

## White Paper

# HOW NOT TO FAIL AT AI

## Notes from the field

- 1** Educate yourself
- 2** Create a common vision
- 3** Pay attention to people and culture
- 4** Choose an AI partner well
- 5** Select initial projects strategically
- 6** Start with minimal data
- 7** Track progress and keep everyone aligned
- 8** Shout about success and avoid "Not Invented Here" syndrome
- 9** Scale Up



# How Not to Fail at AI

Gartner recently estimated that 15% of AI projects are successful. A shocking number. 72% of Citrine Informatics' customers generate value in the first year. In this paper we will draw on the experience of two experts who have been involved in hundreds of AI projects in chemical companies and learn lessons about what works and what doesn't.

## OUR EXPERTS



**Johannes Benkhoff** is an Advisory Partner at SPROUT, a Frankfurt based Innovation & Sustainability Consulting company. He has spent more than 25 years in the Technology and Innovation space in the Chemical Industry, as a Scientist, as Innovation Manager and as an Executive Leader, working for Ciba Specialty Chemicals, BASF, and for 10 years until the end of 2021 with Clariant. Now, at SPROUT Consulting he is putting that experience to work by advising Chemical companies going through digital transformations as an external support to the change management process.



**Kyle Killebrew** is the Chief Operating Officer at Citrine Informatics, the AI software company that enables faster development and deployment of next generation chemicals and materials. In his time at Citrine, Kyle has worked with some of the largest global Chemicals producers to put advanced AI tools in the hands of their product scientists, transforming their product lines. For their work, Citrine has been repeatedly recognized as a global leader in innovation, AI and climate tech by the likes of the World Materials Forum, Fast Company, Time Magazine, and others.

## 1. EDUCATE YOURSELF

### Question:

*Imagine you've been tasked with figuring out what the benefits of AI are, and what requirements your company might have for this new technology. What would be your first step - and why?*



#### Johannes:

It's important to understand what AI or material informatics in product development is, what it is not, and how it is different from ChatGPT. You then need to convey that within the organization. There is little to no "magic" behind it - we need to get people down to earth.

So the first thing I would do is educate myself - not in order to get deep insight, and pretend to be the expert, but to gain an understanding and conviction about what AI could do for us. Only by being convinced myself, will I be able to convince others.

By finding and exploring industry case studies from trustworthy internal and external sources, I will be able to inspire and convince others. And by demonstrating business impact and thinking big, leaders and experts will get enthusiastic, and join in on the AI-journey.

### Question:

*What are common applications and notable outcomes in the Chemicals and CPG space that you've seen?*

#### Kyle:

Our customers span the value chain from producers of intermediates and commodity resin like LYB and Braskem; to companies making specialties and formulated products like Eastman, Syensqo, Synthomer and Lanxess; to end market producers like B Braun, Panasonic and Rolls Royce. A plurality uses AI to quickly reformulate. Accelerating reformulation enables them to quickly win customer RFPs, respond to the market more generally, front-run impending regulation or alleviate raw materials supply chain gaps.

An example of this would be a large push at the moment by many companies to remove PFAS, so-called forever chemicals, from their formulations. A Citrine customer did this for an in-market adhesive in 40% of the time it usually takes them to reformulate a product.

**But customers are regularly finding new ways to apply AI and unlock tremendous value...**

Others use it to **optimize processing** in order to reduce energy costs, reduce waste, or increase yields. One specialty chemicals customer increased yield to the highest they've seen in over two decades in 75% of the time compared to their internal benchmark. They estimate a roughly **~\$1M savings** on that one project alone.



## 1. EDUCATE YOURSELF (cont.)

Several multinational customers have used Citrine to tailor formulations to use **local ingredients** to cut down on supply chain costs and scope 3 emissions, or to rationalize ingredients and reduce inventory costs.

A customer that supplies paints & coatings is using the Citrine Platform in **technical selling** to generate a variety of formulations that meet customer specs, while in the meeting with customers. They recently said in an article in Handelsblatt that this has helped to **increase their revenue by 30%!**

Of course, some customers are developing wholly new products and pushing the boundaries of what's possible in far less time. Because this often receives less focus in industry, it's not typically the primary use case.



### Question:

*And are there common misconceptions about AI that you come across when you have initial interactions with potential customers?*

Kyle:

AI in chemicals and CPG often falls into what I call **"The Valley of Misperception"**. Some conflate AI in chemicals innovation with what we see from ChatGPT, IBM Watson, or Google's Deep Mind. Those models benefit from training on massive datasets, the likes of which do not currently exist in industrial chemicals and product development.

On the other side of the Valley there's a misperception that "small" data environments, like the lab, can't create value quickly. The lab is a unique environment for AI. Data is costly and therefore sparse (relative to the datasets used to train something like GPT).

