Predictive advisory solutions for chemistry management, control, and optimization

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ABSTRACT: Process runnability and end-product quality in paper and board making are often connected to chemistry. Typically, monitoring of the chemistry status is based on a few laboratory measurements and a limited number of online specific chemistry-related measurements. Therefore, mill personnel do not have real-time transparency of the chemistry related phenomena, which can cause production instability, including deposition, higher chemical consumption, quality issues in the end-product and runnability problems. Machine learning techniques have been used to establish soft sensor models and to detect abnormalities. Furthermore, these soft sensors prove to be most useful when combined with expert-driven interpretation.

This study is aimed at utilizing a hybrid solution comprising chemistry and physics models and machine learning models for stabilizing chemistry-related processes in paper and board production. The principal idea is to combine chemistry/physics models and machine learning models in a fashion close to white box modeling. A cornerstone in the approach is to formulate explanations of the findings from the models; that is, to explain in plain text what the findings mean and how operational changes can mitigate the identified risks.

The approach has been demonstrated for several different applications, including deposit control in the wet end, both raw water treatment and usage, and wastewater treatment. This approach provides mill personnel with knowledge of identified phenomena and recommendations on how to stabilize chemistry-related processes.

Instead of using close to black box machine learning models, a hybrid solution including chemistry/physics models can enhance the performance of artificial intelligence (AI) deployed systems. A successful way of gaining the trust from mill personnel is by creating a plain text explanation of the findings from the hybrid models. The correlation between the likelihood of a phenomena and disturbance and the explanations are derived and validated by application and chemistry and physics experts.

Application: The principal idea is to combine chemistry and physics models and machine learning models in a fashion close to white box modeling. A cornerstone in the approach is to formulate explanations of the findings from the models.

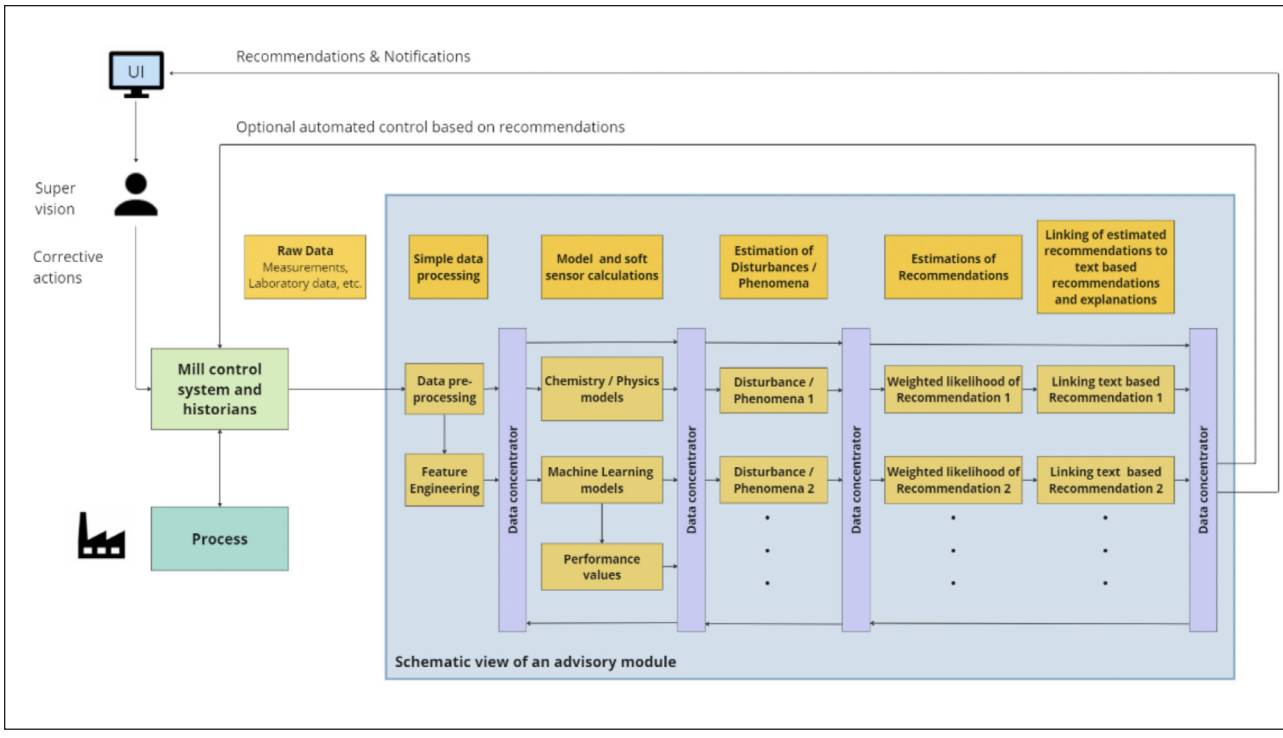
A general trend in the last few years has been to adopt and utilize machine learning models in analyzing and predicting behaviors and phenomena in industrial processes [1]. Many successful implementations have been reported in the past, as in [2], for example. These implementations have mainly been black box approaches where it is unclear how the machine learning models have arrived at a certain prediction. One of the biggest obstacles for the pulp and paper industry in successful implementation of machine learning and artificial intelligence (AI) is the lack of trust in algorithms [3]. The introduction of performance values has helped with the understanding of how the machine learning models weighted the importance of input values at a given point in time, as in [4]. This enables humans to gain insight and spot some irregularities in machine learning models. However, this has, in some cases, not produced a full working model. Also, the interpretation of the performance values is not always straightforward.

