

Alchemite™ Analytics

Product Specification

Alchemite™ Analytics is a web platform that enables multiple users in an enterprise to apply the Alchemite™ deep learning algorithm to:

- Extract more value from sparse, noisy, experimental and process data.
- Gain competitive advantage with optimised formulations, products, and processes.
- Save time and cost with up to 90% fewer experiments.

Using Alchemite™ Analytics, scientists and engineers can develop machine learning models, share these models with colleagues, apply them to company datasets, and analyse the results to extract insight, guide experiment, and inform decision making. This document summarises the features of the platform.

Generate, manage, and share models

- *Automatically 'train' a new machine learning model* in just a few button-clicks from any dataset uploaded in Excel or .csv format.
- *Analyse sparse, noisy data*—through the unique Alchemite™ algorithm, a model can be trained using real-world datasets for which conventional machine learning methods often fail.
- *Get started, fast*—Alchemite™ is highly computationally-efficient. Combined with its ability to handle sparse data, this enables it to quickly generate a model that can then be refined, providing a starting point where other approaches require time-consuming data manipulation.
- *Generate initial data*—what if you have no data? Tell Alchemite™ about your problem (limits, boundaries, etc.) and it suggests what to measure to create the best starting point for your model.
- *Categorical data*—Alchemite™ can handle both numerical data and the unordered discrete values that appear in many experimental data sets.
- *Manage models*—models that have already been trained can be retrieved instantly to be used for new predictions, or to be refined using new data.

	D10	D50	Laser Power (W)	Hatch Scan Speed (m/s)	Hatch Distance (mm)	Tensile Strength (MPa)	Elongation (%)	Density (g/cm³)
	3.670	15.60	46.86	310.0	1.400	0.1200	1179	37.75
	3.660	16.90	49.96	300.0	1.400	0.0800	1065	41.64
	3.150	15.90	48.72	310.0	1.400	0.1000	1248	31.33
	3.340	16.54	48.01	290.0	0.7000	0.09000	1295	33.72
	3.680	16.22	47.32	430.0	0.9000	0.1000	1451	14.70
	3.970	15.70	47.16	390.0	1.900	0.1000	1173	35.64
	3.670	15.54	46.45	470.0	1.900	0.09000	1261	41.83
	3.150	16.88	49.90	420.0	1.900	0.1100	1209	35.32
	3.670	15.76	46.63	230.0	1.400	0.07000	1085	41.83
	3.660	16.43	48.39	410.0	1.400	0.07000	1237	7.876
	2.460	15.19	47.25	230.0	1.800	0.1200	1046	40.05
	2.860	15.00	48.19	450.0	1.400	0.1000	1309	34.98
	3.670	15.54	47.01	490.0	1.900	0.1000	1330	41.83
	4.030	15.70	49.39	210.0	1.400	0.1100	1077	45.95
	3.150	15.27	45.60	480.0	1.400	0.1100	1306	27.75
	2.800	15.98	46.90	290.0	0.7000	0.1100	1296	31.78

Viewing data in the Alchemite™ Analytics web browser interface - the software has identified outlier data (in red) and has imputed missing data and quantified the associated uncertainty (green)

- *Share models* across the enterprise, including the ability to share particular models with specific groups or teams.
- *Control model-building parameters*—options in the user interface enable you to balance speed and accuracy in model building. More advanced control of the algorithm is possible for data scientists using the Alchemite™ Engine API.
- *Optimise the model to its purpose*—choose whether to prioritise predicting outputs from a new set of inputs, or filling in missing data.

