



White Paper

How to get started with AI in Paints and Coatings - and why you need to do that now



#NoDataNoProblem

Some Paints and Coatings companies, and those that sell raw materials to them, have started using AI to great effect. Others are more hesitant. Some are worried that they don't have enough data in the right format to do AI. Others are worried that they don't have the right skill set in-house to get started. This article will outline what value Paints and Coatings companies are already gaining from AI and give practical tips on how to get started and what to look for in an AI provider.

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EASTMAN

electroninks

synthomer

Together more future
dorfner

GRACE

Return on Investment

Moving from being a supplier to a partner

Whether you are a Specialty Coating company selling to an OEM, or a raw material company selling into a Coatings company, you need to deeply understand how your product impacts the performance of that of your customers so that you can recommend the correct product, charge based on value, find a market niche with higher margins.

**Increased
revenue
by 30%**

Citrine's customers are using our software to do exactly this. A [recent article in Handlesblatt](#) outlined how our customer Dorfner, a mining company with a coatings ingredients division, **had increased their revenues by 30%**, using Citrine software to better respond to their customers.

“ [with Citrine] we are able to enter new business models... we are able to get customer lock-in... we were before just a supplier and now we are a development partner... this can't be ROI'ed, it is far beyond”

Mirko Mondan, CEO Dorfner

Accelerated time to discovery

Many customers have seen a reduction in the number of experiments, and therefore time to discovery, needed to hit property targets. A company optimizing properties of a multi-layer polymer coating for an automotive application was able to hit target properties in 2 weeks instead of the usual 10, using the Citrine Platform. This is not unusual amongst Citrine customers. By being able to predict the likelihood of achieving target properties, researchers can concentrate on performing experiments that will work.

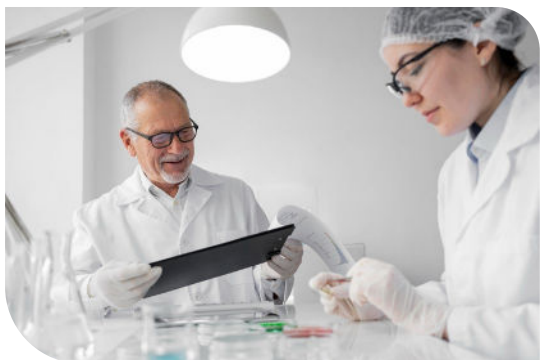
**An 80%
reduction in
time to
discovery**

Dealing with problem ingredients

Other customers are needing to swap out ingredients such as PFAS chemicals from product portfolios. This is where scalable AI comes into its own, once a model is trained on the base formulation, the formulation can be easily adapted for each product in the range, ensuring consistency as well as speed. Citrine's AI platform "featurizes" chemicals, essentially, converting the molecular structure and chemical formulas into extra data such as molecular weight or number of hydrogen bonds. By understanding the fingerprint of the problem ingredient and the role it performs in the original formulation, Citrine's AI can then suggest alternatives.

One customer re-formulated an in-market product, removing PFAS and retaining performance, in under 3 months.

Amplify your expert formulators - reliable knowledge sharing



Deloitte has found that up 25% of the industry's workforce may retire between 2021-26. While AI cannot stop your top formulators from retiring, it can be used to codify their expert knowledge in such a way that it can be reused by more junior staff, now and in the future.

In a data sparse, knowledge rich environment like a paints and coatings lab, it is important that Citrine's AI platform can capture both data and the knowledge of the team and use them in concert to get results. Therefore, Citrine's platform is specifically designed to be used by anyone, whatever their background. The no-code platform can be trained by your experts - just as they would train a new member of their team.

This knowledge is then used to focus the power of the AI model onto unknown areas rather than reinventing the wheel, speeding up development.

Knowledge is captured as:

1. Data uploaded into the system rather than hanging around in a spreadsheet somewhere.
2. In an AI model which is itself a representation of what inputs affect what outputs.
3. In a search space, a description of constraints on formulations e.g. what ingredients can be used, what mixing parameters etc.

Paints and coatings companies are seeing value from AI. AI will become an everyday tool for formulators.

But my data is a mess...

There is a difference between BIG data AI, like ChatGPT and small data AI. In chemicals it costs \$100's or \$1000's to create a sample and test it, which means datasets are small. Citrine Informatics have spent more than 10 years focusing specifically on developing AI that works with small data. They have developed strategies such as knowledge integration (using the expertise of your team to focus the model), chemical featurization (automatically generating extra data), and uncertainty quantification (clever math to calculate the likelihood of hitting targets) to make best use of small data.