In our work, we have explored a variant to pure machine learning models using a combination of chemistry and physics models and machine learning models. By combining these two approaches, it is possible to arrive at more deterministic predictions. Another important factor is to gain the trust of mill personnel to rely on predictions and advice derived from these methods. The main objective of this paper is to demonstrate this hybrid approach and how it can help in arriving at more trusted solutions. A methodology has been derived for translating the outcomes of chemistry/physics models and machine learning models into plain text findings and recommendations that provide mill personnel with advice and corrective actions for detected phenomena so they can make more informed decisions.

GENERAL METHODOLOGY

The approach we have taken is focused on dividing challenges into manageable modules. Each module is concentrated on solving a specific challenge. However, these modules can exchange information and data to optimize performance.

The concept of advisory modules is not limited to chemistry-related processes. It can be used as a general way of guiding and advising mill operators and engineers for any process. As an option, recommendations in the form of setpoint changes can be automated and fed to the mill



1. Overview of the general methodology for one advisory solution.

control system while maintaining full visibility for mill operators and engineers to adjust and change the given recommendations.

The general methodology for one advisory module is shown in **Fig. 1**. This methodology comprises eight steps:

1) Data selection: This is based on process and expert knowledge combined with correlation analysis and performance indicators derived from machine learning models. This approach significantly decreases the need to select hundreds or thousands of tags, as prior qualitative knowledge can help with identifying relevant tags and leaving out non-relevant tags.
2) Loading of raw data from the process: These data include online/offline measurement data, laboratory analysis data, target quality data, machine settings, etc.
3) Data processing and feature engineering: This step includes data format changes, standard statistical calculations, simple logic calculations, delays, and calculated variables, such as mass flows, chemical dosages, mass ratios, freshwater usage, pollutants load, and removal efficiencies like colloids, suspended solids, chemical oxygen demand (COD), phosphorous (P), and hydrophobic contaminants (HF).
4) Model and soft sensor calculations: Here, specific processes and measurements are modeled and estimated. This can be in the form of chemistry/physics models, machine learning models, and performance values derived from machine learning models. The selection of method comes down to a best-fit-for-purpose approach with respect to error optimization, computation complexity, and robustness over time. Examples of the model are mass and water balances, pollutant predictions, deposition risk prediction, and sporulation risk prediction.
5) Estimation of process disturbances and phenomena: This is based on identified correlations between events and disturbances and phenomena. These have been validated by application specialists, operators, engineers, etc.
6) Estimation of weighted likelihood of predefined recommendations to materialize: Again, the predefined recommendations have been validated based on qualitative domain expertise by application specialists, operators, engineers, etc.
7) Linking estimated recommendations to text-based recommendations and explanations: The recommendation and explanations include interpretation of phenomena related to process disturbances.
8) Outcome of an advisory module is displayed in a user interface: This interface allows the mill operators and engineers to follow the processes under supervision. Based on the recommendations from the model, the operators and engineers can take corrective action, such as setpoint changes, initiating inspections, and maintenance. Recommendations in the form of setpoint changes can be automated to be fed to the mill control system, but with the proposed changes visible to mill operators and engineers so they can override them if necessary.

