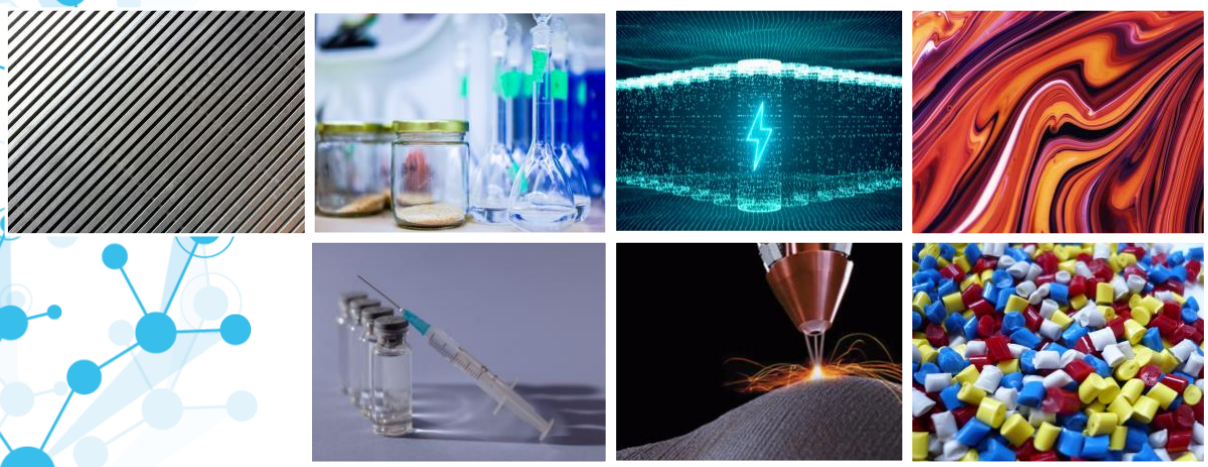
WHITE PAPER

Seven examples of how materials and chemicals companies innovate with AI

Case studies in the use of Alchemite™ machine learning



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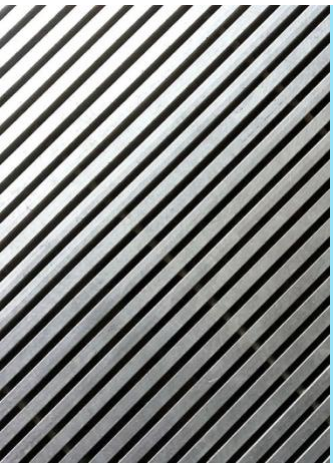
Applied machine learning

Seven examples of how materials and chemicals companies innovate with AI

Case studies in the use of Alchemite™ machine learning



Alloy design

Rolls-Royce designed a new nickel-base alloy, substantially reducing development costs. OCAS NV (ArcelorMittal) gained vital insight into steel properties.

Additive manufacturing

AMRC, Boeing, Constellium, and GE Additive collaborated to optimise AM process parameters.

Formulated products

Domino Printing Sciences saw dramatic reductions in experimental workload for ink re-formulation. Other applications have included food and beverage, specialty chemicals, and paints.

Chemistry

Johnson Matthey (catalysts) and IFF (fragrances) are among companies to accelerate the discovery of new compounds and formulations.

Life sciences

Drug discovery partner Optibrium has had success in projects at AstraZeneca and Genentech.

Batteries

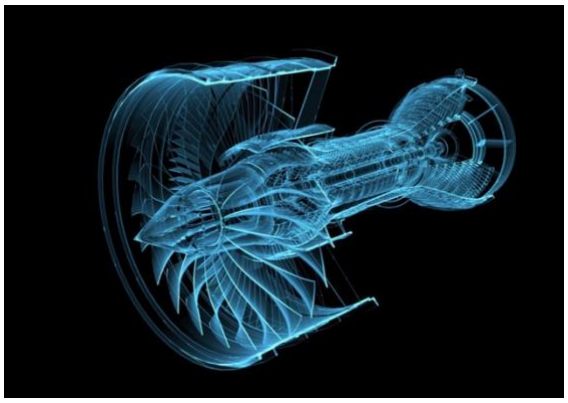
Projects have included novel battery formulations, battery cell and pack design, and predicting key battery management metrics.

Plastics

AI helps to improve performance for plastics and elastomers, to incorporate more recycled material, and to respond to regulatory challenges.

