# Project Deliverable

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<td>Real-time Monitoring and Optimization of Resource Efficiency in Integrated Processing Plants</td>
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## Title

D3.5 Tool for tracking of resource efficiency for batch processing and root cause analysis

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Abstract:
The aim of MORE Task 3.4 was the optimization of resource efficiency in batch production by the utilization of REI that were collected (D1.1), developed and evaluated (D1.2) for the suitability to monitor batch processes. This challenge was addressed by two approaches: (1) the model based optimization approach for online load allocation to improve the resource efficiency by supplying the optimal solution for the given production goal as discussed in D3.6 and (2) The monitoring of resource efficiency by REI to supply information for a root cause analysis in batch-to-batch optimization. The second approach is discussed in this deliverable and was developed for a benchmark process of a sugar plant [1]. The process model is extended by the REI calculation that was developed for integrated batch and continuous processes in D1.3. Furthermore, an offline optimization of the production over a fixed horizon was implemented for the separate optimization of the material and energy efficiency indicators. Finally, a visualization concept was developed that visualized the results and gives advice for future operation, based on the results from D1.4.

Keywords:
Resource efficiency optimization, monitoring, scheduling, Batch-to-batch optimization, Integrated batch-continuous process.

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1. Introduction

Batch plants constitute a significant part of the process industry, transforming base materials such as chemicals into high-value products with special properties demanded by the end-users. These plants are by nature more dynamic than continuously operated plants, as operations on a batch of material have defined durations and are performed in a discontinuous fashion, and because the material is moved between units at discrete points in time.

Mixed production processes contain batch-wise and continuously operated sections. When there is a transfer between the two operating regimes, either batches are created from a continuous stream or batches are mixed with other batches in a buffer tank in order to feed a subsequent continuously operated process. Real-time resource efficiency indicators for continuously operated parts of the plant were defined in the deliverable D1.2. The tracking of resource efficiency in batch processes requires additional considerations regarding the allocation of resources to specific batches and the impact of production logistics on the overall efficiency of the process. For this kind of processes, tailored real-time resource efficiency indicators are needed that were introduced in deliverable D1.3.

This deliverable introduces the concepts of implementation of the MORE methodology to mixed production processes and presents a solution for tracking the resource efficiency for the case study of a sugar plant that incorporates discontinuous and continuous production stages. The plant model originates from Mazaeda et al. [1] and is extended by the resource efficiency analysis and an offline optimization over a fixed time horizon. The detailed modeling of the resource efficiency indicators during the continuous and discontinuous steps in the operation enables a root cause analysis, in case deficiencies of the overall process are discovered in the aggregated plant-wide indicators.

2. Resource Efficiency Indicators for batch processes

Batch processes require the tracking of the batches to ensure the correct allocation of the used resources to the individual batches. Thus the data collection and calculation of REIs require modifications compared to the continuous production. Effects that have an influence on the overall resource efficiency occur on different temporal and hierarchical levels, and specifically designed REIs help to capture the influences on the resource efficiency on different levels (process unit, plant, site). The evolution of the indicators during the production steps of a batch (e.g. a reaction step) can be used to assess the distance to a known optimal trajectory, but only after the completion of the batch the overall resource efficiency can be determined. In order to determine the resource efficiency of the production of a single batch, the resource utilization must be measured with a sufficiently fine resolution so that the resources can be attributed to the individual batches.
Resource efficiency indicators are useful on different layers of the plant hierarchy and therefore have to be aggregated from individual units to the whole site. For indicators on the lower level (individual units or operations), care must be taken that the indicators are not misleading and cause a shift of the burden from one unit to another when the operators optimize them locally. Specifically for batch processes, the information about the amount of material and energy that are introduced to the production process is first collected on the unit level as each batch passes through the plant (see Figure 1, [2]). These local REI are determined for each of the unit operations involved in the production as consumed material and utilities per mass of intermediate product. The propagation of the batch throughout the stages, under consideration of additionally used resources, results in the final efficiency for an individual batch of product. The analysis of aggregated plant specific REI or propagated product specific REI over longer periods delivers an indication of the overall process performance and is exploited for the batch-to-batch optimization presented in this deliverable.

Many operational aspects that may have an influence on the resource efficiency of batch production plants as e.g. the sequencing and scheduling of the unit operations can only be assessed for a larger number of batches. Therefore, in addition to indicators for the single batch, global indicators of the efficiency of the plant over many batches (e.g. production campaigns) are needed. On the plant-wide level it is also possible to identify slow dynamics that call for optimization (e.g. catalyst deterioration).

