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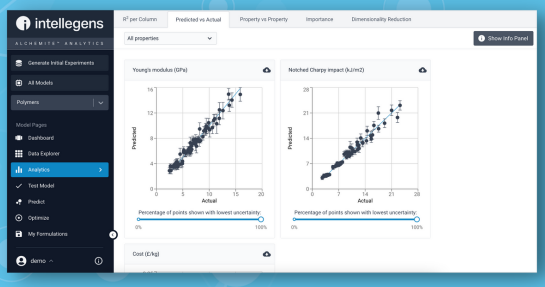
Applied machine learning

Machine learning for plastics and elastomers

Design and optimise polymer blends and formulations, exploiting all available data

Focus experiment and maximise value from results, saving months of work

Find novel solutions to market, regulatory, and environmental challenges



Analysing polymer properties in the Alchemite™ Analytics user interface

Are you developing new polymeric materials? Or improving performance for existing plastics or elastomers? Or researching new packaging options? You might be focused on sustainability goals: incorporating recycled material, using biopolymers, or decreasing energy usage. Perhaps you want to eliminate additives made obsolete by new regulations. Or you could be aiming for a competitive edge with better properties for your plastics at lower cost.

In all of these cases, you must optimise the impact of many ingredient and process parameters on varied outputs such as mechanical and thermal behaviour, appearance, cost, and sustainability metrics. This usually relies on costly, time-consuming experimental programs, plus insights from simulation and production. Data from these sources is often sparse and noisy, making it hard to analyse and use.

Alchemite™ is advanced deep learning software that is able to build models from real-world, sparse, noisy experimental and process data, where other machine learning methods fail. Identify vital relationships in the data. Design new chemistries, blends, and formulations. Propose optimal process parameters. And guide planning of experimental projects to dramatically reduce cost and time.

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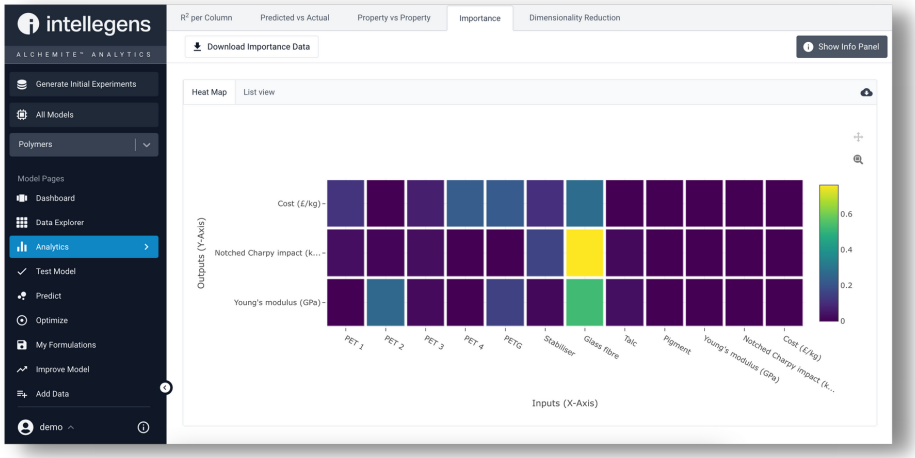

The Alchemite™ Analytics platform provides scientists with quick, easy access to advanced deep learning methods and powerful graphical analytics via a web browser user interface. The Importance Chart provides insight into which inputs drive which outputs.

Example applications

Designing formulations and blends – Alchemite™ is used to predict the combinations of ingredients and processing parameters that will provide the best trade-off between multiple target objectives. Users benefit from such insights into their plastics R&D and in related areas such as inks, paints, foods, and cosmetics. **intellegens.com/casestudies**

Adaptive design of experiments – As well as proposing optimal candidate materials, Alchemite™ is used iteratively within experimental programs to suggest which set of experiments should be done next in order to most efficiently explore parameter space. This adaptive design of experiments has been shown to reduce experimental workloads by up to 90%. **intellegens.com/experiment**

Get more from simulation – Alchemite™ has combined sparse data from experiment and simulation, for example, to predict the physical properties of lubricants. *Fluid Phase Equilibria* **501** 112259 *(2019)*.

Alchemite™ for plastics

With the Alchemite™ software, polymer scientists, chemical engineers, and data scientists can apply powerful deep learning methods to get more from their data. Key features are:

- Gap-fill and validate sparse, noisy data from suppliers, experiment, simulation, and production
- Auto-generate models that identify key ingredient-property-process relationships
- Quantify uncertainty to support a rational business case for key decisions
- Suggest what experiment(s) to do next, increasing the efficiency of experimental programs
- Identify the optimal polymer blend or formulation
- Propose optimised process parameters to improve quality and performance.

Next steps

Contact us to book a demo tailored for your application. Visit our website to download white papers and subscribe to our newsletter. Or follow us on social media.

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