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WHITEPAPER

# Digitalisation in Chemical Production and Process Environments in Flanders

## Why this whitepaper?

From the office's water cooler to innovation-themed webinars and corporate management meetings, digitalisation is on everyone's lips. Yet, digitalisation, or the digital transformation of industrial processes and operations, is not just a buzzword. It is a real revolution taking place across the globe.

In chemical production and process environments, however, the implementation of digital technologies isn't catching on as quickly as anticipated due to a range of sector-specific challenges and hurdles. This whitepaper seeks to highlight these challenges and provide an impetus for companies to overcome these hurdles. Throughout the whitepaper, you will find examples and concrete cases that aim to inform you about possible solutions and inspire you to successfully start, intensify or complete the digital transformation of your company.

Obviously, every company is unique. A one-size-fits-all approach to digitalisation does not exist. While this whitepaper focuses mainly on autonomous production process control, your company might consider moving into this area too complex as a first initiative. In this case, focussing on Operational Technologies equipment and operator-related digitalisation, which represent a lower barrier to entry to Industry 4.0, could be a good starting point. Nevertheless, this whitepaper aims to provide relevant information and inspiration to companies with different digital maturity levels. Moreover, since digitalisation is becoming quite common in discrete manufacturing, there are also more best practices available besides this whitepaper, both in literature and in market.

*This whitepaper was developed within the framework of the Catalisti innovation program Process Intensification and Transformation, which centres on the innovation of chemical processes. Consequently, this whitepaper focuses entirely on digitalisation in production and process environments, and does not discuss digitalisation in terms of HR, supply chains and/or logistics.*

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BASF: Perspectives on IoT sensors
Beaulieu: The importance of process insights
P&G: Digitalisation of the supply chain
Janssen: Advanced data analytics
Cronos: An integrator's perspective
Catalisti: A first digitalisation Catalisti ICON project

# A Revolutionary Shift

The strategic use of advanced digital technologies offers chemical companies broad benefits. Digitalisation fast-tracks innovation, increases productivity, spurs growth, and leads to more efficient and effective management practices. It also contributes to sustainability goals by enabling sustainable production: it allows for the reuse and recycling of chemicals and plastics, a decrease in waste generation, as well as a reduction in energy, solvent, water and/or raw material usage. In short, digitalisation delivers chemical companies a competitive edge on multiple fronts.

Today, many advanced digital technologies have reached a cost and performance level that enables their application in chemical production and process environments. Across the sector, cautious digitalisation steps can already be observed. For instance, companies are exploring and experimenting with certain digital technologies such as data-storing systems, high-performance computing, advanced analytics, 5G and increased levels of automation that lower the threshold for a digital transformation.

Yet, this does not represent the revolutionary shift necessary for a complete digital transformation of chemical production or process environments. Essentially, the adoption of other and specifically more complex digital technologies by the industry, associated with stages 4 to 6 of the Industry 4.0 (I4.0) development path (shown in Figure 1), is still lagging.

The ARC Advisory Group, a leading technology research and advisory firm, reported in 2019 that although more than 75% of companies in the chemical industry invest in digitalisation, less than 25% is moving beyond the pilot phase. These figures are confirmed by the Digital Maturity Model for chemical companies presented in the 2019 Deloitte study “Achieving the next frontier of chemical excellence”.

Although transformational technology is already available for the entire I4.0 development path, the main hurdle for chemical companies appears to relate to seizing the full potential of big data analytics. Identifying this potential is a first prerequisite for digitalising chemical process and production environments.