Alloy design

Challenge



Alchemite™ machine learning was first validated in collaboration with **Rolls-Royce Aerospace** on the computational design of nickel-base alloys for use in aero engines. The aim was to find the material most likely to simultaneously satisfy eleven different physical criteria using a machine model trained from existing data. More recently, **OCAS NV** (a joint venture of steelmaker ArcelorMittal) wanted to gain insight into Processing – Structure – Property relationships, including extracting information hidden in microstructural images. The challenge for these and other metals case studies is to use existing data, which is often sparse and noisy, to build models that can understand alloy systems, propose compositions and processing routes, and reduce the amount of physical experiment needed to achieve goals.

Solution

Alchemite™ generates models from real-world, sparse, noisy experimental and process data, where other machine learning methods fail. It finds relationships between properties and process parameters and exploits these to propose alloy designs and processing routes, and to guide experimental planning. Alloy design teams cite its accurate quantification of the uncertainty in its predictions as a particularly useful tool, enabling informed decision-making.

Outcomes

Rolls-Royce generated and validated a new alloy design, with 90% less experimentation than comparable programs – an estimated cost impact over £10 million.

Savings in development costs of over £10m

Lode Duprez, chief science officer at OCAS, commented that their project "provided insights that can help to improve steel properties and focus valuable experimental resources."

Learn more

Rolls-Royce paper – B.D. Conduit, N.G. Jones, H.J. Stone, G.J. Conduit (2017). Design of a nickel-base superalloy using a neural network. *Materials & Design*, **131**, 358-365.

More on both case studies at Intellegens.com/casestudies.

Chemistry

Challenge

Chemists seek any insight that can lead them to compounds or formulations likely to achieve their target properties while reducing the costs of typical experimental programs. Machine learning can help. Scientists at International Flavors and Fragrances (**IFF**) validated its use for predicting sensory properties – an application where testing can be particularly challenging and costly owing to the subjective nature of experimental measurements and reliance on a panel of human participants. A team at **Johnson Matthey** wanted to design experimental programs that could more efficiently identify catalysts with optimal performance against 16 key performance targets.

Solution

Alchemite™ machine learning can be used to impute missing data from large datasets of chemical property data and structural descriptors, enriching sparse datasets and making it easier to find chemical structures with the required properties. The tool can also propose which experiments chemists should do next in order to maximise their understanding of the systems being studied for minimal experimental investment.

Outcomes

At IFF, the method successfully predicted the sensory properties of compounds using sparse physicochemical and sensory data, outperforming conventional QSAR methods.

At Johnson Matthey, Alchemite™ accurately modelled the catalyst products and proposed experimental routes to new formulations which were then validated.

Faster routes to valuable new chemistries

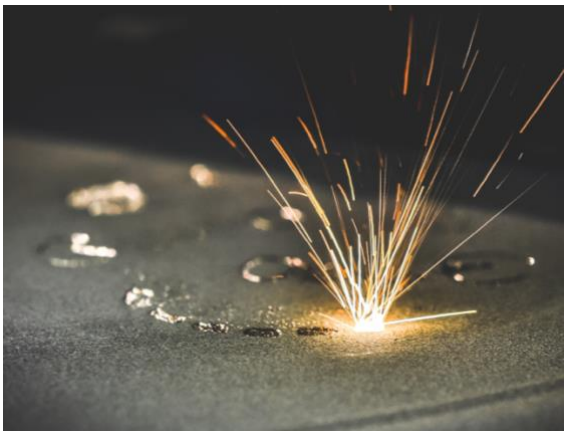
Learn more

IFF paper – S. Mahmoud, B. Irwin, D. Chekmarev, et al (2021) Imputation of sensory properties using deep learning. *J Comput Aided Mol Des,* **35,** 1125–1140.

Johnson Matthey paper – T. Whitehead, F. Chen, C. Daly, G.J. Conduit (2022) Accelerating the Design of Automotive Catalyst Products Using Machine Learning. *Johnson Matthey Technology Review,* **66** (2), 130.

Additive manufacturing

Challenge



Additive manufacturing (AM) could be transformational – delivering lighter, stronger parts and novel product capabilities. But ensuring repeatable AM processes is a challenge, since end properties are notoriously sensitive to small variations in material, process parameters, or the conditions of the AM build. Optimising these factors is complicated by limitations on the available data. Sometimes there is too little data. Or, you may have large project datasets where the data is sparse (e.g., every attribute is not captured for every test) or noisy. Getting the process right for a new material is time-consuming and experimentally-intensive.

Solution

A collaboration involving the **AMRC**, **Boeing**, **Constellium**, and **GE Additive** applied Alchemite™ machine learning to accelerate process parameter optimisation for a new laser powder bed fusion (LBPF) material and process. The project first demonstrated that it was possible to build a machine learning model from historic build data and apply it to predict the results of new builds. The model was then used to guide the testing of a new powder material.

