

Introduction

Chemical Labs are Overdue for Digital Transformation

Chemical labs are critical to every aspect of manufacturing, from R&D through scaleup to operations. While manufacturers have continuously improved product quality and manufacturing productivity through continuous improvement and digital transformation, the lab is often left out of these initiatives. That leaves lab managers with a patchwork of solutions and disjointed processes that burden scientists and technicians with non-value-added work. Poorly integrated lab environments take highly trained lab resources away from innovating and slow down product development, product launch, and product release.

It's time to get the most out of the lab through continued digital transformation. We've identified five dimensions to measure and improve lab integration to optimize lab operations and enhance overall business performance. These dimensions include better integration between people, process, and technology in the lab, including integration of systems around a common data model. We'll look at each of the dimensions in detail and discuss how taking a platform approach helps achieve them.





Table of Contents



The Value of an Integrated Lab Environment

PAGE

The Five Dimensions of Lab Integration

People

Process

Software

Hardware

Data

Next Steps

Acknowledgments 12



The Value of an Integrated Lab Environment

The Challenges of the Status Quo

Before discussing the dimensions of lab integration, let's put them in the context of driving company value through speed, agility, and profitability. The current patchwork state of most labs negatively impacts lab productivity and performance. Even companies that have invested in new lab automation and advanced technologies often struggle with the impacts of poor integration, particularly as they try to become more datacentric.

Disconnected lab environments are characterized by too much non-value-added time entering, transcribing, and finding data. Manual data entry and "copy and paste" approaches lead to poor data quality but, more importantly, a lack of trust in the veracity of the information. When scientists can't trust data, they are more likely to delay approvals, reports, or certificates of analysis (COA) as they verify or duplicate experiments.

The Business Value of Integration

More integration, on the other hand, leads to greater efficiency and fewer mistakes. In turn, it also creates a more reliable digital thread of data that scientists can quickly verify and trust. This allows them to leverage that data for downstream work or reuse it for their own purposes, which increases productivity and leads to faster results and greater agility.

Faster, more productive labs create business value by allowing them to do more with less, freeing up highly valuable resources and allowing more time for innovation. This provides a strategic advantage that drives higher profitability across the product lifecycle through faster new product development, tech transfer, and product release.



The Five Dimensions of Lab Integration

People, Process, and Technology

What does it take to integrate and drive better lab – and business – performance? We've identified five focus areas companies can measure and improve against using a continuous improvement approach. You can look at these "dimensions" across a typical, balanced view of people, process, and technology. This framework provides a proven foundation for developing and introducing more mature operations to drive better outcomes.

Any change effort must start with the people involved. For labs, it's critical to get the most out of highly skilled scientists and technicians. They must be motivated, understand their contribution to the greater cause, and be enabled to collaborate to streamline work, data flows, and innovation. Operator data is also critical to creating a complete digital thread of scientific data.

This leads to process. Peoples' activities must be standardized and optimized into efficient workflows and analytical methods that get the most out of people's effort and create well-documented, trusted scientific data. Both physical and virtual processes, such as simulations, must be standardized and streamlined.

Segmenting the Technology Dimension

The third, fourth, and fifth areas relate to technology. Technology is too complex and too important to consider a single dimension. We'll look at how integrating software, hardware, and data significantly improves lab productivity, throughput, and value.

Acknowledging Overlaps

Note that there are clear overlaps between these areas. For example, trusted test results rely on hardware readings but also validated analytical methods executed by people with the right permissions and certifications. Despite these inherent overlaps, we try to discuss each without too much overlap to give them the attention they deserve.





1 – People



Top Performers have more mature, digital data sharing practices.¹

Enable Collaboration

Companies must integrate people across labs and the enterprise to create and leverage a trusted digital thread of data. Connecting people through an integrated environment enables collaboration in a variety of forms. Collaboration may start by sharing ideas within a team so they can build on findings through additional perspectives and analysis. But collaboration can also include sharing results across teams or creating a virtual team that includes remote labs and third parties such as contract laboratories. Improving tech transfer from R&D to production or across sites is also a high value form of collaboration.

Collaboration can also extend beyond the scientific community. For example, companies could digitally share data with regulators, either directly or by creating submissions in standard formats from underlying data. Even internally, companies may

connect the lab with product management upstream in R&D as results come in against target product specifications.

Enable Discovery

It's ideal to share results directly, but even small companies find it hard to know what happens in different parts of their business. People need to be able to discover the right people to connect to and collaborate with. For example, a team developing a product may be able to use assays or stability tests for ingredients used for an entirely different purpose if they have visibility to the work performed in the other lab. An integrated ecosystem can also allow a scientist to find someone who has done what they're trying to do to learn from their experience, even if they can't directly reuse their findings. Connecting people allows companies to uncover existing scientific insight and knowledge that may not be obvious from the data.



