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SPEEDING UP THE PACE OF CHEMICAL RESEARCH AND DEVELOPMENT

WHITE PAPER

ACCELERATE NEW CHEMICAL DEVELOPMENT

Take the paper out of the lab to accelerate the pace of innovation by streamlining experimentation processes, thus creating process efficiencies and saving time and costs.

SPEEDING UP THE PACE OF CHEMICAL RESEARCH AND DEVELOPMENT

Today's chemical development labs are busy places that create fascinating new chemicals, new formulations and new products that boost the bottom line. But are these labs as efficient as they could be? Not if they're relying on legacy solutions that impede workflows, make it difficult to find and share data and hinder innovation.

This white paper examines the challenges impeding scientific innovation and ways to enable lab researchers to take their research to the next level, thus opening the way to new revenue streams for the organization.

CHEMICAL INDUSTRY SHIFT FROM BULK TO SPECIALIZED

Competitive pressure within the chemical industry is driving a move toward specialized chemical products that differentiate the organization from competitors in the bulk chemicals arena. Bulk chemicals are commodities that produce significant revenues, but specialized chemicals – particularly those protected with patents – are higher margin products and thus highly desirable products that can add significant value to the organization's raw materials.

Specialized chemical products have a market lifecycle, similar to any other product. Profit margins can be mapped against time as the product rises in popularity and use, then falls out of favor when it is replaced by other solutions. The objective therefore is to keep introducing more specialized products to continue generating high revenues in this lucrative area. The tactic to ensure a continuous flow of specialized products is to develop a continuous flow of sustainable innovation.

Sustainable innovation involves research activities, development activities and scale-up activities, each of which can encounter barriers to innovation that slow or halt promising experiments.

BARRIERS TO INNOVATION

Technology has had a tremendous impact on the lab, enabling ever more rapid and frequent experiments to be performed. Lab processes that defined and tracked groundbreaking research were developed, tested and formalized. The research lab emerged as the cornerstone for new chemical product development. Initially, order was imposed with paper lab notebooks that were closely guarded. Instruments were developed to perform ever more precise examinations. As computer technology became the norm, the lab adopted the new tools for research, including standalone software to run those instruments more efficiently and track the results. As technology became more complex, so did the lab's systems.

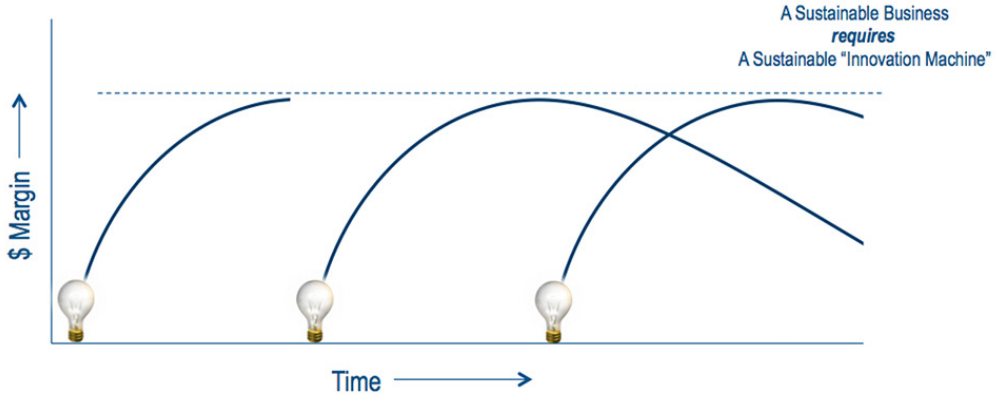

Figure 1: As products in the marketplace lose their competitive edge over time, profit margins erode as well. New product introduction through sustainable innovation processes enable businesses to keep the "innovation machine" flowing as new innovations enhance and replace previous ideas.

