Operational Decision-Making on Desalination Plants: From Process Modelling and Simulation to Monitoring and Automated Control With Machine Learning

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ABSTRACT

This paper describes some of the work carried out within the Horizon 2020 project MIDES (MIcrobial DESalination for low energy drinking water), which is developing the world’s largest demonstration of a low-energy system to produce safe drinking water. The work in focus concerns the support for operational decisions on desalination plants, specifically applied to a microbial-powered approach for water treatment and desalination, starting from the stages of process modelling, process simulation, optimization and lab-validation, through the stages of plant monitoring and automated control. The work is based on the application of the environment IPSEpro for the stage of process modelling and simulation; and on the system DataBridge for automated control, which employs techniques of Machine Learning.

KEYWORDS

Climate Change Adaptation, Drinking Water, Horizon2020 Project, IPSEpro, Low-energy Process, Machine Learning, MDC, Microbial Desalination Cell, MIDES, Plant Monitoring, Treated Wastewater

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1. INTRODUCTION

According to (Thu et al., 2013) and (Knowledge & Tools, 2009), the water demand situation, with increasing population and economic growth is estimated to reach 6,900 billion m³ by 2030. Figure 1 illustrates the estimation of water demand for 2030, considering the needs for agriculture, industry, domestic sectors - taking into account the demand for potable water increases annually by 2% (Thu et al., 2013). This study shows that if business-as-usual practices are continued, it will result in a global water demand that is 40% higher than the available water supply.

Such estimation establishes well the importance of studying solutions based on desalination technologies, which composes the scope of the Horizon 2020 project MIDES (MIcrobial DESalination for low energy drinking water) (2016), upon which the presented developments of the current paper are based.

The MIDES project (running from 2016 to 2020) aims to revolutionize energy-intensive Reverse Osmosis (RO) desalination systems by demonstrating sustainable production of fresh water at three pilot locations in and outside Europe. MIDES is developing the world’s largest demonstration of a low-energy system to produce safe drinking water via the use of Microbial Desalination Cells (MDC), which remove ions from saltwater in an innovative process powered by electroactive bacteria. In a general basis, the project supports: (i) Climate change mitigation by lowering greenhouse gases from current desalination systems; as well as (ii) Climate change adaptation through innovation in providing freshwater resources.

This paper describes the part of the work carried out within the MIDES project, concerning the support for operational decisions on desalination plants, specifically applied to a microbial-powered approach for water treatment and desalination (further outlined in section 2). The supported operational decisions and actions on the implementation of the desalination technology follow a roadmap that starts from the stages of process modelling, process simulation, optimization and lab-validation; through the stages of plant monitoring and automat-ed control. For the stage of process modelling and simulation, the developed work is based on the use of the environment IPSEpro (Perz et al., 1995; SimTech Simulation Technology, n.d.a; SimTech Simulation Technology, n.d.b; SimTech Simulation Technology, n.d.c), while for the stage of automated control, the system DataBridge is applied, employing techniques of Machine Learning (MIDES Consortium, 2018c).

Figure 1. Global Water Demand Gap between 2010 and 2030 (Thu et al., 2013)
The current paper is further structured in the following way: Section 2 presents the overall MIDES project process; Section 3 describes the MIDES roadmap process from Lab to Pilot stages. Section 4 presents the overall process modeling and simulation performed for the MIDES technology using IPSEpro, including the development and implementation of the cloud-based platform that deployed and shared the MIDES process online. Section 5 presents the monitoring and automated control stages of the project (including the Machine learning approach), at lab, pre-pilot and pilot scale. Section 6 discusses the operational decision-making and decision support, given by the developments described in the past sections, in the implementation of the MIDES Pilot Desalination Plant. Finally, Section 7 draws some conclusions about the work carried out in MIDES as a whole and impact of the work presented in the current paper.

