problem that allows for an effective prediction of its appearance that could help in the correct tunning of the operating parameters in order to prevent it.

However, the existing records of data covering the operating conditions of the WWTP, the chemical composition of the sewage, and the observance of bulking, can build the basis for the development of a data-based predictive model. Such a model can generate accurate predictions about the appearance of bulking in future scenarios and can help the plant operator to take decisions.

5.2.2 Energy consumption optimization

The activated sludge process is a very efficient process for pollutant removal, which explains why it is the preferred technology to remove organic matter and nutrients from domestic wastewater. However, this efficiency comes at a cost: the required energy for aeration is quite high, which sometimes makes up to 50% of the total operation's expenses of a WWTP[4].

Nowadays, WWTPs (or Wastewater Resource Recovery Facilities - WRRF) are highly automated thanks to the fact that they are equipped with sensors, actuators, and data acquisition/visualization interfaces. Despite this, the operation is mainly based on the fulfillment of certain set points instead of trying to understand more deeply the underlying mechanisms or correlations that can be derived as a result of the collected data. In other words, the control and supervision of these systems are mostly reactive and not preventive.

To change this paradigm, the data processing procedure must evolve by incorporating the application of a mathematical model, whether mechanistic or data-driven, to draw valuable information related to the state of the process to enable the early detection of process imbalance, undesired microbial population proliferation, inhibition compound presence, or reducing the usual over-operation of the system for energy optimization and chemicals supply.

In a properly designed and well-mixed system, a mechanistic model application, such as the ASM1, can be calibrated to control the aeration levels while keeping the nutrients removal efficiency and having an estimation of the microorganism concentration and its diversity. In a more heterogeneous system but still equipped with several sensors, a Machine Learning approach can be employed for predicting, for instance, energy consumption.

4 Gandiglio M, Lanzini A, Soto A, Leone P, Santarelli M. 2017. Enhancing the Energy Efficiency of Wastewater Treatment Plants through Co-digestion and Fuel Cell Systems. Frontiers in Environmental Science. 5. DOI=10.3389/fenvs.2017.00070

6

WATER RESOURCES MANAGEMENT
Ensuring future availability

Natural resource management helps to preserve and maintain the balance of ecosystems, prevent resource depletion, and meet the growing demands of the human population. This includes implementing sustainable practices for resource extraction, conservation efforts to protect vulnerable species and habitats, and efficient use of resources to minimize waste and reduce negative environmental impacts. By effectively managing natural resources, we can ensure that future generations will have access to the resources they need to meet their own needs and maintain a healthy planet.

6.1 AQUACULTURE

Aquaculture, also known as fish farming, has become increasingly important in recent years due to the growing demand for seafood and the need to support local economies while helping conserve the marine environment. In some regions of the world, such as Asia, most of the seafood that people consume is already sourced from aquaculture.

Figure 11. View of a fish farming site.

Approximately 50% of the global seafood produced for human consumption comes from aquaculture.

Producing more fish in a controlled environment helps ensure food security by providing a reliable source of protein for people in many parts of the world, especially in areas where fishing and hunting are not enough to meet the local population's needs.

On the other hand, overfishing has led to the depletion of wild fish stocks, making it increasingly difficult to catch enough fish to meet the growing demand. Aquaculture provides a sustainable alternative to wild-caught fish, and by reducing pressure on wild fish stocks, it helps conserve biodiversity in marine ecosystems. Last but not least, the GHG emission associated with a kilo of protein coming from a salmon is significantly lower than those emitted by conventional livestock meat.

6.1.1 Modeling to improve the aquaculture process

Design of Culture Ponds and Production Units: Throughout the juveniles' production chain, a diversity of processes and unit operations are required. Modela can virtually evaluate designs and operational conditions to propose improvements while optimizing investment costs.

