# The Batch Optimization Challenge

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## Introduction

A batch process is characterized by the repetition of time-varying operations of finite duration. Batch processing operations are found throughout the industry from specialty chemicals to fine chemicals to food & beverage, consumer products, pharmaceuticals and biotechs, and many others. Operations range from simple blending operations to complex reactions and may be preceded and followed by continuous operations. The scale of operations ranges from very small such as wheeled and skid-mounted process units, to toll manufacturers, to the major chemical companies with large fixed assets. Product values vary considerably, from high volume, low value like polyvinyl chloride (PVC) to low volume, high value, such as biologics, where the quality is critical. This diversity of heterogeneous operations makes batch control and optimization particularly challenging, often resulting in longer cycle times, lower yields, off-spec quality, production loss during grade changes and product changeovers, delayed deliveries, unnecessary waste and recycling, and increased energy usage, all of which means a larger carbon footprint and higher costs.

*Figure 1 - Batch Reactor Train*

The industry has answered this challenge with sophisticated batch control and manufacturing execution systems, built upon industry standards such as ISA 95 and ISA 88. Today these systems do an excellent job of batch execution, including a range of functions from production scheduling, recipe management, inventory management, genealogy tracking, labor tracking, SPC/SQC charts, equipment performance

(OEE), routing and sequencing, trending analysis, and reporting, etc. And of course, they provide supervisory control of the underlying basic regulatory control system, be it through a distributed control system (DCS) or a PLC-based system. These functions are often tightly coupled in on-premise systems but are increasingly hybrid with portions running in the Cloud.

## Batch Optimization Challenges

Despite this progress, the industry still faces a number of problems, some of them due to lacking functionality in the execution system and others due to the way batch processing workflow is managed in many companies. Both of these can lead to a failure to optimize in a timely fashion, if at all.

Consider the case where the MES has limited SPC functionality, that is, univariate analysis of individual variables. This helps detect off-spec products but fails to explain why because it does not look at the interaction between multiple variables. Even more common is that the MES lacks SPC/SQC and this analysis is done offline in a separate analysis tool by production personnel days after the deviation.

For example, multivariate statistical process control can be used to track down the source of variability in batch operations and make mid-batch corrections. The current batch is compared to an average batch. Principal Component Analysis (PCA) can tell if anything in the current batch has changed. Drilling down into the PCA can give the contribution of each batch measurement to the variability observed. PCA along with a process understanding can be used to trace abnormal batches back to equipment and automation system problems. Once the deviation is understood, the process variable setpoints are adjusted by operations but only after one or more batches have deviated for some time. And given the variability in processing equipment and raw materials, the new setpoints may be sub-optimal. This process repeats itself and thus one never gets to optimality in any sense of real-time.

A second issue is that some MESs have non-existent or incomplete data models, thus leading to the lack of a common, contextual view for operations and engineering. No one is looking at the same thing at the same time and as a result, may take actions that are at odds with each other to the detriment of production.

Complicating this landscape is the fact that companies do not have homogenous BES/MES environments. Systems vary by manufacturer, features, and functions, often the result of mergers and acquisitions, and thus the associated difficulty in economically justifying standardizing such environments. And of course, not every plant needs every function, so from simple to sophisticated usually results in multiple vendors.

One very desirable function is the ability to analyze current batches and predict future batches. Few vendors have this functionality, let alone the equivalent functionality in this area. And in those that do, these types of optimization functions are tied to a specific MES and are not open and transferrable i.e., not interoperable. So forget about scaling.

Fourth, optimization techniques common to large continuous processes such as refining and petrochemicals do not apply well to batch processes. Here we are referring to the use of first principles equation-based optimizers layered on top of advanced process control i.e., dynamic matrix controllers, which then drive the underlying control system. While these may be found on the continuous side of large chemical plants, they don’t fit the requirements for batch.