Now, what started as solutions that enabled innovation have often instead become barriers to innovation. Legacy solutions such as paper lab notebooks are causing workflow bottlenecks that impede experiment data access. Hybrid solutions such as aging in-house systems with limited features are often supported with spreadsheet data from different sources. None of these solutions are tied together, and seldom is the information they contain readily accessible or consistently formatted, making it difficult to find and use or re-use information. Data is tucked away in disconnected data silos, whether paper-based or standalone systems, that are time-consuming to search and access, resulting in frustration all around.

The technology in place no longer provides the advantages it used to. Legacy tools that were ground-breaking in their time can not accommodate the level of data sharing and collaboration now required for laboratories to function at maximum efficiency. While there are numerous challenges to innovation, seven key barriers top the list.

Barrier 1: Legacy Record-Keeping Systems

Lab researchers need to know what data is out there, and whether anyone has ever tried an experimental approach. But if scientists can't search and browse other researchers' experiments, that's a big barrier to innovation. Research organizations need to move beyond paper lab notebooks and develop the digital lab. For example, when paper lab notebooks are replaced with electronic lab notebooks, or ELNs, then data becomes instantly searchable by keyword, prior research can be quickly located and evaluated, and researchers can search across other experiments besides their own.

Barrier 2: Too Many Dead Ends in Exploratory Experiments

Along with the frustration of knowing that relevant data is hidden in notebooks, warehouses and other repositories, many exploratory experiments result in dead ends, wasting time and resources. If the researcher(s) had been able to factor in data from prior experiments, the research could have been better targeted to focus on ideas of merit. Physical experiments cost time and money. If ideas can be screened virtually, scientists can stop spending time and money on exploratory experiments that are essentially shots in the dark. With virtual screening, data can be enriched and examined before performing physical experiments.

What started as solutions that enabled innovation have often instead become barriers to innovation.

Barrier 3: Too Many Ideas with No Legs

Beyond repeating experiments that have previously been tried and discarded, there's another frustration: too many ideas with insufficient marketability. A potential line of research often sounds promising in theory, but in practice it just fizzles. For instance, an idea that appears promising in the lab might not scale up well in practice. Or, perhaps a toxic by-product results during manufacture that makes the product unsafe and therefore unfeasible. Time is wasted that could have been better spent if the lab possessed a reference database of the physical experiments that had previously been run. The ideal reference database could be searchable by material ingredients, processing parameters and other decision criteria. Even better would be the inclusion of visualization tools to help explore the highest potential hits of the search.

Barrier 4: Takes Too Long To Innovate

Once a promising research idea is found, product optimization often takes too long. Many research labs find themselves contending with many cycles of experimentation and each cycle takes longer than estimated. Innovation becomes a long, drawn-out process that saps creativity and enthusiasm. What's needed are fewer, faster experiment cycles, coupled with the ability to locate and trust previous experimental results. If data gathering and processing could be efficiently automated, process optimization and scientific innovation could be rapidly enhanced.

Barrier 5: Slow Evaluation of Scale-Up Recipes

Tracing scaled-up samples through all of the required product specification tests is typically a time consuming and manual copy-and-paste operation. Ensuring accuracy and precision during scale-up of recipes is slow and tedious. The entire process needs to be expedited, and can be with end-to-end digital definition of sample screening workflow, tracking of sample through product specification testing and one-click creation of complete product reports. Remove the 'speed bumps' from scale-up; eliminate manual cut-and-paste processes and expedite recipe evaluation.

Barrier 6: Inconsistent Chemical Inventory Management

Beyond the strategic processes listed above, a key tactical process impedes many research labs: inconsistent, inaccurate chemical inventory management. When a material is not available for research despite inventory reports that state the material is on site, research gets put on hold until material arrives. When the lab doesn't know exactly what chemicals are in inventory or where those materials are located, money is spent overbuying chemicals already on site or discarding expired materials that were misplaced. Worse, without accurate knowledge of chemical quantities on site, regulatory thresholds could be exceeded and regulatory reports could be inaccurate, subjecting the organization to noncompliance and potential safety issues and risk, including fines and legal action. Centralized chemical inventory management with built-in knowledge of hazardous substance requirements and one-click access to EH&S reports and safety data sheets can erase this aggravation.