Advisory Solution	Application (module)	Description
Paper/Board Wet End	Deposit control	Improve paper/board quality by decreasing deposit risk in the process. This is the basis for the wet-end solution – the first step towards wet-end stability.
	Retention	Optimize retention chemical usage and prevent retention related runnability issues.
	Internal sizing	Ensure paper/board meets sizing targets and prevent uncontrolled sizing.
	Internal water circulation	Support reducing fresh water usage while maintaining good machine runnability and end-product quality.
	Spore control	Prevent sporulation incidents by running the process in a hygienic manner (with efficient biocide dosing).
Paper/Board Water Treatment	Raw water treatment	Prevent raw water related runnability and quality issues in paper/board production.
	Wastewater treatment	Ensure treated wastewater meets set permit limits for pollutants.

I. Areas/applications where advisory solutions have been developed or are now under development for deployment.

The short list of disturbances and phenomena followed by the creation of recommendations can be seen as a method for capturing process knowledge and developing a common process understanding. This also improves the retention and transfer of process knowledge within a corporation.

Table I lists the areas and applications where the advisory solutions have been developed or are under development for deployment.

SERVICE

One key factor for the proposed implementation is the location where an advisory module is executed. Several options are available. One option is to execute an advisory module in a cloud environment, either in the service provider's cloud or in the corporate cloud. The advantage of the cloud implementation is the availability of large computational engines. Also, no hardware needs to be installed and maintained on site. Naturally, cloud computing also needs software installation and maintenance. Another option is to deploy the advisory module on site. Again, two options are available: in a demilitarized zone (DMZ) running on a server, or in an edge device capable of running containers. The choice of where to run an advisory module comes down to customer preferences, technical computation requirements, costs, security, scalability, and ease of maintenance. **Figure 2** shows an overview of where advisory modules can be deployed.

RESULTS

The hybrid solution (combination of chemistry/physics models and machine learning models) together with text-based recommendations has been successfully utilized for chemistry management in paper and board making processes. The following examples present the results of operational use in paper and board mills. The selected examples are from raw water treatment, wastewater treatment, and wet-end stabilization.

Raw water treatment

The concept in this advisory module is to predict the turbidity level after a water treatment step, prior to a specific operational step in the process. The prediction horizon is about 1 h ahead of time. Based on this prediction and other selected measurements, the target is to give preventive automatic recommendations on process operation and chemistry dosage setpoints. The aim of these recommendations is to prevent or mitigate raw/fresh water runnability and quality issues in paper and board production.

Figure 3 shows an example of how the predicted turbidity (about 1 h ahead of time) follows the measured turbidity.