Outcomes

Ian Brooks of AMRC reported: “Alchemite™ converged on the optimum solution with far fewer experiments. The opportunity for this project is to provide end-users with a validated, economically viable method of developing their own powder and parameter combinations.”

Rapid optimisation of process parameters

Lukas Jiranek at Boeing explained the company’s involvement: “Machine learning has the potential to be a key technology in accelerating further development of AM.”

Learn more

Article – S. Warde (2021) The inestimable value of AI: How Machine Learning can help AM project teams achieve their goals and beyond, *Metal Additive Manufacturing,* 7 (4).

Full case study at Intellegens.com/casestudies.

Life sciences

Challenge

In the vital search for active compounds and new therapeutics, there is great value in any approach that can focus experimental programs on the likeliest success routes, or deliver breakthrough insights. Can machine learning extract more value from existing data to guide drug discovery programs? Datasets are often large, but sparse and noisy. Working with our drug discovery partner, **Optibrium**, **AstraZeneca** sought to predict PK parameters and curves from chemical structure, while the team at **Genentech** aimed to optimise kinase profiling programs.

Solution

The Alchemite™ algorithm has been embedded within the Optibrium drug discovery software, where it is used to analyse small molecule compound data and guide experimental programs. The Alchemite™ software from Intellegens is also applied in areas including biologics, formulation, and clinical trials.

Outcomes

In the AstraZeneca project, Alchemite™ successfully combined descriptors, in silico, and in vitro data to predict PK parameters and curves, generating results comparable to the best in the literature.

Fabio Broccatelli at Genentech commented on their project: “What is nice about this technology is that it uses the chemical information, but also uses the existing experimental information.”

Extract vital insights from existing company data

Learn more

Paper covering AstraZeneca project – O. Obrezanova et al. (2022) Prediction of In Vivo Pharmacokinetic Parameters and Time–Exposure Curves in Rats Using Machine Learning from the Chemical Structure, *Mol. Pharmaceutics, **19**, 5, 1488–1504.*

More on both case studies at Intellegens.com/casestudies.

Formulated products

Challenge

Foods and beverages, paints, inks, personal care products, plastics, pharmaceuticals – these are just some of the commercially-significant products manufactured as formulations. To ensure these products have the right properties, quality, shelf-life, and safety profile, development teams must optimise a complex combination of ingredients and processing conditions, while controlling cost and minimising environmental impact. Testing the full range of possible formulations is usually impossible, so good methods to focus design and experimental exploration are paramount. **Domino Printing Sciences** provide an excellent example in their work to re-formulate inks, seeking to replace additives that were subject to new regulations.

Solution

Domino used Alchemite™ to optimise ink formulations by maximising insights from carefully-chosen experiments.

Outcomes

"We were impressed with the ability of Alchemite™ to identify novel formulations quickly and accurately", commented Dr Andrew Clifton, Director of Marking Materials and Test Engineering at Domino. The work enabled Domino to make more efficient use of lab capacity and run more experimental programs by reducing the number of experiments required in each program. Ultimately, this results in decreased time-to-market and more opportunity for development teams to focus on creative chemistry.

Cut timescales from months to minutes

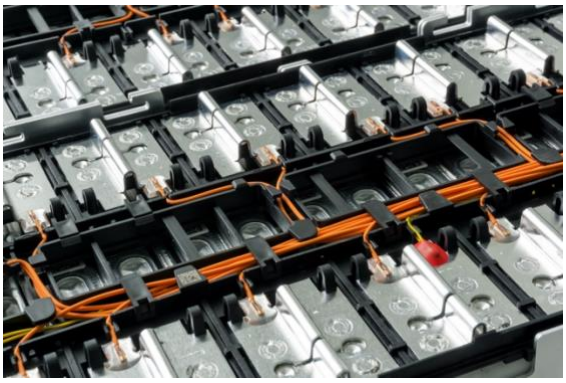
Learn more

More on this case study, including a recorded webinar, at Intellegens.com/casestudies.

Batteries

Challenge

Powering the electric vehicle revolution. Enabling renewable energy sources. Cutting charge times for personal devices. These are urgent drivers to develop new battery technologies, faster. But battery R&D is complex and slow, with many competing factors to balance, and a heavy reliance on time-consuming, costly experiments to fill gaps in data and test prototypes.



Solution

A project including the **University of Birmingham**, **Ansys**, and the **Faraday Institute** applied Alchemite™ machine learning to understand and optimise formulation and manufacturing parameters for lithium-ion battery applications. Battery innovator **Deregallera** has undertaken similar studies of sodium-ion systems. Alchemite™ was also used by researchers at the **University of Cambridge** to predict key metrics for battery management systems.

