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Chemical pulping

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Assessing the value of a diversified by-product portfolio to allow for increased production flexibility in pulp mills

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Abstract: This paper presents a model for design optimization of pulp mill steam utility systems subject to variations in energy prices and steam demands. A Scandinavian Kraft pulp mill is used as case study to investigate investment opportunities in lignin extraction and new turbines. The model enables solutions to be identified that are more flexible than the solutions that would have been identified with a corresponding model using, for example, annual average values for key input data. The results from the case study show that lignin extraction has a potential to contribute to flexibility in pulp mill electric power production under certain conditions provided that the mill invests in both lignin extraction and condensing turbine capacity. However, the potential electric power production flexibility will vary over time. In the studied mill, with a capacity increased to around 1.3 million tonnes/a of pulp, it is estimated to vary between 15 and 30 MW. Furthermore, investment in new condensing turbine capacity only seems to be attractive if electricity prices that are considerably higher than the spot prices of recent years are assumed. Such prices may occur if there is a clear value of tradable electricity certificates or if future electricity prices rise significantly.

Keywords: electricity generation; energy efficiency; flexibility; lignin extraction; steam utility system.

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Introduction

Conventional early-stage techno-economic assessments for screening of energy-related investment opportunities in pulp and paper mills typically consider only one or a few operating scenarios and fixed market prices for fuel, electricity, and mill products. For a traditional pulp or paper mill, which is operated continuously at a stable production rate close to its design capacity, this can be a reasonable approach given that the core operational objective is to maximize the quality and output of one single product.

Recently, the pulp and paper industry has started to shift business models due to the rising demand for sustainable biomass-based fuels and products, which is driven by renewable energy targets as well as increasing pressure on industry to make their processes more resource and energy efficient. Many pulp and paper mills are currently in the process of transforming into forest biorefineries, which, in addition to pulp and paper, also produce traditional energy by-products such as electricity and heat, as well as biofuels, biobased materials and chemicals (Moshkelani et al. 2013, de Blasio 2019). A number of studies have conducted comparative techno-economic assessments of such new technologies and processes (see e.g. Olsson et al. 2006, Benali et al. 2014, Lundberg et al. 2014, Mesfun et al. 2014, Mansoornejad et al. 2017, Akbari et al. 2018). However, the best investment option for valorizing the by-products of the pulp and paper industry will change as a consequence of variations in energy and product prices, policy instruments, etc.

One of the anticipated benefits of the biorefinery concept is that the diversified product portfolio will enable mill owners to respond to changes in product markets (Mansoornejad et al. 2012). Therefore, the value of technological options that provide such flexibility is assumed to increase. Considering the potential benefit of manufacturing flexibility, it could also be beneficial to invest in more than one technology to enable optimization of the product mix depending on the market situation. Svensson et al. (2015) surveyed existing literature on flexibility, controlla-

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bility and operational reliability related to biorefinery process design and also identified several reasons to better consider such operability aspects in early-stage screening of new biorefinery concepts.

One type of flexibility that is of special interest from an electricity system perspective is the potential demand side response of industrial plants on electric power markets (Alvehag et al. 2017). With increasing shares of intermittent electric power production capacity in the system, the demand for technologies that can supply balancing power to the grid is expected to grow. However, adjustments of pulp and paper mills' operation are typically slow. The potential for mills to take an active role on regulating power markets (typically requiring changes within 15 minutes of activation order) is therefore expected to be limited. However, the increasing need for grid services such as demandside flexibility will also be reflected through the day-ahead electricity spot market, which is expected to be characterized by larger price fluctuations in the future. For industrial plants that are able to adjust their operation to variations in the electricity spot price, this can provide a business opportunity.

A few previous studies have considered operational flexibility in decision models for energy systems of pulp and paper mills. Helin et al. (2017) investigated the economic potential of demand side management in a mechanical pulp and paper mill, assuming that the mill could execute power regulating bids by down-ramping of paper production. Their results indicated a notable capacity for demand side management, but with an estimated rational bidding price for regulating power that was significantly higher than the underlying spot price. In the model of Helin et al. the operation was optimized over a 24-hour period and consequently no investment opportunities or seasonal variations were considered. Furthermore, no demand variations were considered. Panuschka and Hofmann (2019) developed a method for flexibility management in a chemical pulp mill's co-generation system. Their model for optimization of plant operation included thermal energy storage units to allow for smoothening of steam demand peaks. Hourly variations in heat and electricity demand over an 8-day period were considered, but variations in energy prices and seasonal demand variations were not. Consequently, this type of model cannot be used to optimize investments in the pulp mill energy system. Siitonen and Ahtila (2010) studied the effect of fluctuating carbon prices on energy investments in a pulp and paper mill and showed that the economic value can be significant. However, Siitonen and Ahtila only considered variations in external market parameters and did not model process variations. Cakembergh-Mas et al. (2010) formulated a model for assessing the economic benefits of different retrofit projects in a Kraft pulp mill and considered monthly planning periods with varying steam demands and prices. However, their model only considered operating benefits of various predefined configurations. Capacities and investment costs of new equipment were calculated only after the optimization, and more short-term variations were not included.

An energy-efficient market Kraft pulp mill will typically have an excess of energy available from the combustion of black liquor. Policy incentives for renewable electricity production (Thollander and Ottosson 2008, Ericsson et al. 2011) have incentivized a number of market Kraft pulp mills in Scandinavia to invest in condensing steam turbines for generation of electric power. Alternative and competing technologies and process solutions are also receiving increasing interest. In a recent article, Akbari et al. (2018) compared different options for converting black liquor into value-added products, and found extraction of lignin as a product to be the most profitable pathway for a Canadian pulp mill. Various approaches have been proposed for extracting and valorizing the lignin from black liquor (see Hubbe et al. (2019) for a recent review). The LignoBoost process, in which lignin is precipitated from the black liquor by means of CO₂ acidification (Tomani 2010), is one of the most mature technologies for such lignin extraction, with experience from commercial-scale operation in two Kraft mills up to date (Björk et al. 2015, Wallmo et al. 2016). Lignin extraction could contribute to pulp and paper industry's opportunities for demand side response to variations in the electric power market (see e.g. Jannasch et al. 2019). By extracting more or less lignin, the steam production, and thereby the steam turbine power generation, can be adjusted to respond to changing electricity prices.

To determine whether the value of flexibility is high enough to motivate the cost of investing in two or more technologies (e.g. both lignin extraction and new turbines), it is necessary to properly model both design (investment) and operating decisions as well as variations in process and market conditions. This is also required to optimize the equipment size, in light of the variations. The design optimization problem for steam utility systems under varying steam demands is most commonly formulated as a multi-period, mixed-integer linear programming (MILP) model (see e.g. Maréchal and Kalitventzeff 2003, Shang and Kokossis 2005, Aguilar et al. 2007, Chen and Lin 2011, Sun et al. 2017). Our own previous studies (Svensson et al. 2014, Svensson 2014, 2015) showed that there can be a value in flexibility of certain investments in pulp mill energy systems, and that a multi-period modelling approach including investment as well as operating decisions is appropriate for being able to capture this value in the investment evaluation.

Our previous studies (Svensson 2014, 2015) adopted a mathematical model of a pulp mill's steam utility system as an example. This model did not represent an existing mill, and therefore no measurements were available for validation of equipment performance models, or for identifying the most important variations affecting the system. For the purpose of the study, the only variations considered were seasonal variations in steam demand, which were assumed to follow a smooth, continuous function representative of seasonal variations for the type of system studied. In reality, steam demand variations are due to a number of factors in addition to seasonal variations. These factors include differences in production rate, product campaigns, or ambient temperatures. Furthermore, such factors do not only affect the process steam demands, but also, e.g., the steam production in the recovery boiler. Market parameters such as electricity and biomass prices also vary over time, which has a significant impact on the optimal operation of the system.

The use of advanced modelling tools for considering variations in design of industrial energy systems is associated with a number of challenges when applied to real industrial cases. These challenges are related to data reliability, the wide range of sources of variations for which correlations are often difficult to identify, uncertainties in cost data, lack of documentation and technical specifications, as well as poor correspondence between literature models and measurement data. In the study presented in this paper, we applied the models developed in previous work to a real industrial case study. We developed the model to include more sources of variations and identified a number of necessary simplifications and developments to overcome the challenges mentioned above.

The aim of this paper is to further develop and adapt a model for design optimization of pulp mill steam utility systems for application to real industrial problems. The model is used to study how variations in energy prices and operating conditions affect investment decisions in a pulp mill's production of fuels and electricity and the mill owner's willingness to invest in additional operational flexibility. A modern and energy-efficient Scandinavian Kraft pulp mill is used as a case study. The investments considered are a new plant for lignin extraction and new steam turbines. Depending on the investment made, a potential energy surplus at the mill can be realised either as bark, lignin or electricity generation. The effects of variations are analysed by comparing the optimal investment when accounting for the varying conditions, with the optimal investment obtained when only considering a single operating and price scenario. By doing this, the paper also illustrates how and to what extent lignin extraction can contribute to pulp mills power generation flexibility in response to daily variations in the electricity market.

The case study mill

The mill studied in this work is a large Kraft pulp mill with an annual production capacity of 750 000 ADt (air dried tonnes) of pulp. The mill has one production line, which is operated in campaigns. Softwood campaigns of three weeks duration are followed by one-week hardwood campaigns, i. e., the mill produces approximately 75 % softwood pulp and 25 % hardwood pulp.