Understand and enhance your data

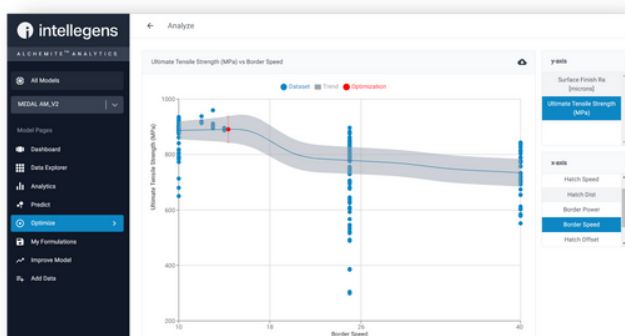
- *View data*—the data associated with a model can be viewed in tabular form and can be sorted, filtered, and downloaded.
- *Outlier identification*—data identified by the model as outliers is highlighted, enabling you to improve data quality or focus on understanding the factors in your system that generate these outliers.
- *Impute missing data*—instantly apply the model to fill in gaps in your data.
- *Understand uncertainty*—where the dataset contains predicted values, a range representing the uncertainty of these predictions is displayed with every value, enabling you to build confidence in the model and use predicted data appropriately.

'Explainable AI' analytics

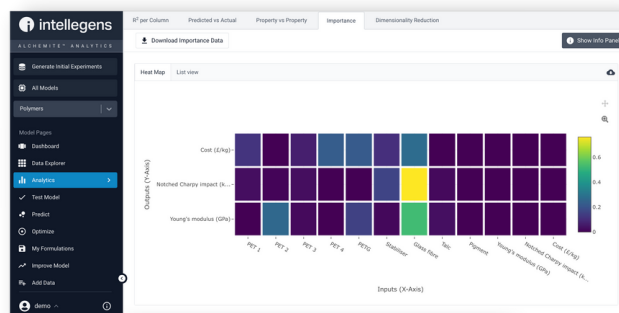
These analytics are a set of graphs that give rapid, visual, and quantitative insight into the accuracy of your models and the relationships identified by the models between the inputs and outputs of your system.

This list of analytics is constantly growing based on feedback from Intellegens customers about which insights are most useful in innovation for materials, chemicals, and manufacturing.

- *R2 per column plot*—a bar chart providing instant visual feedback on the confidence you can place in your model when predicting each of its output variables.
- *Predicted versus actual plot*—a quick visual check on the accuracy of the model when interpolating data.
- *Property vs property plot*—helps you to quickly explore correlations between different properties.
- *Importance chart* - a 'heat map' that shows you which inputs have the greatest impact on which outputs.
- *Dimensionality reduction plot*—projects a high-dimensional dataset onto a two-dimensional surface, enabling you to see clusters of data rows (e.g., materials, formulations, samples, or process runs) with similar characteristics.
- *Sensitivity plot*—helps you to understand how changes in the inputs will impact a specific output for a particular material, formulation, or process.
- *Output tolerance plot*—where it's not possible to exactly specify an input, or inputs, this plot helps you understand the range of outputs that might result.



Analysing an optimisation - the graph shows how an output (Ultimate Tensile Strength) varies with a given input (Border Speed) and where the predicted optimal solution (red dot) lies in this space.



The Importance Chart, one of the 'Explainable AI' analytics, shows which inputs have the greatest impact on which outputs.

Prediction - enable virtual experiments

- *Predict outputs for a new set of inputs*—quickly input a new set of input data and use the model to predict the output, enabling rapid virtual experiments.
- *Predict outputs for many new sets of inputs*—upload many possible input sets, running predictions in batch mode for high throughput virtual experiments.
- *Accurately quantify uncertainty*—Alchemite™ uses an advanced method, based on nonparametric probability distributions for many properties simultaneously, to determine the accuracy of its predictions, enabling you to identify which experimental routes have the highest probability of success.