2. OVERALL MIDES PROCESS

The EU Horizon2020 MIDES project (2016) specifically applies a microbial-powered approach for water treatment and seawater desalination. As published in (Zamora et al., 2019), existing desalination technologies require high-energy input, being Reverse Osmosis (RO) the most widely used technology for seawater desalination with an energy consumption of at least 3 kWh/m³. In this context, the MIDES project aims to go beyond the state of the art in desalination by developing a low-energy sustainable process called Microbial Desalination Cell (MDC).

The MIDES low-energy-powered approach combines MDC technology as pre-desalination step in connection with conventional RO aiming at increasing desalinated water production, while maintaining low energy requirements. The MIDES overall process (as illustrated in Figure 2) includes a pretreatment of the saline stream by ceramic membranes prior to entering the MDC unit, where it is partially desalinated (70-90%) before the RO post-treatment.

As stated in (Zamora et al., 2019), the initial treatment of municipal wastewater in a conventional anaerobic reactor produces an acetate-rich effluent as a fuel for the MDC (illustrated in Figure 2). In the case of saline water, in conventional RO desalination, seawater or brackish water undergoes several pretreatment steps¹ to protect the membranes from pollutants. In MIDES, ceramic submerged membranes substitute this whole pre-treatment, leading to a reduction in chemicals usage and footprint, as well as lowering by 80% the energy demand. The results obtained with a lab-scale MDC has led to significant improvement of water production compared to values reported in the literature (Zamora et al., 2019).

Figure 2. The Overall MIDES Process using Microbial Desalination Cell (MDC)
It is not the intention of this paper to go into details of how the MDC simultaneously treats wastewater and performs desalination using the energy contained in the wastewater. The overall MDC aspects and its performance in MIDES (2016) have been explained in various publications of the project consortium (among them (Arevalo et al., 2017; Ramirez-Moreno et al., 2019; Zamora et al., 2019)), as well as in most of the project’s deliverables (among them (MIDES Consortium, 2016; MIDES Consortium, 2017; MIDES Consortium, 2018a; MIDES Consortium, 2018b; MIDES Consortium, 2018c)). As previously stated, the focus of this paper is to report about the developments of the project work-package concerning Process Simulation & Analysis, Automation & Control, as well as its implications to the operational decision-making process of the overall project implementation and pilot installations, as it will be depicted in the sequel.

3 MDC AND MIDES PROCESS FROM LAB TO PILOT SCALE

As planned in the project, there were three implementation phases in order to test and validate the MIDES MDC and its overall concept. Those three phases included: (1) the Lab-scale MDC; (2) the Pre-Pilot-scale MDC; and (3) the Pilot-scale MDC, including the overall MIDES process in operation.

The roadmap of the implementation of the MIDES technology goes through the testing of the Lab-scale-MDC, up-scaling to the assembly of a Pre-Pilot-MDC, towards the development of the world’s largest demonstrator of the innovative MDC technology at Pilot-scale, which will be validated in three demo-sites: Dénia (Spain); Tenerife – Canary Islands (Spain); and in a demo-site outside Europe (in Egypt). All three Pilot plants will be constructed and operated under real environments in desalination plants operated by the MIDES project coordinator Aqualia (Zamora et al., 2019).

3.1 The Lab-Scale MDC

The Lab-scale-MDC was composed of a 100 cm² electrode area, with the configuration of the MDC press filter reactor assembling 8 elements, as shown in Figure 3.

Figure 3. The MIDES Microbial Desalination Cell (MDC) Elements - Lab-scale version
Figure 4 presents the MDC flow chart used for the mathematical model development, which also illustrates the scheme that was assembled in the Lab.