For crucial processing steps, local indicators can be defined to help the operating staff to assess the efficiency of the individual production stages. However, as e.g. performing a reaction longer to reach a higher conversion may save energy in subsequent separation steps, a full assessment is only possible at the end of the production sequence.

Figure 1: Hierarchical structure of a batch production site on four levels, with the reaction stages R1, R2 and the distillation stages D1, D2.
2.1. Batch Resource Efficiency

As stated in the guidelines all used resources are recorded individually and related to the amount of the resulting product. Figure 2 shows the typically occurring streams crossing the system boundary of the batch where \( m_k \) is the mass of raw material \( k \) fed to the batch, \( Q_{\text{H},i} \) is a heating energy, \( m_{\text{waste}} \) is the material that is discharged to the environment, \( m_{\text{product}} \) is the product material obtained during the batch, \( W_{\text{generated},j} \) is the electrical energy obtained from the batch that is consumed elsewhere, \( W_{\text{el},i} \) is electrical energy consumed, \( W_{\text{cool},i} \) is electrical energy that was consumed to supply the cooling agent, and \( Q_{\text{generated},j} \) is the energy that is discharged from the batch and used elsewhere. It is important to assess all contributions separately in the first step to identify trade-offs that impact the resource efficiency.

![Simplified batch balance](image)

**Figure 2: Simplified batch balance**

In case excess heat or electricity is generated during the production and used in another unit, the resource consumption needs to be corrected according to the following equation:

\[
REI = \frac{\text{Product Output}}{\text{Resource Consumption} - \text{Resource generated}}
\]

This is initially done for each resource separately. If desired, aggregated indicators for the total energy or material efficiency can be derived from the resource and product specific sets of indicators defined in deliverable 1.3.

2.2. Transition from Batch to Continuous Production

In the transition from batch to continuous operation, the material is usually buffered to ensure a constant transfer into the continuously operated section. The buffer tank is assumed to be ideally mixed (see Figure 3, left). Thus the concentrations \( c_i \) of the outlet stream \( m_{\text{out}} \) are equal to the current concentration within the tank.
Figure 3: Buffer tank between batch and continuously operated section (left), timing of transfer operations to and from buffer tank (right)

Figure 3 (right) shows a sequence of two batches that are fed into the buffer tank. Each batch has a known size and the transfer interval is determined by the inlet flow rate. The composition of the arriving material and the amount of resources per unit mass that were needed to produce it may vary from batch to batch. Let $r_{i,n}$ be the entire upstream consumption of a resource $i$ per mass of product in batch $n$, and let $m_p$ be the mass of product in the buffer tank. $r_{i,n}$ and the mass fraction $w_n$ of the product in batch $n$ vary from batch to batch, where $w_n$ relates the amount of product that is contained in the batch to the total mass of the batch. The buffer tank can be modelled as a system of differential Equations describing the states: total mass $m$, amount of product in the tank $m_p$, and specific resource utilization $r_k$ of the resource $k$ per amount of product.

$$\frac{dm}{dt} = \left(\sum_n \dot{m}_n\right) - \dot{m}_{out}$$

$$\frac{dm_p}{dt} = \left(\sum_n \dot{m}_n w_n\right) - \dot{m}_{out} \frac{m_p}{m}$$

The resource consumption that is “carried” by an element of product material is introduced as an additional state variable. The differential equation for a product specific resource utilization $r_k$ can then be derived from the balance for the resource consumption state $m_{cons}$:

$$\frac{dm_{cons}}{dt} = \frac{d(m_p r_k)}{dt} = r_k \frac{dm_p}{dt} + m_p \frac{dr_k}{dt} = \left(\sum_n \dot{m}_n w_n r_{k,n}\right) - \dot{m}_{out} \frac{m_p}{m} r_k$$

Substitution of $\frac{dm_p}{dt}$ and solving for $\frac{dr_k}{dt}$ yields:

$$\frac{dr_k}{dt} = \sum_n \frac{\dot{m}_n w_n}{m_p} (r_{k,n} - r_k)$$

The inlet flowrates $\dot{m}_n$ are assumed to be constant and are defined by total amount $m_n$ and the arrival times $t_{start,n}$ and $t_{end,n}$.