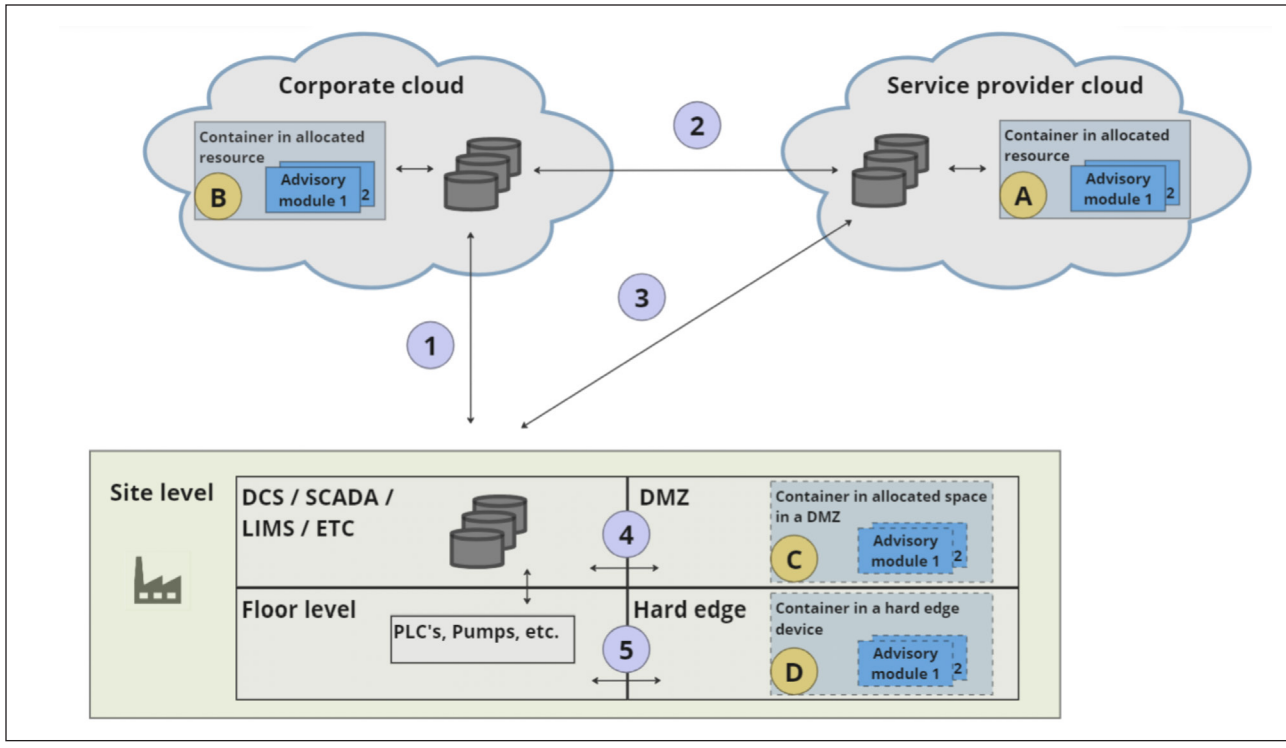
Wastewater treatment

The main target in this advisory module is to ensure that the treated wastewater meets the set permit limits for the pollutants: COD, P, and nitrogen (N). Another target is to bring real-time visibility for the performance of the wastewater treatment plant, showing the effect of the upstream processes on incoming wastewater quality, biological treatment, and wastewater effluent for operators.

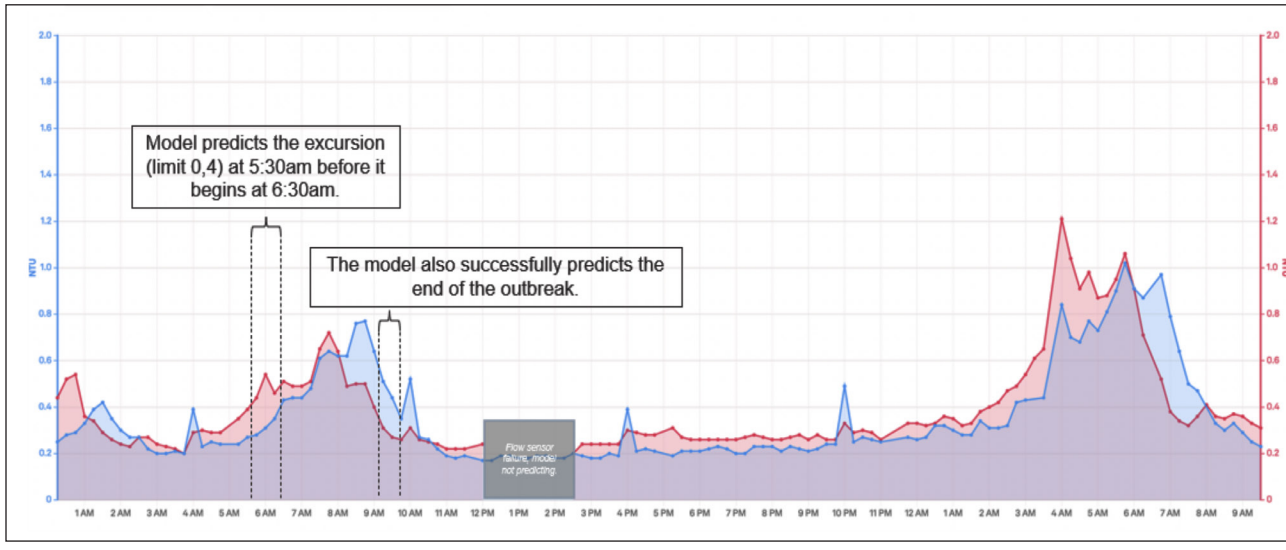
The advisory module includes risk prediction of pollutants (COD, N, P) in the effluent, monitoring of process disturbances (process conditions, water qualities), performance index for the biological treatment phase, and predictions for COD and suspended solids load in the aeration phase.