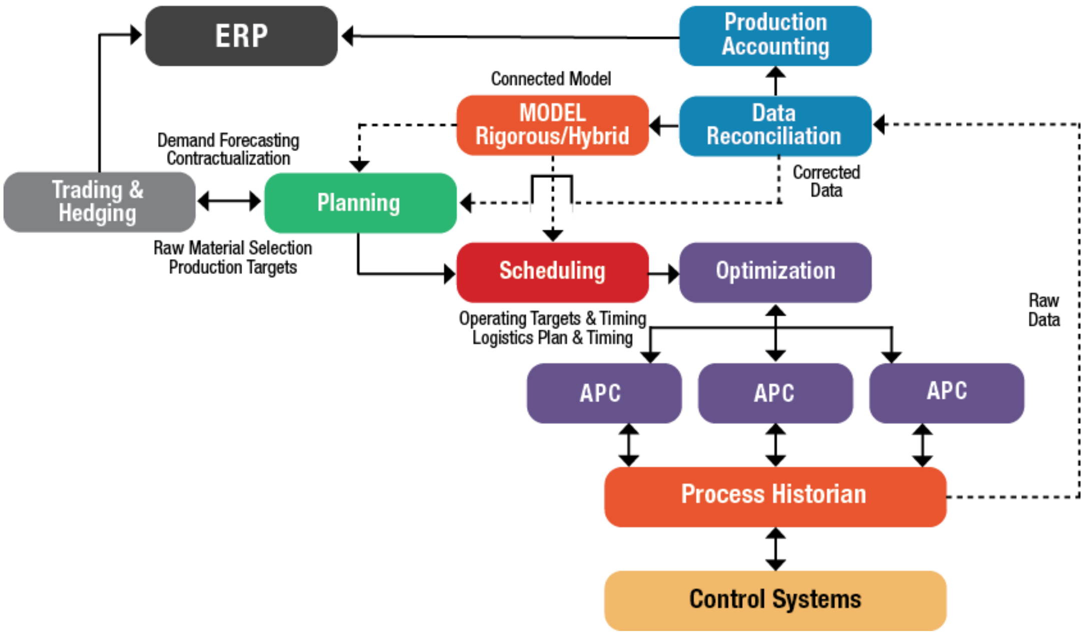


*Figure 2 - Large Continuous Process Optimization Schema*

Fifth, batch records management has been available for some time, typically being an optional feature of historians like AVEVA's PI and AspenTech's IP.21. And while new advanced analytics tools have come to market, such as Seeq and Trendminer, they are workbenches designed for engineers and used in open-loop mode, while ideally, optimization should occur in a closed-loop fashion. In addition, out of the box, they are dependent on underlying historian time series data. As is, they lack direct integration with the batch execution system.

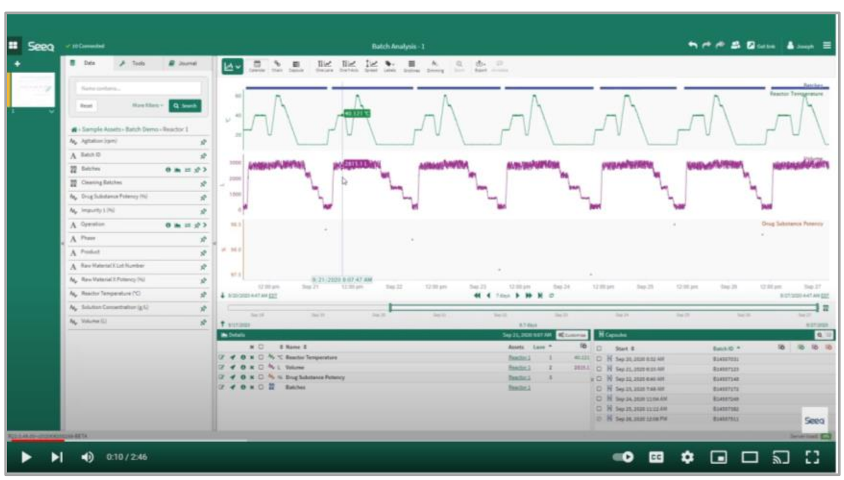


*Figure 3 - Batch Analysis Courtesy of Seeq*

Finally, many facilities lack the right operational data management infrastructure needed to provide the right data in context for optimization to function successfully. Not all plants have historians with automated batch recording. This is a challenge facing all of the industry as we move toward increased digitization of operations. Convincing management to make this investment, which in and of itself provides little return (ROI) until it enables new performance capabilities, is often an uphill battle.