At this stage, besides all the necessary lab tests and procedures for implementation and installation, the MIDES process components and the overall process model were mathematically modelled, simulated and validated in the environment IPSEpro⁶ (SimTech Simulation Technology, n.d.a), by implementing the main engineering/physical laws governing the main processes involved in the system - combined physical, chemical and electrochemical principles, having differential equations used due to their strong ability to embody the dynamics of MDC system (MIDES Consortium, 2016), as well as parameter values and initial conditions setting specific situations to operate the model. A dedicated Desalination/Wastewater-Treatment Model Library with MIDES component-models was created in IPSEpro-MDK (SimTech Simulation Technology, n.d.b) to serve this purpose (as described in Section 4).

3.2 The Pre-Pilot MDC

The Pre-Pilot-MDC was assembled comprising 15 units (modular stack) of 650 cm² electrode area per cell. A first testing phase was performed with one MDC pre-pilot unit in a single lab set-up. The complete MIDES Pre-Pilot Microbial Desalination Cell (MDC) set-up was then built next. Figure 5 illustrates the implementation of the Pre-Pilot phases.

At the pre-pilot stage, apart from all the necessary implementation and installation procedures, the MIDES overall process model was simulated, optimized and validated using IPSEpro (SimTech Simulation Technology, n.d.a); and its automated control stage was built applying the system DataBridge (MIDES Consortium, 2018c) (as described in Sections 4 and 5). For the initial control stage linked to the MDC unit lab-set-up testing phase, the parameters monitoring of the pre-pilot MDC was carried out using a data logger, allowing the visualization of all measured parameter data in real-time.

Figure 6 shows in detail all the components of the complete MDC Pre-Pilot set-up, including its control module. For the control stage linked to the complete MDC set-up of the MIDES pre-pilot system, the parameters monitored were automatically controlled via the system DataBridge from project partner OnControl (as described in Section 5).

3.3 The Pilot-Scale MDC

The Pilot-scale MDC specification comprises of an assembly of MDC pilot-unit stacks of 12 pilot MDC unit cells (4 units per pilot plant) of 0.8 m² electrode area per cell, 50x80 cm. This development represents the world’s largest demonstrator of the innovative MDC technology at Pilot-scale.

Figure 4. The MIDES Lab-scale Microbial Desalination Cell - (a) Schematic (b) Lab set-up
Figure 7 shows the MIDES Pilot-scale MDC at Dénia demo-site, in the installations of the Aqualia Desalination Plant in Spain. The MIDES Pilot-plant at Dénia demo-site was launched in November 2019 and is currently running at operational testing and validation phases, including its controlled operation.

4. MIDeS PROCeSS MODeLLING AnD SIMuLATIOn

The tasks of process modelling, simulation, and process optimization were developed for the project MIDES using SimTech’s simulation environment IPSEpro (SimTech Simulation Technology, n.d.a), (SimTech Simulation Technology, n.d.b). This section briefly presents the IPSEpro system and its use and further development within the project.
4.1 IPSEpro – SimTech’s Integrated Process Simulation Environment

IPSEpro (SimTech’s Integrated Process Simulation Environment) is a heat balance and process simulation software package, which is currently one of the most comprehensive and versatile process modeling systems available. IPSEpro can be applied in a wide range of applications, within the areas of Desalination; Geothermal Energy; Refrigeration; Concentrating Solar Power; and Thermal Power. Since early 90s up to the present times, IPSEpro users have continuously been publishing their results obtained from the modelling, simulation, optimization and validation work using IPSEpro\(^2\) (among them (Aneke et al., 2011; Karellas et al., 2012)). With its various modules, IPSEpro supports users throughout the entire lifecycle of a process plant, from conceptual design to on-line plant performance monitoring and optimization. Due to its unique level of flexibility and its open architecture, IPSEpro is the ideal platform for implementing custom modelling solutions (SimTech Simulation Technology, n.d.a; SimTech Simulation Technology, n.d.b; SimTech Simulation Technology, n.d.c).
In IPSEpro, process models are created using the Process Simulation Environment (PSE). In PSE, the user sets up the process model graphically by drawing a flowsheet using components from a model library. Required data is entered directly in the flowsheet. By drawing the flowsheet and entering the data, the user implicitly creates a system of algebraic equations, which is then solved by the IPSEpro’s solver core. Results are displayed graphically in the flowsheet. The modelling approach has been described in detail in (Perz et al., 1995).

