WHITE PAPER

Title: What to consider when selecting a Production LIMS

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What to consider when selecting a Production LIMS

Abstract: The role of Production Laboratory Information Management Systems (Production LIMS) in providing data for Industry 4.0 technologies is gaining significant attention. This whitepaper delves into the unique challenges of collecting and managing sample data before outlining nine key considerations when selecting and implementing a Production LIMS.

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Introduction

Laboratory automation has been a theme in the cement industry since the commissioning of the first blend control systems in the 1970s. The first automated laboratories followed as cement plants sought to improve the consistency and quality of their analysis – and thus of their finished product.

In recent years, the Industrial Internet of Things, Cloud computing, artificial intelligence (AI), and machine learning have reshaped manufacturing. Known as Industry 4.0, this transformation has delivered various benefits for cement producers, including real-time decision-making, process, energy, and quality optimisation, predictive maintenance, and improved environmental performance. Against this background, cement plants are asking how their laboratories can support Industry 4.0.

The answer to this question lies in the fundamental building block of laboratory automation: the Production Laboratory Information Management System (Production LIMS). The reason for this is data. All Industry 4.0 systems require data; the higher the data quality, the better the Industry 4.0 outcomes will be. Because the Production LIMS collects, organises and tracks essential sample data in the cement laboratory, selecting an appropriate Production LIMS is critical to the cement industry's Industry 4.0 ambitions.

The second part of this paper will return to this point and consider key factors when selecting a Production LIMS. However, it will first be helpful to understand the complexities of LIMS and sample data as the context within which that selection sits.

Production LIMS vs Overall LIMS

Within the broader industrial context, different LIMS exist for different specialist applications, e.g., pharmaceutical laboratories, scientific laboratories, and commercial laboratories. However, when it comes to cement plants specifically, there are two LIMS to be aware of.

- Production LIMS: This is the primary Laboratory Information Management System on which laboratory automation systems are based and which receives data therefrom. Production LIMS specifically target the production laboratory environment, offering a set of LIMS features relevant to running many standardised routine samples every day.
- Overall systems, either in the form of an Overall LIMS (if managing laboratory data only) or a Plant Data Management system (PDM) (if combining process data and laboratory data).

Cement plants often separate LIMS functionality between the Production LIMS and the Overall LIMS / PDM system, which raises questions regarding system architecture (see further discussion below).

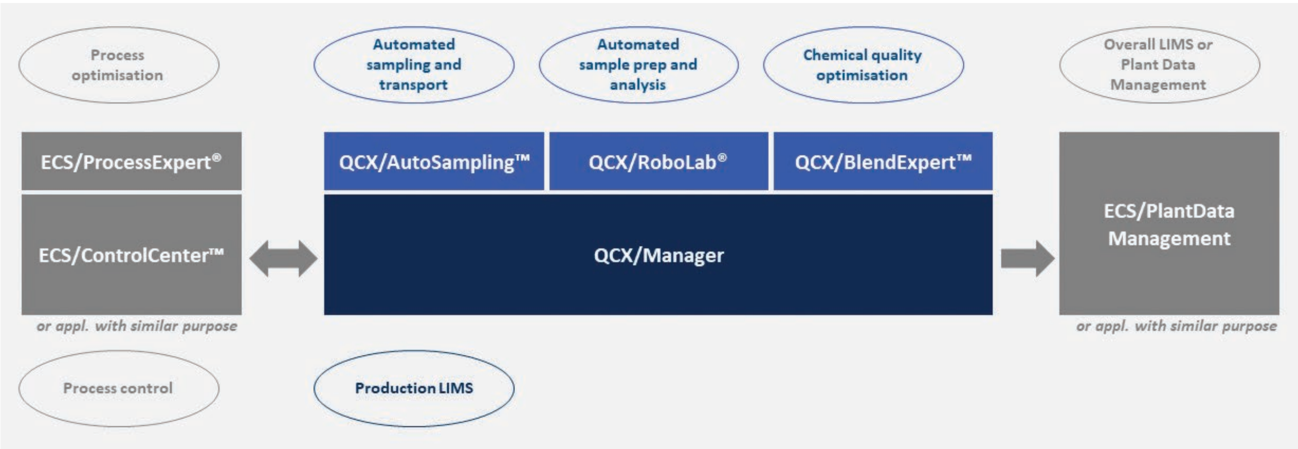


Figure 1: Typical cement plant software layout with process control system, Production LIMS, expert systems, and an overall plant data management system.

Sample data is not process data

There are two main points to be aware of when considering sample data:

- The methodology of sample data collection.
- The nature of sample data.

Sample data collection

Consider sample data's cousin: process data. Sensors in the plant automatically collect and send these data to the plant control system. This process is standard, consistent, and replicable and delivers data without human intervention. In contrast, sample data collection processes vary widely between cement plants and require different degrees of human intervention.

Fully automated sample collection, transportation, and analysis lie at one end of the scale. This delivers dependable, well-structured, accurate data but requires a higher initial investment. However, even in such highly automated systems, procedures outside the automated laboratory remain, requiring a degree of human intervention. Typical examples of actions that are difficult (or infeasible) to automate are setting time tests in the physical laboratory and various tests in the chemical laboratory. Compressive strength testing is an even more complex example involving mixing, moulding, curing, and testing at different ages up to 28 days.

At the other end of the scale are laboratories that still rely entirely or partly on manually operated processes, from sample collection and handling to operating laboratory equipment and data entry. This is labour-intensive and involves a substantial risk of human error creeping into the system. Whatever the level of laboratory automation, however, all sample data should feed into a common Production LIMS if these data are to support the effective use of Industry 4.0 technologies.

