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Assessment of the Plantwide Control Structure in a Pectin Production Plant

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Abstract: Real application studies constitute a relevant part of academic plantwide control research, as they promote industrial awareness and ideally acceptance. Especially in the area of bio-based processes, few works have been documented. These processes are characterised by large uncertainties, batch-operated units, and time-delayed measurements, which ultimately results in comparably low levels of automation. This work features the application of a stepwise plantwide control structure synthesis framework to an industrial bio-based production plant. Firstly, this is to give an indication of whether plantwide control is apt for this type of process. Secondly, it highlights specifically where substantial challenges arise during the application.

Keywords: Plantwide Control; Biotechnology; Industrial control; Manual Control; Inventory control

1. INTRODUCTION

Control of bio-based processes is a topic of ongoing academic research with more than 200 publications per annum in the field of engineering. There seems to be academic focus on the product formation step, but downstream processing can be costly, not lastly due to capacity, yield, or quality bottlenecks. Plantwide control (PWC) deals with the derivation of robust control structures for large-scale continuous processes. In real-life industrial plants, this often requires that quantitative means and engineering heuristics are combined. Plantwide control has been referred to as an automation philosophy (e.g. Larsson and Skogestad (2000)), as it is often not straightforward to assess whether one candidate structure is superior to another, especially on a long-term basis. With regard to bulk chemical production, Foss (1973) states: "And it is well recognized that no amount of detailed study will ever replace all uncertainties with certainties. Rather, it is for the control system designer to recognize the significant uncertainties and to conceive controls that function effectively nonetheless."

This is still true, and bio-based processes are known both for uncertain conditions as well as raw materials. In general, PWC is not well defined in a bio-context. A reason for that might be batch operation. Some unit operations, but also entire plants are operated discontinuously, especially in pharmaceutical production. Here, cross-contamination is to be avoided by means of cleaning and sterilising equipment between batches. Obviously this complicates the application of frameworks designed for continuous processes, and furthermore caps plant throughput significantly. The latter renders de-bottlenecking the predominant plantwide task (Amaran et al. (2016)), however as a matter of scheduling rather than control. Beyond that, a traditional focus on feed-forward statistical control, frequent manual control by operators, and not lastly the absence of high-fidelity plantwide numerical models complicate the application of PWC to bio-based processes. Still, a conclusive plantwide feedback control strategy plays a vital role in the U.S. Food and Drug Administration (FDA) endorsed 'Quality by Design' approach (Yu (2008)). However, only few applications are documented. There are model-based studies of bio-PWC (e.g. Ochoa et al. (2010)), but especially industrial cases (e.g. Van Dijk et al. (2009)) seem to be scarce.

Pectin, a gelling and thickening agent derived from citrus peels, is generally produced in large-scale continuous processes. An acidic, hot process regime relieves the bioburden, as most units are in essence self-sterilising. Therefore, pectin plants share many features with bulk chemical plants. However, uncertainties are large, manual control common, and the integration of batch units into the continuous process is challenging. Thus, pectin production is located somewhat at the interface between bulk chemical- and bio-based production. This motivated a case study to analyse plantwide operations in a real pectin plant with the ambitions of pointing out

- Potential control structure shortcomings.
- Difficulties that arise when applying a PWC framework to this type of process.

To protect classified information, the investigation is limited to the extraction-purification-concentration section of the plant. Real quality attributes will be used to assess optimality, but no quantitative product data can be enclosed. This is not expected to distort the conclusions drawn in the article which is structured as follows: section 2 gives a brief overview of plantwide control and motivates the choice of framework. Theory is succeeded by an outline of the case study scenario as well as the application of a step-wise PWC methodology (section 3). This includes

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the discussion of possible control structure shortcomings as well as arising methodological challenges. Hereafter, the work is concluded.

2. BACKGROUND

Plantwide control (PWC) refers to the systematic control structure synthesis for complete chemical plants. While single-loop controller tuning was formalised early-on, control system architectures have been configured by experts based on experience or belief for many years - and, many places, probably are still today.

Challenges stem from uncertainties as well as the combinatorial complexity in the choice of technology, hierarchical structure, and input-output pairings - but also from the requirement for robustness to process changes and longevity in the context of an evolving production environment. PWC offers tools that support this complex decision-making process which often requires taking qualitative elements (company policies, expected future trends, cost and realisability) into account.