The performance of the online COD prediction in the aeration phase is presented in **Fig. 4**. The online prediction (solid blue line) correlated very well with the laboratory values (light blue dots). This online prediction is valuable for the operators, because the laboratory value is measured only once a day from a small grab sample.

The advisory module gives recommendations for the operators to decrease or increase the chemical dosages in primary sedimentation. The recommendations are based on the online COD and suspended solid predictions.



2. Possible options for installing advisory modules in: (A) service provider's cloud; (B) corporate cloud; (C) demilitarized zone (DMZ) on site; or (D) hard-edge device on site. The options (C) and (D) are under development (DCS: distributed control system; SCADA: supervisory control and data acquisition [system]; LIMS: laboratory information management system).



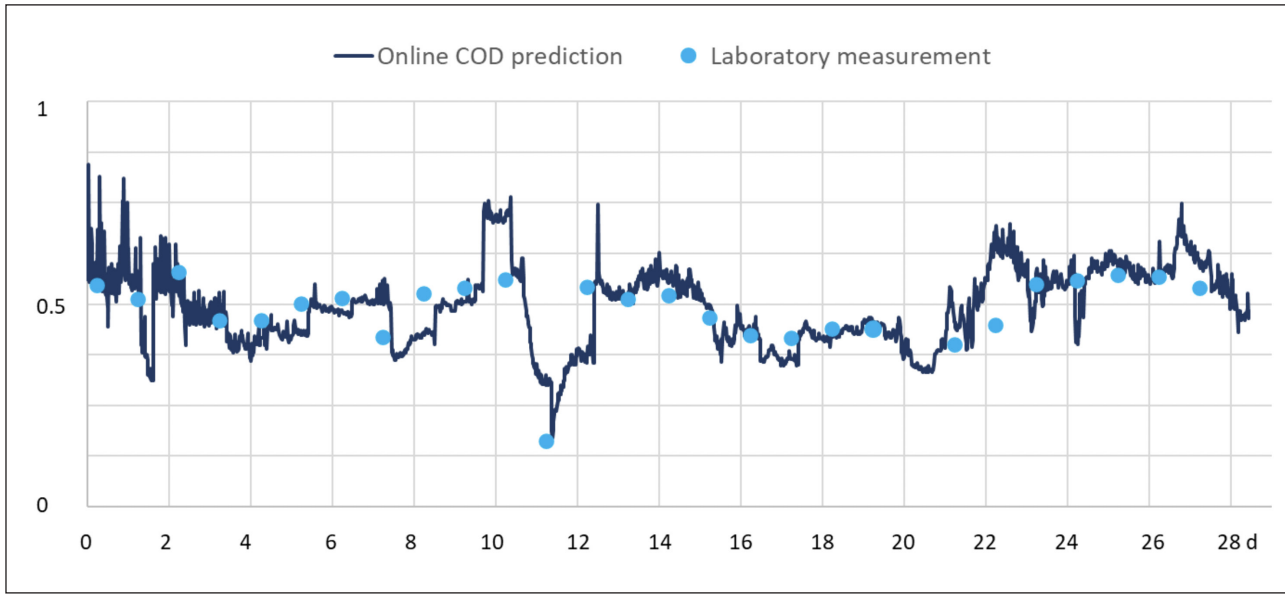
3. Predictive turbidity model accuracy. The red line is the predicted turbidity (1 h ahead of time), and the blue line is the measured turbidity.