Some AI projects start with no data

Sometimes, either by necessity, or choice, projects start before any data in the relevant area has been gathered. In this case an initial set of experiments are carried out, similar to a Design of Experiment (DOE) matrix but stripped down to cover the search space in the fewest experiments possible. The aim is to prime the AI model so that it can guide future experiments. Sequential Learning (the process by which groups of 5 or so experiments are suggested, run, the results inputted, and the AI model retrained and used to suggest the next set of experiments) is then used to get closer and closer to the objectives of the project. This methodology still requires fewer experiments than trial and error or DOE.

Started with no data:
Read a case study



AI-Driven Development of Additives for
Carbon Fiber Manufactured Process

Some companies have data in silos



It may be that commercial information on ingredients is in an ERP system and rheological measurements are in a LIMS. Or perhaps, your IP is stored in handwritten notebooks on a shelf? By running a short timescale AI project first, you will see exactly which data is useful for your AI model and therefore worth the time to digitize. Citrine Informatics have an experienced team that can help you create a data strategy and get your historical data into their platform. Data pipelines can be set up to ensure all future data goes in automatically.

Citrine's data model is scalable. It can easily accept data from new data sources over time. Unlike an SQL based data model that needs to have

data in one big rigid table, Citrine's graphical database structure grows with you as you learn more and want to add new properties, or if you get data from your raw material suppliers.

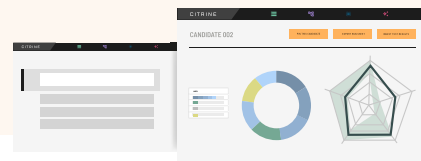
In summary, learn by doing. By starting with a small but valuable AI project you will understand better which data you need and can put a data strategy in place that shows immediate value without boiling the ocean.

But I don't have any data scientists...

AI platforms have come a long way in the last 5 years. While they were once the domain of data scientists, the best ones can now be used by anyone. In fact, you want your formulators using them directly. Cutting out the middle man means that formulators can easily add their own knowledge into the platform and iterate faster when they have a good idea. They can also learn what the AI model is finding important and thus deepen their own understanding.

“We understand our own laboratory more than before. It's fun to work in this way”