During normal operation, the steam generation in the recovery boiler is enough to cover not only the process demand of steam, but also to produce an excess of heat and power. The mill is a net exporter of electricity and delivers excess heat to the co-located sawmill and the local district heating network.

Over the years, significant efforts have been put into improving the pulping process of the mill, to improve the pulp quality and increase the production capacity. Additionally, the energy efficiency of the pulping process has also been continuously improved. For example, the mill has a very high degree of process heat recovery, and further measures have been proposed to increase the use of secondary heat for preheating of combustion air and feed water to the boilers. While pulp is still the core product, the mill has successively developed into a multi-product plant, with electricity sales contributing significantly to overall revenues. Consequently, it has become of greater interest for the pulping company to further improve their resource efficiency and develop a product portfolio that allows for maximizing the combined revenues from a variety of by-products.

The steam utility system

A simplified flow sheet of the mill's steam utility system is illustrated in Figure 1. The recovery boiler is the primary steam production unit. The steam production in the recovery boiler varies over time depending on variations in flow and heating value of the black liquor (see also Process data and capacity constraints for the pulp mill section). During



Figure 1: Simplified layout of the steam utility system of the case study mill. Condensate return and feedwater systems are omitted for clarity. Steam header pressures are approximate.

most operating conditions, the steam production from the recovery boiler would be sufficient for covering the process steam demand. However, to manage the steam balances of the mill in the presence of variations in steam supply from the recovery boiler as well as variations in process steam demand, a supplementary boiler fired with bark is also constantly in operation.

Lignin extraction

This study includes the possibility for the mill to invest in a lignin extraction plant. The extraction of lignin enables conversion of surplus energy from the wood raw material into a value-added product by removal of lignin from the black liquor in the evaporation plant via acid precipitation. Extracting lignin would provide the pulp mill with an opportunity to generate a new by-product that could potentially be used for various applications (Gellerstedt et al. 2013, Téguia et al. 2017). Previous work has also shown that lignin extraction may provide a great opportunity for indirectly increasing the flexibility of the pulp mill's utility system in response to steam demand variations (Svensson 2014, 2015). It does so by providing a way to adjust the load of the recovery boiler, thereby achieving a larger operating range for steam production that does not rely only on the limited capacity range of the bark boiler. Lignin extraction has also been shown to be of interest for debottlenecking the recovery boiler in case of a pulp production increase (Axelsson et al. 2006, Laaksometsä et al. 2009, Wallmo et al. 2009, Välimäki et al. 2010, Périn-Levasseur et al. 2011).

Production increase

The pulp mill company is investigating the opportunities for a strategic investment in a new production line, which would significantly increase the pulp production capacity. Different options for the pulp product of the new line are being investigated. We consider one of these options, where the new line extends the production capacity of one of the pulp products currently produced in the mill. However, all options are based on approximately the same increase in pulp production (about 80%). The decision about the production increase is based on a number of criteria, most of which are beyond the scope of this study. The design of the new production line, and the resulting mass and energy balances based on spreadsheet calculations made by a consultancy company, were therefore used as input to this study. With regards to the steam system, the new production line will affect mainly the amount of black liquor being processed and the demand for steam at 4 and 12 bar(a) (all of which will increase by approximately 80 % on average). In addition, a change is planned to replace the current use of high-pressure steam (61 bar(a)) for soot blowing by 27 bar(a) steam. When the black liquor heat flow increases as a result of the pulp production increase, the existing recovery boiler becomes a bottleneck. However, an older recovery boiler, that is currently not in operation, is still available at the mill, and is planned to be started up again in connection with the production increase. However, the two recovery boilers together are nevertheless insufficient to handle the entire black liquor flow during high production after the production increase. Therefore, a lignin extraction plant is planned as a debottlenecking option.

In this work, an optimization model is used to determine the optimal capacity of the lignin extraction plant, and the best investment in new turbine capacity given predefined changes of black liquor heat availability and process steam demands. It is assumed that the pulp production increase is given, and not affected by changes in the lignin extraction rate above that required for debottlenecking the recovery boiler. This is a reasonable assumption if. when increasing the lignin extraction so that the recovery boiler is no longer a bottleneck, other parts of the process such as the digester, evaporation or bleaching plants, also have limited capacity for further production increase. It is further assumed that if debottlenecking of the steam main pipelines is required, this is included in the given pulp production investment plan, and no further optimization is considered.

Optimization model

The optimization model used in this work is a multiperiod, mixed-integer linear programming (MILP) model. The MILP model is used to identify the optimal design decisions (capacity invested in lignin extraction and/or new turbines) considering an optimal response in steam production and turbines operation given the investments made and variations in prices and process steam demands.

The optimization model, which is described in the following sections, was developed from previous models, which were applied to model mill examples (Svensson 2014, 2015). However, the application of the optimization model to a real mill revealed some requirements for adjusting some parts of the model. The changes were made to consider additional operational constraints, to handle lack of or uncertainty in equipment performance data, and

to enable tuning of models to measured data. Furthermore, the possibility to turn boilers or turbines on or off on a dayto-day basis was excluded from the model after discussion with mill staff, who considered it technically and economically infeasible to start-up and shut down boilers, turbines and lignin extraction equipment for the purpose of operational optimization.

The objective of the optimization is to:

where the total investment costs *InvCost* are annualized by the capital recovery factor r, *BarkCost* represents the annual fuel costs for bark, *LigRev* the annual operational revenues from lignin extraction and *ElecRev* the annual revenues from electricity production. The objective is achieved by optimizing the investments, the steam production in the bark boiler, the lignin extraction rate and the steam flows through turbines.

Investment costs

The total investment costs *InvCost* may include investments in new turbines and a lignin extraction plant (Equation 2). The cost function $Cost_x(Y_x)$ for investment in equipment *x* is expressed by a piecewise linear function (in n linearization intervals) of the capacity, Y_x , of the equipment (Equation 3). $C_{inv,x}(i)$ is the investment cost at the *i*th breakpoint, of the piecewise linear function, $\overline{Y}_x(i)$, is the equipment capacity at that breakpoint, and $k_x(i)$ is the linear slope between $\overline{Y}_x(i)$ and $\overline{Y}_x(i+1)$. The binary variable z_x is 1 if investment is made in technology *x*, and 0 otherwise. If investment cost function, i. e. between starting point of the first linearization interval $\overline{Y}_x(1)$ and the end point of the last $\overline{Y}_x(n+1)$. This is given by Equation (4).

$$InvCost = \sum_{x} Cost_{x}(Y_{x})$$
⁽²⁾

$$Cost_{x}(Y_{x}) = \begin{cases} 0, & Y_{x} = 0 \\ C_{inv,x}(i) + k_{x}(i)(Y_{x} - \overline{Y}_{x}(i)), \\ \overline{Y}_{x}(i) \le Y_{x} < \overline{Y}_{x}(i+1), i \end{cases}$$
(3)

$$z_{\chi}\overline{Y}_{\chi}(1) \le Y_{\chi} \le z_{\chi}\overline{Y}_{\chi}(n+1)$$
(4)

Operational costs and revenues

The year is divided into time periods t, of duration d_t , which represent the total annual operating time of the mill.

BarkCost is the annual bark cost as a function of the bark price, $p_{bark,t}$, and use of bark as fuel in the bark boiler, $Q_{Bark,t}$, both of which may vary between the time periods *t* (Equation 5). Similarly, the annual lignin revenues, *LigRev*, associated with lignin extraction, $Q_{Lig,t}$, are a function of the lignin price $p_{lig,t}$ in different time periods (Equation 6).

$$BarkCost = \sum_{t} d_t p_{\text{bark},t} Q_{\text{Bark},t}$$
(5)

$$LigRev = \sum_{t} d_{t} p_{\text{lig},t} Q_{\text{Lig},t}$$
(6)

ElecRev represents the annual revenues from electricity production, $E_{\text{prod},t}$ (Equation 7). Electricity produced in the steam turbines, $E_{\text{prod},t}$ can either be used at the mill, thus leading to reduced purchase of electricity from the grid, or be sold to the grid. Variations in own consumption of electricity due to variations in boiler and turbine loads, e. g. air fans and steam condenser pumps, have been neglected. The same electricity price, $p_{el,t}$, is assumed for selling and purchasing electricity. The model could easily be adapted for differentiated purchase/sales prices if the mill electricity consumption is available with the time resolution of the model, by including an additional constraint for the electricity balances of the mill.

$$ElecRev = \sum_{t} d_{t} p_{el,t} E_{prod,t}$$
(7)

A share of the total electricity production is eligible for so-called green electricity certificates, which can be sold to generate additional revenues. However, the price for electricity certificates is assumed to drop significantly in the near future, and this revenue is therefore neglected in the base case. Appendix C describes the modelling of electricity certificates for an alternative scenario that assumes high prices of certificates.

The total electric power produced in the mill in a given time period, $E_{\text{prod},t}$, is given as the sum of electric power outputs, $E_{T,t}$, of all turbines *T* (Equation 8).

$$E_{\text{prod},t} = \sum_{T} E_{T,t} \tag{8}$$

Boiler operation, bark use and extraction of lignin

Part-load operation of boilers is represented by the use of marginal efficiencies that are estimated to be valid as long as the boiler load is kept above the minimum load limits set in the model. While boiler efficiencies typically decrease at part-load conditions, the marginal efficiencies (i. e. the change in steam production divided by the change in fuel input) are almost constant. However, the use of constant marginal boiler efficiencies is based on the assumptions that the minimum load of the bark boiler has been set to have an acceptable efficiency over its full range of operating conditions.