The nature of sample data

Consider, again, process data. This presents a regular time series, with measurements typically taken at equal intervals. Again, sample data is more complicated. Sample collection intervals may not be equal, and there may be lengthy delays between sampling and analysis. Samples are typically divided into multiple preparations and provide complex analysis results, where each sample may be analysed on multiple instruments, and each instrument may deliver multiple data values. Sample data also typically cover a production timespan and an underlying tonnage. All this means database structure and metadata are far more important considerations for sample data than for their process equivalent.

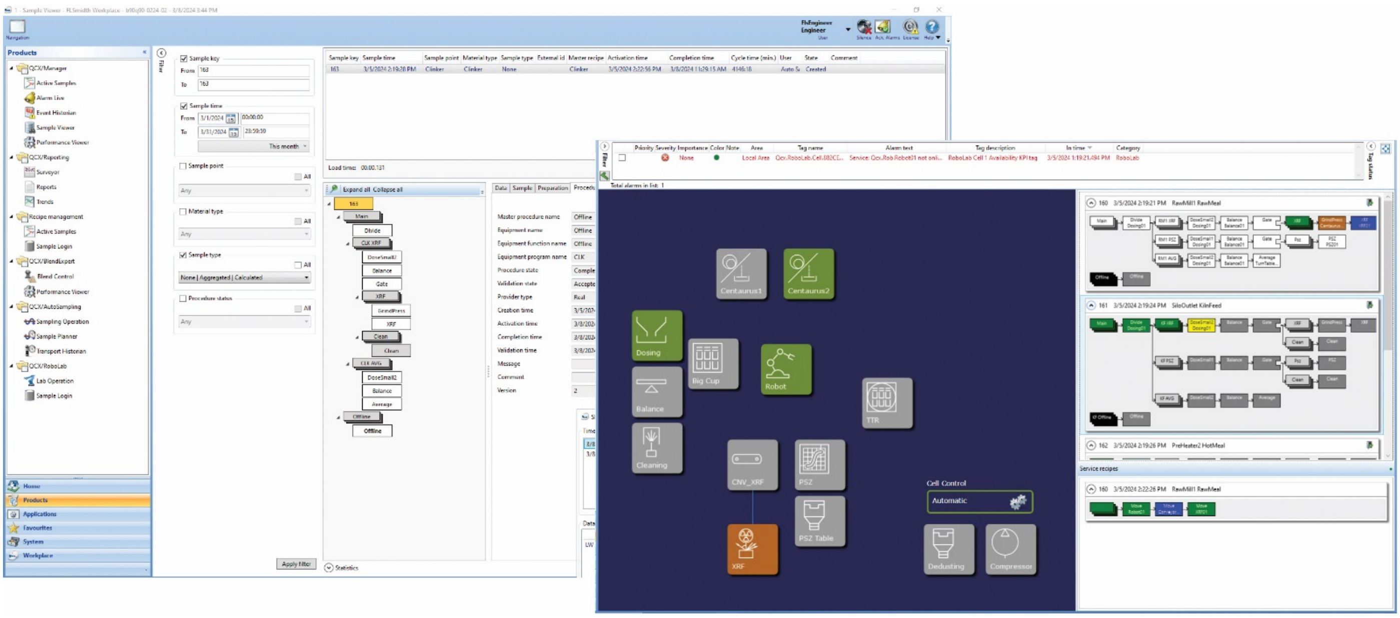


Figure 2. Production LIMS and laboratory automation hosted in a common software environment.

LIMS selection checklist

The authors have compiled the following checklist of considerations when planning and selecting a Production LIMS. The checklist is based on conversations with cement plants and the authors' multi-decade experience implementing laboratory systems in the cement industry. It is relevant for automatic and manual laboratory systems while also considering future Industry 4.0 requirements.

1) System architecture
2) Metadata
3) Sample database
4) Sample data integrity
5) User interfaces, reporting and trending
6) Export features
7) Online analysers
8) Equipment performance tracking
9) Initial and maintenance costs

1) System architecture

Cement plants with an automated laboratory will typically use a Production LIMS for recipe management, equipment control, and the acquisition of analysis results. This Production LIMS may be sufficient for smaller plants to cover all LIMS requirements. However, larger plants typically only use the Production LIMS at the front end, exporting sample data to an Overall LIMS or a PDM system. Such an overall system may cover a single plant or span several plants.

When the laboratory contains manual equipment, should this connect to the Production LIMS or feed results to the Overall LIMS / PDM system? For routine samples, the authors suggest linking to the Production LIMS, as the Production LIMS will already know about and have fully defined the sample in the sample database (as it is likely to be a subsample of a sample scheduled automatically).

Whatever the decision, it is essential to ensure every sample is unambiguously identified across both the Production LIMS and the Overall LIMS / PDM system via a unique sample key. When samples are scheduled automatically, it is easiest for the automated system to assign these keys to every new sample scheduled. In most Production LIMS, the keys will be a number that increases by one for every new sample scheduled throughout the lifetime of the systems. The Overall LIMS / PDM system may reuse the keys from the Production LIMS as-is, extend them with a prefix, or generate another numerical key, which links to the Production LIMS via a cross-referenced list.

Finally, but crucially, sample and process data must be accessible to optimisation software solutions via effective export functionality and a well-considered data infrastructure. This is true regardless of whether the optimisation solutions are based on AI or other technologies and whether they are standard products or more experimental and site-specific trial systems.