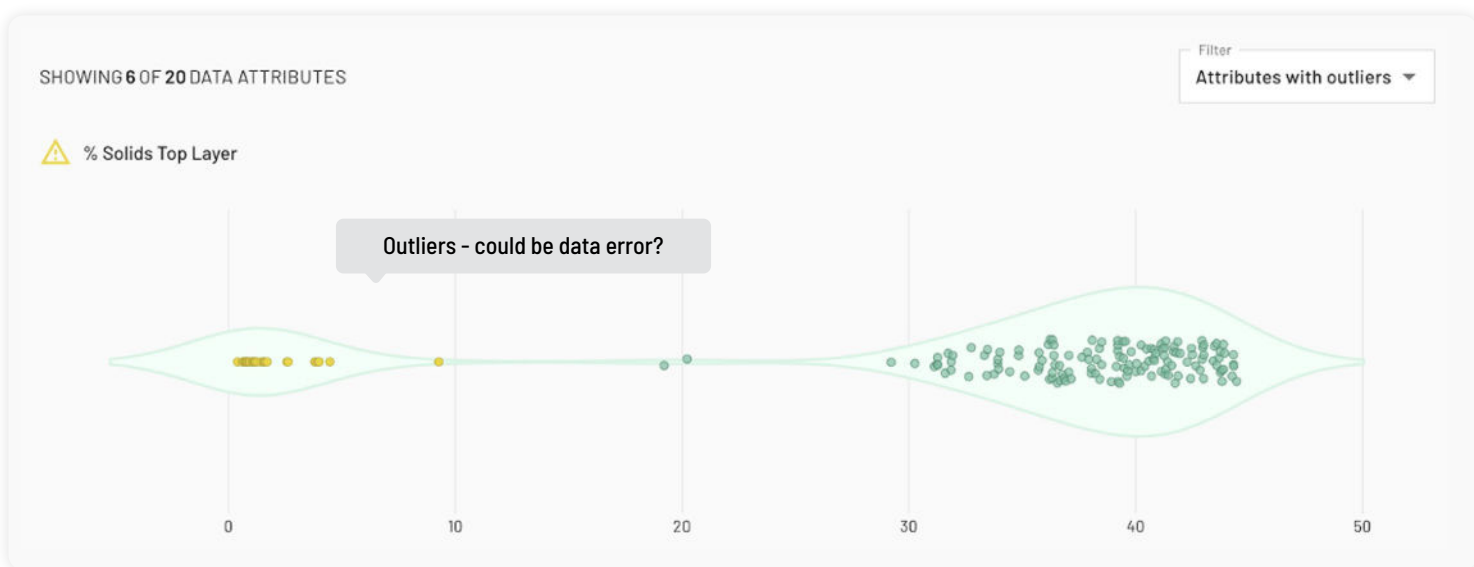
Oliver, Technical Application Lead



No-code, graphical user interface is essential

While the Citrine Platform does have an API (code-based interface) that data scientists can use if they want to, making the graphical user interface intuitive and easy to use is a priority. It enables formulation experts to add information such as relationships and equations directly to AI models accelerating progress and giving your team ownership of models, leading to quicker adoption. AI models are generated automatically from the data set chosen, using some assumptions. A formulator then just has to add their knowledge and sense check the model.

Review your data graphically



Tick a box to say that the amount of surfactant is important

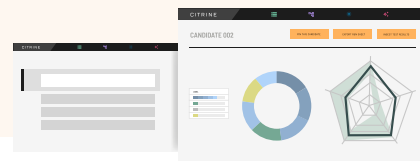
☒ Select All

Custom Formula

☐ Surfactant Fraction


Ingredient Fractions

- ☒ Acrylic-A share in Flat Formulation
- ☒ Acrylic-B share in Flat Formulation
- ☒ APEO Surfactant A share in Flat Formulation
- ☒ APEO Surfactant B share in Flat Formulation
- ☒ APEO Surfactant C share in Flat Formulation



Make sure your team can learn from the AI platform

AI models work by figuring out connections between input and output properties. Your team will benefit from understanding these connections more deeply. If you can show that an ingredient has no effect on the target output properties, that is really useful information. Sometimes unintuitive connections will be made and by reviewing the features that the AI model finds important you will find out something new.

 **AI lets us solve problems with less work. It's like having a flashlight in a dark room."**

FEATURE IMPORTANCES ⓘ

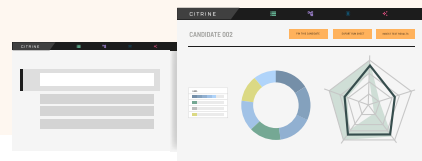
surfactant share in Flat Formulation	36%
HEUR share in Flat Formulation	18%
surfactantFraction	17%
coalescent share in Flat Formulation	3.6%
binder share in Flat Formulation	3.3%
solvent share in Flat Formulation	2.9%
thickener share in Flat Formulation	2.9%

The team can review the feature importance to both sense check the model and perhaps learn something new.

Change management

Adopting AI is a change to people's day-to-day working styles and as such, of course presents a challenge. However, it is a small part of an overall digital transformation for many companies and an excellent way to show the value of good data management. By doing high-value, AI projects first, you can show your team the value of their data and motivate them to participate in wider data digitization programs. Over the last 10 years, Citrine has built up an experienced team of change managers, who have learnt from over 100 engagements to develop a solid methodology for rolling out AI.

AI shouldn't be made available like a bowl of fruit. While it sounds good to make something freely available to those that could benefit from using it, in reality a bowl of fruit in an office sometimes goes moldy because people don't have the time to pop downstairs and peel an orange. And so it is with AI. Even though researchers know that a new tool could potentially save them time in the long run, they may feel too busy to stop and learn something new. Citrine's expert customer success team have developed strategies for helping groups adopt the technology, by training a network of champions and ensuring high level buy-in for the business goals of projects.



What to look for in an AI provider

- Deep experience in AI for paints and coatings
- An experienced change management team that can smooth the adoption process
- A platform that is chemically-aware and provides chemical featurization
- A graphical data model that can accept data from lots of different sources and is scalable
- A no-code easy to use platform that can capture and leverage your team's expert knowledge
- Easy ways to search, filter, visualize and share data between team members so that no one reinvents the wheel
- AI tailored to work with small data sets

**AI is inevitable. It is a great step forward in all sorts of disciplines. In the end, it is just math.
But pick an easy-to-use platform backed up by an expert team to help you get started.**



**Contact us for both a demo of the platform and a more detailed, tailored
return on investment calculation for your business.**