A number of excellent reviews on the matter exist; the reader is referred to Vasudevan and Rangaiah (2012) for a relatively recent and exhaustive example. There are generally three trends in PWC. Firstly, one finds heuristic / process-oriented approaches with little to no reliance on numerical models. In contrast, mathematically-oriented approaches (optimisation-based or algorithmic) need high-fidelity models. According to Downs (2012), due to a lack of PWC experts and a growing base of available plantwide models, these approaches are promising future topics. Lastly, hybrid frameworks contain elements of both.

During the formative years of plantwide control research, Stephanopoulos (1983) wrote: "Sequential arrangement of processing units offers no particular control problems and the plant can operate easily and smoothly. Capital and operating costs are, in such case, rather high." Looking at downstream lines in today's bio-based production plants, a sequential paradigm is descriptive.

In-process inventory is not always suboptimal, as the otherwise required process control solutions can outweigh the arising costs (Zheng and Mahajanam (1999)). In a scenario with high raw material variability, it can furthermore be desirable to have equalisation throughout the downstream line. However, in a continuous multi-product plant, inventory generally prologues costly changeovers. This calls for an inventory control strategy that functions also with moderate amounts of material in the loop. Furthermore, in an increasingly competitive global market, a holistic perspective on plant operations and automation (including planning) is necessary, especially for plants situated in high wage countries.

Purely model-based approaches seem inappropriate for most bio-based processes. Anticipating section 3, also in the pectin plant it quickly became evident that the absence of a high-fidelity plantwide numerical model is a reality that has to be faced. Still, it seems unnecessary to exclude model-based tools stringently. Therefore, section 3.2 is based on the hybrid framework developed for the most part by Skogestad, Postlethwaite, Larsson, and Havre in the late 1990s (Skogestad (2012)). It offers a clear, stepwise structure, room for quantitative methods, but also a large heuristic base. Not lastly, application studies with process-oriented reasoning in a real-life industrial context are documented (e.g. Downs and Skogestad (2011)).

3. PECTIN PLANT CASE STUDY AND APPLICATION OF PWC METHODOLOGY

Pectin is ordinarily extracted from citrus peels that are residuals of juicing processes. Peels can be processed fresh if the plant is located in proximity of a juicer. High quality and yield make dry citrus peel the raw material of choice also in Europe, despite of the required cutting, drying, packaging, and transporting. Furthermore, as not every product can be derived from every raw material, it can be desirable to have a stock of dried peels for on-demand production. Consequently, it should be the ambition of a producer of specialised pectins to operate flexible plants that can shift from one specialised product to another at low changeover cost - which is a plantwide challenge.

Satisfying product performance requires that the chemical properties (i.e. degree of methyl-esterification (%DE), distribution of functional groups and side-chains, length of polymers) are set appropriately. These are process and raw material dependent, and some of them correlated. There are a number of qualitative final product attributes such as 'mouth feel' or 'taste experience'. They are of superordinate importance for the customers, yet inherently difficult to quantify reliably. Inferential measurements exist, but can only be determined in slow, manual laboratory experiments. One of these is syneresis, the ability to retain water. Overall, raw material and product specifications define the - hardly predictable - downstream processability, where especially product concentration and molecular weight influence the rheological properties of the highly viscous, shear-thinning fluid.

3.1 Case Study Process System Description

In general, operators play a key role in day-to-day operations as active parts of the control structure. Furthermore, it was deemed unrealistic to rigorously model either plantwide process or disturbance profiles in a way that would allow drawing meaningful conclusions from simulations. In that, the work at hand differs from many model-based plantwide control studies. The disparity between effort and expected return-of-investment was as much a limiting factor as the lack of crucial measurements and non-deterministic behaviour by the operators. Therefore, focus in the following is put on understanding the structural links in the context of process-oriented plantwide control.

Pectin extraction: The process is depicted schematically in figure 1. Upstream, parallel extractions evolve on a batch schedule. Extraction time is thus not a degree of freedom, even though the end-time constraint can be relaxed in extreme cases (at the cost of upsetting quality and/or throughput). The amount of peel loading, pH as well as temperature are the manipulated inputs and iteratively tuned in batch-to-batch manner. A first guess is based on laboratory and pilot peel pre-processing, but also on previous experiences with peel, producer, and region.