$$\dot{m}_n(t) = \begin{cases} 0, & t < t_{start,n} \\ \frac{m_n}{(t_{end,n} - t_{start,n})}, & t_{start,n} \leq t \leq t_{end,n} \\ 0, & t > t_{end,n} \end{cases}$$

For the example described in Figure 3, the trajectories shown in Figure 4 were obtained. The same batches are introduced into the buffer tank with different transfer times (slow-fast). Under the assumption that the buffer tank is ideally mixed, the resource efficiency of the constant outflow is characterized by the current state $r_k$. Thus, it is possible to propagate the resource efficiency of the batch material to the continuous outflow.
2.3. Transition from Continuous to Batch Production

In case of the transition from a continuous section into batch operation, the total resource consumption associated with the new batch \( n \) can be computed by the integral shown in the following equation:

\[
r_{k,n} = \int_{t_0}^{t_f} \dot{m}_{p,\text{out}}(t) \ r_k(t) \ dt.
\]

Additional contributions that are introduced during the production as a batch can be attributed in the previously discussed fashion for pure batch processes.

3. Case Study

As a case study the MORE framework was applied to the benchmark problem that was published by Mazaeda et al. [1]. The considered factory produces food grade sugar from the juice of sugar beets by evaporation and crystallization (see Figure 5).

In the first section the fresh juice passes through a cascade of three evaporators and is concentrated by the removal of excess water. The first stage is heated by an external steam supply and evaporates part of the water that is contained in the juice. By this step, steam is generated that can either be used to heat the next effect or to heat any of the crystallizers. Steam that is not used will be vented and its energy content is lost to the environment. The energy integration from effect to effect is possible because of the increasing vacuum from effect to effect, making the separation less and less energy demanding. The sugar concentration in the rich juice is measured and controlled indirectly by the condenser pressure.

Subsequently, the concentrated juice is transferred to the melter where it is blended with recycle streams that are also rich in sugar content. The melter is a continuously stirred vessel that blends the materials to feed them back into the crystallizer section. After the liquid deposit, which is acting as a buffer tank, the syrup is charged into the discontinuously operated crystallizers which are operated in an alternating fashion. During the course of the batch-crystallization, more water is evaporated to obtain a supersaturated mixture and to initiate crystal growth. The heating energy for this task is supplied either by the first or by the second effect of the evaporator section.

The suspended crystals from all units are collected in the receiver after the end of each batch. From there the mixture is continuously fed into the centrifuge via another buffer tank. The centrifuge is continuously operated and produces the product stream of sugar crystals and two additional syrup streams. The higher
concentrated syrup is directly recycled to the melter, while the poor syrup is transferred to the recovery section.

Figure 5. Flowsheet of the sugar plant for the production of food-grade sugar from sugar beets

In a sugar plant, the recovery section usually consists of two sequential crystallizer sections that are identical in construction to the previously described crystallizer section. For the sake of simplicity these two stages are approximated by a continuous black-box model of the recycle in the analysis of the benchmark problem.

The additional modeling effort described in section 2.2. for calculations of nonstationary buffer tanks is required for two tanks in the sugar plant example. The melter continuously blends streams of different sugar concentrations at varying volumes, since the brix target value and thus the operational state of the evaporation section is subject to changes. Furthermore, the strike receiver acts like buffer tank receiving the batches from the three crystallizers and is continuously feeding the mixture to the centrifuges via the distribution channels.

3.1. Resource Efficiency Indicators

The system boundary on the highest hierarchy level for the case study investigated here is the complete plant with the three sub-sections: the evaporator section, the crystallization section, and the recovery section. Water and the sugar juice are the only raw materials that are used in the production of the one single product: food grade sugar. The waste stream (molasses) contains water, sugar, and impurities originating from sugar beets and is nontoxic, with little environmental impact. The indicators describing the resource efficiency of the process are defined as follows:

$$HEE_{evaporator} = \frac{m_{sugar}}{Q_{H,steam} - (\sum_i Q_{generated,1,i} + Q_{generated,2,i})} \quad \forall \ i = 1,2,3$$
Energy is introduced into the process at the evaporator section as steam $Q_{\text{H,steam}}$. The heating of the crystallizers is supplied with excess heat from the evaporator section ($Q_{\text{generated,1}}$ and $Q_{\text{generated,2}}$).

$$CEE_{\text{evaporator}} = \frac{m_{\text{sugar}}}{W_{\text{cool,condenser}}},$$

$$CEE_{\text{crystallizer,}i} = \frac{m_{\text{sugar}}}{W_{\text{cool,condenser,}i}} \quad \forall \ i = 1, 2, 3$$