As IPSEpro is an open and flexible framework, component equations and physical property methods are not part of the core software. Instead, application-specific information is contained in model libraries, which can be created and modified using a special Model Development Kit (MDK). For instance, a model library specifically developed for ORC (Organic Rankine Cycle) processes (Perz & Erbes, 2011) includes a comprehensive set of component models based on working fluids used, as well as models for the part-load behaviour of the components, so that the user can analyze the off-design characteristics of ORC plants. The same applies for Desalination plants, using a dedicated Desalination Model Library (SimTech Simulation Technology, n.d.c). Figure 9 below illustrates IPSEpro Simulation Package general architecture (SimTech Simulation Technology, n.d.a; SimTech Simulation Technology, n.d.b).

4.2 IPSEpro in MIDES

IPSEpro Process Simulation Environment (PSE) (SimTech Simulation Technology, n.d.a) and IPSEpro Model Development Kit (MDK) (SimTech Simulation Technology, n.d.b) were both used in the development of MIDES component models, with the creation of a customized model library called MIDES_Lib, as well as in the creation of the overall process model including the MDC.

The IPSEpro simulated models support understanding the performance of the involved processes. The MDC mathematical simulation model was a useful tool to predict the behaviour of MDC systems in different conditions. Hence, the mathematical process model was able to simulate accurately the quantitative influence of different parameters on the MDC performance. Figure 10 shows the first version of the Microbial Desalination Cell Model, as the core of the MIDES process in an IPSEpro model. It describes the process in one membrane stack based on published material (Zamora et al., 2019).

The complete MIDES process (originally shown in Figure 2) was implemented, simulated and optimized in the IPSEpro-PSE Process Simulation Environment (SimTech Simulation Technology, n.d.a), as illustrated in Figure 11, including the MDC and the other customized desalination and wastewater-treatment components created using the IPSEpro-MDK (SimTech Simulation Technology, n.d.b) for the MIDES_Lib.

This MIDES process model was validated by project partners, taking into consideration the parameter values of the mathematical models and the measured data from the pre-pilot set-up. This
paper gives an overview of the whole development, not dealing with technical details. Hence, the calculated results of the simulated process model are not presented.

4.3 IPSEpro Online Platform - Implementation

The ability to collaborate with others online has become a vital element of the modern workplace. Cloud-based systems for collaborative work on documents have made it much easier to develop projects with contributors in distributed locations. Cloud-based systems often do not need to install any software locally. Instead, a standard web browser functions as the user interface. From a user’s perspective, using such systems generates several key benefits, like:

- Since the documents are stored in the cloud and can be accessed from different locations, this enables collaborators to contribute to documents without the need to send copies to each other via e-mail or other communication means.
- Since a standard web browser serves as the user interface, the system is to a large extent hardware independent and can be used from a wide range of devices.
- It is not necessary to license and install software locally. It may be necessary to sign up for a service agreement, but typically this is often more cost effective than the purchase of local software licenses. It also ensures that any new functionality that becomes available can be used instantaneously by all users.
A requirement of the project MIDES was to present its overall process model in a shared online platform, in order to allow better collaboration among developers and project partners. By using the solver core of IPSEpro (illustrated previously in Figure 10), it was possible to base the implementation of the cloud-based platform on a web modelling approach. Using the same solver core and the same model library as in the original IPSEpro environment ensures that the results obtained with the cloud-based platform are identical to those previously obtained with IPSEpro.

The work described hereafter concerns the development of the IPSEpro online platform (MIDES Consortium, 2018b), with the characteristics described above for creating and solving process models, without the requirement to install any software locally. All interaction with the model, from defining the model to reporting results, is done via a web browser. Taking advantage of recent developments in browser technology, in particular HTML5, a browser-based user interface has been developed, as included in the general IPSEpro online platform concept in Figure 12; and in the system architecture at implementation-level, shown in Figure 13.