## Elements of Success

So how do we address the batch optimization challenge? What are the necessary elements for success?

There are five key elements to success:

1. Ready-to-use visualization and insights
2. Sophisticated and secure, yet easy to use
3. Open, interoperable, and scales to any environment
4. Capable of closed-loop supervisory control
5. Cost-effective; easy to license and support

### *Ready-to-Use Visualization and Insights*

The ideal optimization system should provide visualization that both informs and advises the shop floor as well as production management personnel. The key is "insight into performance." This means more than just showing which recipe is being executed and the batch status i.e., how it is proceeding, but the ability to project its finish and compare it to other batches. This also allows operations to see the sources of variability in real-time. The system should support access to standard BI tools like PowerBI.

### *Sophisticated and Secure Yet Easy to Use*

The system should have advanced capabilities, incorporating not only multivariate statistics but artificial intelligence, including machine learning techniques, yet hide this sophistication from the user. These techniques should not only be applied to batch control but to equipment performance i.e., reliability. The system should also be able to incorporate first-principles equations and calculations where appropriate. Data models should be fast and easy to train without coding. The system should predict the batch trajectory and indicate in real-time the parameters that are influencing performance. In essence, the system should be ready-to-deploy and self-tuning. Most biotech and pharmaceutical companies are adopting Process Analytical Technology (PAT), so the ability to intake spectral data (a list or array of values) is also a desirable feature.

The system should also comply with ISA 95 and ISA88 standards so that it can align and integrate with the execution systems (MES & BES), and where there is no execution system, interpret context from the streaming data and events. It must be ISO9001 SOC2 for quality auditing as well as meet GxP and CFR 21 part 11 requirements. And course, it must be cyber-secure compliant with IEC62433.

### *Open, Interoperable, and Scale to Any Environment*

Open, interoperability is the key to scaling. Such an optimization solution should be able to handle the small, low-volume, high-value batch processing in the pharma and biotech industries as well as the range of batch processes found in specialty and fine chemicals. This means it should scale from an R&D pilot environment to large-scale batch operations. This allows companies to build libraries of models for all their batch processes, starting in R&D where the optimization solution can be piloted and then scaled. And it should be MES and control system agnostic, yet be able to integrate with such systems via APIs, SDKs, and standard protocols such as OPC UA and MQTT supporting access to a variety of data sources and systems. At a minimum, it should run on both Azure and AWS, and be customizable using Python and other coding tools.

### *Capable of Closed-Loop Supervisory Control*

While most companies will start out optimizing in open-loop supervisory mode, where the operator approves and makes the changes in setpoints recommended by the system, the system should be capable of fully-closed-loop supervisory control, becoming an integral part of the overall manufacturing execution system. The idea is to drive toward autonomous batch operations.

### *Cost-Effective, Easy to License and Support*

The system should be cost-effective to allow scaling across a range of batch processes. Licensing should be simple, typically by the batch process, and not be encumbered by complicated arrangements such as tokens, or the number of users or interfaces. It should be available as a Software-as-a-Service (SaaS).

Finally, services should be available to train personnel and transfer the ability to use the platform to the acquiring company.

## Market Alternatives

What are the options in the market for addressing the batch optimization challenge?

First, let's remember that the status quo installation for most companies is typically an aging MES, which may or may not have univariate SPC, combined with the use of an offline statistics software package. Some vendors have upgraded their software to implement multivariate SPC, but this still falls well short of optimization. And ditto for some of the off-line software packages that can now be placed online.

A review of the newer MESs that can handle batch processing reveals that as of this writing, there are only one, maybe two vendors, who have the analytics capabilities that are even close to fulfilling the success elements. Unfortunately, this means one has to purchase the entire MES and/or associated control system to get these capabilities. Thus, for most existing facilities, this is not an option, likely would prove to be quite costly, and may not scale down to smaller processes, however valuable they may be.