The bark use, $Q_{\text{Bark},t}$, is consequently given by the steam production in the bark boiler $M_{\text{BB},t}^{\text{prod}}$, the marginal boiler efficiency η_{BB} and the enthalpies of HP steam and feed water, h_1 and h_{fw} (Equation 9). (The steam headers are numbered $j = 1, 2, \ldots$, starting from the highest pressure.) Lignin extraction reduces the steam production in the recovery boiler, $M_{\text{RB},t}^{\text{prod}}$, from the reference steam production $M_{\text{RB},t}^{\text{ref}}$, which also varies between time periods, mainly due to variations in the flow and heating value of the black liquor fuelling the boiler. The lignin extraction $Q_{\text{Lig},t}$ is therefore a function of the resulting steam production reduction, the enthalpy increase over the boiler and the recovery boiler's marginal lignin efficiency, $\eta_{\text{RB}-\text{LIG}}$ (Equation 10). Part-load efficiency effects of the lignin extraction plant are assumed to be negligible.

$$Q_{\text{Bark},t} = (h_1 - h_{\text{FW}}) M_{\text{BB},t}^{\text{prod}} / \eta_{\text{BB}}$$
(9)

$$Q_{\text{Lig},t} = (h_1 - h_{\text{FW}}) \left(M_{\text{RB},t}^{\text{ref}} - M_{\text{RB},t}^{\text{prod}} \right) / \eta_{\text{RB-LIG}}$$
(10)

Previous model versions have included an opportunity to start and stop the bark boiler depending on the steam demand. However, according to mill personnel, the bark boiler is always required to be in operation for safety reasons. Consequently, both the recovery boiler and the bark boiler must always operate within the minimum and maximum load limits, here defined by the minimum and maximum steam production M_b^{min} and M_b^{max} (Equation 11).

$$M_{b,t}^{\min} \le M_{b,t}^{\text{prod}} \le M_{b,t}^{\max}$$
(11)

The lignin extraction, $Q_{\text{Lig},t}$, is, furthermore, limited by the available heat content of the black liquor, which is directly proportional to the reference steam production in the recovery boiler. The maximum lignin extraction can therefore be expressed as $\rho M_{\text{RB},t}^{\text{ref}}$, where ρ is a constant parameter (Equation 12). The lignin extraction is also limited by the capacity invested in the lignin extraction plant, Y_{LIG} (Equation 13).

$$0 \le Q_{\text{Lig},t} \le \rho M_{\text{RB},t}^{\text{ret}}$$
(12)

$$Q_{\text{Lig},t} \le Y_{LIG} \tag{13}$$

Turbine models

The turbine models are linear functions relating the power output $E_{T,t}$ of a turbine *T* in time period *t* to the steam

flow $M_{T,s,t}^{\text{turb}}$ through the turbine stages *s* (Equation 14). The power output is a function also of the maximum inlet steam flow to the turbine. For existing turbines, this maximum inlet flow, M_T^{max} , has a known value and can therefore be incorporated in a generic constant, $b_{T,0}(M_T^{\text{max}})$. However, for new turbines, the maximum inlet flow is a variable to be optimized, M_T^{cap} .

$$E_{T,t} = \sum_{s(T)} \mathbf{a}_{T,s} M_{T,s,t}^{\text{turb}} + \begin{cases} \mathbf{b}_{T,0} \mathbf{\gamma}_T & \text{if T existing turbine} \\ \mathbf{b}_{T,2} M_T^{\text{cap}} + \mathbf{b}_{T,1} & \text{else} \end{cases}$$
(14)

The estimation of parameters $a_{T,s}$, $b_{T,0}$, $b_{T,1}$ and $b_{T,2}$ is described in Appendix A, which also discusses the validation of the turbine model for existing turbines.

After discussion with mill staff, it was considered unrealistic to allow for turbines to be taken on and off operation in different time periods. However, the opportunity to replace existing turbines with new, more efficient ones, should be considered. Therefore, the model includes a variable y_T representing the option to permanently turn off existing turbines. If investments are made in new turbine capacity, these new turbines are assumed to always be in operation. If an existing turbine is kept in operation, the binary variable γ_T takes the value one. Equation (15) then ensures that the inlet steam flow is kept between minimum and maximum flow limits, where the parameter μ_{T}^{\min} defines the minimum inlet flow to a turbine as a fraction of the maximum inlet flow. A corresponding constraint for new turbines is given by Equation (16). If, instead, an existing turbine is taken off operation, the variable y_T takes a zero value, which sets the inlet steam flow to zero according to Equation (15), and thereby the power output of the turbine is also zero as given by Equation (14).

$$\mu_T^{\min} \gamma_T M_T^{\max} \le M_{T,1,t}^{\text{turb}} \le \gamma_T M_T^{\max} \quad \text{for existing turbines T}$$
(15)

$$\mu_T^{\min} M_T^{\operatorname{cap}} \le M_{T,1,t}^{\operatorname{turb}} \le M_T^{\operatorname{cap}} \quad \text{for new turbines T}$$
(16)

Finally, some constraints are added to represent maximum turbine extraction flows and maximum power output. The extraction steam flow after turbine stage s(T) of turbine T, $M_{T,s,t}^{\text{ext}}$ is given by Equation (17). For existing turbines, the steam extraction is limited by a maximum extraction flow, $M_{T,s}^{\text{maxext}}$ according to Equation (18). Corresponding constraints for maximum extraction flows of new turbines are not included. Since the maximum extraction flow should depend on the size of the installed turbine capacity, it cannot be a fixed parameter. However, to include it as a variable would not make any sense as long as there is not any cost associated with increasing its value. Instead, for new turbines, the maximum power output, $E_{T,t}$, is limited by a design capacity, E_T^{max} (Equation 19), which in turn is used to determine the turbine capacity used in the investment cost function, see further below.

$$M_{T,s,t}^{\text{ext}} = \begin{cases} M_{T,s,t}^{\text{turb}} & \text{if } s(T) \text{ last turbine stage} \\ M_{T,s,t}^{\text{turb}} - M_{T,s+1,t}^{\text{turb}} & \text{else} \end{cases}$$
(17)

 $M_{T,s,t}^{\text{ext}} \le \mathbf{M}_{T,s}^{\text{maxext}}$ for existing turbines T (18)

$$E_{T,t} \le E_T^{\max}$$
 for new turbinesT (19)

In order for the linear formulation of the turbine model (Equation 14) to hold with fixed coefficients, a turbine *T* should be either a back-pressure extraction turbine or a low-pressure condensing turbine. In principle, a wide variety of different combinations of back-pressure and condensing turbines, which inlets and extractions connected to different headers can be considered. While the above turbine constraints are generic, some more specific constraints are needed to describe the investment opportunities for specific new turbines in the mill. For the case study three main alternatives for new turbine investments were considered, namely:

- TURB1: A back-pressure extraction turbine (BPETa) with extractions at header 27, 12 and 4 bar(a).
- TURB2: A low-pressure condensing turbine (LPCTa)
- TURB3: A combined turbine with inlet at the high-pressure steam header (header 1), extractions at header 27, 12 and 4 bar(a), and a condensing tail. This is modelled as a combination of a 3-stage back-pressure extraction turbine (BPETb) and a low-pressure condensing turbine (LPCTb).

Additional constraints (Equations 20–22) are added to relate the maximum power output of individual turbines to turbine capacities used in the investment cost function. In practice, TURB3 is modelled as two separate turbines according to Equations (14–19) above, with a constraint that limits the inlet flow to the condensing stage to be less than or equal to the outlet flow from the last stage of the highpressure section of the turbine (Equation 23).

$$E_{BPETa}^{max} \le Y_{TURB1} \tag{20}$$

$$E_{LPCTa}^{max} \le Y_{TURB2} \tag{21}$$

$$E_{BPETb}^{max} + E_{LPCTb}^{max} \le Y_{TURB3}$$
(22)

$$M_{LPCTh1t}^{turb} \le M_{BPETh3t}^{turb} \tag{23}$$

Mass and energy balances

The steam header data are assumed to be constant and not optimized by the model. The steam headers are numbered

j = 1, 2, ..., starting from the highest pressure. Mass balances for steam pressure headers *j* are formulated in Equations (24)–(26). $M_{T,s,t}^{\text{turb}}$, $M_{v,t}^{\text{vlv}}$ and M_t^{vent} denote the steam flows through the turbine stages s(T), expansion valves *v* and atmospheric vent, respectively; the notation *in*() and *out*(), refers to the inlet and outlet headers of turbines, turbine stages and valves, as relevant, and is used to mark subsets of turbines, turbine stages and valves, for which the steam flows should be included in the mass balances for a certain header. $M_{j,t}^{\text{proc}}$ denotes the process steam demands and $M_{j,t}^{\text{qw}}$ denotes quench water added for saturation purposes to steam header *j*.

The mass balances, as formulated in Equations (24–25), are not mill-specific, but still not fully generic. In particular, it is assumed that turbines may only have inlets at the highest-pressure steam header or the lowest-pressure steam header, and the atmospheric vents are only placed at the lowest pressure header. However, the mass balances can be used to represent any number of steam headers, valves and turbines, with inlets and outlets of valves and outlets of turbines at any header.