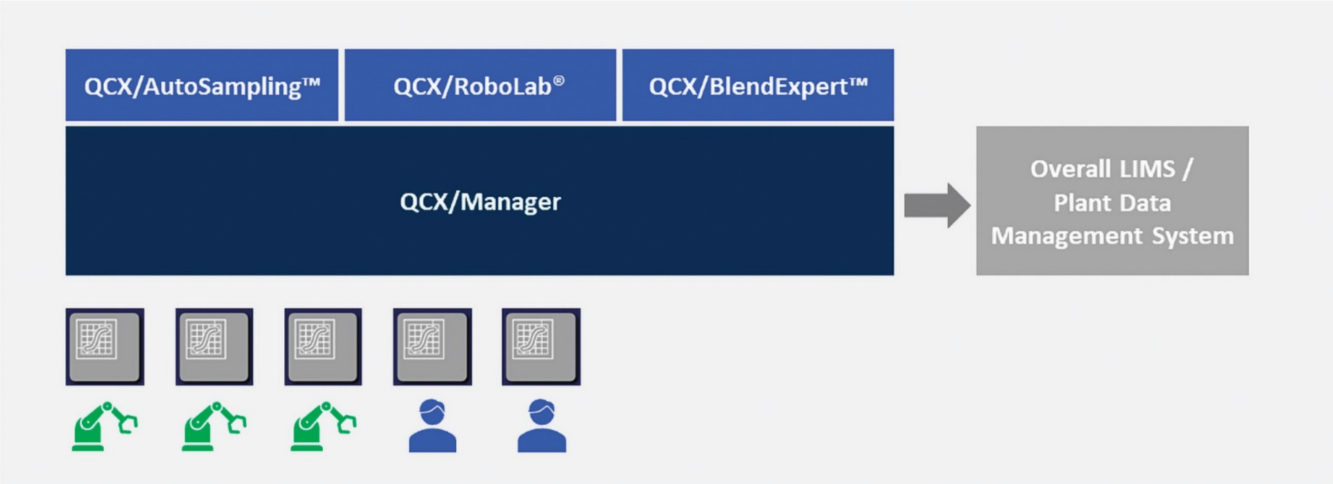


Figure 3. Manual laboratory equipment connected to the Production LIMS.

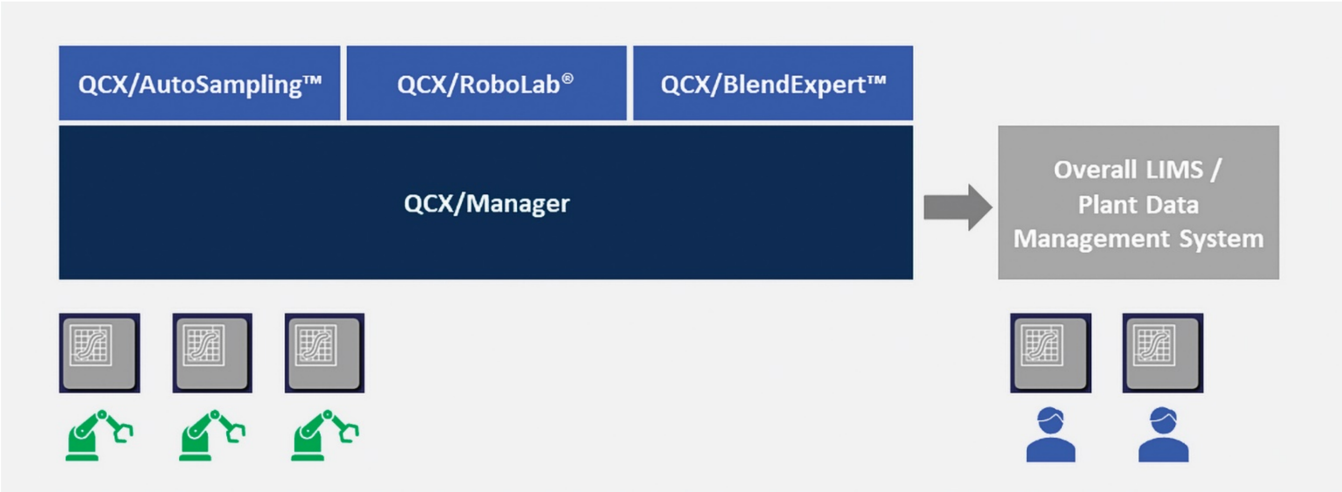


Figure 4. Manual laboratory equipment connected to the Overall LIMS or Plant Data Management system.

2) Metadata

Metadata are data about data. When it comes to sample data, significant metadata include:

- Sample time: the time and date of sample extraction.
- Sample point: the process location where the sample was extracted, e.g. Cement Mill 2.
- Material type: the product produced when the sample was extracted, e.g., 'CEM III A.

However, this is far from a complete list. Additional sample-related metadata include when the sample arrived at the laboratory and when the analysis occurred, while metadata for manually introduced samples (manually input) may include batch number or truck ID.

When considering the specific analyses each sample undergoes, most analysers provide additional relevant metadata, e.g., the analytical program used. Further, and especially for systems that span several sites, it may be beneficial to record analyser-specific metadata, such as instrument make, model, serial number, calibration date, and a free-text field with additional calibration info.

All these metadata are valuable when managing sample data and may gain even more significance when implementing Industry 4.0 solutions. Deciding how they are handled is thus a crucial factor in planning and implementing a Production LIMS, which should be able to manage metadata gracefully and make them available alongside sample data through data export features.