Outcomes

The University of Birmingham manufactured a new electrode formulation which showed excellent lifecycle and capacity, as predicted by the machine learning.

Deregallera discussed the use of Alchemite™ in focusing their experimental work at an Intellegens webinar.

A paper published by the University of Cambridge team showed the promise of machine learning for prediction of battery state, including State of Health (SOH), State of Charge (SOC), and Remaining Useful Life (RUL).

Solutions throughout the battery value chain

Learn more

Electrode formulation paper – S.X. Drakopolous et al (2021) Formulation and Manufacturing Optimisation of Lithium-ion Graphite-based Electrodes via Machine Learning. *Cell Reports Physical Science,* **2**, 100638

Deregallera recorded webinar available at intellegens.com/webinars.

Battery management review article – M-F. Ng, J. Zhao, Q. Yan, G.J. Conduit, Z.W. Seh (2020) Predicting the state of charge and health of batteries using data-driven machine learning. *Nature Machine Intelligence*, **2**, 161-170.

Plastics

Challenge

Developing new polymeric materials. Improving the performance of existing plastics or elastomers. Incorporating more recycled material. Eliminating additives that have become obsolete due to new regulations. Or simply improving performance or lowering cost. These are all typical plastics R&D objectives and, in all cases, development teams need to optimise the impact of multiple, interacting ingredients and processing variables. They are doing this based on data from experiment, simulation, or production that they are constantly seeking to understand and improve.

Solution

Polymer R&D organisations use Alchemite™ to more effectively mine their experimental and proess data. They seek relationships in this data that provide clues on how to change their materials or processes. They identify where it would be most beneficial to focus experiment or simulation, saving time and cost. They even build models of their systems that might be used to manage polymer production – for example, to change process parameters in response to the inevitable variability in the composition of incoming recycled feedstock.

Outcomes

Typical project outcomes:

- Reducing the experiments in a program to explore new polymer formulations by 50-80%.
- Cutting time-to-market for a revised product that removes a newly regulated additive.
- Capturing understanding of a polymer system in a model, avoiding the loss of vital knowledge when domain experts leave the business or retire.

Solve market, regulatory, and environmental challenges

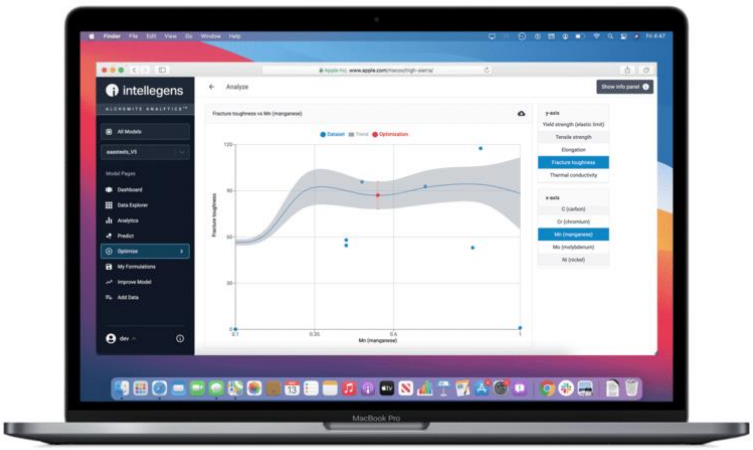
Learn more

View a recorded webinar on machine learning for polymer R&D at Intellegens.com/webinars.

About Alchemite™

Alchemite™ deep learning software from Intellegens solves real-world, sparse, noisy data problems where other machine learning methods fail. The Alchemite™ Analytics web browser interface provides fast, easy access to this powerful technology, and valuable graphical analysis of the results, tailored to the needs of scientists in materials, chemicals, and manufacturing. Alchemite™ Engine provides fully flexible API access for data scientists to apply the methodology and integrate with their own tools and workflows.

- Extract more value from sparse, noisy data
- Win with optimised formulations, products, and processes
- Save time and cost with up to 90% fewer experiments
- Deploy advanced deep learning for maximum impact.



About Intellegens

Our mission is to be the leading machine learning solution for real-world, sparse and noisy data problems in industrial R&D and manufacturing processes. Our focus is on making it easy to apply machine learning to accelerate innovation. Alchemite™ originated at the University of Cambridge and development is on-going at Intellegens, in close collaboration with our growing community of Alchemite™ customer organisations. These represent sectors including alloys, additive manufacturing, aerospace, batteries, ceramics, chemical processes, composites, consumer products, cosmetics, drug discovery, energy, food and beverage, formulated products, paints, plastics, and printing technology.

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