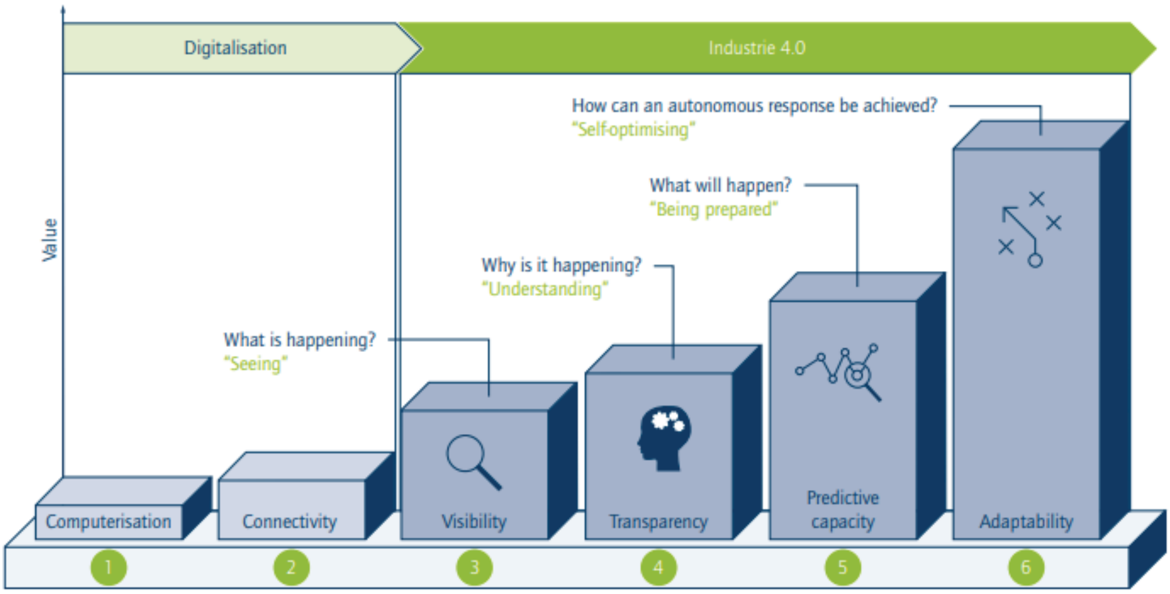


*Figure 1: Stages in the I4.0 development path (Source – Acatech I4.0 Maturity Index)*

# The Data Loop

**Transforming data into knowledge and actions**

The Industrial Internet of Things (IIoT) is expected to become a predominant tool in unlocking potential intelligence from the huge continuous data flows that can be captured. IIoT devices transmit data between connected equipment without human interference and can streamline many parts of industrial companies. Such data architecture, converting **physical information into digital records**, is associated with the first digital revolution (I3.0) that occurred in the latter half of the 20th century. Since then, the quantity of stored data has grown rapidly (so-called "big data"). Meanwhile, computing power has substantially increased and machine learning algorithms have continuously been optimized. These evolutions enabled a second digital revolution (I4.0), introducing a second conversion: from **digital knowledge to physical actions**.

Both the I3.0 and I4.0 conversions are reflected by the data loop in Figure 2. This constant loop includes data capture (generation and validation), data architecture (central data management) and advanced data analytics.

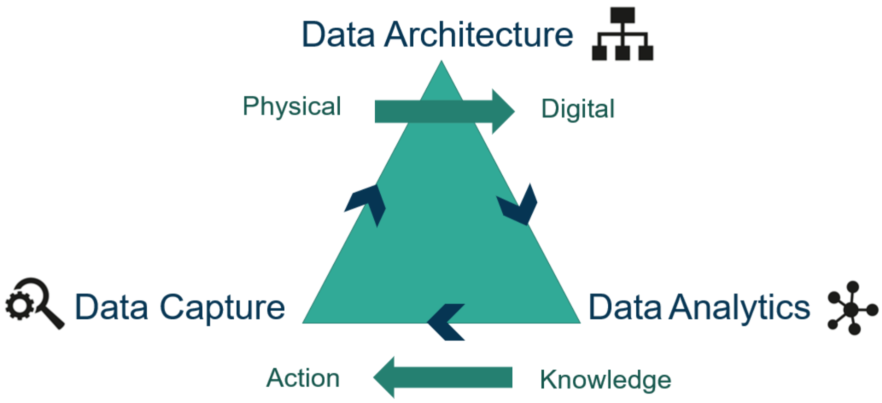


*Figure 2: Transforming data into knowledge and actions is key in gaining a competitive edge.*

Let us dive deeper into the challenges chemical companies encounter throughout the different stages of the data loop!