Contributions to the cooling energy efficiency are considered at the condenser of the evaporator section ($CEE_{\text{evaporator}}$) and at each of the crystallizers ($CEE_{\text{crystallizer,}i}$) to condense the steam produced during the crystallization process.

$$ME_{\text{sugar}} = Ml_{\text{sugar}} = \frac{m_{\text{in,sugar}}}{m_{\text{product,sugar}}}$$

The material efficiency relates the sugar in the juice that is fed to the process to the amount of solid sugar crystals that are exported from the crystallizer section.

$$WU = \frac{m_{\text{water,in}}}{m_{\text{sugar}}}$$

The water usage indicator captures the amount of water used by the process in the centrifuge of the crystallizer section and in the recovery section.

$$WP_{\text{molasse}} = \frac{m_{\text{waste, molasse}}}{m_{\text{sugar}}}$$

The waste production is determined by the amount of molasses emitted by the recovery section which is necessary to discharge the impurities introduced to the system with the raw material.

### 3.2. Offline optimization

Because of the availability of a full dynamic model of the process, it is possible to calculate the exact resource efficiency of the intermediate product at any stage of the process by balancing and propagating pseudo components as described above in the section on the transition of REIs between continuous and batch production. This approach has the advantage that closing the recycle streams does not pose any difficulties, because information on the resource consumptions is available for all streams that enter the melter. If the amount of resources consumed per unit of the stream is below the current state of the pseudo component in the melter, then the stream is reducing the value of the pseudo state in the melter. This process is analogous to a stream of water diluting a reaction medium.

The environmental indicators are only of minor interest for the overall resource efficiency in this case, since the waste stream does not have a large environmental impact. Thus the most important aspects for this process are the material and energy efficiency. The CEE and HEE are coupled in this set-up and can be
aggregated to the TEE without any loss of information, i.e. a minimized HEE will also yield a minimal CEE, because all the required cooling capacity in this process is directly proportional to the amount of heating applied. In order to obtain the resource optimal operation, the process was optimized for the total energy efficiency ($TEE$) and the material efficiency ($ME_{sugar}$) and compared to the base-case operation from the benchmark description. Here the variables $r_i$ denote the resource intensities that are calculated from the resource utilization per product throughout the process (the inverse of the REI):

$$\min_{B, P_i, P_{steam}} \frac{\int_0^t r_{HEE} \dot{m}_{product} + r_{CEE} \dot{m}_{product}}{\int_0^t \dot{m}_{product}} dt$$

$$\min_{B, P_i, P_{steam}} \frac{\int_0^t r_{ME} \dot{m}_{product}}{\int_0^t \dot{m}_{product}} dt$$

The decision variables for the operation of the process are shown in Table 1, also indicating their limits and their base-case values. $B$ is the Brix set point for the stream of juice after the evaporation section. The Brix value is the mass based concentration of the amount of solid material that is dissolved in water, here it includes sugar and impurities. The P-factors determine the actual pressures in the crystallizers during the execution of the recipes, the factors are multiplied with a pressure set point trajectory in the crystallizers and increase or decrease the pressure. P-factors above one increase the pressure and thus the temperature within the crystallizers, resulting in shorter batch times. The Brix and P-factor control inputs are parameterized by 12 piecewise-constant values each over the time horizon of 72 300 seconds (20 hours). The steam pressure of the imported steam can be varied between the bounds, but remains constant over the entire time horizon considered.

### Table 1. Decision Variables for optimization

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<th>Lower Bound</th>
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<td>B</td>
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<td>Fresh steam pressure</td>
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The three crystallizers are started in an alternating fashion that is determined by a given schedule (see Figure 6). The length of the crystallization steps is varying according to the chosen P-factors. Due to the heat integration of the evaporation and crystallization sections, the pressure in the evaporators (and thus also the energy that is reused) is affected by the chosen P-factors.
3.3. Results

The model of the sugar plant includes the calculation of the resource efficiency calculation. It is a DAE system with 151 differential and 1162 algebraic equations and is solved using the DASOLV solver for sparse DAE systems. The results of the optimization are summarized in Table 2. The minimization of the total energy intensity improved the TEE by 1.2 % and also slightly improves the ME in comparison to the base-case. The optimization for the ME of the raw material improved the indicator by 0.34 % while also improving the environmental indicators. This was expected since an improved extraction of sugar from the raw material to the product reduces the sugar waste and reduces the water consumption for the recovery section. The overall improvements are relatively small because of the tight constraints on the controlled variables. Nevertheless, the obtained information about the process can be exploited to supply a monitoring and decision support solution to the operators by displaying the current value in reference to the obtained optimum.