Barrier 7: Lack of Flexible IT Solutions

Finally, where technology is used, it is often inflexible and limited in scope. Every group of scientists needs their data in a different way, but often the current IT system is too rigid to accommodate these needs. In many cases, the platform cannot accommodate research requirements that could streamline activities or the software tools are incompatible with the in-house IT system. This inability to accommodate the needs of the lab and IT is a huge barrier to innovation. What's needed is a flexible, scientifically aware data processing and reporting system with the ability to quickly build custom functionality and plug into other applications products that also address corporate IT goals and objectives.

The answer lies in transforming manual, legacy processes into real-time digital activities.

These seven barriers highlight the challenges to chemical development innovation. They include outdated workflows, tools and systems that get in the way of being efficient, productive and innovative. These legacy processes can be replaced with state-of-the-art digital solutions that streamline workflows, eliminate research roadblocks and set the lab onto a sustainable path fostering continuous innovation.

The answer lies in transforming manual, legacy processes into real-time digital activities. It means a focus on sustainability. It means accessing data in real-time – from published literature to prior experiments to current results – regardless of who performed the research. Once this access is available, companies effectively break down these barriers, streamline productivity and speed innovation.

BREAKING DOWN THE BARRIERS

The need is high for sustainable innovation to stay ahead of the competition and develop breakthroughs and new technologies.

Yet sustainable innovation is difficult to achieve when data deluge makes it difficult to find, manage and share data. Whether its old data or someone else's in the organization, the inability to easily search and browse experimental data is a big barrier to innovation.

Centralize Data in Digital Solutions

Research organizations that migrate data management to centralized systems achieve instant access to all experiment data. To collaborate effectively, scientists need to be able to easily search and browse prior research and related experiments. Time-consuming activities such as cutting and pasting materials and graphics into paper lab notebooks should be replaced with a single, centralized digital system that all researchers use.

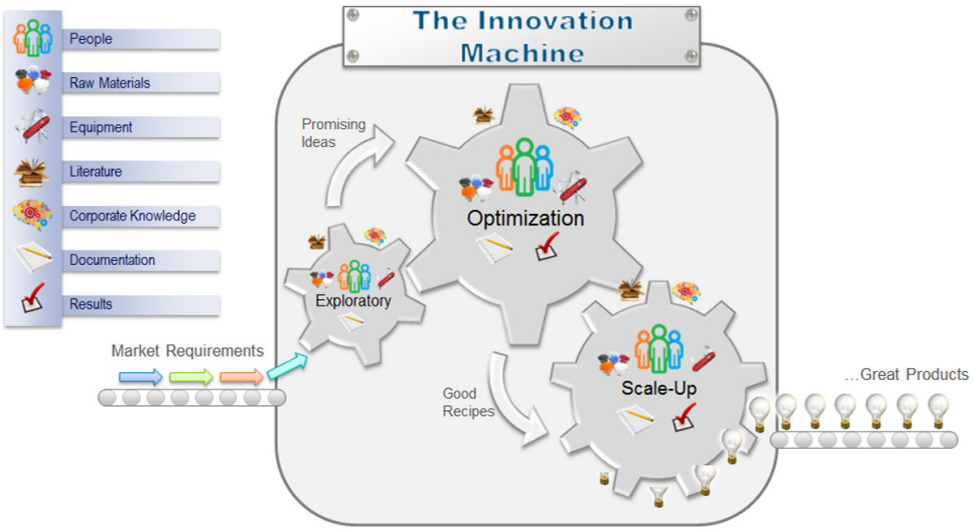

Figure 2. The combination of people, resources, research literature and testing tools used to streamline the three critical phases of experimentation -- exploratory, optimization and scale-up -- create the backbone of an organization's "Innovation Machine." The successful use of these variables throughout the experimentation phases can take thousands of disparate ideas and convert them into a manageable number of viable candidates – thereby reducing the time to innovate while developing only the best candidates that can scale up into production.