## 1. Data Capture

**Digitalisation of industrial processes requires the accessibility of large amounts of useful and accurate data to feed model-based algorithms.**

Correctly capturing data, that is where it all starts. Currently, many data sources exist in production and process environments. Data is captured, for example, by sensors, process control systems and maintenance activities. The way data is captured and validated has a major impact on the later implementation of data analytics and the generated knowledge leading to a physical action, as illustrated in Figure 2.

### Challenges

As **safety standards** in chemical processing are quite strict, the tolerance for error is low. The margin for making a wrong decision based on inaccurate data should always be minimal. Therefore, many chemical companies question how the accuracy of data capture technologies will impact safety, and specifically adherence to existing safety standards.

Secondly, companies cannot always rely on existing sensor technologies for capturing data, especially with respect to industrial processes that involve **challenging circumstances** (e.g. high speed, low concentrations, aggressive environments, inaccessible locations, etc.). For data capture on such processes, advanced inline/online sensing technologies are required. Unfortunately, these advanced technologies do not exist for all of the challenging and harsh environments present on Flemish production floors. Commercial sensing technologies are currently being developed and tested for some of these circumstances, but not necessarily for all specific environments or with sufficient accuracy specifications.

**BASF: Perspectives on IoT sensors**
There are already a lot of sensors in (petro)chemical installations, especially for the critical process parameters, where it is worth the investment. Further development will focus on more complex measurement principles, such as Process Analytical Technology (online measurement of chemical composition/product quality) and the use of, for example, video or hyperspectral imaging. IoT-like sensors, where there is also a focus on (wireless) infrastructure, are typically used as a supplement to existing sensors, often for diagnostic or secondary monitoring. We may see more of a shift to critical process parameters in the future, which is also why we are gaining experience now. A general requirement for IoT-like sensors is that they must be robust and ATEX-certified. Many suppliers, especially start-ups and scale-ups, are lagging behind, delaying the deployment of these innovations.

Even though most companies see major benefits in sensors for e.g. predictive maintenance and automated replenishment, it remains expensive to equip all plants and production lines. Therefore, success stories in the chemical sector, in terms of **return on investment**, are needed for companies to consider the investment.

Lastly, detailed analysis on what is needed (and what is not) is essential to create **added business value** with data capture. To this end, companies should effectively reflect on and think through their plant model. Crucial questions which need to be answered are: what knowledge should the measurement build up? And what do we want to measure: the process or a consequence of it?

**Beaulieu: The importance of process insights**
Without a good physical model, backed by the necessary scientific models (e.g. the gas law, heating and cooling behaviour,...) data science does not achieve much, other than ending up with a full set of hard drives. A very complicated viscometer could, for example, be incorporated to determine the chain length of polymers. However, perhaps this insight could also be gained based on the reaction time and temperature, without the investment, calibration, complexity, etc. associated with an advanced sensor. In short: think, then act!

## Solutions?

The impact of data accuracy on employee and environmental safety is highly company- and process-specific. Research focusses on the generation of high-quality data and the calibration of sensors in a network. Currently, self-configurating sensors with automatic calibration are commercially available. Both wireless and wired connections are feasible. Although sensors with lifetimes of years are commercially available, battery challenges remain a point of attention.

The digital transformation increases the need for advanced inline sensing techniques. In order to find the right technique, it is crucial for companies to match potential sensors with their particular data needs. Sensors provide a lot of information, but if one does not know what the information will be used for, this will not solve anything. A first step would be to extract the added value of existing data obtained by existing sensors integrated in the infrastructure. Feedback can then be generated on potentially missing data points or levels of detail, before implementing new sensors and progressing to the next level.