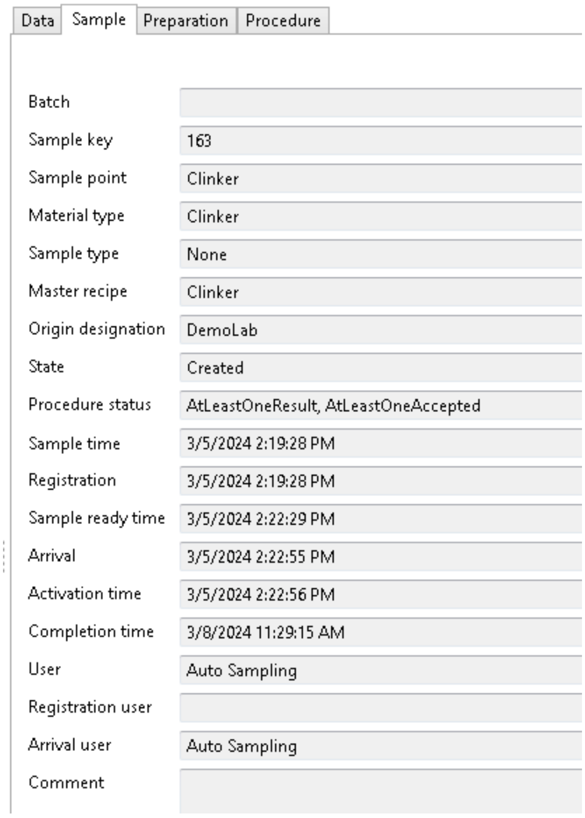


Figure 5. Example of sample-related metadata.

3) Sample database

As mentioned, sample data are far more complex than traditional time-series process data. This triggers specific requirements for the sample database's structure in a Production LIMS, most notably whether samples are stored in a flat or hierarchical database.

In the author's experience, a Production LIMS in an automated laboratory environment works best when mimicking the real world, e.g., implemented as a hierarchical database with a main sample and preparations. This provides an intuitive and direct relationship between the recipe, which controls how the main sample and subsamples propagate through the laboratory and the sample database, which stores the results and metadata. The authors have also found it helpful to adopt a similar principle for results from manually operated equipment.

Laboratories that export sample data to an Overall LIMS or PDM system typically prefer to convert to a flat data structure during the export. Although this makes sense in terms of simplicity, it does result in a loss of detail. An extended data storage horizon in the Production LIMS may make sense here, so the full details remain available in the primary system.

How long should the Production LIMS store data? When data is exported to an Overall LIMS or PDM system, the authors consider three months sufficient. When plants operate a Production LIMS only, two years is usually adequate, as PDF reports will be generated along the way and remain available for long-term documentation. However, these guidelines may change as documentation/reporting requirements evolve and the need for sample data as the basis for AI increases. It is thus realistic to expect future data preservation requirements of 10 years or more.