Configuration of Antibloom Systems: Bloom of microalgae causes million-dollar losses to the industry. Technologies are offered to minimize this

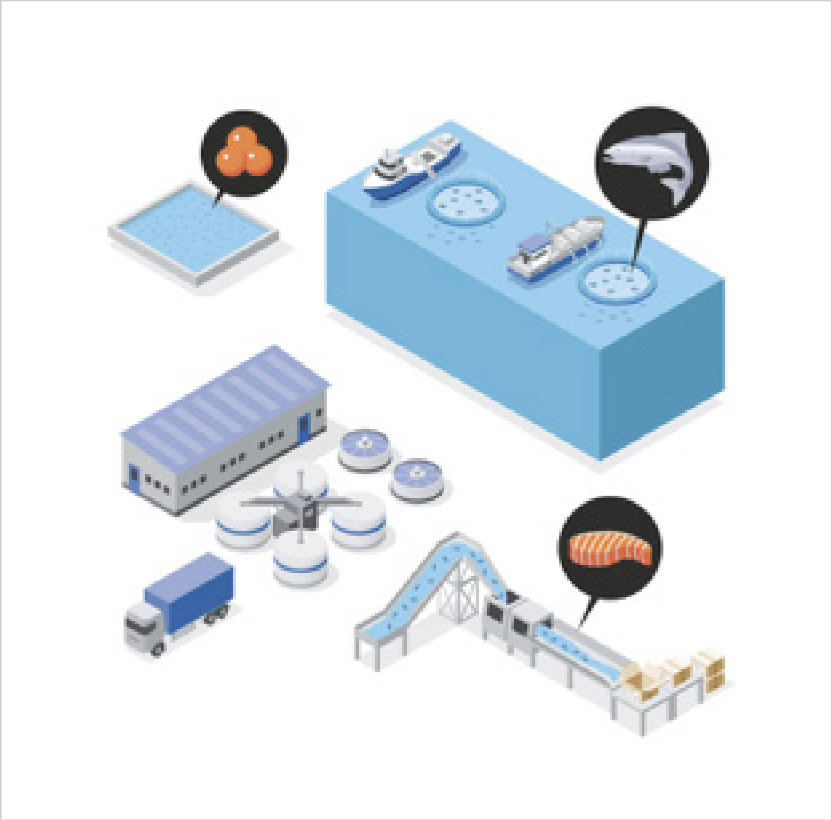


Figure 12. Aquaculture process stages.

effect without evidence of their actual effectiveness. Modela can build virtual prototypes to test the antibloom performance.

Biofiltration optimization for RAS Systems: Nutrient removal is a key biological process that makes recirculated water safe for fish culture. Modela can assist in monitoring and controlling its operational and environmental variables by applying mechanistic modeling.

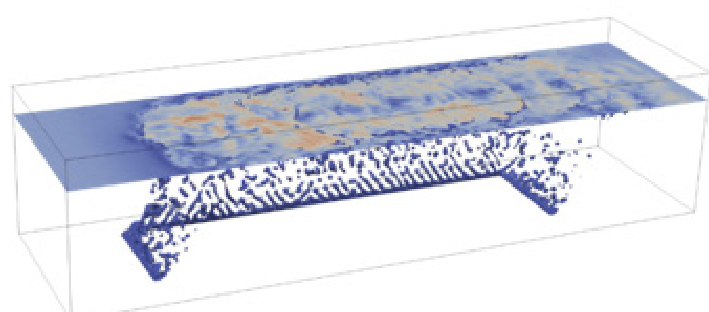
Configuration of Surgency Systems: Diseases negatively affect fish farming. One way to reduce these risks is by diluting and mixing the farm water with fresh water from deeper zones. Modela can assess these systems' designs using CFD to optimize the upwelling process.

6.1.2 Selecting a suitable technology

Several technological solutions based on air diffusers are commercialized for aquaculture, however, deciding which one is the more appropriate for a particular farming site is challenging. The characteristics of the diffuser and the sea conditions will affect the antibloom and/or surgency effects.

Using CFD-based models, the effect of critical variables, such as airflow rate, perforations size, diffuser depth, and sea current, on the effectiveness of the systems can be evaluated, to compare them and choose the more suitable technology.

Figure 13. Virtual prototype for analyzing a bubble curtain



"ModSim has provided us with an objective evaluation of the impact that the anti-bloom systems of interest can have to protect our farms".

Camanchaca

Pablo Albistur González, Regional Farm Site Manager in Salmones Camanchaca.