The process steam demands, $M_{i,t}^{\text{proc}}$, are calculated according to Equation (26). The reference steam demand, $M_{i,t}^{\text{proc, ref}}$, represents the steam demands of the mill if no lignin extraction or new condensing turbine is implemented, i.e. the reference demands that are not affected by investments or operating changes in the steam utility system as optimized by the model. For the production increase scenario, this reference steam demand is given by the estimated future process steam demand. If lignin is extracted, washing water used in the lignin extraction process is returned to the evaporation plant, causing an increased steam demand there to evaporate the added water. Therefore, in the model, a low-pressure steam demand is added to the reference steam demand if lignin is extracted, which depends on the lignin extraction rate Q_t^{Lig} and the specific increase in low-pressure steam flow per MW lignin extracted, σ . The potential effect of increased condensate flows to the feedwater system due to this steam demand increase is neglected. However, there will also be an increase in steam demand for condensate heating if the steam flow through condensing turbines, $M_{T,s,t}^{\text{turb}}$, is increased compared to the reference turbine condensate flow, M_t^{refcond} . The enthalpies, h_{fw} , h_{cw} , h_j , refer to the enthalpies of feed water, condensate water and steam at header j.

$$M_{\text{RB},t}^{\text{prod}} + M_{\text{BB},t}^{\text{prod}} = M_{1,t}^{\text{proc}} + \sum_{\substack{T:in(T)=1\\T;in(T)=1}} M_{T,1,t}^{\text{turb}} + \sum_{\substack{v:in(v)=1\\v;in(v)=j}} M_{v,t}^{\text{vlv}} \quad (24)$$

$$\sum_{\substack{T,s(T):\\out(s)=j}} M_{T,s,t}^{\text{ext}} + \sum_{\substack{v:\\out(v)=j}} M_{v,t}^{\text{vlv}} + M_{j,t}^{\text{qw}}$$

$$= M_{j,t}^{\text{proc}} + \begin{cases} \sum_{\substack{V:\\ in(V)=j\\T:\\in(T)=j}} M_{T,s,t}^{\text{turb}} & j = 2, \dots, j_{\text{max}} - 1\\ \sum_{\substack{T:\\ in(T)=j}} M_{T,s,t}^{\text{turb}} + M_t^{\text{vent}} & j = j_{\text{max}} \end{cases}$$
(25)
$$M_{j,t}^{\text{proc}} = M_{j,t}^{\text{proc}, \text{ref}} \\ + \begin{cases} 0 & \text{if } j < j_{\text{max}} \\ \sigma Q_t^{\text{Lig}} + \left(\sum_{\substack{T,s(T):\\out(s)=cw}} M_{T,s,t}^{\text{turb}} - M_t^{\text{refcond}}\right) \frac{(h_{\text{fw}} - h_{cw})}{(h_6 - h_{\text{fw}})} & \text{else} \end{cases}$$
(26)

Some process steam demands, such as steam used for feed water pre-heating, vary with boiler load. This boiler load-dependency has been neglected in the model (see Model simplifications and development needs section for a discussion about this simplification).

Energy balances for steam headers are given by Equation (27), where $h_{T,s}^{ext}$ represents the estimated enthalpy of the extraction flow from a turbine stage. In reality, this will vary with the steam flow through the turbine stage, but to keep the linearity of the model, a constant estimated value is applied.

$$\sum_{v:out(v)=j} M_{v,t}^{vlv} \mathbf{h}_{in(v)} + \sum_{\substack{T,s(T):\\out(s)=j}} M_{T,s,t}^{ext} \mathbf{h}_{T,s}^{ext} + M_{j,t}^{qw} \mathbf{h}_{qw}$$
$$= \left(\sum_{v:out(v)=j} M_{v,t}^{vlv} + \sum_{\substack{T,s(T):\\out(s)=j}} M_{T,s,t}^{ext} + M_{j,t}^{qw}\right) \mathbf{h}_{j} \quad j > 1$$
(27)

Model input data for the case study

The model was run with 352 time periods of 24 hours. The remaining days of the year were excluded due to production maintenance stop or disturbances with the assumption that any operating costs or revenues related to fuel use or electricity production could be neglected.

Process data and capacity constraints for the pulp mill

Data for steam production and consumption at the mill was collected from the mill's data information system. However, not all steam flows are measured and, consequently, some steam demands were calculated from mass and energy balances.

The heat content of black liquor fuelling the recovery boiler varies over time. The main causes of this variation



Figure 2: Reference steam production in the recovery boiler (RB) and process steam consumption at different pressure levels. Daily averages according to measurements 2017. Days which deviate significantly from normal operation are excluded.

are the different raw material campaigns, which lead to different compositions of the black liquor, and variations in the pulp production rate. The operation of the recovery boiler is determined by the need to process black liquor for regeneration of cooking chemicals. The steam production therefore varies according to the variations in flow and heating value of the black liquor (see Figure 2).

Figure 2 also illustrates the variations in steam demand. For the low-pressure (4 bar(a)) steam demand a slight seasonal variation can be noticed in addition to the day-to-day variations. The demand as well as magnitude of variations are much lower for other steam pressures.

As a source of data for the prospective new mill with the new pulp production line, mass and energy balances were available for four different operating scenarios. However, data for day-to-day variations were not available. Since current variations in steam production and consumption are due to a large extent to changes between hardwood and softwood campaigns, and the new production line will operate only on softwood, it is not reasonable to scale up current variations to the new production level. Instead, and partly due to lack of other information, we chose to neglect any potential new variations in operation above those already occurring at the mill. Consequently, the production increase was modelled by adding a constant demand of steam at the steam pressures needed for the new production line and a constant increase in black liquor heat flow to the recovery boilers (see Production increase section).

More input data for the pulp mill is presented in the Appendix section. This includes, e.g., performance data for turbines (Appendix A) and boilers etc. (Appendix B).

Investment costs

The investment cost data used in the model is presented in Appendix B, Table B.1. This includes the investment costs for turbines and the investment cost for the lignin extraction plant. Cost functions for turbine investments are based on literature (Axelsson et al. 2006) and updated using the Chemical Engineering Plant Cost Index (CEPCI). However, the investment cost function for lignin extraction from the same literature source is more uncertain, since it was estimated at an early stage of technology development before the first actual commercial-scale investments were made. In this analysis, the cost function based on Axelsson et al. (2006) was therefore updated using CEPCI and thereafter adopted using a cost-correction multiplication factor of three. This was based on more recent indications from industry, ongoing research projects and press releases from the first commercial plants (Stora Enso 2013), all of which indicate that there are reasons to expect the investment cost to be substantially higher than suggested by the early estimations.

Energy market data

It was assumed in this study that the mill will continue to have a positive bark balance in all scenarios studied. This means that the mill will continue to export bark, and not have to purchase any additional wood fuel for operation of the bark boiler. We assumed a sales price of bark that is about 20% lower than the market price of wood by-products in Sweden during 2018 (16 €/MWh (Swedish Energy Agency 2019a)). In practice, the price for selling bark varies over the year, mainly due to variations in the demand for solid biofuels for heating purposes in Sweden. The price can be as low as 10 % of the market price of higher quality wood by-products during extreme periods. However, it is possible to store bark for short periods of a few weeks. It was therefore assumed that during periods of low market demands, the bark storage is filled, to allow for selling the bark at a higher price once the demand increases again (see also Uncertainty in market parameters and costs section).

Lignin was considered to be valued higher than wood fuels, due to its potentially more valuable uses, for example as a raw material for production of biofuels, materials and chemicals (Gellerstedt et al. 2013, Téguia et al. 2017). Instead of explicitly modelling the direct operating costs for chemicals and electricity consumption in the lignin extraction plant, a net operating margin (= lignin price - operating costs for electricity, CO₂ and chemicals) was used. As a reference case, this operating margin was assumed to be 20 €/MWh, implying that the lignin needs to be sold for a somewhat higher price to be able to cover operating expenditures and still make the operating margin of 20 €/MWh. For comparison, the assumed lignin operating margin of 20 €/MWh is about 25% higher than prices for wood fuels in Sweden 2019 (Swedish Energy Agency 2019a) and in the lower range of estimated future willingness-to-pay for biomass (Pettersson et al. 2020). Note that changes in steam and power production due to lignin extraction are explicitly included in the model and therefore not reflected in the lignin value. Neither is the value of the potential for pulp production increase captured in this value. This follows from the assumption that the pulp production is given, and not affected by variations of the lignin extraction rate.

For electricity prices, the reference price variation profile was determined based on daily average prices from the NordPool spot market (price area SE4) for the year 2017. However, the spot prices were relatively low during 2017. To construct alternative price profiles, new electricity generation capacity at the mill was assumed to be eligible for green electricity certificates (Swedish Energy Agency 2019b) (see Appendix C for more information) and the higher electricity spot prices and certificate prices from 2018 were applied. Note that the price of green electricity certificates is expected to drop significantly in the near future (Energimyndigheten 2018) which is why revenues from sales of certificates were not included in the standard model and base case price profile. The different price profiles considered are shown in Figure 3.

Results

Model validation

The model was validated for current operating conditions by running the optimization with data for 2017, a constraint that sets all investments to zero, and constraints that fix the bark boiler steam production to the measured values for the same year. Since the recovery boiler steam production is fixed by default, the total steam production and process steam demands are then given, implying that the electricity production calculated by the model can be expected to be close to the measured electricity production. Figure 4 shows the calculated and measured electricity production.