The IPSEpro cloud-based simulation platform has been implemented as a web application and as such typically defined as a client-server computer program, which the client (including the user interface and client-side logic) runs in a web browser. Consequently, the components of web applications can be divided into the categories: client-side components and server-side components, and a middleware which manages the communication between client and server. Figure 13: IPSEpro Online Platform - System Architecture at Implementation-level illustrates the overall implementation.
level architecture of the IPSEpro cloud-based simulation platform, partially developed under the MIDES project.

- **Client-Side Component:** In the cloud-based simulation platform, the client side comprises two major components, a project management component and the flowsheet editor. The project management component enables the user to log into the system, to create new projects, or select existing projects to use in the flowsheet editor. It also includes functionality to enable users to share projects with other users and to delete existing projects, managing this way the data stored on the server. The flowsheet editor enables the user to create and modify the flowsheet of the process model, to edit process parameters, to execute the system solver and to display results.

- **Server-Side Components:** The server-side of the cloud-based simulation platform includes two major components: (1) A web server with a database server, which stores all data about users and user projects. The web server also provides all parts of the interface which are not specific to a particular model library; and (2) a Library Server, which is responsible for providing all model-library-specific information required by the client side and which provides the capability to solve a process model that it receives. Additionally, the server side includes a reverse proxy server which directs client requests to the appropriate back-end server.

- **Flowsheet Editor:** The flowsheet editor is the central component of the cloud-based simulation platform. It enables the user to create and modify the flowsheets of processes, to edit process parameters, to execute the system solver and to display results. Once the basic functionality of the flowsheet editor is loaded, it requests from the library server all the information about components in model library which is required to configure the user interface. This includes information about the graphical appearance of the available components (icons), as well as information about the user-accessible data in the components (i.e. variables, parameters, etc). After this information is loaded, the user can graphically edit the flowsheet in the same way as with a desktop application.

When the flowsheet is configured, the user can trigger the solution of the flowsheet. The flowsheet editor sends the request for solving the system to the library server. When it receives the results, it automatically displays them back in the flowsheet.

In order to ensure the long-term usability of the system on a wide range of platforms, it was decided to base the flowsheet editor on HTML5 (W3C, 2014), which provides a rich set of capabilities that allows the system to implement interactive graphic functionality as required in the flowsheet editor. Moreover, the use of HTML5 allows the system to implement dynamic web pages without the need to use any browser add-ins and it is sufficiently well supported by all major web browsers and the IPSEpro cloud-based simulation platform has been successfully tested with all of them.

- **Library Server:** The Library Server provides two services: (1) upon the respective request from a client, it returns the information about all component in a model library which is required to configure the user interface for using it with the respective model library; and (2) it also handles the request to solve a project. The information about the system components that are required by the flowsheet editor is extracted from the model library description used by IPSEpro. When the client requests to solve a process, it includes with the request a complete description of the structure and parameterization of the system. The library server feeds this information to the solver core, which converts it into a system of algebraic equations, which it then solves. The results are then sent back to the client to be displayed graphically.

- **Performance Aspects:** The usability of a cloud-based platform is, to a large extent, determined by the system performance. Slow and unresponsive interaction will inevitably reduce acceptance by users. Several individual aspects have been evaluated during the development of the IPSEpro cloud-based simulation platform. They are:
◦ Time for opening a project/storing projects.
◦ Responsiveness of the user interface/browser.
◦ Time required for solving a system.

Unlike with locally installed software, the performance of a cloud-based system depends on a wide range of factors, where the speed of local hardware is only of moderate impact. Some of these factors are: (i) the browser which is used on the client side; (ii) the speed of the internet connection; and (iii) the speed of the cloud server.