Optimisation - find new solutions

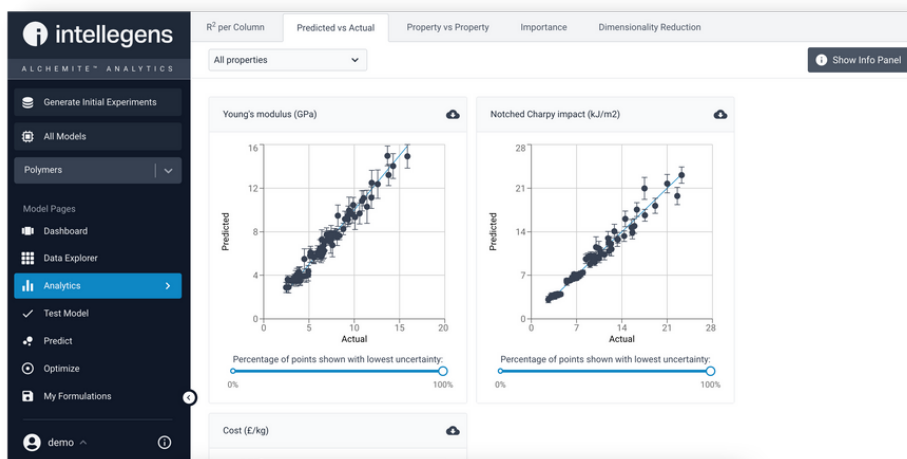
- *Optimise system inputs for a target set of outputs*—Alchemite™ will find a new set of input parameters that best satisfy your specified target outputs - e.g., to design a new formulation, or select an optimal set of process parameters.
- *Impose constraints*—you can fix specific inputs, limit them to lie within a range, or constrain combinations of inputs - e.g., to ensure that the percentages of each component in a formulation or material add up to 100%.
- *Flexibility in specifying targets*—required outputs can be specified as numbers, ranges, or as maximum or minimum values.
- *Analyse optimisations*—explore the results by plotting (left) how outputs vary based on changing inputs, and where the optimised solution lies in this space.

Improving models—enabling 'Adaptive Design of Experiments'

- *Guide data acquisition*—whatever the physical process or system that your model represents, you may be able to improve the performance of the model by gathering more data and using it to refine the Alchemite™ model. Alchemite™ can tell you which data to gather in order to maximise model improvement and minimise effort.
- *Adaptive Design of Experiments*—when you are modelling an experimental program, this model improvement becomes a 'Design of Experiments (DoE)' method, because it tells you which set of experiments to do next. We call this 'Adaptive DoE' because, used iteratively as new data is added, it continually improves its guidance. Such approaches have led to experimental goals being met with 90% fewer experiments.
- *Define your search space*—specify your target properties, any constraints you want to place on your inputs, and how many experiments you want to do next. Alchemite™ will recommend the input values to use for those experiments.
- *Specify your purpose*—you can ask the algorithm to either recommend a set of experiments that will help the model to increase its accuracy within the space already explored, or to suggest experiments that will widen the exploration of design space.

Enterprise deployment

- *Simple web user interface*—any user can log in securely via a portal and use the system within their standard web browser technology.
- *Flexible licensing*—specify the number of users, with the ability to distinguish between admin users, model builders, and model users.
- *Enable collaboration*—models and data can be shared between Alchemite™ Analytics users.
- *Advanced configuration and integration*—the Alchemite™ Engine API enables data scientists more advanced control over the Alchemite™ algorithm and integration with in-house software and workflows.
- *Model deployment*—models developed via Alchemite™ Engine can be deployed into the Alchemite™ Analytics web user interface, enabling data scientists to easily share their work with scientist and engineers across the business.
- *Easy, secure, web-based deployment*—options include a secure cloud-based system hosted by Intellegens, deployment on your organisation's cloud-based infrastructure or installation within your corporate firewall.
- *Support for standard corporate IT*—successful implementations on corporate systems have included AWS, Azure, and Google Cloud.



Predicted vs Actual plots are one of a range of 'Explainable AI' analytics that give you confidence in your model and help you to understand its accuracy.

More information

Download our white paper on Alchemite™ deep learning for more background information, including a reference list.

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