The small deviations that are shown between measured and calculated electricity production can be explained by the following arguments:

- The model optimizes the distribution of steam between the different turbines and assumes no unnecessary steam flow through let-down valves. In reality, the turbines might not be operated optimally, and some let-down valves might be open.
- The model uses daily average values for the steam flows. In reality, the steam flows might vary significantly during a day. The non-linear relation between turbine efficiencies and steam flow might then cause a different average efficiency compared to what is estimated in the model.
- Measurement errors could be an additional source of deviations.

Overall, however, the model was judged to perform satisfactorily, considering especially the limitations to accuracy set by using daily average values (Mean Square Error = 10 MW^2 , $\text{R}^2 = 0.94$). The modelled and measured total electricity generation summed over all time periods considered differ by less than 2%.



Figure 3: Daily electricity prices during 2017 and 2018. Prices from the NordPool spot market (SE4). In one series, the monthly spot close price for green electricity certificates is added to the electricity spot price. Sources: (Nord Pool 2017, 2018, Swedish Energy Agency 2018).



Figure 4: Model validation. Calculated and measured total electric power generation.

Optimal investments for current pulp production

First, the model was run with data representing pulp production levels and market prices of 2017. For this case, the investment cost for lignin extraction is too high in relation to the value of lignin and no investment is proposed by the model. Furthermore, the relatively low electricity prices in 2017 favours a reduced use of bark over electricity production, which causes the model to set the bark boiler operation at minimum load for most of the time, providing no incentives for investments in new turbines. When the bark boiler is at minimum load, the large variations in steam production from the recovery boiler due to shifting wood campaigns end up in the existing condensing turbine (T6), see Figure 5.



Figure 5: Optimized electric power generation in existing turbines. Current operation of the mill.



Figure 6: Comparison between optimized and measured steam production in the bark boiler for the reference case representing current operation of the mill.

In reality, the bark boiler was operated well above the minimum load from March to August, as seen in Figure 6, while the model suggests minimizing the bark use during those months. Currently, no optimization-based decision support system is used at the mill for operating decisions in the steam boiler and turbine system. However, fuel and electricity prices are monitored continuously, and general relations between bark boiler and turbine loads are used together with rules-of-thumb to guide operational planning. According to mill personnel, the actual operation of the bark boiler (and condensing turbine) is at least partly explained by a low demand for bark on the biofuel market during the summer period, which together with difficulties associated with storing bark makes it better to combust the



Figure 7: Optimized electricity generation, lignin extraction and bark use for the mill after the production increase and optimized investment in lignin extraction.

bark on-site (see also discussion in Uncertainty in market parameters and costs section).

Production capacity increase

Validation of required lignin extraction capacity

The model for the production increase was first solved for four time periods representing different characteristic mill operating scenarios (softwood/hardwood campaigns and summer/winter conditions). For these four scenarios, detailed energy balances were calculated for the mill with a new prospective production line. The result obtained by the model was that the production increase requires a minimum lignin extraction rate of approximately 55 000 tonnes/year for debottlenecking of the recovery boiler. This is a little lower than the lignin extraction capacity assumed for the prospective new line's energy balances (60 000 tonnes/year). However, the prospected energy balances are not optimized and it is reasonable to assume that the prospected capacity is somewhat over-dimensioned. Furthermore, at least one of the scenarios include quite substantial direct reductions of steam through let-down valves in the energy balances, which can be completely avoided if steam flows are optimized through the turbines. Overall, the model results compare very well with the detailed energy balances and were thus considered reliable enough for further assessments.

Production increase – Reference case

This case applies the same basic assumptions as for the case of current pulp production, but adds increases in steam demands and black liquor heat representing the operation of a new production line (see Production increase section). Mill operating conditions were assumed to vary according to data from 2017, and market prices for 2017 were assumed.

Figure 7 shows the optimized lignin extraction, electricity generation and bark use over the year. Due to low electricity prices, relatively high lignin prices, and the requirement to invest in at least a small lignin extraction plant, this scenario strongly favours the investment in lignin extraction. This results in a solution with investment in a 209 MW lignin extraction plant, corresponding to a lignin extraction capacity of approximately 258 000 tonnes/year. This is more than four times the prospected capacity of 60 000 tonnes/year. Investment is also made in a new 37.5 MW back-pressure turbine.

With this huge capacity of the lignin extraction plant, the extraction rates become limited by the available black liquor flow and the assumed maximum lignin removal from black liquor as specified by Equation (12). This means that care must be taken about the uncertainty in this limit to ensure that stable recovery boiler operation can be maintained. Nevertheless, according to the model, most days of the year, the lignin extraction is maximized, either



Figure 8: Optimized operation of new back-pressure turbine and steam vent resulting from shutting down the condensing turbine. Production increase scenario with investment in a huge lignin extraction plant.

against the capacity of the lignin extraction plant (Equation 13) or against the available black liquor flow (Equation 12). Similarly, the bark boiler load is also typically minimized. This means that the total steam production is minimized, which leaves very little or no excess of steam for condensing power production. As a result, the model shuts down the existing condensing turbine in order to maintain the high lignin extraction rates while avoiding operating the turbine at too low loads. Note that the model does not allow for on/off operation of the turbines, i. e., the turbine must either always be on, or always off.

As a consequence of shutting down the condensing turbine, there will be significant amounts of steam vented to atmosphere during certain periods (see Figure 8). However, in some periods, depending on the operating conditions, the minimum steam production is not sufficient for covering the process steam demands. In these periods, the load of the bark boiler is increased, and if this is not sufficient, the lignin extraction rate must be reduced to allow for more steam production in the recovery boiler.

Production increase – Higher electricity prices

The results above indicate that with the applied assumptions there is little value in generating electric power in a condensing steam turbine considering that not even the existing condensing turbine is utilized. However, electricity prices were low during 2017. To analyze the effect of the electricity price the model was run with electricity prices from 2018. Here, we also included the 2018 prices of tradable green electricity certificates for any electricity generation above the currently established normal year production (see Appendix C). Note that the price level for certificates observed in 2018 are not expected to be representative of future values. Nevertheless, these were included to simulate a price scenario with significantly larger price variations over the year.

In this case, electricity production is strongly favoured over lignin extraction. The optimal investment in lignin extraction is at the minimum capacity required for debottlenecking the recovery boilers (39.2 MW) and investment are made in both a new back-pressure turbine (50.9 MW) and in a new low-pressure condensing turbine (16.5 MW). A clear trend can be seen over the year with increasing electricity production and decreasing lignin extraction rates due to increasing electricity prices (see Figure 9). In particular, the price of tradable green certificates increased substantially during the second half of the year (see Figure 4). Lignin extraction even goes down to zero in periods when no debottlenecking is required, typically, during hardwood campaigns when the black liquor heating value is lower.

These results represent an especially interesting case for two reasons. Firstly, during the second half of the year, operation of the lignin extraction plant contributes to



Figure 9: Optimized electricity generation, lignin extraction and bark use for the mill after the production increase and optimized investment in lignin extraction plant assuming a low investment cost for lignin extraction and electricity prices from 2018.

adapting the mill electricity production to electricity price variations. The variations in lignin extraction are not explained directly by electricity price variations, but above a certain electricity price, lignin extraction is no longer kept constant at maximum rate. In fact, the lignin extraction rate is reduced at high electricity prices, either until the point where no more steam can be accommodated by the condensing turbines, or until the minimum needed for debottlenecking the recovery boiler is reached. Secondly, since the optimal operation varies over the year, the investment decision needs to be optimized to obtain the flexibility to respond to market variations. Therefore, the capacity of 39.2 MW for lignin extraction is required even if the annual production of lignin reaches only 28.5 MW. This scenario is therefore a good example of when a simpler model assuming annual averages would not have been able to predict the value of investing in larger new steam turbines in combination with the investment in lignin extraction.

Power generation flexibility to varying electricity prices

The results presented above (for the scenario with production increase and 2018 prices) indicates that under certain conditions it could be profitable for a mill to invest in steam turbines for condensing power generation even if also investing in the lignin extraction plant. This way the mill gets increased flexibility to steer energy production towards either biofuels or electricity, depending on the market prices. It should be recognized that these operational adjustments are likely to be slow, and that this flexibility is probably only obtained for variations on hourly to daily scale.

Some of the variations in electricity generation given by the model are due to variations in electricity prices, but the variations in electricity generation are also a result of varying process conditions. To estimate the magnitude of the power generation flexibility for the mill if it invests in a lignin extraction plant and a new low-pressure condensing turbine, the model was solved with fixed investments according to the solution presented in Production increase - higher electricity prices section, i.e., investment in a 39.2 MW lignin extraction plant, a 50.9 MW back-pressure turbine and a 16.5 MW low-pressure condensing turbine. The model was then solved once with a constant high electricity price, and once with a constant low electricity price. This way, two distinct operating modes were simulated, one in which fuel use is minimized given the investments made (by maximizing lignin extraction and minimizing the load of bark boiler), and one in which electricity generation is maximized. The resulting electric power generation over the year is shown in Figure 10.

The difference in electric power generation between the two operating modes in Figure 10 would be the potential production flexibility given this investment package.



Figure 10: Resulting optimized electric power generation for a given investment (39.2 MW lignin extraction capacity, 50.9 MW back-pressure turbine, 16.5 MW low-pressure condensing turbine) assuming a constant, high electricity price (max electric power generation) or a constant, low electricity price (max lignin extraction).