We have already mentioned the new AI/ML-powered analysis tools that have come to market. They do a better job than the statistics-only packages but still don't optimize per se. They are under some pressure to expand their functionality to real-time control, but they would still fall short of all the elements. For now, we believe that they will "stay in their lane" providing process data analytics.

Next, we looked at several new manufacturing production optimization software solutions, be they implemented as a system or as a series of composable components designed to execute specific tasks. We found that the vast majority of the solutions are designed for continuous or discrete processes, and not batch. They could modify their offering for batch, but this has yet to happen substantially.

Finally, one has the option to DIY one's own solution, either using a software vendor who offers an analytics suite, contract a solution from an IT services firm, or developing in-house by the company itself. None of these are attractive in terms of cost, time to market, productization, and support.

So where is one to go? Where can we find a productized solution offered by a company with the domain knowledge to apply it successfully in batch operations?

## Introducing the Quartic.ai Operations Automation System

Quartic.ai is the best--class company offering an enterprise-scale AI platform that makes fully optimized manufacturing a reality for batch processes in the chemicals, life sciences, consumer product goods (CPG), and food and beverage industries.

Quartic's Batch Operations Automation system is unique in that it can combine machine learning and first principles models along with subject matter expertise to optimize batch manufacturing.

- Integrates every possible type of data source at enterprise scale and applies advanced data analytics to add context to your asset parameters.
- Develops accurate and insightful models, through automated AI, and gain insight into your manufacturing operations, with a high degree of accuracy and fidelity.
- Deploys readily available AI models or integrate your own AI models and predict the current and future state of your manufacturing operations.
- Provides visibility to and insight into the performance of the manufacturing process and its equipment, and explains the sources of variability.
- Predicts the optimal batch trajectory and recommends changes to control setpoints to achieve optimal results.
- Scales cost-effectively to any batch environment

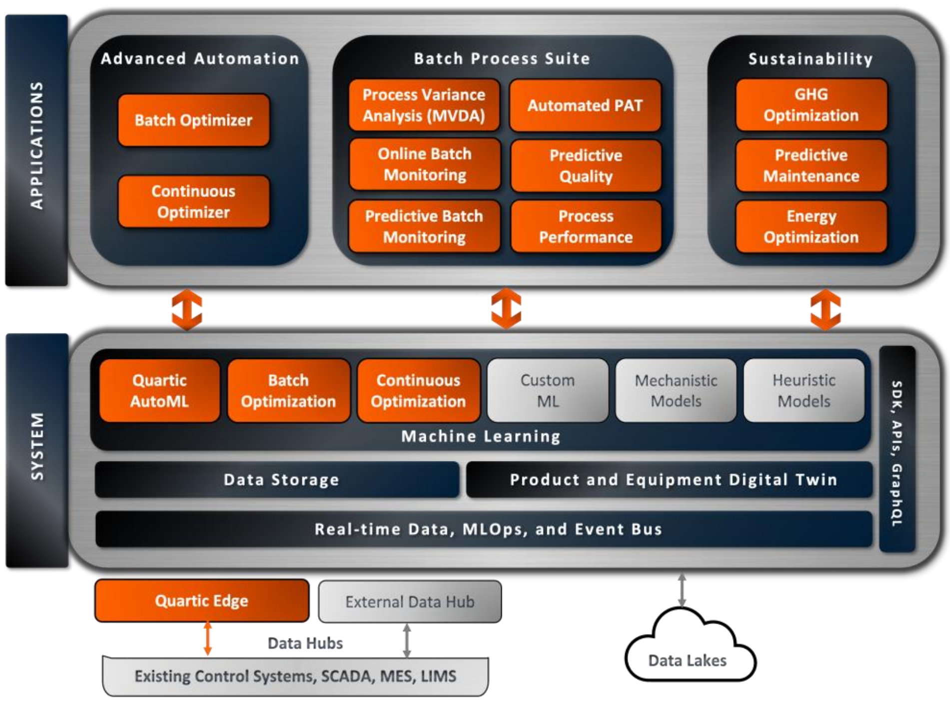


*Figure 4 - The Quartic Q.Platform*

To learn more about Quartic.ai and what it can do for your company, visit: https://www.quartic.ai/