Luckily, Flanders has expertise with regards to the development of advanced sensors, its compatibility with AI-driven technologies, as well as the integration of sensors in industrial environments. To design and implement these sensors, however, different actors must be brought around the table: from sensor manufacturers to system integrators and mechanists.

**P&G: Digitalisation of the supply chain**
Acquiring good quality data from sensors, positioned in critical places of a process in a manufacturing plant, is important. Yet, it is only the first step in a series of requisites. Data has to be structured and stored using the right OT/IT infrastructure. This, however, is not always enough to translate this data into knowledge.

While this data will convey information about the manufacturing process itself, it misses the equivalent type of process data coming from, for example, the supplier that provides the raw materials used in your manufacturing plant. What can be done if, for the quality of the products you make, process data from a supplier is equally critical as the data from your own process?

When it comes to leveraging digitalisation, we have gone beyond the boundaries of our own company and have merged our and our suppliers' data bases, whilst maintaining structured and traceable data. This has enabled us to access data, analyse it, and generate the knowledge needed to resolve many technical problems. This would not have been possible based merely on our own data. This is the digitalisation of the supply chain.

## 2. Data Architecture

**Converting data into knowledge requires a solid data architecture that stores data from multiple sources, both internal and external, in a consistent, standardized and centralized manner.**

As indicated by Figure 2, data architecture plays a key role in the data loop. Architectural interconnectivity, facilitated by the introduction of IIoT, is a basic requirement for a successful digital transformation.

### Challenges

Many chemical manufacturers have already invested in infrastructure for data generation and IT systems. However, the rapidly growing number of sensors, embedded systems and connected devices results in a **huge continuous data flow**. As a result, process equipment-based data are often being ignored because there is simply too much of it, making it difficult to identify important relationships.

In the past, data might have been stored in different systems. Additionally, **historical (legacy) data** might have been labelled or normalized incorrectly, or exhibit substandard data quality. These challenges complicate their use as part of a streamlined data architecture.

Another barrier to a well-functioning data architecture might be a **company IT landscape** that has evolved over time, making production systems incompatible or giving rise to communication delays when data architectures are located at different sites. A big challenge is setting up a good interface between all existing equipment and systems, as not all equipment can be easily connected. Moreover, different IT applications need to be integrated in such a way that optimized data exchange can be done.

Just like data capture, implementing a good data architecture can also be hindered by **safety aspects**. In general, data architecture should always be secure in order to avoid hacks that might endanger the safety of production processes. A second problem specific to IIoT systems is that bugs, unforeseen interactions, or device/communication failures, can cause unsafe and dangerous situations. As such, operating a closed feedback loop might not be possible based on internal and external guidelines for data integrity and process safety. Furthermore, process automation without any human interaction might require extensive assessment and risk-mitigation actions, which could widen the time, budget, and resource requirements.

### Solutions?

In order to guarantee a good data architecture, correct normalisation, periodisation and labelling of all, both historical and contemporary, data is key.

By knowing and understanding processes, the frequency with which a parameter needs to be logged and, as a result, the data flow too, becomes clear. For example; it makes no sense to log the temperature every 100 ms in a 10 $m^3$ reactor. Perhaps every 10 s is enough, which reduces the amount of data by a factor of 100, but will still yield the same amount of information.

When historical data appears to be incorrectly captured or stored, it is often much more convenient to collect new data. This is especially beneficial for cases where the captured data originates from in spec monitoring or maintenance activities as feed for predictive control. However, in particular cases (mainly in R&D environments) historical data can be highly unique and thus difficult or costly to recollect, both in terms of time and resources. In these cases, it is worth the effort to enable historical data as feed for advanced data analytics.

Solutions for production system incompatibilities are highly company-specific. Some chemical companies have sites at different locations causing communication delays between different parts of the systems. Although fast processes that require interaction on an ms-s-min basis typically do not require a cross-site or inter-site approach and are therefore covered locally, it should be evaluated if certain data architecture parts need to be located on the same site. Supervisory activities, or planning/scheduling (hours-days-months), can be done on a site-wide basis. Those types of “technical” delays for which systems should be on-site are, however, less relevant.

