# How the cloud helps manage chemical reactions

**Digital twin and real-time simulation using high-performance computing in the cloud**



## About Orion Engineered Carbons

Orion (NYSE: OEC) is a leading global supplier of carbon black, a solid form of carbon produced as powder or pellets. The material is made to customers' exacting specifications for tires, coatings, ink, batteries, plastics and numerous other specialty, high-performance applications. Carbon black is used to tint, colorize, provide reinforcement, conduct electricity, increase durability and add UV protection. Orion has innovation centers on three continents and 14 plants worldwide, offering the most diverse variety of production processes in the industry. The company's corporate lineage goes back more than 160 years to Germany, where it operates the world's longest-running carbon black plant. Orion is a leading innovator, applying a deep understanding of customers' needs to deliver sustainable solutions. For more information, please visit orioncarbons.com.

## Summary

Orion Engineered Carbons has migrated its highly complex simulations of chemical processes to the cloud. Its IT partner AllCloud was tasked with preparing the company's cloud journey and helped resolve security questions about the protection of intellectual property. The result: up to 20 percent faster calculations and sufficient computing capacity available at the touch of a button to meet the growing need for simulations. Powered by high-performance computing, a digital twin of the production systems delivers insights that go far beyond those of traditional measurement technology. The results of real-time analytics enable Orion to change production parameters during the manufacturing process to fine-tune quality parameters.

### Protection of sensitive data in the cloud resolved

The carbon black manufacturer Orion has decided to implement an extensive project involving the migration of many of its IT workloads into the cloud. This marks an instrumental component of the company's digital transformation program which was initiated three years ago. One that has already gone live is the simulation area, which requires an especially high level of performance and computing power. Simulations of chemical reactions help optimize areas such as production processes and product quality. The cloud is ideal for this project due to the high-performance computing (HPC) requirements, as the company can book computing capacity based on demand.

At the beginning of its digital journey in 2020 Orion started to think about using HPC in the cloud but came up against a few challenges that needed to be resolved. "The biggest challenge was to clarify whether and how we could protect our expertise (IP) if we were to migrate calculations for the operational production environment to the

cloud," notes Arndt-Peter Schinkel, Vice President of Innovation at Orion. The simulations comprise a wealth of specialized knowledge and experience. "The protection of our intellectual property was ensured on-premises, while in the cloud we needed to establish the relevant framework with AWS and providers and set up the corresponding agreements," explains Ben Scherer, Vice President Global IT at Orion. It took sometime, but the company was able overcome all the hurdles.

## Highly complex production environment

"We operate so-called carbon reactors, which are flow reactors in which chemical reactions take place," says Schinkel. "It is key to understand when and why an aspect of the production process isn't running the way we want it to – for example, if a product's characteristics don't turn out as we envisaged." He says it is crucial for staff to be alerted to potential problems as soon as possible because that is the only way they can intervene immediately in the real-time process. One issue is that these processes run at extremely high temperatures of about 2000°C and, in the worst case, could even burn a hole in the reactor if the flow is defective. Using root cause analysis, staff can find out the possible causes of any anomalies. This process also helps prevent damage from the outset. Previously, Orion ran these tests on-premises, but the resource consuming simulations increasingly led to speed and capacity bottlenecks.

## Increasing requirements for calculations

"We need large and expensive servers in our datacenters for these type of calculations," explains Scherer. "In addition, there's a constantly growing need for us to run more simulations simultaneously for our 14 factories. The cloud enabled us to achieve significant performance benefits for these workloads." Right from the start, the performance in the cloud was over 20 percent higher. Although the huge jump in speed at the beginning is put into context as time goes on, the cloud migration still brings the company major benefits. "In the cloud, we're continually using the latest, state-of-the-art processors so we don't lose out on performance as technology progresses," notes Scherer. That is a key difference compared to companies buying hardware, which must be used for many years.

Using high-performance computing in the cloud also enables the company to avoid the not insignificant delivery times for hardware, especially as these have recently increased considerably. "On-premises, the delivery, the IT support required for implementation, and the sourcing approval often took an average of up to six months. Delivery can take a lot longer now due to the current supply chain disruptions. In the cloud, it just takes a few seconds and a couple of mouse clicks – that's a major benefit. Another advantage is that we have the flexibility to scale up or down whenever we need to," says Ben Scherer. The needed hardware is always available. While the company used to have to postpone less urgent calculations, the capacity it needs is now available to run everything faster and simultaneously.