Figure 11: Load-duration curve of potential power generation flexibility for a given investment (39.2 MW lignin extraction capacity, 50.9 MW back-pressure turbine, 16.5 MW low-pressure condensing turbine), calculated as the difference in electric power generation between an operating mode with maximized electricity production and an operating mode with maximized lignin extraction and minimized load of the bark boiler.

To highlight the distance between the two curves, the difference in electric power generation is plotted and sorted according to magnitude in a load-duration curve, see Figure 11. Figure 11 shows that the potential power generation varies between approximately 15 and 30 MW, and that it is above 20 MW for about 3/4 of the year.

Influence of variations on optimal solution

Could the results presented above have been obtained by a simpler investment model accounting only for annual average process conditions and market prices? For some of the scenarios this is likely. However, whether the variations influence the results or not depends on a number of different parameters and assumptions and it is difficult to predict a-priori if the more advanced model proposed in this paper will give a different result than a single-period model.

To illustrate the differences that can result from using this model compared to a single-period model, a few scenarios with different combinations of lignin and electricity prices were investigated in some more detail. For every such scenario, the multi-period model was solved, as well as the corresponding single-period model using annual average process data. The solutions obtained were compared with regards to optimized lignin extraction capacity, optimized new turbine capacity, and annual bark use, lignin extraction and electricity generation. The results are shown in Table 1.

In the price scenarios with higher lignin prices and electricity prices from 2017, the annual-average model identifies a lignin extraction capacity and an annual electricity production that are similar to the results from the multi-period model. The single-period model does slightly underestimate the new turbine capacity required to reach

		Multi-p	eriod mo	odel			Single	period a	nnual av	verages		Single- minimu extract	period a um investion	nnual av tment in	verages I lignin	with
Electricity price After the second s	//EDR	E Lignin extraction capacity	ス Annual lignin extraction	ର S Annual bark use	 New turbine capacity 	S Annual electricity production	E Lignin extraction capacity	것 Annual lignin extraction	A Annual bark use	 New turbine capacity 	S Annual electricity production	E Lignin extraction capacity	な Annual lignin extraction	A Annual bark use	 New turbine capacity 	A Annual electricity production
icui	MWh		A	01111		01111		A	01111				A	01111		01111
2017	15	39.2	48.0	336	39.1	1295	0	0	530	45.8	1426	39.2	48.3	329	35.2	1314
(no cert)	20	209.3	247.6	407.4	37.5	893	202.3	249.1	329	33.6	887	202.3	249.1	329	33.6	887
	25	210.4	248.0	407.5	37.4	892	202.3	249.1	329	33.6	887	202.3	249.1	329	33.6	887
2018	15	39.2	18.9	761	72.2	1521	0	0	823	64.4	1583	39.2	0	823	64.4	1583
(incl cert)	20	39.2	35.1	758	67.4	1482	0	0	823	64.4	1583	39.2	48.3	823	50.9	1469
	25	134.4	159.4	760	37	1189	0	0	823	64.4	1583	82.8	102	823	35.9	1342

Table 1: Comparison of optimization results for multi-period and single-period models under different price scenarios.

this annual electricity production. However, the most notable difference between the single-period and multiperiod model results in these two scenarios is that the bark use is significantly underestimated. In the multi-period model, the bark boiler load is used to cover steam deficits in time periods when the recovery boiler steam production is low compared to the steam demand while in other time periods, steam is produced in excess and vented. In the single-period annual average model, on the other hand, the bark boiler operation can be exactly matched to balance the constant recovery boiler steam production and process steam demands and no heat is lost for venting.

Table 1 also shows that the single-period model fails to capture the required capacity for lignin extraction for off-loading the recovery boiler. By averaging the heat flow to the recovery boilers over softwood and hardwood campaigns, the available recovery boiler capacity is falsely determined to be sufficient. Consequently, the optimum lignin extraction capacity is determined to be 0 MW for several scenarios using the single-period model. To improve the quality of the solution from the single-period model, it was also solved with an additional constraint requiring that the capacity of the lignin extraction plant should be greater than or equal to 39.2 MW. The resulting solutions are shown in Table 1. However, with this constraint, the single-period model instead underestimates the turbine capacity required to reach a certain annual electricity production. Note especially that the condensing turbine investment is overlooked in the 2018 scenario with 20 EUR/MWh lignin price. Furthermore, this model cannot reliably predict the annual lignin extraction given a certain lignin extraction capacity, which is particularly apparent in the 2018 scenario with 15 EUR/MWh lignin price, where the annual lignin extraction is zero despite the forced investment.

Discussion

Uncertainty in market parameters and costs

No detailed assessment of the bark balances was made in this study. The use of bark as fuel in the bark boiler was simply associated with an alternative cost representing the lost sales of bark on the fuel market. After optimization, we checked that the resulting bark use can be covered by the bark available (roughly estimated) at the mill. As mentioned in Energy market data section, the price for selling bark is characterized by significant seasonal variations, since the bark is mainly used for heating purposes, and the demand therefore varies significantly with the outdoor temperature. In our model it is assumed that bark can be stored at the mill site, to allow for sales at a higher price level. However, while bark can be stored for short periods of up to a few weeks, there are challenges associated



Figure 12: Electricity price duration curves for current (solid line) and possible future conditions in 2030, 2040 and 2050 (dashed lines). Current electricity prices refer to spot prices for Swedish price area SE4 for year 2018. Future prices represent modelled scenarios for the short-term marginal electricity generation cost for the same price area in different years assuming strategic collaboration between sectors. Data is extracted from results generated using the model presented in Göransson et al. (2019).

with longer storage such as risk of self-ignition. In reality, there might therefore be incentives for burning bark at the mill instead of storing it when the demand is low. This could, for example, be part of the explanation for the results shown in Figure 6. Currently, effects related to varying bark demand, bark balances and storage are not captured in the model. Possible developments could be explicit modelling of bark generation and storage capacity, or a price model representing the seasonal demand variations, or a constraint representing different maximum bark exports during different time periods.

The market for lignin is also highly uncertain. The value of lignin could range from its fuel value to significantly higher values, especially in potential future applications. However, the latter might also require additional investments at the mill for further processing of the lignin. Depending on the application considered, and the corresponding assumed value of lignin, the market demand will also be different. In our model runs, we have tried different values of lignin, but in this article, we have not shown any results from these sensitivity analyses. The assumed lignin value is quite high for a wood fuel, but not very much higher. However, even with this modest lignin value, a very large lignin extraction capacity (209 MW), which corresponds closely with the assumed maximum lignin removal from black liquor, is identified as the optimal solution for the production increase (see Production increase – Reference case section). A more important uncertainty with regards to the lignin extraction investment is the capital cost, which has a strong influence on the optimal solution. In our model, an increase of this investment cost would quickly lead to results where the lignin extraction capacity is simply minimized.

It should be noted that without investment in a lowpressure condensing steam turbine, the possibility for flexible electricity production is drastically reduced. The electricity production in the back-pressure turbines is closely connected to the process steam demand and not flexible in the same way. With the electricity prices assumed in this work, investment in a low-pressure condensing turbine is, however, only favourable if rather high prices are assumed for green electricity certificates. Considering that prices of such certificates are expected to drop significantly in the near future, the power generation flexibility of pulp mills might not become very pronounced after all. Nevertheless, the mill is considering investment in a condensing turbine. Such a decision could be explained by the large uncertainties related to investment in lignin extraction, in combination with the above discussed difficulties to sell excess bark. The investment cost assumed for the condensing turbine in the model may also differ from the costs assumed by the pulping company.

The spot price for electricity can also be expected to change in the future. In Figure 12, the daily average elec-

tricity spot prices from 2018 are plotted as a price duration curve, which is compared to examples of possible future scenarios for short-term marginal electricity generation costs based on models developed by Göransson et al. (2019) with a 3 hour resolution. In the future scenarios, the shares of intermittent electric power generation from solar and wind increase due to successively more stringent targets on greenhouse gas emissions as well as an assumed cost reduction for wind and solar power plants. This leads to more hours with low prices (when it is windy and/or sunny), but also to higher prices when the capacity is limited. For these particular scenarios, it was assumed that there will be strategic collaboration between the electric power generation sector, an electrified steel plant, the electrified transport sector in the form of passenger electric vehicles, and residential heat supply, which enables severe price peaks to be avoided.

Based on our results, the pulp mill will only exploit operational flexibility towards the electricity market if the prices are high enough during a sufficient length of time to motivate investment in a condensing turbine and also low enough during a sufficient length of time to not simply maximize the utilization of that turbine capacity throughout the year. Figure 12 indicates that in 2030, the price between approximately 1000 and 4000 hours is estimated to be at a similar level to the prices of 2018, which were used in our model. However, for about half of the hours of the year (4000 hours and above), the prices are estimated to be notably lower, which means that it will be less attractive for the mill to invest in a condensing turbine. Admittedly, the price peaks are also higher in the 2030 scenario, but only during a limited number of time periods, and are therefore not expected to significantly increase the willingness to invest in electric power generation capacity in the mill. The scenarios for 2040 and especially 2050, involve many hours (>3000) of prices that are significantly higher than the prices of today, while also showing many hours of low (and very low) prices. Under such conditions, the high price periods might motivate investment in a condensing turbine, while the low price periods would favour lignin extraction.