In fact there are long-standing models and techniques that Citrine deploys that enable our customers to **start training models with 20 to 30 - maybe 100 data points**. And not hundreds of thousands. The data we work with is often messy - handwritten, unstructured, or locked up somewhere in cupboards - and often stored in different silos. Here again we combine a variety of longstanding approaches and techniques to make quick use of this data.

Despite not having an abundance of structured data, Chemicals developers do have a wealth of **knowledge in the heads of their experienced product experts**. Citrine AI can and does learn from that, not dissimilar to how a new team member out of grad school might. The AI doesn't need to reinvent the laws of physics, in some cases it's already pre-trained to understand them. In more niche cases the user can impart those laws by typing or verbalizing them to Citrine.

This point is important to underscore: **Citrine AI is built to work alongside product experts** like any one of their other teammates.



## 1. EDUCATE YOURSELF (cont.)

We do this for three reasons,

- i. It means there are **quick iterations** when the product expert has a cool idea, there is no middle man to wait for. We typically see that Citrine AI learns a product's chemistry in 2 or fewer experimental iterations.
- ii. It means that you can easily scale the use of AI, **data science resource is no longer rate limiting**.
- iii. It means that the product **expert's knowledge gets captured** just in the course of working the software. Codified in the platform, so that less experienced employees can easily use it, and learn from it in the future.

**This is Citrine's secret sauce** - combining a variety of AI techniques and an intuitive user experience to enable product developers of any level of experience to quickly train and learn from the Citrine Platform with minimal data and **minimal learning curve**.



## 2. CREATE A COMMON VISION

**Question:**

*OK, we have educated ourselves, what's the next step?*



**Johannes:**

Actually we often see that organizations don't overcome this initial step, a critical hurdle - what we call the **"getting started dilemma"**. People and organizations keep talking about "AI" - experts talk about science and technology. There's buzz at all levels, yet, no necessary steps are taken to move ahead.

What's missing is a common vision for the organization

It's important to translate what AI can do in general to what it can do for your organization - and to "paint a picture", a bright future for your company. The ultimate rationale for using AI is to advance the organization's competitive edge, and create new and lasting business.

To overcome this critical hurdle, it is crucial to bring decision makers from the business side and product experts together to identify the landscape of opportunities: map possible areas, assess how AI could provide value in the short and long term. From there, develop an **inspiring and realistic vision** for the company. This will spark enthusiasm in teams and individuals, and help gain **resources, budgets and engagement** in the organization. People will want to join.



### 3. PAY ATTENTION TO PEOPLE AND CULTURE

#### Question:

*How do you move from the inspiring vision to create the necessary dynamics internally? What are the next steps?*



**Johannes:**

It is important to understand the current situation within the organization. Not only processes and data **but also, very importantly, people!**

Early on, you need to identify people who are enthusiastic about using new technologies – those that will be leading the change – **innovative early adopters**. But also those that can potentially hamper the initiative. It's important to be very conscious about this. You need to understand the **concerns and potential threats** and fears people may see both inside and outside the team, and address those. Actively maneuver the change process.

I guess, we all recall Peter Drucker's quote: **"Culture eats strategy for breakfast"**. It's the culture of openness and willingness to listen and to address people's concerns which can mobilize or, if not done, actively dis-engage people.

I have learnt my lessons on this!

When I first started in this area, my naive misconception was that scientists would naturally be excited by new technology and open to learning something new. But **researchers are human** just like everyone else!



**Let me tell you a "funny story"**

We aimed for an initiative among our scientists to train and build new capabilities by bringing more advanced experimental planning tools into the organization. Simple things we thought. Tools such as DOE – design of experiments. Replacing what I refer to as „Excel Sheet Planning“ – to get faster, unbiased, and more scientific approach to experimentation. To speed up lead generation and time to market via fast, directed development cycles.

We thought, **"let's train them, and let them run"**, and let them play around. They'll like it, they'll see success, and they'll advance.

**That was a failure:** What happened?

After initial training, and capability building, and even providing ongoing support through coaching by expert teams, it took only a few months until we noticed that **only few scientists were regularly using the new tool** and had anchored it in their working habits. The majority had gone back to the original "easier" methods.

So apparently, ... surprise! ... even scientists are human beings. Change is scary. In essence – it is critical for success to understand, and actively maneuver the change process.

### 3. PAY ATTENTION TO PEOPLE AND CULTURE (Cont.)

**Question:** *How do you actively manage the change?*



**Johannes:**

It's important to focus on early adopters, those people who are highly motivated early on, and then tackle those who may follow at a later stage.

**Select the first cross-functional teams**, a diverse group of employees, composed of key people and skills, to map out the first roadmap for initial projects in the organization. People who are eager and willing to get the necessary technical and business questions, challenges and opportunities understood and addressed, and translate this to move from an inspiring vision of "what's possible?" ... to **"what is realistic and doable within my organization?"** ... and at "what price tag" and at "what timescale".