6.2 DESALINATION

Desalination is a process that removes salt and other minerals from seawater and brackish water, making it safe and usable for various uses, including drinking, irrigation, and industrial purposes. This process helps to fight water scarcity by providing a new source of fresh water in areas where water resources are limited or suffering from over-extraction. For instance, desalination can provide relief to coastal communities where seawater is readily available but the access to fresh water is limited, and also during droughts and emergencies, such as natural disasters, when freshwater supplies are disrupted.

Several desalination methods are available but, in general, they can be classified into two types: thermal and membrane processes. The thermal processes require heat transfer to achieve the evaporation or solidification of the water. Within this group, distillation plants stand out as they produce more than 50% of the desalted water worldwide[5]. The membrane processes use a semipermeable membrane to remove the salt from the water solution at high operation pressure, such as is done in reverse osmosis which is used in most desalination plants[6]. Each of these technologies has its pros and cons, and the best choice for a particular application depends on several factors, such as the location, size of the plant, and energy cost.

5 Referencia: https://www.britannica.com/technology/water-supply-system/Fluoridation#ref1084838

6 Fuente: https://www.britannica.com/technology/desalination#ref301632

Desalination technology has advanced significantly in recent years, making the process more affordable and efficient. However, it is still an expensive option compared to other sources of fresh water, and important challenges remain to be addressed in order to achieve a commercially efficient and environmentally harmless process[7]:

7 Fuente: https://www.asme.org/topics-resources/content/8-engineering-challenges-for-desalination-technologies

- Membrane performance: reducing energy consumption and costs.

- Seawater conditions: improving the water quality for the intake pretreatment system.

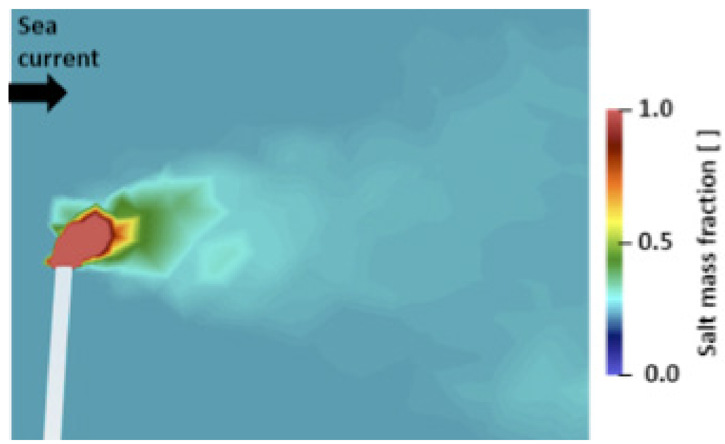
- Brine disposal: mixing and diluting the brine to be discharged into the environment.

- Energy recovery: recovering the pressure energy applied in reverse osmosis.

In this context, the use of modeling and simulation can be of great help. CFD-based virtual prototypes can provide detailed information on the flow, temperature, and concentration fields within the desalination system, as well as on the heat and mass transfer processes taking place. This information can be used to optimize the design of the system, characterize the process, and predict its performance under different operating conditions. For particular desalination processes, for instance, in the case of reverse osmosis, models can be used to simulate the flow of water and salt through the membrane, predict the salt rejection rate, and evaluate the effect of various parameters on the process performance, such as membrane permeability, pressure, and temperature.

Overall, CFD simulations provide a powerful tool for understanding and optimizing the performance of desalination processes and guiding the design and operation of these systems in a cost-effective and sustainable manner.

Figure 14. Virtual prototype for analyzing the impact of brine discharge.



Discharge and intake system
Evaluation of different geometrical designs, locations, and operating conditions to select the optimal configuration.

Coastal conditions
The simulations can take into account the effect of the velocity, pressure, and temperature profile of the sea current on the brine mixing.

Brine plumes
Characterization of the spatial and temporal evolution of the brine plume dilution by estimating the salt concentration profile.

Heat exchanger
Study of the heat and mass transfer between phases to select the configuration that optimizes the system efficiency.

TAKE-HOME MESSAGE

7

Modeling and simulation are becoming ubiquitous, embedded in all the activities that are currently undertaken, from pattern detection from internet use to selecting preferences for streaming movies or digital twins for airplane design.

The fourth industrial revolution is underway, and the modeling tool must be embraced and exploited wisely so that a more sustainable, circular, and controlled industrial sector can be attained.