No optimization runs were performed for the future price scenarios. Such a long-term perspective would require reconsidering a number of other assumptions in the model, e. g. future development of bark and lignin prices, future investment costs, and future financial incentives. Because of this uncertainty, and the large number of possible future scenarios, it was determined that such simulations would not add a significant value to the current study.

Model simplifications and development needs

Our previous models (Svensson 2014, 2015) allowed for starting and shutting down boilers and turbines as a response to daily variations in steam demand. However, potential costs or difficulties associated with starting and stopping equipment were not considered, and even if the steam demands and energy prices fluctuate significantly between days, it will not be technically or economically feasible to frequently start-up and shut down boilers, turbines and lignin extraction equipment. For this work it was therefore decided to not allow for any on/off operation of equipment. Further work could be motivated to include the costs and time required for start-ups and shut-downs in the model, to enable on/off operation for more long-term operating scenarios, such as seasonal variations. It could, for example, be motivated to have a boiler in operation during winter, but shut it down during summer.

The models of turbines and boilers could potentially be further developed also in other respects. Examples include how to constrain the steam flows through individual turbine stages and extractions. For example, a minimum extraction flow might be as relevant as the maximum extraction flow used for existing turbines. Similar constraints for new turbines should also be considered. but need to be associated with some cost function to be relevant. The effect of variations in cooling water temperature on the power output of condensing turbines should also be included in future models. Other examples of potential future developments include a more detailed modelling of steam condensates and boiler feed water preparation systems, as well as internal steam demands of the boilers and own electricity consumption that depends on turbine and boiler loads.

As described in Model input data for the case study section, the model was solved for 352 days of one year. Some of the other 13 days were excluded because of a maintenance stop at the mill, where the entire production was stopped. The remaining days were excluded because measurement data deviated too much from normal operation for different reasons, which lead to violations of constraints in the model. For example, days were excluded for which the daily average of a boiler or turbine load was less than the minimum load limit set in the model. In reality, the load has probably not been constantly below the minimum load, but for example, a boiler may have been out of operation during part of the day, and at part-load during the rest of the day, which leads to the observed constraint violations when averaging the measurement values. Better model accuracy could be obtained by dividing these

days (and other days with big changes in operating conditions) into shorter periods. However, this improvement in accuracy was considered to be negligible in comparison to other large uncertainties affecting the model results, e.g. prices and investment costs.

The current version of the model has a time resolution of one day, and process data as well as prices are averaged over these time periods. While this approach leads to some problems since conditions may change significantly during a day, there are other challenges associated with using shorter time periods. One challenge is related to the computational effort required if solving the model with significantly higher number of time steps, especially since some model instances are already cumbersome to solve on a standard desktop computer. However, this could be handled by modelling time slices as, e.g., representative hours. Since no storage is considered in the model, this would be rather straightforward modelling-wise. However, identifying the representative time slices could be difficult due to the large number of varying parameters, with different and sometimes uncertain degrees of correlations. Furthermore, while it would be beneficial to use a higher time resolution to capture, for example, hourly electricity spot price variations, this is not necessarily advantageous for capturing different process conditions. Changes in the process, such as a change in production campaign to another type of raw material, may take several hours to propagate through the different process units. For a single hour during such a transition, it is likely that steady-state balances do not accurately represent the system. While it may be motivated to put large efforts into identifying representative time slices (of various duration) for an energy systems model used, e.g., in regional energy policy planning or scenario analysis (see e.g. Poncelet et al. 2017, Reichenberg et al. 2018), this is more doubtful for investment optimization in an individual mill where other uncertainties (such as investment costs) are likely to be more important for the investment decisions.

Conclusions

This article presented a novel modelling approach for investment decision optimization in pulp mill energy systems, which considers the value of a diversified energy byproducts portfolio for achieving a more flexible system. The proposed model explicitly considers potential operational flexibility towards variations in energy prices, steam production and process steam demands. It was applied to a case study of a large Kraft pulp mill assumed to plan for a significant production capacity increase. For the existing design of the steam system, the modelled operation was validated against measured values before the model was applied to investigate possible investment options. It was shown that the multi-period approach suggested here may identify solutions with more flexibility than the solutions that would have been identified with a corresponding single-period model.

The results from the case study suggest that lignin extraction has a potential to contribute to flexibility in pulp mill electric power production under certain conditions provided that the mill invests in both lignin extraction and condensing turbine capacity. At each given point in time, the potential power generation will, however, be limited by the mill's internal energy balances and demand for offloading the recovery boilers. The potential electric power production flexibility will therefore vary substantially over time; in the studied mill it varies between 15 and 30 MW.

The optimal investments in the mill depend on several factors such as the lignin price, the electricity price and the magnitude of variations in electricity price. The optimal investment also depends on capacity limitations in boilers and existing turbines, variations in steam demand and black liquor flow and composition, as well as on the assumed investment costs. Depending on the prices of lignin and electricity, it will be preferable to maximize either the lignin extraction (favoured by a high lignin price and low investment cost for lignin extraction and/or low electricity prices) or the electricity generation. Note, however, that based on our assessments, investment in new condensing turbine capacity only seems to be attractive if assuming that new electricity production will be eligible for tradable green electricity certificates with a price well above the expected future value of such certificates. However, with large variations in electricity price, it will sometimes be beneficial to extract as much lignin as possible while sometimes it will be more favourable to extract less lignin and produce more electricity. Under the right conditions, such variations may therefore motivate investment in new turbines, despite the fact that these will not be fully utilized, and despite the fact that the lignin extraction process will not be continuously operated at maximum load.

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Property/coefficient	Turbine					
T	T3	T4	T5	Т6	BPETa/b	LPCTa/b
Inlet header, <i>in</i> (<i>T</i>)	1	1	1	1	1	6
Extraction headers, <i>out</i> (<i>T</i>)	4,5	2,6	3, 4, 6	cond	2, 4, 6	cond
a _{7,1} [MW/(kg/s)]	0.4902	0.2726	0.3936	1.0421	0.2838	0.6344
a _{7,2} [MW/(kg/s)]	0.1638	0.3714	0.0791		0.1735	
a _{7,3} [MW/(kg/s)]			0.1712		0.1726	
b _{7,0} [MW]	-5.4536	-5.8090	-7.1326	-2.6924		
$b_{T,2}$ [MW/(kg/s)]					-0.1057	-0.0554
b _{7,1} [MW]					0	-0.0605
$\overline{M_T^{\text{max}}[\text{kg/s}]}$	42	50.8	56.4	52.1	var	var
μ_T^{\min} [-]	0.61	0.54	0.79	0.23	0.5	0.25
$M_{T,1}^{\text{maxext}}$ [kg/s]	15.7	6.2	7.4	52.1		
$M_{T,2}^{\text{maxext}}$ [kg/s]	28	46.3	11.2			
M ^{maxext} _{7,3} [kg/s]			42.5			
h ^{ext} _{T.1} [MJ/kg]	3.033	3.231	3.105	2.417	3.239	not used
h ^{ext} _{7.2} [MJ/kg]	2.872	2.871	3.027		3.057	
h ^{ext} _{7.3} [MJ/kg]			2.859		2.876	
h _{cw} [MJ/kg]				0.088		0.088

Table A.1: Data for existing and new turbines.

cobsson provided valuable input on formulations and descriptions in parts of the manuscript.

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Appendix A. Turbine model parameters and validation

The parameters $a_{T,s}$, $b_{T,0}$, $b_{T,1}$ and $b_{T,2}$ in the linear turbine model (Equation 14) are coefficients estimated by assuming that part-load operation is achieved by throttling the inlet steam flow to the turbine. A simplified model of the power production as a function of steam flow based on the isenthalpic pressure reduction over the inlet valve and turbine constants is assigned, and finally linearized using the isentropic efficiency as a tuning parameter to match the linear model to daily averages of measured flows and power outputs. (Days when turbines were out of operation or were subject to other major operational disturbances were excluded from the data set.) The resulting turbine model parameters are presented in Table A.1. (Inlet and extraction headers are defined according to Figure 1.)

Given measured steam flows, the model predicts the power output of the existing turbines T3–T6 (Figure 1) with sufficient accuracy considering the inherent uncertainty in measurement data (Figure A.1). The reason for the poorer accuracy of the condensing turbine T6 is mainly that the influence of variations in the temperature of cooling water used in the steam condenser is not accounted for in the model.

Appendix B. Model input data

Valves inlet and outlet headers are defined according to Figure 1.

Reference process steam demands, $M_{j,t}^{\text{proc, ref}}$ and steam production in recovery boiler(s), $M_{\text{RB},t}^{\text{prod}}$ are illustrated in Figure B.1 for the projected future production levels.

The extra steam demand in the evaporation plant when lignin is extracted, σ , is 0.0234 kg/s LP steam per MW of extracted lignin. The maximum lignin extraction rate as a function of the reference steam production in the recov-



Figure A.1: Prediction of turbine power using the linear turbine model compared to measured values. Calculated and measured power values are based on the same measured steam flows through turbine stages.



Figure B.1: Reference steam production in the recovery boilers (RB1 + RB2) and process steam consumption at different pressure levels. Projections for mill after production increase.

ery boiler, ρ , is 0.723 MW lignin for every kg/s of HP steam produced. This corresponds to a lignin extraction rate of 0.182 tonnes/ADt, which is in the same range as values reported in literature (Välimäki et al. 2010, Wallmo et al. 2009).

Other model data are shown in Tables B.1–B.2.