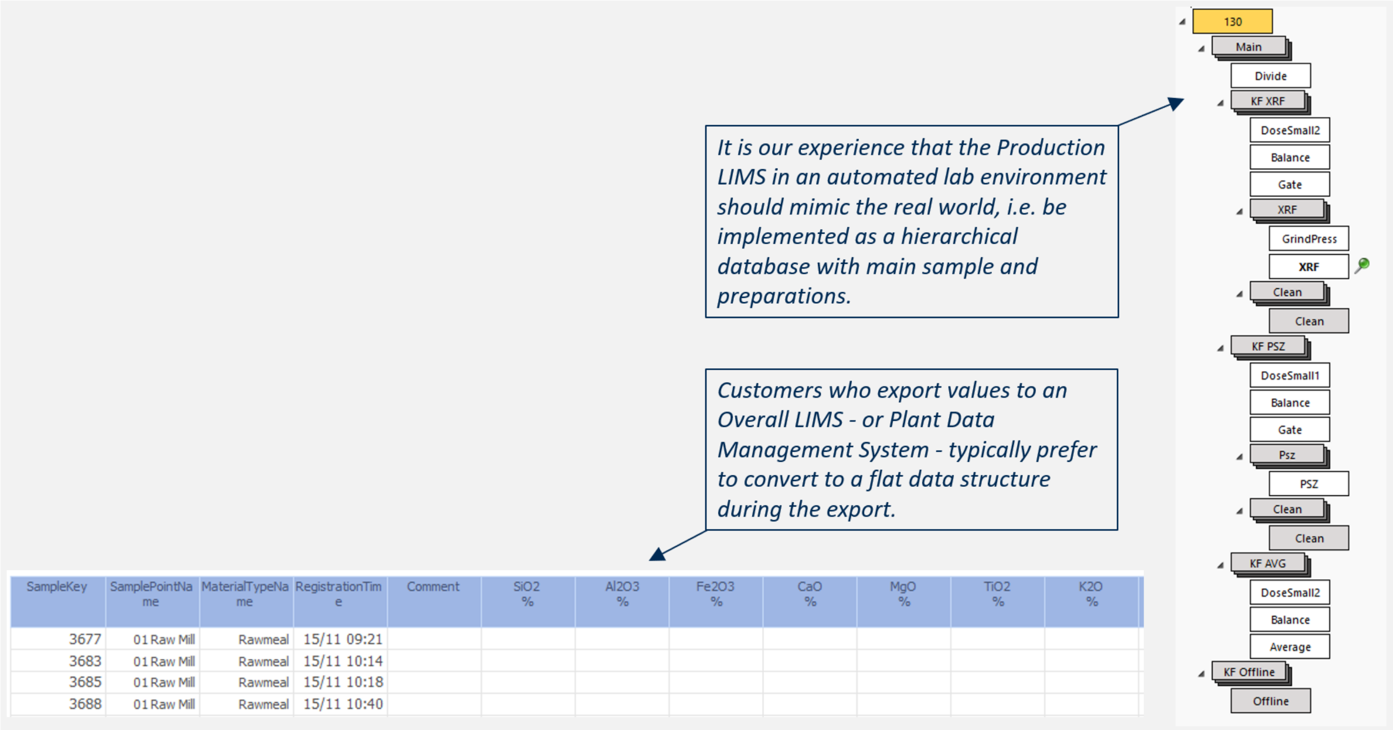


Figure 6. Hierarchical vs. flat database structure.

4) Sample data integrity

Next for consideration are the features required to ensure sufficient sample data integrity. For example, should it be possible to remeasure a sample without overwriting the original sample data? Furthermore, should the Production LIMS provide an audit trail to track who accepted a sample, invoked a remeasurement, or changed an analysis result?

Many LIMS packages offer an audit trail or change log, which documents all user activities influencing the sample data. While this is essential in some industries (e.g., pharmaceutical laboratories) due to regulation, it is typically a lower priority for cement plant laboratories; however, the authors expect this to change as documentation requirements increase in future.

While this information is undoubtedly useful, an audit trail comes at a price. User rights and passwords must be carefully managed—not only during the commissioning of the Production LIMS but also during everyday use. Detailed tracking of user actions necessitates more restricted user rights, with operators required to provide credentials whenever they perform an action affecting sample data. The days of the single operator station, with a generic lab user continuously logged in, are gone.

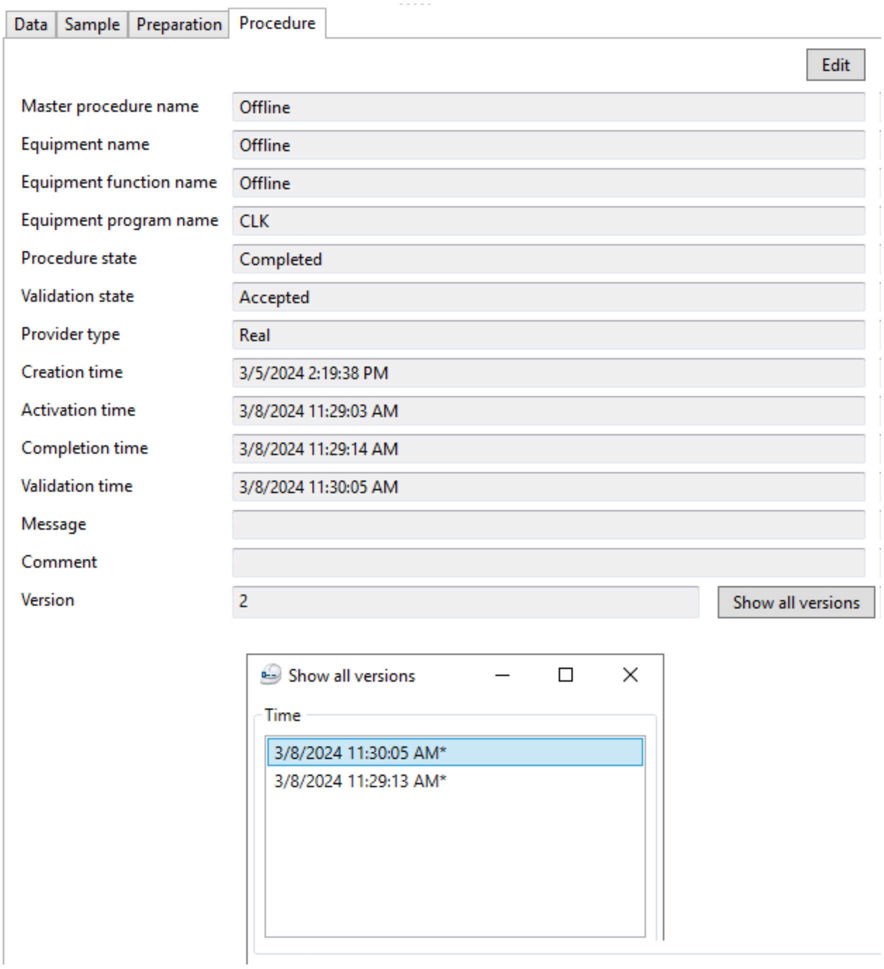
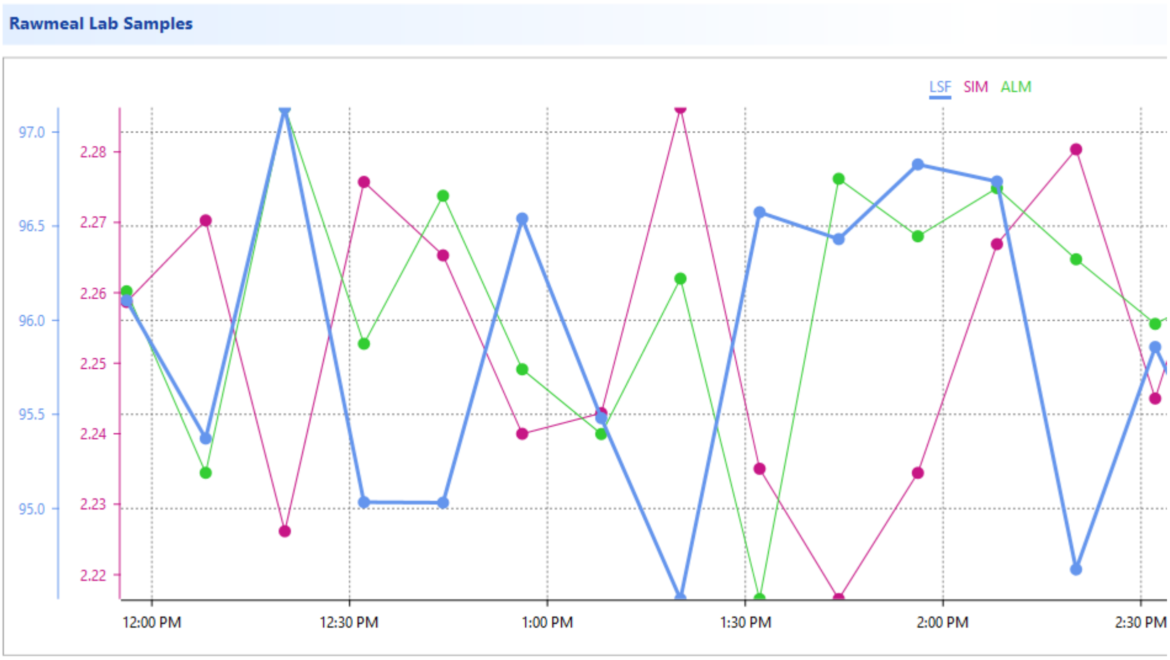


