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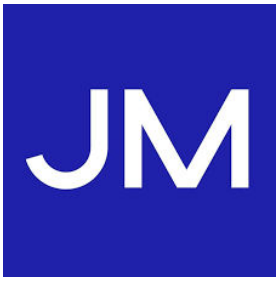
CASE STUDY

Designing improved catalyst technologies at Johnson Matthey



Executive summary

In an Intellegens webinar, **Johnson Matthey**, specialists in sustainable technologies based on catalysts, described the deployment of Alchemite™ machine learning to unlock the potential of in-house data. In a project focused on clean air applications, machine learning was able to improve formulation designs, providing insights that could **halve the amount of physical testing** required in future work in this area. Work with the Life Science Technologies unit identified changes that resulted in a **4% increase in yield** for a key reaction and, in another project, proposed an experimental route that is **five times faster** than the traditional approach. Alchemite™ has facilitated this effort through its easy-to-use web user interface, which enables chemists to engage with advanced machine learning with no need to code or develop a deep data science background.

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The challenge

Johnson Matthey (JM) are specialists in sustainable technologies based on catalysts and related products and services that deliver cleaner air and healthier environments. The company recognised, in the words of R&D Director Liz Rowsell, that "JM is a company rich in data but not always rich in the insights we could gain from our valuable data resources".

One part of the solution was that "the application of quality digital systems could unlock this data mine." As part of this effort, JM has deployed the Alchemite™ [1] machine learning software for chemicals, materials, and manufacturing applications from Intellegens. The aim was to support an approach in which more of its team are 'hybrid scientists' – comfortable combining domain expertise in areas such as chemistry with an aptitude in data science.

At an Intellegens webinar [2], Claire Hatfield, Digital Analyst at JM, presented two case studies in the application of Alchemite™ machine learning to chemicals R&D.

Clean air project

The first application area was **clean air** technologies for catalytic converters. The JM team analysed legacy data from around 600 complete datasets which provided data on over 70 different variables.

Results were improved catalyst formulations and the potential to cut experimental workloads in half for future projects

Alchemite™ was able to build models based on this data that provided detailed understanding of the factors governing catalyst performance, leading to **improved formulation designs** that were experimentally validated. This work has been published in the *Johnson Matthey Technology Review* [3].

In addition to these insights, the machine learning model was shown to be highly predictive of experimental results in a low temperature regime when results from high temperature experiments were provided as a model input (figure 1, overleaf). This creates the potential to focus future testing programmes on high temperatures, **halving the amount of physical testing**.

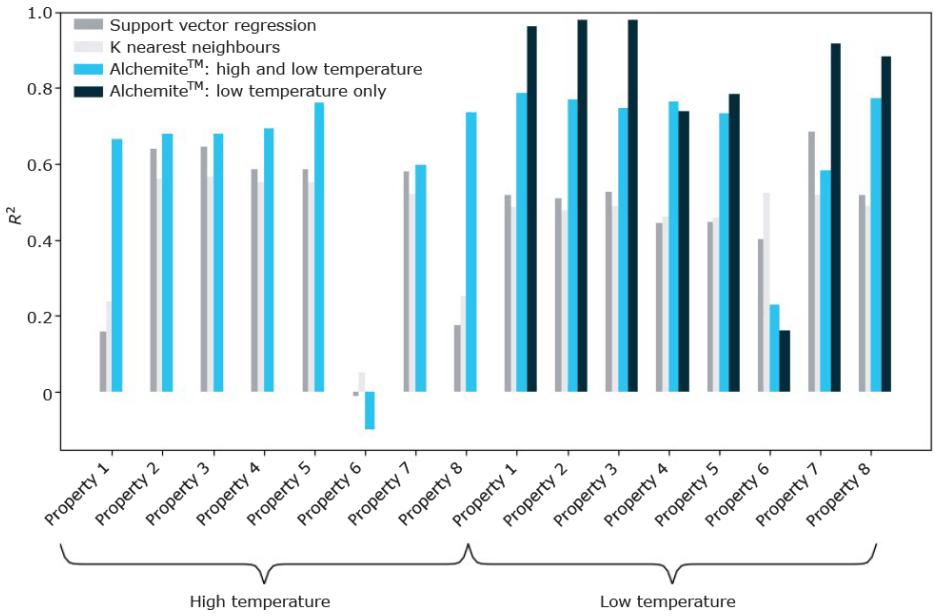

Figure 1. Alchemite™ outperformed other modelling methods on the clean air dataset. And, when data from high temperature experiments were used as an input, the model was highly predictive of low temperature experimental results (dark blue bars).

Life sciences technologies project

JM's Life Science Technology unit was able to identify changes that resulted in a **4% increase in yield** for a key reaction. Claire Hatfield explained: "Our scientists had carried out about 170 experiments for a specific reaction where they were trying to maximise the yield. They were fairly convinced they had the maximum yield that they could obtain. Alchemite™ Analytics suggested six more formulations to try - things like varying temperatures and trying different additives. The scientists went back into the lab, made these formulations, and one gave a yield 4% higher than they had previously obtained. A 4% yield, when scaled up, can give significant cost savings and environmental footprint reductions."