Later other people will join in, ... once first success is demonstrated.

Once success is made visible people will want to follow, once they see the benefit for themselves - to advance, to be successful and to "shine".

### 4. CHOOSING AN AI PARTNER WELL

**Question:** *If you were selecting an AI technology provider to work with - what 3 things would you look for?*

**Kyle:**

First, look for an AI platform that **works with your existing team and data**, aiming to create value quickly. (I'm talking weeks, not months or years.)

Second, while I'm assuming you will cover the standard aspects like information security and business longevity, it's crucial to **ensure the software can scale rapidly**. This includes verifying whether they use a data model that can grow with your AI usage. Make sure it will be easy to incorporate new business units into the system.

Third, choose a provider with an **experienced team** that understands change management and will partner with you to achieve business success, rather than just selling you software.



## 5. SELECT INITIAL PROJECTS STRATEGICALLY

Question:

*How do you select the right initiatives to work on?*

Kyle:

This is a very important question. Over the last decade, we've learned two critical lessons: 1) How you start may be one of the greatest predictors of future success, and 2) There is a wrong way to start.

Citrine has a disproportionately large and experienced team to ensure that both of these points are well addressed. Even before we kick off implementation, we work closely with customers to ensure that their goals for using AI are specific, measurable, and attainable.

We build a plan that clearly articulates how we'll achieve those value-based outcomes and by when. This plan stratifies AI applications based on: 1) The **potential business value**, and 2) **The ease of application**. "Ease of application" is determined by the availability of experts, data, and lab time.

Making experts, data, and lab time available, as well as aligning on goals and a plan to achieve them, are all dependent upon **leadership buy-in**.

The greatest determinant of future success is **leadership engagement**.

We'll launch the highest stratified applications and in parallel help to get the lower ones ready for later launches.



## 6. START WITH MINIMAL DATA

Question:

*There are many advisors out there who recommend investing first in strategizing and preparing data before ever attempting to apply AI. But given your points about working with sparse data, is that what you'd advise?*

Kyle:

Our customers who achieve the highest returns, 3-5x in the first year, work on data and AI simultaneously. **Prepared data on its own yields minimal return**. It's when you start training AI and running analytics on the data that it becomes truly powerful.





## 6. START WITH MINIMAL DATA (cont.)

High-ROI customers begin with whatever minimal data they have, even if it's only enough for a single project. This approach allows them to create initial value, learn which data is worth digitizing (thus starting to accumulate returns immediately), and simultaneously prepare more data.



Much of the historical data might be outdated, and irrelevant for digitalization!

By choosing some initial application with high return and getting that done quickly, you drive more interest and support across your organization that enables you to propel additional data digitization and new AI applications.

## 7. TRACK PROGRESS AND KEEP EVERYONE ALIGNED

### Question:

*If first project success is crucial for the success of the entire initiative - how do you ensure those initial projects will be successful? How do you keep such a project on track?*



Johannes:

The first 1-2 projects need to succeed - **failure is not an option** - as it may massively slow down, or even put the entire initiative at risk. The mindset which is needed from top and senior leaders in the organization - is the readiness to do **"anything to make it happen"**.

The **organizational and project framework** to ensure success **will be key!**

3 levers are critical for this:

- i. Deeply engaged **people & teams** getting the journey started with a realistic execution roadmap.
- ii. A **business leader** who's in the trenches and "pulls" and supports this starting team as much as possible, helping to overcome any roadblocks.
- iii. **Top executives** - eventually the CEO - who stand for the initiative, from the top. Ideally such transformational initiative is led from the very top, and the entire organization is continuously inspired by the **vision and through reported progress from senior leaders** - "talking the walk, and walking the talk".

## 7. TRACK PROGRESS AND KEEP EVERYONE ALIGNED (cont.)



Close attention and coaching of the initiative is needed:

- **Capability building** to support project teams to learn, practice and play their new roles.
- **Agile working practices** should be considered as classical project management methods tend to fail for such exploratory initiatives.
- Continuously **aligning the organization** - horizontally across departments, and vertically across hierarchies.
- **A cross-functional steering framework** to keep the project focused to value and technically realistic.

Independent external support and coaching - if internally not available - has proven to be very effective.

## 8. SHOUT ABOUT SUCCESS AND AVOID "NOT INVENTED HERE" SYNDROME

**Question:**

*Success! What are the next projects, what obstacles do you see?*



**Johannes:**

It's great to see first success, but that doesn't always translate to further success. There are some "human nature things" going on here. People often assume that their area is more complex and different from other areas. What worked elsewhere doesn't work here.

That's what is often referred to as **"NIH" - not invented here syndrome!**

Human beings like to try out things themselves, rather than "stealing with pride" ...or applying working solutions from elsewhere. **Unfortunately human psychology is not in favor of learning by positive example**, but way more effective by failure or pain!