Predictive wet end solution in a paperboard process

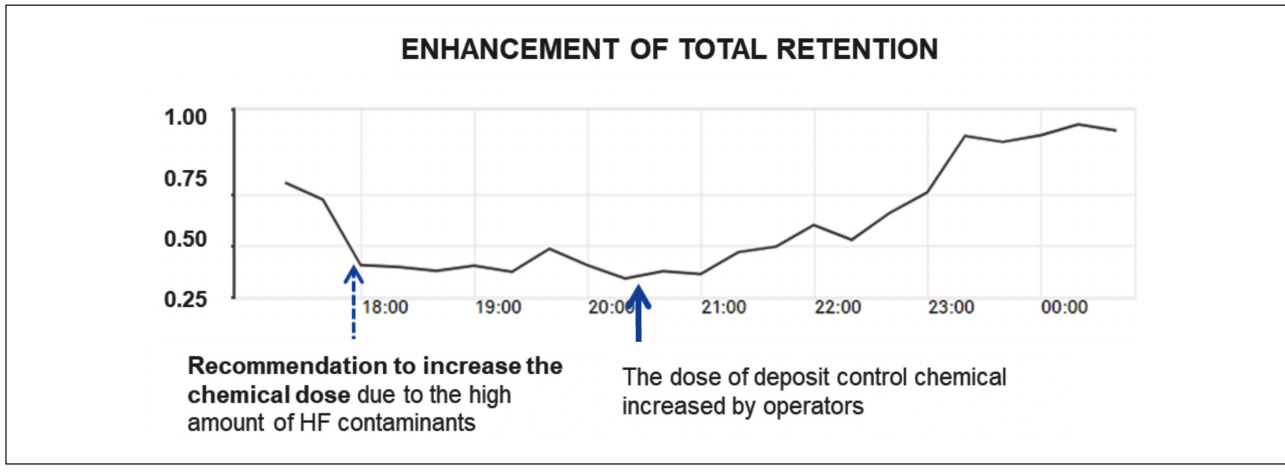
The main target here is to stabilize the wet-end chemistry and to improve both machine runnability and end product quality. The aim is also to train operators for chemistry management and to make chemistry statuses visible to the mill personnel.

This advisory module is based on prediction of deposit risk in the machine and monitoring of the overall chemistry status in several sub-processes (pulps, broke, wet end, water circulation). In addition, the solution shows root causes for instability in the wet end.