"Alchemite™ found a 4% increase in yield, which can scale up to significant cost and environmental benefits"

JM experience aligns with expectations that Alchemite™ delivers 50-80% reductions in experimental workload

Results from the Alchemite™ analysis for another experiment enabled the team to identify a route to the optimal formulation that requires five times fewer experiments than the traditional approach. Combined with the clean air project results, this means that the JM experience aligns with the expectation established by the Intellegens team across a wide range of different industry projects that, depending on the details of the system being studied, Alchemite™ machine learning delivers a 50-80% reduction in experimental workloads.

Deployment experience

The positive project outcomes in these two application areas were important, but equally significant was the experience of deploying and using the Alchemite™ software, since is what will enable JM's strategic goals of implementing quality digital systems and supporting the development of data analysis skills for their scientists.

"The biggest success that we've seen is in how easy the platform is to use"

During the webinar, Claire Hatfield described this experience: "The biggest success we've seen is in how easy the platform is to use. We have scientists now using it who previously didn't have much interest in analysing data." She highlighted in particular the straightforward user interface (figure 2), documentation, and support from the Intellegens Science Team in establishing how best to apply the machine learning to JM's problems.

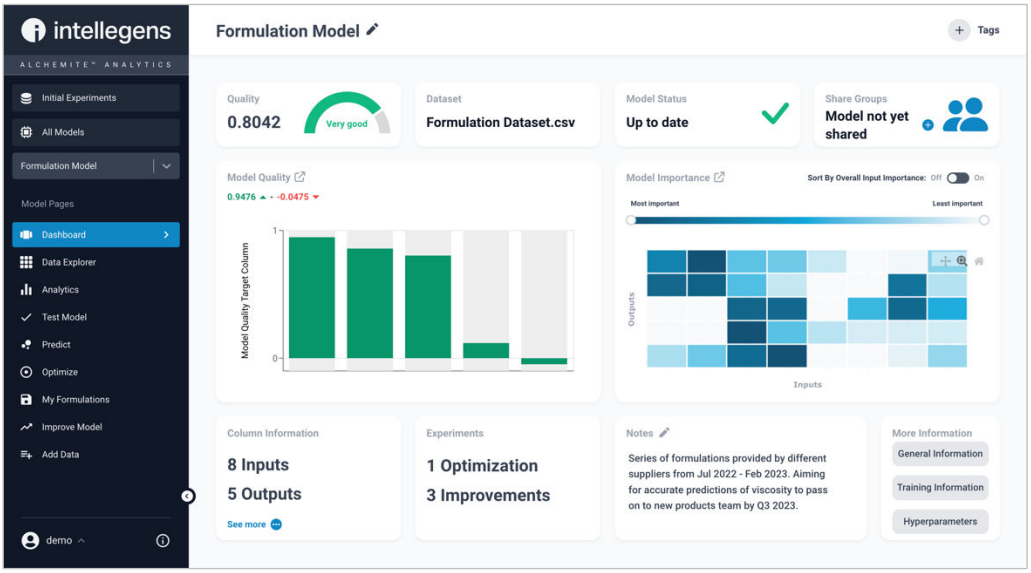

Figure 2. Alchemite™ Analytics web browser use interface.

Summary and next steps

Johnson Matthey have successfully applied the Alchemite™ machine learning software to the development of catalysts for clean air and life science applications:

- Ease-of-use of Alchemite™ machine learning makes it ideal for wider deployment involving both chemists and data scientists.

- Modelling catalysts for clean air applications identified improved formulations and potential to double experimental efficiency.
- A project in life science technologies delivered a 4% yield improvement in a key process and identified a 5 times speedup for another experiment.

In the clean air area, JM intends to expand use of Alchemite™ to other groups and projects, including the improvement of Nox emissions from catalytic converters. Next projects in the life science group include further improvements of reaction performance, faster surveys of literature data, and enriching analysis through the use of 3D descriptors for chemical structures.

About Johnson Matthey and Intellegens

Johnson Matthey is a global leader in sustainable technologies, applying cutting-edge science to create solutions that make a real difference to the world. Leaders in catalysts and related fields for more than 200 years, JM applies unrivalled scientific expertise to enable cleaner air, improved health, and the more efficient use of natural resources. Its strategic focus includes accelerating the big transitions needed in transport, energy, chemicals production, and creating a circular economy. **matthey.com**

Intellegens, originally a spin-out from the University of Cambridge, provides unique machine learning software, Alchemite™, that is applied to accelerate innovation in industry sectors including chemicals, food and beverage, life sciences, and materials. **intellegens.com**

References

1. Alchemite™ machine learning software, Intellegens Limited, Cambridge, UK. https://intellegens.com/products-services/

2. Webinar: Case studies of machine learning for sustainable technologies, Intellegens Limited, Cambridge, UK (April, 2023). Recording available at: https://intellegens.com/case-studies-of-machine-learning-with-johnson-matthey/

3. Tom Whitehead, Flora Chen, Christopher Daly, Gareth Conduit, Accelerating the Design of Automotive Catalyst Products Using Machine Learning, *Johnson Matthey Technology Review* **66**, (2), 130 (2022)

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