Figure 7. One sample, measured twice, with both results available.

5) User interfaces, reporting and trending

The question of user interfaces may seem basic, but it is integral to facilitating reliable and accurate system use. The basic requirements will include a sample viewer and reporting and trending functions, which are viewable on-screen and via PDF export. For the latter, the Production LIMS may offer scheduled, automatic PDF report generation in addition to on-demand creation; it may also allow emailing PDFs to relevant contacts within the organisation. Remote access, e.g., in the plant control room for live monitoring of critical production and quality data, could be another interesting feature.



Sample key	Sampling time	Si	Al	Fe	Ca	LSF	SIM	ALM	Limestone %
4935	3/8/2024 3:44:04 PM	13.4	3.10	2.81	41.0	95.28	2.27	1.10	57.31
4922	3/8/2024 3:32:04 PM	13.3	3.10	2.83	41.2	96.43	2.24	1.09	54.99
4909	3/8/2024 3:20:04 PM	13.4	3.09	2.82	41.3	96.21	2.26	1.10	58.12
4896	3/8/2024 3:08:04 PM	13.3	3.11	2.81	41.1	96.37	2.24	1.11	55.99
4883	3/8/2024 2:56:04 PM	13.2	3.09	2.82	41.1	96.67	2.24	1.10	58.76
4870	3/8/2024 2:44:04 PM	13.5	3.11	2.81	41.1	94.98	2.28	1.10	55.09
4857	3/8/2024 2:32:04 PM	13.4	3.12	2.83	41.2	95.86	2.25	1.10	55.95

Figure 8. User interface for live production and quality data monitoring in the control room.

6) Export features

Sample data provide no value when left in the Production LIMS. It is thus vital to consider data export requirements. These will include what systems the Production LIMS will export to (e.g., Overall LIMS, PDM system, control room, optimisation software packages) and the required export format (e.g., XML, CSV, Microsoft Excel, direct database link).

It is equally important to consider the structure of the exported data. These will typically fall into one of these three categories:

a) **Tag-oriented:** Sample data are exported from the Production LIMS as tags (e.g., via OPC), typically with one tag per sample-point/material-type/analysis-item combination (or sample-point/material-type/calculated-value combination). The received values are handled as time-series signals and do not include sample-related metadata. While this approach may be acceptable for real-time display, e.g. in a control room, it will usually be too rudimentary for export to an Overall LIMS or PDM system.
b) **Sample-oriented, flattened structure**: Sample data and metadata are exported from the Production LIMS in a sample-centric format. Each sample is represented by a flat record that contains all relevant sample information (e.g. sample key, time sample taken, analysis items, calculated values, etc.). This is the preferred format for export to most Overall LIMS and PDM systems.
c) **Sample-oriented, full hierarchical structure:** This is like (b), but data are exported in the full hierarchical structure of the Production LIMS. This format increases the complexity on the receiving side and is, in most cases, considered overkill today. However, the authors believe this could change as requirements for access to complete, detailed information in the overall systems increase.