Again, I learnt about this the hard way!



## 8. SHOUT ABOUT SUCCESS AND AVOID “NOT INVENTED HERE” SYNDROME (cont.)



### Let me tell you another story.

We were planning an AI-based initiative to accelerate product development and to step-change performance of next-gen materials in an important business segment.

1. We identified a high rank business leader who was eager to explore and invest. Good starting point. A business sponsor, an owner, who pulled.
2. We selected a top notch external partner to cover the computational science part. And by combination of computational science and historical data we successfully modeled a very complex formulation.
3. We created High Throughput Experimental workflows, and could run many experimental iterations creating lots of new data in fast development cycles. After a few months we had a true „in silico screening” tool.
4. We got new deep and unprecedented insight into the mode of action of the active materials, and a stepchange performance increase.

A true success story – so far ! Failure! ... to cut it short - unfortunately this impactful lighthouse success story did not scale!

### Why was that?

We had **focused too much on data and technology**, and selected applications, where we had good confidence that technology, data and approach would have a very high likelihood of success. This meant that other product experts each found “good” arguments why this would not work in their environment, their applications ... **and they would not even try !!!**

**We had not been successful in building a convincing story** to pull in the next leaders and get them excited about supporting the initiative.

So, maybe against first intuition, it's more important to win strong business leaders, who will be supportive and who will send clear, and inspiring signals - than having the “perfect project” with the “perfect data”.

Therefore the scaling approach should not be very different from the initial approach mentioned before:

- Creating an inspiring and convincing picture of how value and success for the business can be created.
- Ensuring you have engaged leaders supporting & leading teams.
- And continuous communication of progress & success from top leadership.

### Exciting results are infectious

It's important that top executives broadcast lighthouse successes and provide clarity on how people can contribute to success. “Public praise” can serve that purpose - very effectively. People will volunteer to join-in.

## 9. SCALE UP

### Question:

*How does Citrine help its customers scale – get to the next level?*

We often work with the customer to broadcast the success of that first project across more of their organization and start to generate interest from other product experts that could organically drive additional scaling and value.



From a technology point of view, the aspects of our platform that enable scaling now come to the fore.

Several of our customers have attempted to DIY and failed when it came time to scale their solution. Their data scientists have not developed a system easily used by product experts and they struggle to deploy and manage hundreds of models. They work with us now because we solve scaling.

The Citrine Platform has been built as a piece of enterprise software. It uses a graph data model so it is easy to bring together diverse datasets, it uses state of the art usability techniques so that you don't need any code to create and run AI models, all of Citrine's 11 years of experience have been poured into the software so that it creates a smart first pass model automatically, products experts can then easily add their own knowledge into the platform, which means that projects are not limited by data science resource, and of course as you would expect from enterprise software, it is built securely and has an authorization system, it is regularly updated and as we learn more about materials informatics we add new features.

This all means that product experts are not involved in deploying and maintaining software, they **concentrate on what they are good at**.

For them, the platform is easy to use, and it's fun.

### Question:

*How are Citrine involved on an ongoing basis, once AI workflows are embedded in the day-to-day?*

**Kyle:**

The team that helped the customer get started (a mix of data engineers, data scientists and change management advisors) continue to be available, if there is an issue or the customer wants advice about a new project.

Our customers are capable of autonomously kicking off and working on new projects. Because our team has a relevant scientific background as well as a vast experience integrating data sources, our customers will at times ask us to become more involved again as new teams and / or products come on line.



### Summarizing the top tips from Kyle and Johannes



#### Johannes:

1. To get things going in the organization, educate yourself and build a **compelling picture of business value and the future**, to engage leaders, experts and teams.
2. **Identify and empower the front-runners** - people who are eager to start and to pave the road for the next. Help them, support them, train them, and coach them for success.
3. **Showcase successes** and provide clarity on how people contribute to success, and how this will lead to a bright future for them - as individuals - and for the organization. **That will foster imitation.**

#### Kyle:

1. AI for Materials, Chemicals and CPG innovation is AI that works on small datasets to reduce the number of experiments needed to do R&D. It has **proven success** and in the future it will be pervasive across the industry.
2. Find an AI provider that can **use the data, knowledge, and skill set you already have**, rather than making you do a big data project or hire data scientists first.
3. **Make sure the AI you choose can scale**, so that once you have success, you can get the most out of it across your organization. Is the data model graphical? Can all the assets be easily reused? Is the software easy to use?



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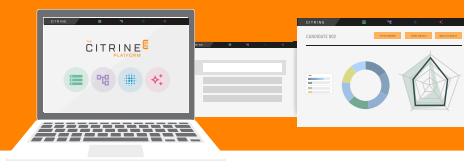
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