First stage filtration: The extraction slurry is drained gravitationally to a battery of continuous filters that remove the coarse cellulose remnants. Extraction tanks are emptied one-at-a-time without interruptions, otherwise filter

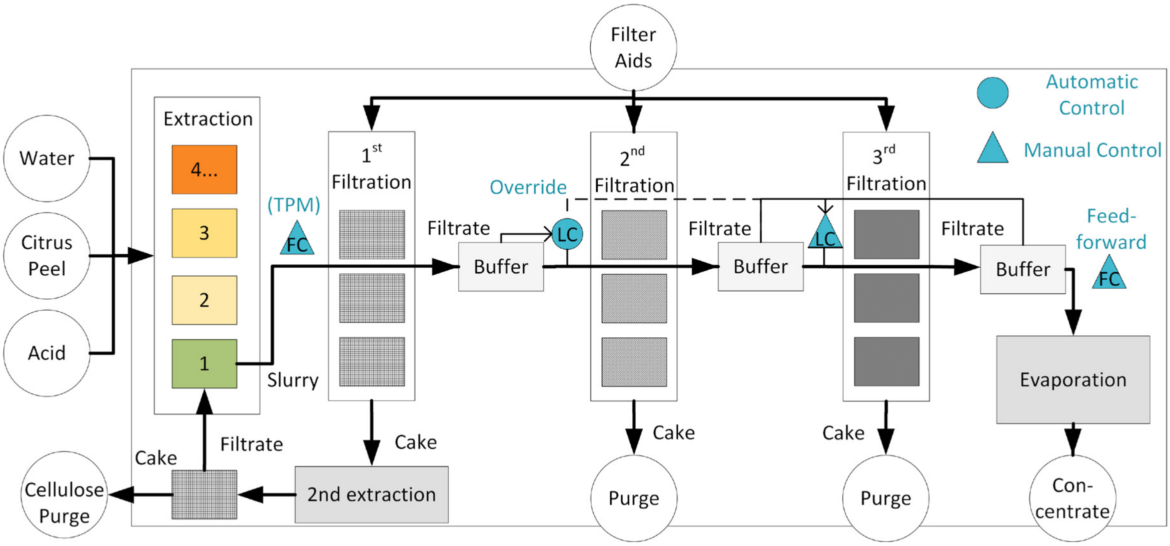

Fig. 1. Extraction-purification-evaporation sub-system with indication of automatic and manual inventory control.

cake integrity degrades, reducing capacity. This cake is fed to a number of re-extraction tanks to increase yield. Some re-extraction broth and extraction broth are mixed before a batch is fed to the first stage filtration. Due to lower pectin concentrations as well as further degradation of the pectin molecules, the re-extraction broth is less viscous, which improves the processability of the mixed slurry. A filter before this mixing purges most of the solid phase from the system.

Second stage filtration: The filtrate is fed to a further system of parallel continuous solid-liquid separators. The filter flow rates can be adjusted flexibly, and the inflow is determined by the flow rates of the upstream filters which are adjusted by an operator such that the extraction tank content is steadily processed.

Third stage filtration: Lastly, vertical perlite-precoated pressure leaf filters remove remaining impurities. The separation by means of size-exclusion is robust, given that the perlite precoat is distributed properly. An operational challenge arises as these filtrations are batch processes with strongly varying cycle times (Bähner et al. (2017)). The arising period of inactivity induces significant variability into flow rates and buffer tank levels. A detailed description of the work-flows as well as simulations of the tank levels around the filters can be found in Bähner et al. (2018), but are not necessary in a plantwide context.

Evaporation: The pectin extract is concentrated to reduce the amount of agent necessary during precipitation (omitted from this analysis) which is economically desirable. Thus, it is preferred to run the evaporator close to the point of sticking. However, sticking material eventually burns, which upsets product clarity due to the appearance of black particles. This leads to a quality downgrade or scrap material and calls for a conservative back-off strategy. Due to oscillatory behaviour, the operators dislike interfering once evaporation and precipitation are aligned.

3.2 Application of a Plantwide Control Structure Synthesis Method

In the following, Skogestad (2012)'s step-wise plantwide control structure synthesis framework is applied to the pectin process. It explicitly contains a top-down analysis (steps 1 - 3) from the superordinate production target, meant to yield ideal candidate structures. The bottom-up analysis (steps 4 - 7) systematically identifies the static and dynamic constraints of the existing physical system realisation, revealing which candidate control structures are implementable in practice.

By applying this framework, potential deficiencies in the plantwide control structure are to be identified. Furthermore, it is meant to demonstrate where application of the methodology to this type of process is most difficult.