## Digital twin of production systems

The company is still using the on-prem machines in order to prepare the cloud simulations. "There's a range of different criteria we need to comply with so that a simulation runs properly," says Schinkel. "We need to set a lot of parameters, such as checking that the flow will develop as planned or adjusting the geometrics to answer certain questions. Questions might be whether the resolution is as it should be or whether iterations and calculations will run according to plan. The data is only sent to the cloud once it has been checked and validated, at which point the scenario is calculated. This process practically creates a digital twin of each reactor. Before anything goes live, the staff run multiple detailed experiments to ensure that the virtual computing models also work in the physical world.

Modeling the simulations means the staff gain more insights while enabling them to directly recalibrate production to enhance various characteristics.

## HPC simulations deliver completely new views of the process

"With these calculations, the resolution is much greater than what is possible with traditional measurement systems," says the manager of the modeling department. "That gives us a far better understanding of the process compared to what we would have without high performance computing." This is because the high temperatures make things very difficult for measurement systems. Simulations, on the other hand, enable Orion to have different perspectives of the process. Product characteristics are always the result of a complex flow process. If it looks like they are not going to turn out as planned, staff need to intervene in the manufacturing process at that exact moment and set the parameters to put the issue right. "We can only get an idea of what needs to be changed if this development is visible to us," explains Schinkel. For example, they may add more flow in certain places or reorganize positions and temperatures for the addition of certain feedstocks like oil. This helps ensure better product quality as well as higher output from the feedstock they are using – and that also boosts sustainability.

## Significantly less work for IT

The IT department has provided the production team with a user interface with which it can encrypt everything and transfer the data in the form of templates to the cloud. "From the maintenance and deployment viewpoint, the workload is significantly smaller and everything is considerably more flexible and agile than before," reports Scherer. The operational teams do have an extra task in sending the data to the cloud. "But that's compensated by the provision of an extensive workbench in the cloud that helps them identify the ideal equipment. There are more options, more tools and features," says Scherer. He adds that the cloud delivers an additional advantage too: an internal on-prem server with a certain specification is not always the best solution for all simulations. He says the cloud lets the team try out more things to ensure they are running calculations or simulations on the most suitable hardware. Schinkel mentions the example of product post-processing. "Some customers prefer pellets or granules to the powder format. This type of question requires a different set of hardware to that needed for reactor simulations."

## A broader AI workbench for experiments

Schinkel says that the team sometimes needs to run calculations in parallel or even to work on an entire domain. For example, they need completely different hardware to work on a heat transfer problem than for flow calculations. "The hardware they use has a major influence on the time it takes to run a simulation," comments Schinkel.

Orion uses the AWS Marketplace that offers ready-to-use simulation environments, unlike on-prem where they had to work directly within a Linux environment. The company is also using its own container solutions in the cloud. The program's source code has been adapted so that certain features are embedded in it and grouped together in a container. If staff want to try out something quickly, they look for a solution in the Marketplace. "If we see that it works along the right lines, we set up containers and adapt the code using our own modules," reports Schinkel.

## Cloud competence of internal specialists is essential

"AllCloud helped us to build our business case while explaining and preparing our cloud journey for us – we found that extremely helpful," notes Schinkel. From Scherer's perspective, the training for the approximately 30 team members on basic cloud functionality was a big success. "On a cloud journey, it's important not only to focus on the technical enablement but also to keep an eye on building competences among staff from the different departments involved," he says. Alongside training on the basics, the team underwent AWS training courses on architecture, SysOps, developerment and security. All these areas were relevant to the HPC project, which involved a higher level of complexity than a "normal" cloud migration.

The company chose an agile setup for its project methodology and worked in sprints. "We prefer agile delivery as it helps us split work into smaller blocks and iterations and see tangible results quickly," says Scherer. "The collaboration and communication with AllCloud were always very straightforward and efficient," he adds. Schinkel agrees and says that AllCloud finds a solution right away if any questions should arise.

## AWS standard tools underpin security policy

In order to manage cloud security and protect its intellectual property, the team set up a framework with an appropriate policy. Next, a process was implemented in production to follow the security concept – not a trivial task. "An important part of the package AWS provides is setting up a landing zone. That includes a higher level of security with encryption as well as a channel security setup for the AWS mobilization phase," explains Scherer. He adds that high-performance computing also requires deeper security and that AllCloud provided a lot of support for that particular need, as well as for the mobilization phase. The AWS concept has three steps – assess, mobilize, migrate – with which the migration of business applications is so well-prepared that it is much quicker and more scalable.

In the next few months, the company will be transferring additional workloads to the cloud, including AI-related initiatives such as predictive maintenance for the production systems. The last item on the list is the migration of SAP to the cloud. Orion has already successfully completed the first step, which demonstrated that it is certainly worth the effort.

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