Share Data in a Secure Environment

A centralized digital system can deliver a secure environment where all data is consistently formatted, readily accessible and easy to read and report. Role-based access permissions make it possible to control who can view, access or change data. Data can be searched by keyword or any other parameter, putting relevant information on the researcher's desktop in seconds.

Once the data is centralized in a single system, intellectual property (IP) is protected and secure. Experiment data can be quickly accessed, examined and qualified. Ad hoc experiments, including both exploratory experiments and optimization experiments, are available for review. Reference data can be obtained and shared in a few quick keystrokes.

Access Past Experiment Data

A centralized digital system streamlines record-keeping processes so that all experiments related to a project are available from one place and stored permanently in a digital interface. Users can attach multiple file types to the record, such as PDFs, images, spreadsheets and documents, making it easy to manage large quantities of data and files.

Making experiment data available from a centralized source accelerates access to previous experiment data, enabling significant time savings. Scientists no longer waste time on dead-end theories and tests when they can rapidly search by material ingredients, processing parameters, results, genealogy and more.

Reduce the Number of Physical Experiments with Virtual Screening

Digital capabilities deliver the ability to perform virtual screening and thus greatly speed up the experimental process. Virtual screening saves significant time and money by enabling fewer physical experiments because data is enriched and examined first.

Collaboration Tools Enable Team Participation

Research labs aren't relying only on in-house scientists to develop products. Numerous other researchers may well be involved in the product research and development processes. These experts may be found within a single organization or at collaborating firms around the world. An ELN, for instance, can help promote multidisciplinary collaboration on projects by providing a central digital location to deposit data and communicate. Users can access the record in real-time through a web browser, thus avoiding time zone barriers to communication.

As research organizations develop new chemical products, developers may be concerned with how to protect their investment. An ELN provides the option to include e-signatures for signing and countersigning notebook entries with time/date stamps to support potential intellectual property disputes.

Shorten and Reduce Experiment Cycles

By incorporating a detailed structured database of past experiments and results into an ELN, researchers can avoid dead-end ideas and only explore the best possible ones with sophisticated searching and visualization tools. No more committing large amounts of time and money. Accelerate experiment cycles through automated data gathering and processing. Further, a database of past experiments enables fewer experiment cycles. You can also streamline the evaluation of scale-up recipes when the digital system delivers the ability to define sample screening workflows and track samples through complete one-click product reports.

Streamline Scale-up

Beyond exploratory experiments, a centralized system can streamline scale-up of the most promising ideas. While scale-up is very similar to optimization, researchers are optimizing for different criteria at this stage in the development of a new potential product. Despite only one sample to focus on, the data generated can still be significant and rapidly become unmanageable – particularly in the case of long-term testing conducted over several months. The data management can become more complicated when several different types of tests on the same product occur simultaneously. Advantages that can streamline workflows during scale-up include end-to-end tracking of product specification tests and complete product reports generated by a few keystrokes.

Leverage a Scientifically-Aware Data Processing and Reporting System

Lack of flexibility in existing IT solutions is a key barrier to innovation. Every group and scientist needs their data in a different way since each is pursuing different experiment parameters. This includes specialized needs for how data is viewed, how the data is manipulated and which protocols are used. When all the functionality resides in a centralized scientifically-aware data processing and reporting system, research teams and individual scientists alike have a framework that very quickly builds the requisite scientific tools.