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<tr>
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<th>Value (ME)</th>
<th>Value WU</th>
<th>Value WP</th>
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<td>min (ME)</td>
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<th>Value WP</th>
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<tr>
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<tr>
<td>min (ME)</td>
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<td>- 0.34%</td>
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<tr>
<td>Base-Case</td>
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Figure 6: Crystallizer schedule
4. Visualization of Resource Efficiency

The resource efficiency indicators can mainly be used in three ways: in online optimization or optimizing control, [3] [4] to derive control structures from the REI analysis, and to provide guidance to managers and operators for a more resource efficient operation. As most batch plants are not fully automated and the decisions of managers and operators have a large influence on the performance of the plant, the latter aspect is very important. Deliverable D1.4 outlined considerations that need to be taken into account during the design process of operator dashboards. The most important points are summarized below and applied to the given case of study.

Resource efficiency is a multi-dimensional concept that can only be represented by a set of indicators that describe the energy efficiency, material efficiencies and environmental performance for different products on multiple levels in the plant hierarchy. To represent a number of indicators that are computed on different aggregation levels requires efficient dashboard concepts with visualization elements that are best suited to highlight the intended relations and that are easily comprehensible with little effort for interpretation. We propose to use a monitoring approach that gives an overview of the resource efficiency at first glance and subsequently breaks down the contributions further to enable the user to conduct a root cause analysis. The structure of the interface, the graphical elements that are used their design (e.g. color coding) are important to achieve acceptance by the operators and to influence their decisions by the visualization of the resource efficiency indicators.

Since the representation of complex chemical systems requires multiple REI and supporting information, multiple plots and graphs are needed. Grouping in rows and columns increases the ease of perception and reduces the time required to find the required information. Ergonomically designed dashboards should follow the reading direction the user is accustomed to, hence for western users the most important information should be displayed in the top left area and the least important on the lower right.

To go beyond the possibilities of classical two- or three-dimensional representations, the use of additional attributes like color, orientation, size and a smart combination of specialized visualization elements should be considered [5].

4.1. Dashboard Concept for the Sugar Plant Case-Study

Figure 7 shows a dashboard concept including a control panel for the navigation through the plant hierarchy with efficiency indicator bars for the three plant sections, indicating the resource efficiency of each section (upper-left). Upon user interaction, the different plant sections can be activated, which triggers an update in the historical trends (lower-left) and the detail view (upper-right) for the selected subsection- and resource-specific REIs. The lower-right field is intended to give supplementary information about the visualization elements to increase the user acceptance. For the example shown in Figure 7, the user can identify a suboptimal performance of Pans A1 and A2 in the crystallizer section.
Below the detailed view of the pans in the crystallizer section, the predicted optimal operation inputs are displayed. They were obtained from the offline optimization described in section 3.2, and considered the last known production goals and external influences. In a real application, the operators can use this information to manually adjust these parameters to improve the future production. In case the process is affected by effects that are not included into the model, they cannot be regarded during the optimization, but since the visualization of measured historic and current values shows these effects the operators are able to take corrective measures.

5. Conclusions

In this deliverable, a solution for the monitoring and optimization of resource efficiency in a mixed batch-continuous processing plant example was presented. All inputs of materials and energy are considered and related to the amounts of product and intermediate products. The indicators were propagated through the plant for individual batches and the continuous processing stages. The resulting indicators for the material and energy efficiency were then used in the cost function of an offline optimization to find the most efficient operating conditions. Finally, a dashboard concept was developed that on the one hand serves as a monitoring tool to servile the efficiency measures of the process and enables the user to perform a root cause analysis. Furthermore, the results from the offline optimization are included into the dashboard design to give guidance to the operator in the decision making process for a better performance in the future.

The developed modules for resource efficiency tracking, root cause analysis, and offline optimization in batch processes can be connected to the Intexc Suite environment that was developed by LeiKon. The Intexc Suite offers the connectivity to the systems on site, in order to retrieve the necessary data for the resource efficiency analysis and optimization, and a flexible browser-based visualization interface.
6. References