Evidently, the chemical industry requires high accuracy. Methodologies that do not depend on labelled data, such as unsupervised learning, use no feedback signal to evaluate the quality of the output. Although, they may lead to the discovery of patterns which have not been previously considered, they may lack indication of accuracy. Therefore, research focusses on methodologies that require as few labelled data as possible, i.e. with minimal supervision while still being able to statistically evaluate the outcome (precision and accuracy).

Within Flanders, expertise is available, both within IT companies and research institutes, to investigate/propose potential solutions to deal with the practical aspects of data preparation and databasing, as well as establishing interconnectivity with maximized cyber privacy and security.

## 3. Data Analytics

**After data has been accurately captured and stored in a fit-for-purpose data architecture, data should still be converted into knowledge.**

This conversion can occur based on human input, fully AI-driven or at different points in between those two extrema. Both human and AI-driven data analysis and decision-making have their pros and cons. There are cases where they coexist as complementary tools. However, due to the increased real-time production data, today’s manual way of data analysis is generally avoided if there is no real requirement. AI-driven data analytics is thus gaining more attention to generate more process knowledge in less time, leading to increased level of product developments, process optimisation and scale-ups in a cost-efficient and sustainable manner.

janssen

**Janssen: Advanced data analytics**
In the manufacturing of active pharmaceutical ingredients, the particle size distribution (PSD) after crystallisation is of crucial importance for the tableting process and for the release profile. A data analysis tool was developed to actively trace trend correlations within all available process data, divided into specific data windows of interest via recipe-based breakpoint functions and analysed via dynamic time warping algorithms, to identify root causes for PSD variations during the different scale-up processes. Combined with specific plant operations expertise, this data analysis tool helped to unveil new critical process parameters much faster. It also allowed us to scale up from lab to the commercial facility, with the updated critical parameter set swiftly resulting in stable and robust PSD. This secured the commercial launch of new active ingredients.

## Challenges

An important challenge that currently receives a lot of attention is the **interpretability and explainability of AI-driven technology**. White box models and system identification techniques have been developed to model processes and predict the closed-loop performance. Though having many advantages such as stability guarantees, such models are often simplistic, capturing only part of the behaviour of the process. While the complexity of black box models results in a large degree of flexibility allowing them to learn highly non-linear functions, it also complicates a human interpretable understanding of how these models reason and reach a decision. Relating back to the previously mentioned safety aspects, the tolerance for error is quite low in various chemical processes. It is thus of high importance that the response to novel input data is somehow predictable within acceptable bounds.

Another challenge regarding data analytics, is the **limited availability of multidisciplinary profiles** able to give digital outcomes a physical interpretation and vice versa; translate technological needs towards the data scientist. If this translation fails, many uncoordinated individual initiatives pop up that do not manage to go beyond a proof-of-concept stage due to difficulties in convincing management on their return on investment. Ideally, such multidisciplinary skills are thus developed in all layers of the company structure, ranging from CEO to technical operators, assuring successful digital transformation. The demand for such multidisciplinary talents is expected to increase further in coming years. No wonder that Belgian companies cite 'availability of staff' as the most important barrier to investment in digital technologies according to the 2019 DigiChem study by Catalisti, Centexbel and Sirris.

CRONOS GROEP

**Cronos: An integrator's perspective**

As an integrator, we are currently less involved with the chemical industry than, for example, with discrete manufacturing. To some extent, the markets upon which integrators call is driven by the technology providers they work with. I4.0 OT and IT convergence is, in terms of knowledge and competence requirements, rather centred on OT and IT mechanics, electronics and software development. A world apart from chemistry. Hence, most sales and engineering staff from companies who sell I4.0 solutions have little or no understanding of chemistry. Combined with the limited availability of multidisciplinary staff in chemical companies, this results in the value proposition of digitalisation not being well positioned in this industry. This works the other way around too. While I4.0 product providers heavily solicit integrators, they hardly see or hear from the many simulator and PAT tool providers the chemical industry typically works with. Conclusion: both parties should engage and get more out of the I4.0 value proposition by investing in multidisciplinary staff.