Step 1: Define the Operational Objectives and Constraints

Profit is not only defined by the sales volume, as quality (functionality) has a significant influence on gelling properties. An optimal region for degree-of-esterification exists for a product - raw material coupling, and a small amount of optimised product can have the same gelling power as a larger amount of sub-optimally configured pectin. A plantwide objective function including product performance therefore reads

$$J = \min -p_P \, \eta_P \, P + \sum p_{F_i} \, F_i + \sum p_{Q_j} \, Q_j \, , \qquad (1)$$

where η_P denotes the gelling potential, P, F and Q product, raw / auxiliary materials, and heat / energy flows, respectively; p_P the price of the current product, p_{F_i} and p_{Q_j} prices of all raw materials i and utilities j, respectively. Objective functions, e.g. by Skogestad (2012) or Zheng et al. (1999), the latter including an explicit term for personnel, ordinarily do not include a quality factor. Ultimately, this is a matter of convention, as quality could be priced into achievable sales revenue. However, it was deemed more intuitive to introduce a further factor rather than having to deal with prices that do not correspond to the product-specific list price. A quality-quantity trade-off arises as pH, temperature and extraction time not only affect the performance-defining KPIs, but also pectin yield. It is however not easy to quantify this trade-off reliably, i.e. due to the vastly changing nature of the raw materials, which is why specialists often pinpoint the

Table 1. Overview of constraints affecting the pectin production process.

Constraint on	Type	Reason
Extraction		
Temperature	$T > T_{extr_{min}}$	Sterilisation purposes
Flow (soft equality const.)	$Q_{out_{average}} = \frac{V_{Fill}}{t_{I,B}}$	One tank emptied at all times ($t_{I,B}$: interval between batches)
Draining time	$t_{drain} > t_{drain_{min}}$	Gravitational draining
First-stage Filtration		
Power	$p < p_{max_{F1}}$	Maximum power of generator
Third-stage Filtration		
Pressure	$p < p_{max_{F3}}$	Pump power limited
Cycle Time	$t_c < t_{c_{max}}$	Forced re-initialisation after unusually long cycle
Cycle Time	$t_c > t_{c_{min}}$	Minimum feasible re-initialisation frequency (manual work)
Re-initialisation	$t_r > t_{r,min}$	Re-initialisation takes a minimum time
Quality		
Clarity	$c_P > c_{P_{min}}$	Customer requirement or standard product specs
Gel potential	$\eta_{P_{min}} < \eta_P < \eta_{P_{max}}$	Product performance (performant, yet homogeneous gel)
Syneresis	$s_{P_{min}} < s_P < s_{P_{max}}$	Customer requirement or standard product specs

optimum location based on experience. In practice, the bill of materials gives an indication of the cost factors, but a refined break-down to single production campaigns is difficult and uncertainty-afflicted. In the regarded sub-scenario, the units most costly in terms of utilities (i.e. energy uptake) are evaporator, solvent / precipitant recovery columns, generators and pumps. Auxiliary material streams aside from water are solvent, filter aids, and acids / bases. The dominant constraints on process and products are summarised qualitatively in table 1.

Step 2: Determine the Steady-state Optimal Operation

The second step of Skogestad's framework deals with optimal steady-state operation. However, in the multi-product pectin plant, transient periods arise regularly due to a quickly evolving production cycle. The economic implications of producing changeover material are mitigated by skilled post-processing (blending). As a consequence of the transient nature, optimum conditions are changing regularly - as are active constraints. This leads to a scenario where controlled and manipulated variables are coupled according to the most pressing needs, which is possible by including operators as highly adaptive control system elements. For instance, clarity feedback can lead to adjustment of the raw material (new peel / adjustment of peel blend / reduction of re-extraction intensity) as well as the filter aid feeding strategies. This decision is made based on multiple factors whenever a new laboratory measurement is available. Similarly, both temperature and pH in the extractions are used to steer the gelling properties based on expert knowledge and experience. The evaporator runs at maximum efficiency, if incoming product concentration is at the stickiness constraint. This in turn depends on viscosity and product concentration, and thus is used to determine the maximum amount of raw material loading per tank. But, aside from evaporator sticking, peel loading is limited by the cycle times on the pressure filters. At this point, it is unrealistic to automate the decisions that need to be taken when an active constraint shifts. Still, generally, the optimal operating point is found when the

I Degree-of-esterification is adjusted to raw material, resulting in maximum possible gelling potential.
II Gel exhibits the highest acceptable syneresis.
III Clarity is at the low end of the product specs.
IV The evaporator viscosity (stickiness) constraint OR the pressure filter lower cycle time constraint is active.