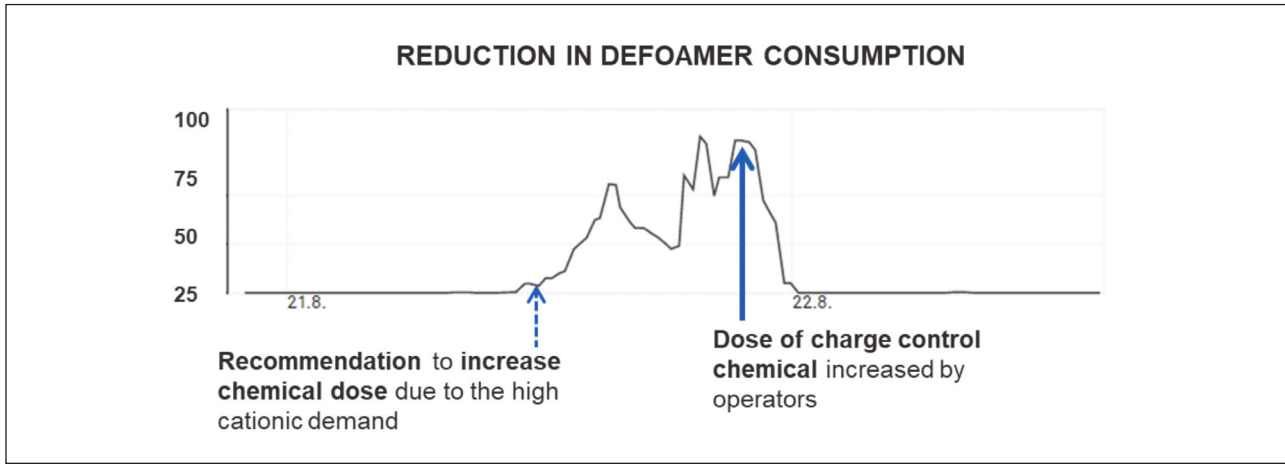
In a trial, the advisory module gives recommendations for operators to optimize the dosage of several deposit control chemicals. The operators actively utilized the recommendations and implemented up to 90% of all recommen-



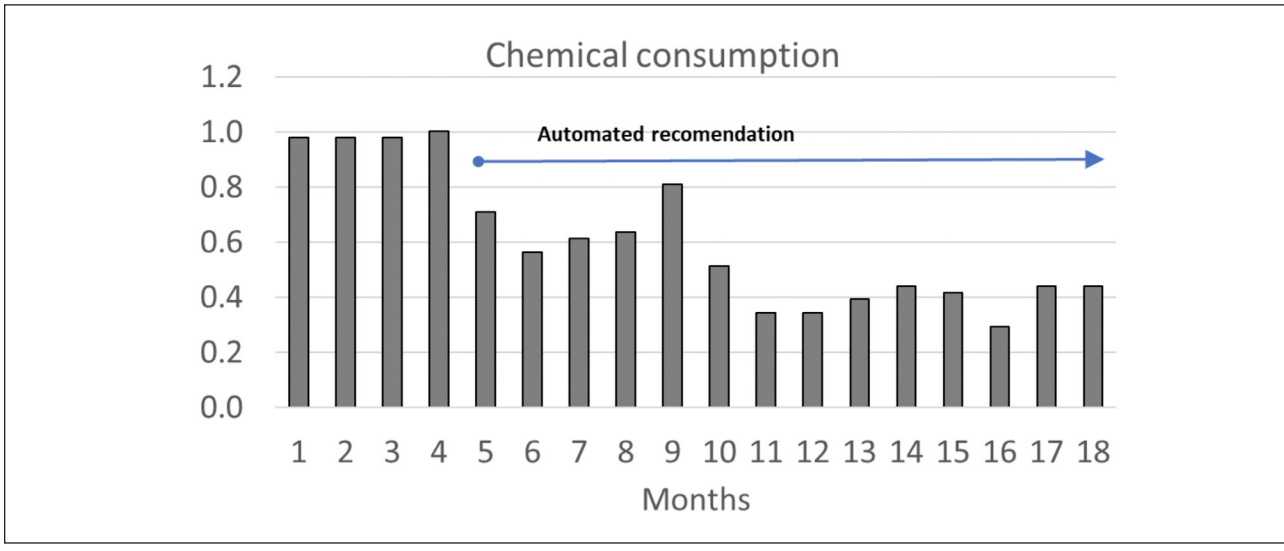
4. An example of the accuracy of the online chemical oxygen demand (COD) prediction in an inlet stream to an aeration unit. The dark blue line is the predicted value, and the light blue dots are the measurement values (scaled values between 0–1).



5. Improvement in total retention (scaled values between 0–1). As a result of the operators following the recommendations given by the advisory module, the retention improved around 1% (HF: hydrophobic contaminants).



6. Defoamer consumption (scaled defoamer dose between 0–100%).



7. Effect of automated recommendation on the overall chemical consumption (scaled values 0–1).

dations for several months. Overall, the chemical changes were beneficial, with clear responses seen in the stability of the wet end and the performance of the wet-end chemicals (e.g., sizing agent, defoamers). Some examples of the responses are shown in **Fig. 5** and **Fig. 6**.