The time required for opening and storing a project is determined by the speed of the internet connection. The project shown in Figure 14: MIDES Process Model simulated in the IPSEpro Online Platform takes about 3.5 seconds to open. The responsiveness of the user interface is crucial for convenient use of the platform. Comparison between different hardware and software configurations show that the choice of web browser is a major influence, due to the highly interactive nature of the user interface.

The overall time required to obtain a solution for calculation of a project is determined by the speed of the internet connection for transferring input data to the library server and returning results from the server back, as well as the time required by the library server to actually solve the system of equations. The solver core used by the library server is fast. The actual solution for the project shown in Figure 14: MIDES Process Model simulated in the IPSEpro Online Platform takes about 0.5 seconds. Measurements show that, on average, about twice this time is required to transfer data between the client and the server, so that the overall time for solving a system is about 1.5 seconds.

- Platform Implementation Risks and Mitigation: Using a cloud-based system can present some risks due to the dependency on a public networked system. The system may have to cope with network failures, as well as with security threats. The implementation of the IPSEpro cloud-based simulation platform has addressed those risks and their mitigation measures. It is inherent in the system architecture that a network failure will result in severe restrictions on the use of the simulation platform. For example, in the case that it is impossible to reach the library server for obtaining simulation results. However, the implemented functionality of the platform ensures that even in the case of a network failure, no data is lost. Likewise, security procedures have been implemented to protect user data from unauthorized access.

4.4 MIDeS Desalination Process Model Used Online

Figure 14 shows the MIDES process model within the IPSEpro Online Platform (MIDES Consortium, 2018b). It is possible to identify on the left side of the environment, the icons of the customized desalination and wastewater-treatment components created for the MIDES_Lib model library and used in the simulation of the overall MIDES process. Results of the simulation are automatically displayed in the data-crosses placed along the process components’ connections; and within the parameter boxes in the flowsheet.

5. MIDeS MONITORING AND AUTOMATED CONTROL

The control and monitoring systems presented here were implemented and optimized by the partner OnControl, along the development of the MIDES project, starting from the field devices up to the high-level control tools. All sensors and actuators were selected considering the principal process variables to be monitored and controlled. Such selection was made based on commercial solutions already available in the market, taking into account the financial viability of the project and future scaling up. Moreover, with the selection of the sensors, the actuators and the desired behavior for the process, the low-level control architecture was developed, which comprises of a Programmable
Logic Controller (PLC) and a Human Machine Interface (HMI). The final element of the control architecture is the high-level control layer that is composed by OnControl software systems used to read, process and visualize data in real-time. The overall architecture of implemented system is depicted in Figure 15.

As illustrated in Figure 15, the data module Databridge is responsible for all acquisition and processing of the data, which includes all the tools that will provide and expert control of the system. The main Databridge plugins used were the following: (1) Expert Fuzzy Control system: software that allows the incorporation of expert human knowledge about the process in the system to be controlled using “if-then” fuzzy rules. The user can construct the controller and adapt it using a user-friendly graphical interface; (2) Statistical Modeling System; (3) Ontrend Plugin: software that allows the creation of historical data of the process, saving it in a PostgreSQL database; and (4) PostgreSQL: Database used by the Ontrend plugin of the Datacube to show/monitor the historical data of the process.
In addition to Databridge, the systems Datacube and Dashboard were also used in order to achieve unattended control architecture and process monitoring.

The Dashboard technology is used for real-time process monitoring in a single webpage interface, where the main information from process is made available.

Datacube is a high-level user interface platform that is used for: Historical analysis of the process using the plugin Ontrend; as well as for Analysis of the Key Performance Indicators of the process. The Datacube system is a modular and extensible software, which creates an interface between the operator and the process. It allows for a historical view of the process, online and historical analysis of the energy consumption and automatic creation of reports.