Due to correlations between variables, not all outputs can be steered independently, thus the above is an idealising scenario. Furthermore, as a cause of the delayed laboratory analyses, iterative adjustments of the inputs take time, and fast product changeovers can make it impossible to reach optimal conditions. Due to variance within the peel lots and during processing, a further challenge lies in identifying the appropriate back-offs - often, operators follow heuristics. In conclusion, the process is subject to severe disturbances and by nature often in transient regimes. It is therefore not possible to stringently define steady-state optimal operation as indicated by the framework.

Step 3: Select Economic (Primary) Controlled Variables

Due to the fairly large share of raw material costs in the total product price, it is of high importance to enable the full application-specific peel performance by setting the chemical composition appropriately. This can only be done reliably in a feedback manner, and can thus be a long-lasting endeavour as the gel-test is ultimately the longest feedback loop. The evaporator is one of the largest energy consumers in the plant, thus product concentrations should at all times be high. In conclusion, the primary controlled variables are all strictly optimal at their constraints and amount to

- Gel strength & syneresis (maximise yield)
- Viscosity (maximise energy efficiency)
- Clarity (minimise filter-aid usage)

Step 4: Select the Location of the Throughput Manipulator

The optimal location of the throughput manipulator (TPM) lies in the proximity of the bottleneck with flow rate propagation radiating outward via local inventory control loops (Aske and Skogestad (2009)). During nominal operation, the evaporator is not a bottleneck - it can still be driven to the point of sticking. However, in a maximum throughput scenario, it denotes a hard constraint that needs to be approached iteratively due to a tendency to oscillate. Pressure filtration can limit throughput also during phases of nominal operation. As Skogestad (2002) points out, bottlenecking during nominal operation is not necessarily a problem, if future surplus capacity can be utilised to make up for the loss. However, in the pectin plant, bottlenecks are generally undesirable due to upsets to the batch extraction schedule.

Therefore - theoretically - flow rates close to pressure filters and evaporator constitute good TPM candidates. As each of the parallel pressure filters needs to be assigned a set point individually, they are inapt for facile throughput steering. On the other hand, the evaporator feed is likely a good candidate. However, as any persistent downstream flow rate change ultimately calls for an adjustment of the batch schedule, a number of batches ($N_{aff} \leq t_{extr}/t_{drain_{prev}}$) will be affected by a disturbed duration. This induces quality or yield losses.

Therefore, even though total upstream capacity is not the rate limiting step, throughput is consciously set at the front-end, accepting that it is more difficult to ramp-up to full capacity, defined by batch filter cycle duration or evaporator sticking.

Step 5: Select the Structure of the Regulatory (Stabilizing) Control Layer

Only the buffer tank levels are not self-regulating, calling for type-2 (regulatory) control. In classical chemical processes, one might furthermore expect quality KPIs (here especially gel strength and clarity) to be controlled in the regulatory layer. However, due to the lengthy laboratory analyses, the frequency of the implemented (manual) control actions resembles that of the supervisory layer (multiple hours) and should be seen as such. The appropriate choice of raw material and skilled initial guesses for the extraction conditions usually guarantee that product is on-spec (blendable). However, product concentration and gel strength can be estimated using chemometric inference. This allows detecting uneconomical operating points if the peel pre-analysis was imprecise. At this faster rate, it constitutes a form of regulatory control. Still, the economically optimal operating point can only be identified after the laboratory measurements are obtained - if peel and product properties have not changed in the meantime.

Due to the inactive phases of the 3rd filters, the buffer tank levels around them are inherently oscillatory, rendering automatic level control using proportional controllers infeasible (Bähner et al. (2018)). (Rapid level changes would lead to frequent significant flow rate adjustments and upset the evaporator.) Thus, operators are in charge of closing the mass balance, which they can as the residence time in the surge tanks is large enough to enable manual control. The evaporator flow rate is ultimately set in a feed-forward manner - which is also a form of propagating the front-end TPM flow rate downstream. This is possible as the liquid throughput is known with some accuracy. As a consequence, the operators must regulate both buffer tank levels using only one (the cumulative) pressure filtration flow rate. This under-actuated system is often feasible for long periods of time, and only rarely upstream or downstream flow rates need to be adjusted. Furthermore, if the buffer tank upstream of the 3rd filtration approaches overfill, an automatic override reduces inflow, shifting material upstream and thereby easing the workload on the pressure filters for some time. The interplay of manual and automatic control on the regulatory layer is indicated in figure 1. All in all, it seems that the automatic level control that can be implemented in a straightforward manner has been implemented. The structure of the regulatory layer is then as follows:

Quality / yield control:

- Manual feedback control based on chemometric inference leads to manipulation of extraction conditions (pH, temperature, seldom: duration or peel type)

Inventory control:

- Batch schedule is TPM, defines 1st filtration flow rate
- 1st buffer: aut. level control def. 2nd filter flow
- 2nd buffer: manual manipulation of 3rd filter flow, automatic override of 2nd filter flow
- 3rd buffer: manual manipulation of 3rd filter flow, manual override of liquid throughput (usually set as feed-forward guess) on evaporator

Step 6 & 7: Select Structure of Supervisory Control Layer and Structure of Optimization Layer (RTO)

As the decisions on both levels are taken by the same operators or engineers at low frequencies, a separation of the two levels does not seem adequate. The optimising adjustments that assure energy efficiency and yield have been discussed in the previous section. The structure of the layers could refer to, for example, the intervals at which stakeholders meet to evaluate, plan, and adjust operations, or an alignment of laboratory shifts and the production wheel. This is not necessarily an area where PWC is the most viable tool, but operations research and company-specific knowledge matter.

3.3 Discussion

The ambitions of this work were to identify existing shortcomings in the plantwide control structure, but also to understand whether this hybrid PWC framework can be applied sensibly in a bio-based production context. Clearly, the absence of a high-fidelity mathematical model with high information density is inconvenient in the plant analysis. Core issues of PWC (selection of controlled variables, input-output coupling) need to be addressed based on process understanding. Due to the decoupled dynamics (sequential arrangement of unit operations), this is possible. Overall, the analysis does not seem to indicate significant shortcomings in the control structure implemented by engineers through iterative ad-hoc adjustments. During the examination of throughput and inventory control strategies, aspects of feed-forward flow rate control, override-, and under-actuated inventory control are found. These are not often discussed in PWC literature, and it is interesting to point out that there seem to be no better obvious solutions.

Overall, the prevalence of transient states indicates that control-affine production planning could alleviate the burden on control system and operators. Furthermore, trying to match existing plant operations to the standardised functions in the the PWC framework helped in understanding plantwide operations in a more structured way. Therefore, as a turnout of this collaboration, a more consistent terminology within the company will in the future facilitate collaboration with process control consultants and researchers.

In the applied methodology, a handle for analysing / optimising batch-continuous interaction could not be identified. Furthermore, it appears that the (here essential) role of operators is paid little regard. While Rijnsdorp (1986) dedicates high relevance to operators in a plantwide context, many of the recent frameworks focus on models and algorithms - again, not without reasons (Downs (2012)). However, in a biochemical context, the terms multi-variable- and plantwide control cannot be used interchangeably. Instead, in a manual control context, economically optimal utilisation of on-site operators is an issue.

Piechottka and Hagenmeyer (2014) as industrial members (BASF) of the control engineering community, among many, point out a gap between process control research and practice. One reason for this might be that industrial processes are not organised in a form that encourages the application of PWC. If so, guidelines for a sustainable plant automation trajectory with a focus on enabling future plantwide optimisation should be helpful in closing the gap. Hopefully, this work raises the question whether this an issue that should be addressed by PWC researchers. Furthermore, it is not clear whether there should be a dedicated sub-category dealing with plantwide control of bio-based processes, acknowledging their particularities.

4. CONCLUSION

In any case, the above challenges and the lack of identified improvements raise the question whether academic plantwide control with a focus on integrated systems is a viable tool in the analysis and optimisation of bio-based processes. On the other hand, in an increasingly competitive global bioeconomy, restricting optimisation and engineering projects to unit operation level does not seem attractive - there is ambition to change on the industry side. Producers of biotechnological products tend to employ lean production specialists (or seek external consultants) rather than advanced- or plantwide control experts. As many bio-based production sites resemble those of the discrete industries for instance in scale, handling of raw materials and final product, or the amount of personnel on-site, this is not far fetched. On the other hand, the unit operations are often those found in classical chemical process industries, and the control system vendors are the same. Not lastly, advances in process analytical technology should enable more feedback control also in bio-based processes in the future. Therefore, there is opportunity both for industrial and academic researchers, but it seems that the roles are not yet clearly assigned, and that collaborations are rather uncommon.

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