2 - Process

Standardize and Centralize Processes

The manufacturing industry has proven the value of standardizing, automating, and continuously improving processes to improve outcomes. The lab shouldn't be an exception. Science relies on repeatable lab methods, and companies may have invested in creating processes, SOPs, and analytical methods. Too often, however, scientific methods are standalone and don't create a continuous, digital flow of action and information. Creating streamlined, user-friendly workflows is a start, but it's also important to automate and capture procedure details as tasks are executed. This completes the digital thread, allowing experimental results to be shared and trusted because the approach is known, validated, and documented in an integrated way.

It's also important to remember that the lab doesn't exist in a silo. Lab operations should also be an integrated part of workflows that extend up and

down the product lifecycle. For example, test results should be routed appropriately to automate reviews and approvals. Creating digital process continuity from the lab lets companies provide data that is fit for purpose, for example, to validate claims, ensure product safety, or satisfy regulators.

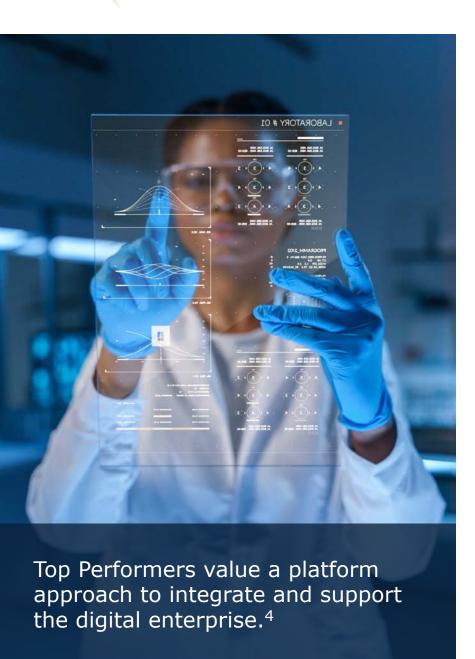
Include Virtual Processes

Not all processes happen in the lab. Many are performed in silico. Operations like modeling and simulating molecules, compounds, and processes should also be integrated into the broader lab environment. This allows companies to leverage physical and virtual test results combined with the audit trail necessary to trust the results. Processes may also span both virtual and physical realms, for example building a model to predict results, validating the simulation with actual tests, and then improving and reusing the model. Integrating physical and virtual processes, over time, allows scientists to conduct fewer wet experiments because models are more valid and supported by empirical data.

Top Performers have invested in more digital lab best practices such as consistent lab methods and processes across geographies and employing process automation.²



3 - Software



Enable the Lab with the Right Tools

Technology has multiple components including software, hardware, and data. Companies must integrate each as well as integrate them together across the technology stack. Integrating lab technology allows for digital continuity and creates a digital thread of information that companies can leverage across the enterprise.

First, it's essential to have the right solution capabilities to give the lab the right tools to do their iobs. Modern lab software should allow them to quickly find validated analytical methods so they can stop reinventing the wheel. Our research on improving lab performance shows that Top Performers are more likely to use specialized systems focused on R&D and the chemical lab, including LIMS, ELN, Chemical MDM, and Laboratory Execution.³ Having the right systems is important, but many companies are less hampered by a lack of systems. Instead, they struggle with multiple systems that do the

same job for different organizations or locations. For example, it's not uncommon for a company to have more than one LIMS and ELN, sometimes in the same lab, for different types of experiments.

Take a Platform Approach

Beyond simply having too many systems, companies typically have too many point solutions to support the lab. Each may provide value but requires scientists and operators to switch between systems and pull data from each to complete the full picture for their project. These standalone software solutions lead to disconnected workflows and pockets of data that aren't contextualized. On the other hand, a more integrated approach creates more harmonized processes and a common dataset that scientists can leverage for other purposes. For example, a single system integrates test results with validated methods and equipment calibration documentation to create efficiency and increase trust and reusability of the findings.



4 - Hardware

Integrate Lab Equipment

The lab is equipment intensive, and much of it is becoming automated. Modern lab equipment unlocks tremendous advantages from robotics and automation. For example, automation can allow scientists to accelerate and iterate repetitive tasks and experiments to optimize a recipe across a set of target parameters. However, companies commonly implement these technologies as islands of automation. To best leverage automated lab equipment, it must be connected and integrated to bring the physical environment into the digital thread.

At a minimum, integrating lab equipment eliminates the need for manually transcribing, copying and pasting, or transferring results via thumb drives. This is valuable even for simple equipment like scales or a pH meter. Connecting equipment eliminates NVA work and reduces opportunities for error, allowing the lab to do its science and have it automatically documented. Integration also enables scientists to capture experimental findings combined with other supporting data like digital signatures and important hardware information like processes, service records, and calibration.