In order to monitor the performance of the MIDES process, a tool for the implementation and monitorization of the Key Performance Indicators (KPI) of the process was created. Using this platform, it can be implemented the most varied KPIs: overall process efficiency, production flow, energy management system, among others. As can be seen in Figure 16, the software offers a graphical interface using the Datacube that allows the user to monitor the KPIs and check its historical data. Such tool is particularly important to support decision-making processes within the project implementation procedures.

5.1 Monitoring Control System in the Pre-Pilot

The monitoring automated control system deployed in the MIDES pre-pilot installation within the IMDEA lab set-up is shown in Figure 17. The development of the control system was an iterative process that starts from the selection of the system requirements. The next step was the design of the electrical diagram for the construction of the switchboard. From this electrical diagram, the switchboard was assembled. Its Overall, the main characteristics of the control system-module are:

- IP66 Wall-mounting polyester enclosure;
- Safety equipment for devices and people protection;
- Power supply of the automation equipment, sensor and actuators;
- Power supply of the MDC; and
- Automation Equipment: PLC and HMI.

In parallel to the construction of the switchboard, the programming of the PLC and HMI was performed, as illustrated in Figure 18. In the visual interface of the pre-pilot the user can control the peristaltic pumps, the liquid and gas solenoid valves and monitor the potentials and current of every MDC cell.

Figure 16. DataCube Key-Performance Indicators
As a sub-area of Artificial Intelligence (AI), Machine learning (ML) focuses on studying algorithms and statistical models used by computer systems to perform a specific task, relying on patterns and inferences. ML algorithms build a mathematical model based on sample data (training data), in order to make predictions or decisions without using explicit programmed instructions (Bishop, 2006). ML can be used in various applications across business problems, together with Data Mining (Friedman, 1998), focusing on exploratory data analysis for predictive analytics.

In MIDES, a Machine Learning (ML) approach with Statistical implementation was developed using the Databridge model to predict the Chemical Oxygen Demand (COD), by means of a software sensor (aka. soft sensor). The collected data as “training data” came from a total of 12 monitored variables, which included: conductivity, pH, redox, temperature, current generated, pump velocity, etc. (in catholyte, anolyte, saline tanks). Those parameters were measured every 1 minute. Data from COD laboratory measurements were also considered, which have scarcely and infrequently measurements, of approximately twice a day. The COD soft sensor allows the estimation of COD in real-time every 1 minute, allowing the operators to make fast decisions on the process.

To predict the COD, the variables parameters from saline, anolyte and catholyte tanks were used as input variables. Those were: the conductivity, pH, redox and temperature, for which a total of 16 samples were used to learn the COD predictive model. For such purpose, a partial least squares (PLS) model was used as the predictive model and deployed for operation in the Databridge module.

5.2 Machine Learning Using Databridge

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The PLS was chosen as the predictive model, because it is robust to noise, correlated and irrelevant features, which are common issues in industrial applications.

Figure 19 shows the coefficients of PLS model, and the prediction comparison, between real and estimated COD. Figure 19(a) shows the relevance of each input variable regarding the COD values. It can be concluded that conductivity in anode has the strongest correlation concerning COD (which is in line with MDC operating conditions, since the conductivity is related with ionic conductivity of organic matter in anode tank), and also the saline redox (in MDC technology, the redox values tend to positive when oxidising species appears in solution. For example, oxygen or Fe(III) that can be reduced into water and oxidise other molecules). Figure 19(b) shows the coefficients of PLS model for COD prediction. For the project particular case, the results of the predicted model were assessed as pertinent. This way, the ML approach was validated, as the relation between prediction and real values did not compromise the overall MDC behaviour at the given operating conditions.

6. THE OPERATIONAL DECISION-MAKING SUPPORT IN THE MIDES PILOT DESALINATION PLANT

Operational Decision Support Systems have been extensively studied, including use-cases (Nurminen et al., 2008) (InteGRail FP6 Research Project, n.d.), and show to offer decision makers accurate and appropriate conditions for better decisions, as they are provided with the needed information and results from simulated models of their analyzed processes, in order to optimize operations as well as further implementation phases of respective systems and installation plants.