Example of response to retention

The amount of hydrophobic contaminants (i.e., wood pitch from incoming pulp) increased strongly in the wet end. In this case, the operators received a recommendation to increase the dosage of a deposit control chemical to fix the wood pitch in the fibers. Although the high concentration of hydrophobic contaminants had already weakened the retention, the increase in chemical dose implemented by operators improved the chemistry stability in the wet end and enhanced retention (Fig. 5). When the process disturbance in the pulping process had subsided, the operators were advised to reduce the chemical dosage.

Example of response to defoamer consumption

A high amount of dissolved anionic compounds caused foaming in the machine and high consumption of defoamer chemicals. The operators received the recommendation to increase the dosage of the charge control chemical. After the implementation of the recommendation, a clear response was seen in defoamer consumption (Fig. 6). An overall chemical savings was achieved by lower defoamer consumption.

Example of automated recommendations to mill control system

The recommendations for chemical dosages were automated and integrated into a mill control system. The automatic dosing control resulted in a cost-efficient chemical treatment (**Fig. 7**). The chemicals were dosed on an as-needed basis, hence avoiding overdosing. As a result, wet-end stability improved, and less contaminants such as pitch, white pitch, dissolved anionic compounds, and colloidal particles were concentrating in the wet end. Still, the operators had full visibility to the recommendations and could at any time switch the chemistry dosing to the mill's own control loop or manual dosing.

BENEFITS

The new advisory modules have clearly improved the visibility of the chemistry and process performance for operators and mill engineers. These online solutions have enabled proactive process improvements. Consequently, it has increased work efficiency in the mills, e.g., decreased manual laboratory work and reduced time required to troubleshoot issues.

Some examples we achieved together with customers are:

- Improvements both in process and chemical performance of paperboard making processes.
- Wet-end stability improvements, e.g., with respect to variations in quality measurements.
- Runnability improvements, e.g., retention increased around ~1%–3%, and chemistry-based wet-end breaks decreased around 25%. Chemical consumptions were optimized based on needs (no underdosages or overdosages), with a chemical decrease of up to 30%.
- Less defects with optimized chemistry.
- Clear improvements in sustainability.

CONCLUSION

In this paper, we have demonstrated an alternative approach to utilizing machine learning models. As opposed to using black box machine learning models, a hybrid solution including chemistry and physics models can enhance the performance of AI deployed systems. A successful way to gain trust from mill personnel is to create a plain text

explanation of the findings from the hybrid models. These explanations have been derived and validated by application and chemistry and physics experts. In cases where it shows benefit, automating the recommendations and linking the mill's automation system is possible. Further optimization with automation continues to provide mill personnel full visibility of the reasoning behind the proposed actions and deeper explanations of the chemistry and physics phenomena related to the process in question. **TJ**

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About this journal

ABOUT THE AUTHORS

In this paper, we present a systematic approach on how to use machine learning algorithms in conjunction with chemistry/physics models, measurements, and domain expertise. It forms a holistic approach on how to form practical, usable explanations about identified phenomena, as well as recommendations for how to respond.

In this study, it became clear over time that instead of using machine learning algorithms as black box solutions, more transparent and informative solutions could be of better use. We also saw that involving mill operators and engineers at an early stage was key to the success of such a project. Most interestingly, we found that by using explanation values for machine learning algorithms and validating them with domain expertise, it is possible to get acceptance for forming hybrid solutions.

For mills, the information here can be used as a basis for forming strategies on how to use machine learning algorithms in a hybrid implementation. A next step would be to formalize how to integrate such a hybrid solution to traditional mill supervisory control and data acquisition (SCADA) systems.

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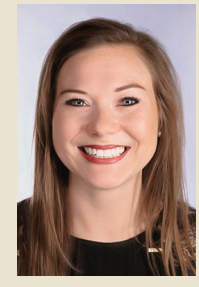
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