Integrate Hardware into the Lab Ecosystem

Automating data collection saves time in the lab, but integrating across equipment provides even greater benefits. Integration should go beyond data capture from a single source. It should consolidate and contextualize data centrally and get data flowing securely. An integrated hardware ecosystem allows companies to capture test results alongside audit trail information to incorporate it into a cohesive digital thread of information. For example, results can be contextualized with other data like reagents, temperatures, validated equipment procedures, operator training details, and equipment calibration records so the results are trusted and reusable.

Integrating equipment further into the lab ecosystem extends the value by streamlining review processes downstream, allowing automated review and approval on an exception basis, knowing that scientists can trust the results.



5 - Data

Top Performers are 42% more likely to have fully captured and reusable knowledge.⁶



Digitalize Data, the Heart of Science

Data is the last dimension, but it is an underlying theme for all of the previous dimensions. That's no surprise because science is inherently data-driven. Our research suggests that data-centric labs have higher productivity and get more value from their data.⁷

Lab data can be a valuable corporate asset, but too much "dark data" is inaccessible and provides no value. Although most labs have moved from paper, most have not made the leap to fully digital data. Non-digital data like scanned information or data embedded in documents, spreadsheets, forms, files, or authoring tools that requires a human to interpret it is not readily retrieved and reusable. Companies must digitally capture, integrate, and contextualize lab data so they can leverage it strategically.

Top Performers are more than three times as likely to have "fully digital" data in the Lab than Others.9

Capture data in a Holistic Model

With technological advances like AI, digital data is becoming even more critical. For example, analytics can leverage scientific data to find correlations and insights that may not be obvious. However, the data has to be in a reusable state. Our research shows that difficulty correlating data from multiple sources is one of the most commonly reported challenges in the lab.8 Automation helps, but companies must also standardize how they store information. As an example, they should develop common taxonomies and ontologies for lab measurements and implement effective data governance to manage changes and consolidation over time.

A holistic, integrated data model is crucial, and companies can potentially base theirs on developing industry standards such as Pistoia or Allotrope. The goal is to create a deep scientific dataset to provide everything needed in context. This can support processes like submissions or release by exception because the data is organized and trusted. This data asset also creates an environment to drive further value from advanced analytics, AI, ML, and natural language processing.



Next Steps

Recognize the Opportunity

Today's lab environment is ripe for improvement. Most chemical labs' productivity hasn't continuously improved on par with other operations in the manufacturing enterprise. There is still too much inefficiency, inability to find and reuse data, and patchworks of solutions. Lack of integration leads to inefficiency, delays, and a lack of agility in the status quo. It's time to digitally transform and integrate the lab across people, process, and technology using a platform approach to speed up the lab and resulting product development, launch, and release.

Get Started

Ultimately, companies should integrate from ideation to production in the plant, creating a data continuum or digital thread with effective data governance across the product lifecycle. Most companies should start small. It's essential that they understand their starting point by objectively evaluating their capabilities and identifying what must be improved. But, they shouldn't expect to change everything at once and they don't have to reinvent the wheel; they can reuse existing methods and processes already developed. Further, they can extend these with simple, out-of-the-box methods.

Plan for Success

Lab managers have to look at increasing integration across people, process, and technology programmatically with an emphasis on data. It's critical to get management support for their effort and communicate the value in business terms. They must also make sure the lab is involved, sees the advantage for them, and feels empowered to make needed changes. It's important to recognize that this is a journey. Effectively updating people, process, and technology takes time. It's OK to start small but have a plan that leads to fully digital, integrated people, processes, and technology to drive speed and accuracy. But it's time to get started.



Acknowledgments



Jim Brown
President
Tech-Clarity, Inc.

About the Author

Jim Brown founded Tech-Clarity in 2002 and has over 30 years of experience in the manufacturing and software industries. Jim is an experienced researcher, author, and speaker and enjoys engaging with people with a passion to improve business performance through digital enterprise strategies and supporting software technology.

Jim is actively researching the impact of digital transformation and technology convergence in the manufacturing industries.









Tech-Clarity is an independent research firm dedicated to making the business value of technology clear. We analyze how companies improve innovation, product development, design, engineering, manufacturing, and service performance through the use of digital transformation, best practices, software technology, industrial automation, and IT services.

References

1-5, 9 Jim Brown, *The Digital Chemical Lab*, Tech-Clarity, 2018
7, 8 Julie Fraser, *Leveraging New Technology in the Lab*, Tech-Clarity, 2022

Copyright Notice Unauthorized use and/or duplication of this material without express and written permission from Tech-Clarity, Inc. is strictly prohibited. This eBook is licensed to Dassault Systèmes / https://www.3ds.com