## Solutions?

According to the Gartner classification, data analytics can be subdivided into 4 categories presented in increasing order of complexity, which can be projected on stages 3 – 6 in the I4.0 development path as illustrated in Figure 1; (1) descriptive analytics (based on historical data: determines what is happening in the moment and in the past and allows to classify, this is the most deployed form of data analytics), (2) diagnostic analytics (combining data with insights: explains descriptive analytics by searching for the origin of a cause, this is a less deployed form of data analytics), (3) predictive analytics (combining data with AI-driven predictions: looks to the future using algorithms based on historical data) and finally (4) prescriptive analytics (combining data with both insights and AI-driven predictions: formulates advice based on predictive analytics, which is the most optimal, yet most complex choice, which explains why it is currently least deployed).

Despite all the advantages AI brings to chemical engineering, among others by introducing predictive and prescriptive capacities, it is used only for single process units and/or for estimating the optimum value of a single parameter. Building these online, multidimensional decision-making expert systems have the potential to improve fault tolerance, reduce waste due to out-of-spec products while substantially improving energy efficiency. It is important to emphasize that no models have been developed for a complete multi-parameter process and no known chemical industry unit has ever been adapted to be controlled by this method. Once again, the uncertainties on return on investments delay the implementation of AI-driven data analytics in chemical process and production environments. Newly developed AI-based technologies should have a quantifiable added business value compared to existing technologies such as advanced process control in order to be relevant.

**A first digitalisation Catalisti ICON project**
A recently started research project (i.e. the Catalisti ICON DAP$^2$CHEM project) focusses on the development of real-time optimisation models for two chemical test cases: a telescopic continuous flow reaction and a continuous solvent switch distillation. Besides researching adequate models for self-optimized control, attention is paid to the explainability of these algorithms' behaviour, based on which insight can be gained about the conditions under which the model is safe to use. It is vital to emphasize that no modern AI algorithm has ever been employed for active fault-tolerant control of chemical processes in real time. This pioneering Catalisti project represents a first step which can be used as a blueprint for other chemical and pharmaceutical companies in Flanders and Europe.

Partners in this project are Ajinomoto Bio-Pharma Services, Cronos, Flanders Make, imec, Janssen, KU Leuven, and P&G. The project is expected to end on 30 September 2022.

## From Talk to Action

Although the implementation of digitalisation itself is accompanied by major challenges, many hurdles and several currently unanswered questions, companies can and should start implementing digitalisation to secure a competitive edge. As substantial investments and their associated uncertainties make it hard to define a solid digitalisation strategy, and it is impossible to tackle everything at once, **a gradual approach is required** to reduce complexity and identify relevant subprojects.

Does your company wish to take on the next step in digital transformation? Does your company face a challenge or a hurdle that seems insurmountable without external support? Does your company seek the right partner to implement certain digital technologies, from sensors to data-storing systems and AI-driven decision-making software? Catalisti is your point of contact! From partner search to bilateral contacts and multilateral innovation projects: **through our broad network, we have access to multi-disciplinary partners than can support the digital transformation of your business**. Together, we find the answers to your digitalisation questions. Together, we move from talk to action!

Now is the time to join the digital revolution and secure a competitive edge! As a neutral partner within the Flemish chemical landscape, Catalisti stands ready to support you and your company in this exercise.

**Questions?**
Questions about this whitepaper, about the digital transformation of your company, or about aspects of I4.0 that were not discussed in this data-focussed whitepaper? Please contact us at info@catalisti.be or through your Catalisti contact person.

# Sources

Several companies within the Catalisti network provided valuable input for this whitepaper. Furthermore, the following sources were accessed:

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