When implementing a new Production LIMS that will export to an existing system, it may be an appropriate time to change or fine-tune the interface. It is also important to consider potential future requirements to futureproof the Production LIMS.

```
          <MatName>Silica </MatName>
        </xsl:when>
        <xsl:when test=".='Silica Sand'">
          <MatName>Silica Sand</MatName>
        </xsl:when>
        <xsl:otherwise>
          <MatName>
            <xsl:value-of select="." />
          </MatName>
        </xsl:otherwise>
      </xsl:choose>
    </xsl:template>
    <!-- Site Specials -->
    <!-- Translation from QCX MaterialTypeName to KM MatName -->
    <!-- If not found QCX MaterialTypeName is send as KM MatName -->
    <xsl:template match="SamplePointName">
      <xsl:choose>
        <xsl:when test=".='Cl_3'">
          <LocName>Clinker #3 Hourly</LocName>
        </xsl:when>
        <xsl:when test=".='Cl_4'">
          <LocName>Clinker #4 Hourly</LocName>
        </xsl:when>
        <xsl:when test=".='FM 1'">
          <LocName>FM1 Hourly</LocName>
        </xsl:when>
        <xsl:when test=".='FM 2'">
          <LocName>FM2 2Hourly</LocName>
        </xsl:when>
```

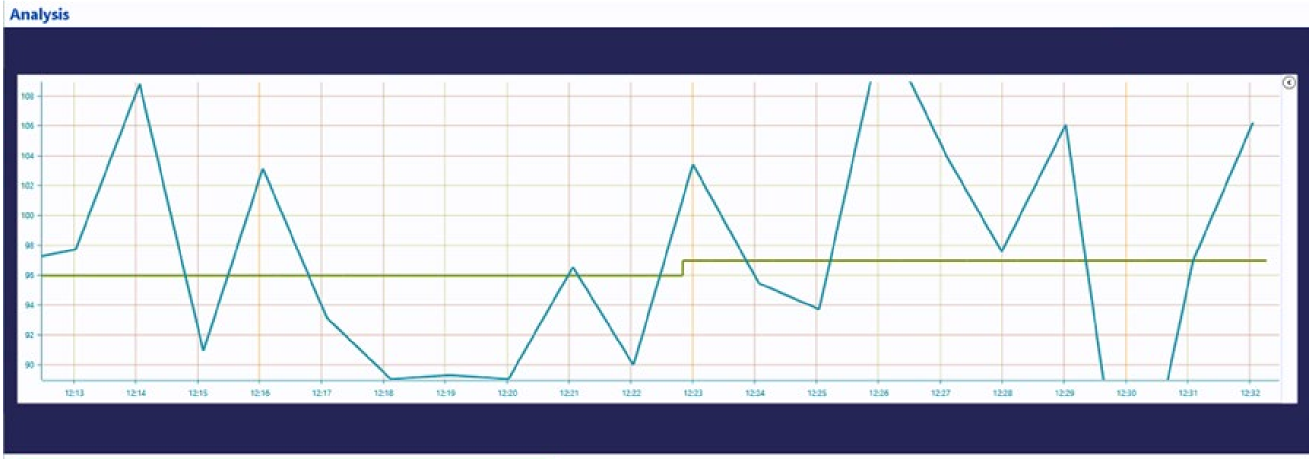
Figure 9. XSLT is a powerful tool for customising the format of XML export files.

7) Online analysers

Online analysers are becoming increasingly prominent in the cement industry. Located near the sampling point, such analysers provide results faster and more frequently than traditional centralised systems. The trade-off is lower accuracy; however, the right software can counter this by implementing dynamic calibration based on more accurate but less frequent results from the central laboratory. This way, it is possible to create results that deliver the best of both worlds, boosting the performance of optimisation software packages.

A pivotal point is whether online analysers should connect to the process control system or the Production LIMS. The answer is not always straightforward and often depends on how a plant uses its online analysers.

The authors believe that online analysers used for *chemical quality optimisation*, e.g., online XRF, PGNAA, or PFTNA analysis, should connect to the Production LIMS, as such equipment typically relies on the dynamic calibration noted above. The Production LIMS is where online and central laboratory results most obviously meet, and this dynamic calibration can occur. On the other hand, it makes more sense to connect online analysers used for *process optimisation* to the process control and optimisation system. Typical exceptions here would be cases where dynamic calibration based on central laboratory analysis is needed or where there is a desire to store online results alongside central laboratory data in the Production LIMS.



Item	Raw	Corrected	Aggregated	Current Account	Last Account	Last Reference	Bias
Timestamp	12:32:02 16-01-2023	12:32:02 16-01-2023	12:32:02 16-01-2023	12:32:05 16-01-2023	12:21:57 16-01-2023	12:21:53 16-01-2023	12:23:11 16-01-2023
SiO2	11.2 %	12.2 %	12.2 %	13.3 %	13.7 %	13.4 %	-1.0
Al2O3	2.65 %	3.17 %	3.17 %	3.21 %	3.15 %	3.09 %	-0.52
Fe2O3	2.92 %	2.72 %	2.72 %	2.68 %	2.40 %	2.50 %	0.20
CaO	43.5 %	42.2 %	42.2 %	41.9 %	41.9 %	41.5 %	1.4
MgO	0.584 %	0.582 %	0.582 %	0.728 %	0.936 %	0.892 %	0.002
LSF	119.88	106.23	106.23	97.70	96.24	97.15	-
SIM	2.01	2.07	2.07	2.27	2.46	2.39	-
ALM	0.91	1.16	1.16	1.20	1.31	1.23	-

Figure 10. Dynamic calibration, aggregation, and monitoring for online analysers.