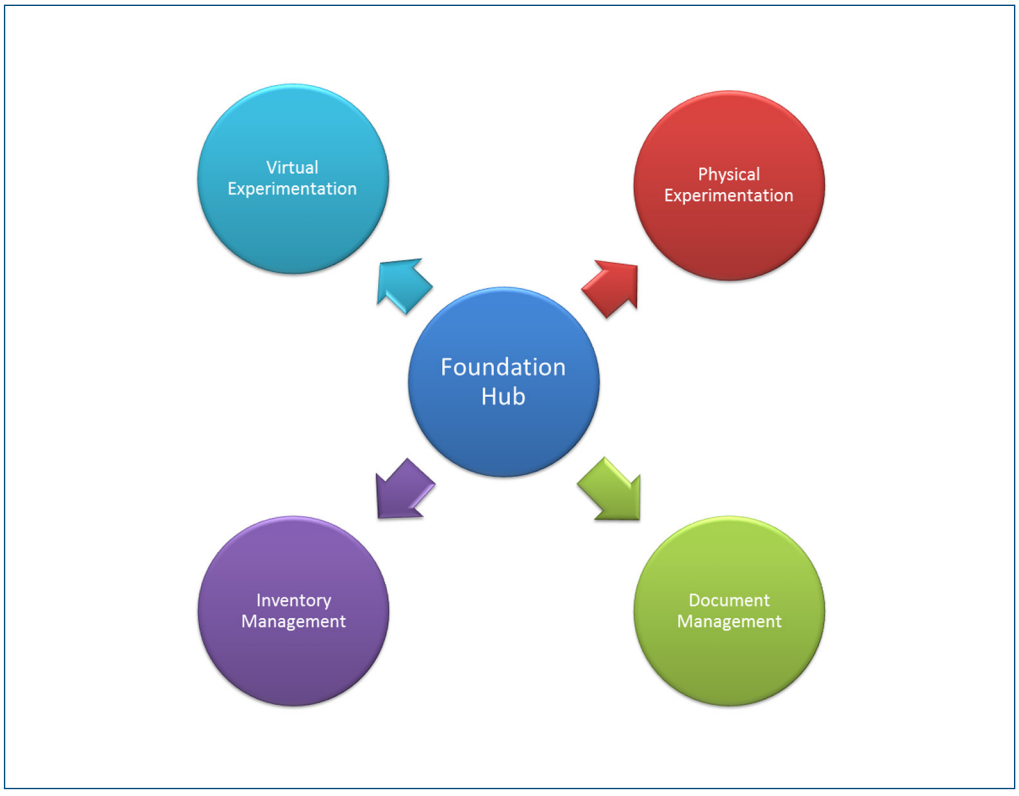

Figure 3. A centralized system for data processing and reporting enables integration with other important lab tools: virtual experimentation; physical experimentation; inventory management and document management. These tools provide powerful capabilities that improve lab performance and optimal lab efficiency.

SUMMARY

When product optimization takes too long because it takes too many cycles of experimentation and each cycle takes longer than it should, that process is broken. The fix is to implement a solution that enables fewer, faster experiment cycles along with the ability to find and trust previous experimental results. Such a system will provide automated data gathering and processing. In support of the system, a well-managed chemical inventory system can help keep research on schedule by expediting the search and procurement of raw materials. In short, capabilities like these expedite the pace of innovation.

When everyone in the lab can access data in real-time – whether published literature or prior experiments or current results or reagents on hand – barriers are removed, productivity improved and innovation enabled.

BIOVIA solutions deliver all of these functions and capabilities… replacing disparate, disconnected legacy systems with centralized electronic lab notebooks; providing instant access to data and experiments at collaborating research sites; enabling real-time document management; comprehensive chemical inventory management; optimized virtual experimentation and physical experimentation. Chemical organizations can confidently implement BIOVIA digital tools to speed up product innovation and boost lab productivity – all within an easy-to-use electronic workspace.

Learn more about specific BIOVIA solutions your chemical development lab can implement now. Request a no-obligation web demo at **http://www.3ds.com/products-services/biovia**.

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