Within MIDES, the operational decision-making support provided by the simulation analysis of the MDC and its process, as well as its automated operational control was of vital importance for the accuracy of its performance and data validation, as well as for the mitigation of risks in the pilot implementation stages.

The mathematical model of the Microbial Desalination Cell MDC provided by the results of the project work-package concerning “Microbial Cell Design Engineering and Testing” were further implemented in IPSEpro and integrated in the customized MIDES component-model library (MIDES_Lib), which augmenting the existing IPSEpro Desalination Model Library (SimTech Simulation Technology, n.d.c). The MIDES_Lib was then used in the IPSEpro Process Simulation Environment PSE to create the comprehensive MIDES process model, which was simulated, optimized and validated by all involved technical partners.

The concept of using IPSEpro as a Decision Support System (DSS) or coupled with a DSS for operational applications has its origin described in (Dargam & Perz, 1998) and has been source of insights for further investigations in the DSS area (like in (Kazim & Aydin, 2011), for instance).

Figure 19. (a) Coefficients of PLS model for COD prediction. (b) Predicted and real COD.
Specifically, the analysis planned to support operations in MIDES was based on the insights and results of the respective simulated process model, as well as of its monitored control system. Figure 20 shows the considered steps used in MIDES for operational decision support, in order to allow pertinent actions to be taken to improve system performance envisaging more accuracy in the implementation phases of the project. Steps 1 to 6 were planned to be taken using the MIDES mathematical model and the simulated process model in IPSEpro. Step 7 relates to the actions implemented in the pilots implementation phase. Finally, steps 8 and 9 relate to the performance of the automated control & monitoring system built within the pilots. A feedback from step 9 to step 4 was in some cases needed to re-start the process with updated values.

The overall simulated model implemented via SimTech’s process modelling package IPSEpro, including its developed and deployed online platform, was then a useful asset for the project, in providing a decision-making tool concerning the integration of the MIDES process from Lab-scale to Pre-Pilot scale. The use of the simulated model of MIDES allowed the confirmation of expected parameters and values of the project implementation that then validated its implementation phase. Moreover, the simulation model of the overall process provided valuable insights at all stages of the project (lab, pre-pilot and pilot scales).

Furthermore, the results obtained in the analysis of the MIDES Pre-Pilot-scale MDC could also be used for assessing the impact of up-scaling of changed component parameters in the next phase of the Pilot-scale MDC, and even analyzing the performance of the pilot plants.

Likewise, the results of the MIDES Monitoring System allows project managers, end-users and decision-makers to have a clear picture of the operational situation of the pilot plants in order to be granted assistance on assertive potential decision-making options, whenever needed.

7. SUMMARY AND CONCLUSION

A cloud-based simulation platform for the IPSEpro process & simulation modelling environment has been implemented and its capabilities have been demonstrated. The experience gained with the system shows that it is well suited for realistic applications and can be particularly useful for collaborative project development, like MIDES.

In terms of the developed IPSEpro Online Platform, a major benefit of the cloud-based simulation platform is the fact that no software needs to be installed locally. This makes the system access easier, which is of particular benefit in collaborative research projects where a larger number of users needs to access the models. Additionally, there is no risk of version conflicts that can occur with locally installed software. Another advantage is that process models can be readily shared, and changes are available to all authorized users virtually instantaneously.

Considering the implementation aspects of the IPSEpro Online Platform described in subsection 4.3, and the Control Monitoring System described in section 5, we can assure that the shared MIDES process model for development collaboration among project partners is robust and accurate in performance and security aspects; and that the automatically monitored data presented to the end-users and pilot developers, including ML & statistical analysis, serve as important tools of decision-making.
making with accurate levels of assertiveness. Those features enforce a rapid decision-making process on potential changes to be implemented in the model as a whole, impacting all stages of the project implementation from lab-scale, through pre-pilot to pilot stages.

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