Appendix C. Modelling the eligibility for electricity certificates

Essentially all electricity generated at the mill is renewable since it is based on the biobased wood raw material. In

Sweden, renewable electricity production can be approved for award of tradable green certificates during a time period of 15 years (Swedish Energy Agency 2019b).

Production plants where the generation capacity was taken in operation more than 15 years ago can be approved for new awards of certificates if the electric power generation capacity is increased. In that case, a fixed award factor will be determined based on a demonstrated increase in normal year production, which represents the share of production eligible for certificates. This means that if the studied pulp mill increases its electricity generation capacity, it will be approved for a new award of electricity certificates, and a new award factor will be established. Note that if the award factor is determined to be, for example, 20 %

Investment cost parameter	Lignin extraction	Back-pressure turbine	Condensing turbine	9	
r [1/y]		0.2			
x	LIG	TURB1	TURB2	TURB3	
\overline{Y}_{x} [MW]	[33, 73, 113, 153, 216]	[10, 28, 46, 64, 82]	[4, 8, 12, 16, 20]	[10, 34, 58, 82, 106]	
C _{inv,x} (<i>i</i>) [10 ⁶ €]	$3.0 \overline{Y}_x(i)^{0.6}$	1.3 $\overline{Y}_{x}(i)^{0.6}$	2.3 $\overline{Y}_{x}(i)^{0.6}$	2.3 $\overline{Y}_{x}(i)^{0.6}$	
k _x (<i>i</i>) [€/MW]	$\frac{(C_{inv,X}(i+1)-C_{inv,X}(i))}{(\overline{X}(i+1)-\overline{X}(i))}$				
		$(I_X(l+1) - I_2)$	x(1))		

Table B.1: Investment cost data.

Table B.2: Performance data for the boiler.

Boiler parameters b	Rec. boiler RB1	Rec. boiler RB2	Bark boiler BB
$\eta_{\rm b} \left[\frac{\rm MW \ steam}{\rm MW \ "fuel"} \right]$	0.92 ^a	0.92 ^a	0.88
M ^{min} _b [kg/s]	100	60	12
M _b ^{max} [kg/s]	180	105	30
$h_{fw} = h_{aw} [MJ/kg]$		0.504	

^aMarginal lignin-to-steam efficiency = Steam output decrease/heat content of extracted lignin

the mill will be awarded certificates for 20 % of its electricity production independently of whether the electricity is generated in the new or in the older part of the plant. Every month, the mill reports its actual electricity production and receives certificates for the share of the production corresponding to the award factor. The current award period for the studied mill expires in 2022. For evaluation of an investment that will be made today or later and therefore mainly operate after 2022, it is therefore reasonable to assume that the award factor will be 0 % if no new installations in electricity generation capacity are made.

However, if investments in, e.g., new turbines are made so that the electric power generation capacity is increased, the mill can be approved for a new award period. In the model, the electricity that is eligible for certificates, $E_{\text{cert},t}$, generates revenues at a certificate price of $p_{\text{cert},t}$. To consider the revenues from sales of green certificates in the model, Equation (7) is replaced by the following constraint:

$$ElecRev = \sum_{t} d_{t}(p_{el,t}E_{prod,t} + p_{cert,t}E_{cert,t})$$
(C1)

In the case of a new award period, a new award factor will be determined. To correctly determine $E_{\text{cert},t}$, the award factor, based on an increase in normal year production would therefore be needed. However, in the proposed modelling framework, it is not straightforward to obtain the normal year production, since this would depend on the investments made and the full capacity of potential turbine investments might not be utilized under the varying prices and steam balance conditions. The model

would quickly become highly non-linear, if all dependencies were included explicitly. As a simplification, any electricity production above the daily average corresponding to the current established normal year production, E_0 , of ca 800 GWh is assumed to be eligible for certificates. This leads to the constraint formulated in Equation (C2).

$$E_{\text{cert},t} \le E_{\text{prod},t} - \frac{E_0}{\sum_t d_t}$$
 (C2)

Note that this constraint is only valid if the electricity production summed over each month is actually higher than the monthly reference production. Otherwise, the revenues from electricity certificates would become negative in the model, while in reality, the mill would simply not receive any certificates and the revenues would be zero. With respect to modelling, this could be further improved, by introducing monthly periods and "bigM"-constraints to avoid negative values of the monthly sums of $E_{cert,t}$. However, since the price of certificates is assumed to drop drastically in the near future, the electricity certificates were not included in the standard model formulation. Therefore, it was also decided that it was not worth the added model complexity to further improve the modelling of this special case.

Nomenclature

Abbreviations

ADt	Air-Dried tonnes
BPET	Back-Pressure Extraction Turbine
CEPCI	Chemical Engineering Plant Cost Index
LPCT	Low-Pressure Condensing Turbine
MILP	Mixed-Integer Linear Programming

Indices

b	boiler
i	linearization interval

j	steam headers
S	turbine stage

- *t* time period
- T turbine
- x potential technology/equipment for investment (turbines or lignin extraction plant)
 v expansion valve

Parameters

- $a_{T,s}$ slope of the linear function that describes the power output of turbine *T* as a function of the steam mass flows through the turbine stages *s*
- $b_{T,0}$ intercept of the linear function that describes the power output of an existing turbine *T* as a function of the steam mass flows through the turbine
- $\mathbf{b}_{T,1}$ constant in the linear function that describes the power output of a new turbine *T* as a function of the steam mass flows through the turbine and the maximum inlet steam flow rate
- $b_{T,2}$ constant in the linear function that describes the power output of a new turbine *T* as a function of the steam mass flows through the turbine and the maximum inlet steam flow rate
- $C_{inv,x}(i)$ investment cost at the *i*th breakpoint of the piecewise linear cost function for investment in equipment *x*

 d_t duration of time period *t*

E ₀	current normal year electricity production re-
	ported in the electricity certificate system
h _j	enthalpy of steam at header j
h _{cw}	enthalpy of cooling water
h _{fw}	enthalpy of feed water
$h_{T,s}^{ext}$	enthalpy of extraction steam from the stage <i>s</i>
	of turbine <i>T</i>
$k_x(i)$	slope of the i^{th} linearization interval for the
	piecewise linear cost function for equipment <i>x</i>
M_b^{min}	minimum steam production in boiler b
M_b^{max}	maximum steam production in boiler b
M ^{ref} _{RB,t}	reference steam production in the recovery
	boiler in timer period <i>t</i>
$M_{j,t}^{\text{proc,ref}}$	reference process steam demand at header <i>j</i>
	in time period <i>t</i> without investments or oper-
	ational changes
M_T^{max}	maximum inlet flow of existing turbine T
$M_{T,s}^{maxext}$	maximum extraction flow after turbine stage <i>s</i>

of existing turbine T

$M_t^{refcond}$	reference condensate flow from condensing
	turbines in time period <i>t</i> without any invest-
	ments or operational changes
n	number of linearization intervals
p _{bark,t}	bark price in time period <i>t</i>
p _{cert,t}	price of tradable green electricity certificates in
	time period <i>t</i>
p _{el,t}	electricity price in in time period t
p _{lig,t}	lignin price in in time period <i>t</i>
r	capital recovery factor / annuity factor
$\overline{\mathrm{Y}}_{x}(i)$	capacity/size of equipment x at the i^{th} break-
	point of the piecewise linear cost function for
	that equipment
η_b	marginal fuel-to-steam efficiency of boiler b
ρ	maximum lignin extraction rate per mass flow
	of high-pressure steam produced
μ_T^{\min}	minimum fraction of the maximum inlet flow
	to the turbine T that can go through the turbine

Variables and variable functions

BarkCost	annual fuel costs for bark
$Cost_x$	investment cost for equipment <i>x</i>
$E_{\text{prod},t}$	total electricity production in in time period <i>t</i>
$E_{T,t}$	electric power output of turbine T
E_T^{\max}	design capacity of new turbine turbine T
$E_{\text{cert},t}$	electricity production eligible for tradable
	green certificates in time period <i>t</i>
ElecRev	annual revenues from electricity production
InvCost	total investment costs
LigRev	annual operating revenues from lignin extrac-
_	tion
$M_{b,t}^{\text{prod}}$	steam production in boiler b in time period t
$M_{j,t}^{\text{proc}}$	process steam demand at header <i>j</i> in time pe-
	riod t
M_T^{cap}	maximum inlet flow of new turbine T
$M_{T,s,t}^{ m turb}$	steam flow through stage <i>s</i> of turbine <i>T</i> in time
	period <i>t</i>
$M_{T,s,t}^{\text{ext}}$	extraction steam flow after turbine stage s of
	turbine <i>T</i> in time period <i>t</i>
$M_{j,t}^{\mathrm{qw}}$	quench water added for saturating the steam at
	header <i>j</i> in time period <i>t</i>
$M_{v,t}^{\rm vlv}$	steam flow through expansion valve v in time
	period <i>t</i>
M_t^{vent}	steam vent to atmosphere (from low-pressure
	steam header) in time period <i>t</i>
$Q_{\mathrm{Bark},t}$	bark fuel used in the bark boiler in time period
	t
$Q_{\mathrm{Lig},t}$	lignin extracted in in time period t
Y_{χ}	capacity/size of equipment/technology x

- z_x binary variable, which is 1 if investment is made in technology *x* and 0 otherwise
- γ_T binary variable, which is 1 if the existing turbine *T* is kept in operation, and 0 otherwise
- σ specific increase in low-pressure steam demand for black liquor evaporation when lignin is extracted

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