8) Equipment performance tracking

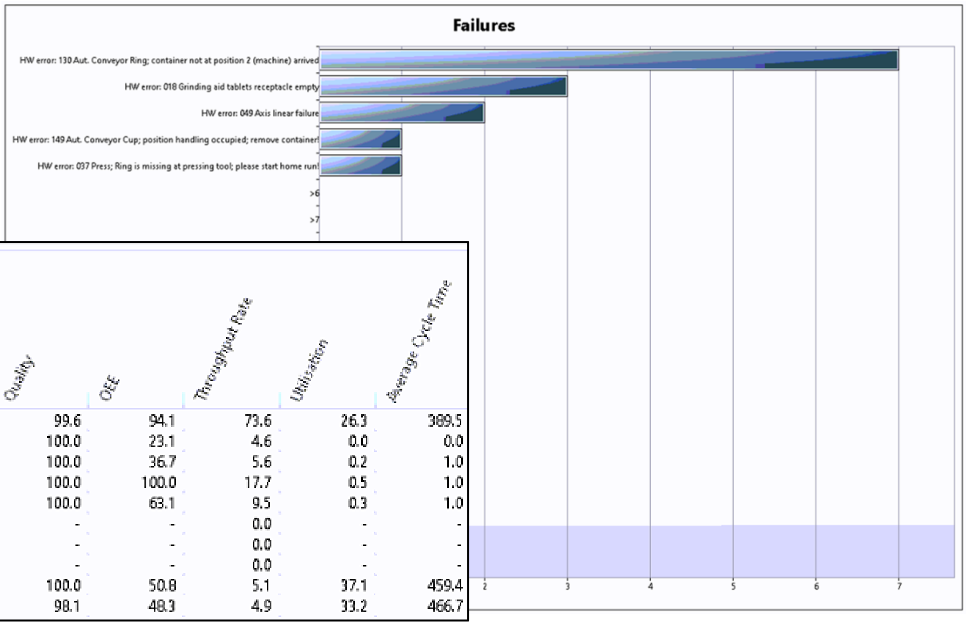
Tracking equipment status and performance is an increasingly valuable tool for securing uptime and ensuring efficient use of equipment.

- **Status monitoring** typically provides a live view of the operational status of all connected equipment, e.g., ready, operating, waiting, or unavailable. It may also indicate information on equipment failures and warnings. In its simplest form, changes to the colour/shape of icons on an overview picture indicate changes to equipment status. In more advanced forms, faceplates or sub-screens provide much more detailed information.

Figure 11. Status monitoring. The basic system indicates status via colour-changing symbols (left). More advanced systems include detailed faceplates (right).

- **Equipment performance monitoring** takes status monitoring a step further. Recording equipment status over time makes it possible to display a more comprehensive selection of performance metrics, often as key performance indicators (KPIs), e.g., availability, good samples, bad samples, throughput, and sample processing time. More advanced statistics also now play a role, e.g., a failure top ten that lists the most frequent equipment failures over a specific period. This has proven to be a simple yet valuable tool for root-cause downtime investigation.

While some Production LIMS have integrated features to monitor equipment performance, others require an external system to manage such monitoring.



	Availability	Performance	Quality	OEE	Throughput Rate	Utilisation	Average Cycle Time
RoboLab Preparation Cell	94.4	100.0	99.6	94.1	73.6	26.3	389.5
AverageRack01	100.0	23.1	100.0	23.1	4.6	0.0	0.0
Balance01	98.9	37.1	100.0	36.7	5.6	0.2	1.0
Balance02	100.0	100.0	100.0	100.0	17.7	0.5	1.0
Balance03	99.4	63.4	100.0	63.1	9.5	0.3	1.0
BigCupStock01	100.0	-	-	-	0.0	-	-
BigCupStock02	100.0	-	-	-	0.0	-	-
BigCupStock03	100.0	-	-	-	0.0	-	-
Centaurus01	100.0	50.8	100.0	50.8	5.1	37.1	459.4
Centaurus02	98.7	49.9	98.1	48.3	4.9	33.2	466.7

Figure 12. Equipment performance monitor showing typical KPIs and a list of most frequent equipment failures.

Regardless of the LIMS's capabilities, an obvious limitation arises when not all equipment can report status information in real-time via a remote-control interface—a prerequisite for capturing meaningful performance metrics. In the authors' experience, equipment designed for automatic sample handling often provides relevant functionality, while equipment designed for manual sample handling often does not. However, this is a generalised statement, and the authors would always recommend investigating the remote capabilities of specific equipment options.

9) Initial and maintenance costs

A final consideration concerns initial investment and ongoing annual maintenance costs. Influencing factors include initial implementation costs, flexibility, future maintenance, and software licences.

- Initial cost: The cost of the software package is an obvious and important parameter. So, too, is the cost of implementation. For example, will the system need to be programmed for the application, or does it come with out-of-the-box functionality? How does this impact implementation time? What configuration and set-up will the vendor provide, and what must plant staff manage themselves between initial commissioning and full operation?
- Maintenance: It is difficult to estimate the exact maintenance costs for a Production LIMS; however, there are questions to ask up front that can provide an idea:
    - Can only the vendor change configurations/add equipment, or can the customer do this?
    - Is it possible to create communications scripts to interface with new equipment?
    - Can sample recipes be changed on the fly, or are they hard coded in the system?
- Software licences: As in other industries, cement is moving toward a subscription model for software. This is because software must update regularly to stay safe and secure and to benefit from improvements and new features. Software subscriptions manage these updates as predictable OPEX items rather than major CAPEX projects every n^{th} year. However, for crucial plant operations, such as the Production LIMS, plants may not accept running on ‘rented’ software; then, an alternative hybrid route is a perpetual licence backed by an ongoing software maintenance agreement.

Conclusion

Production LIMS play a vital role in the front-end acquisition and storage of sample data at cement plants. However, we expect this role to become increasingly important as the need for detailed and well-structured data grows to support Industry 4.0 advances. Careful planning and selection of the sample data infrastructure—considering the above considerations—is thus essential to supporting Industry 4.0 goals.

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