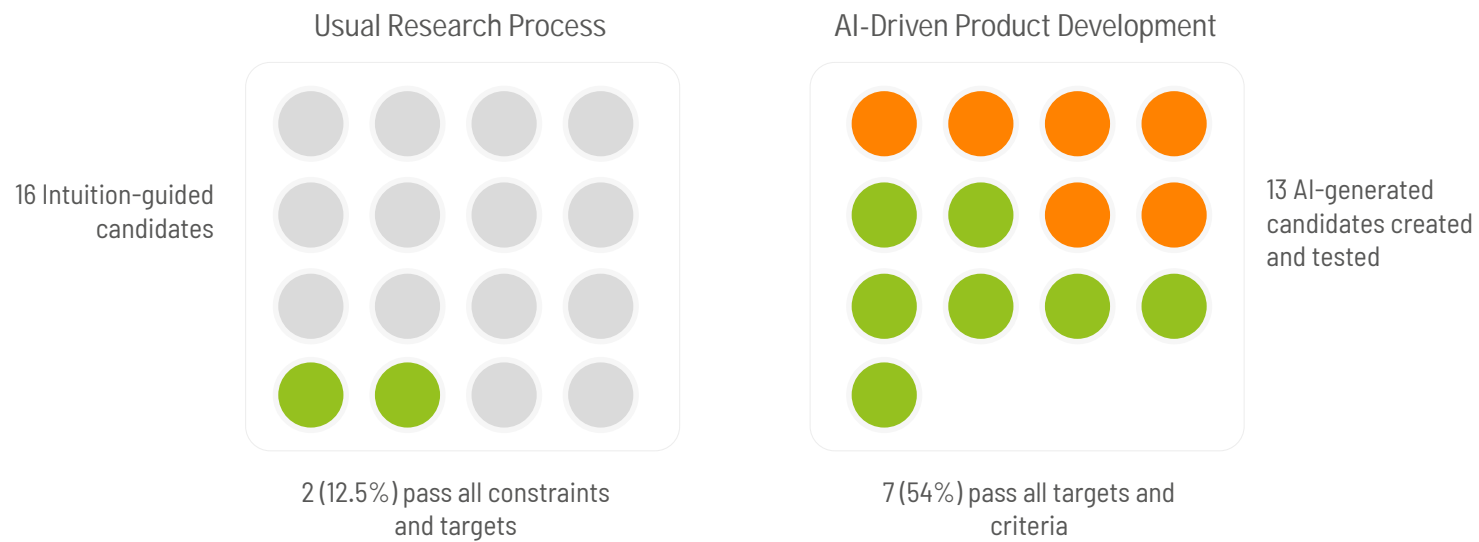


There were 16 formulation candidates suggested by the usual research process and 13 suggested by the initial simple PDFK model on the Citrine Platform. The IRBODWR suggested by the Citrine Platform passed DO constraints at a rate 4 times that of the candidates suggested using the usual research process.



Next Steps

After the success of the first model, the team wanted to co-optimize a property that affects the efficiency of manufacturing composites with other properties. The customer team again incorporated domain knowledge into the modeling approach, using process effectiveness property (B) as a latent variable in the second model. A latent variable is an intermediate property whose data can be modelled from the inputs and whose values may be used as inputs to the main model.

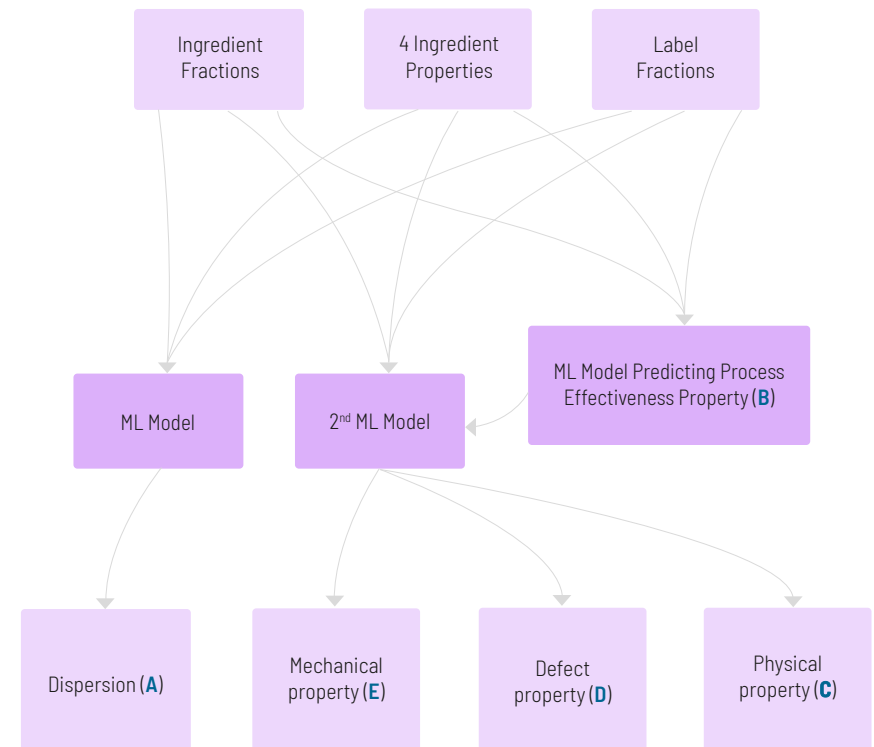
The second model found fewer candidates that met the dispersion and processing effectiveness constraints, and no candidates met the new physical property (C) target. While this was disappointing, it was also useful information. The customer now knows that the current search space does not contain candidates that can co-optimize all 4 properties.

New Product Development Insights

The project produced valuable insights for the customer. They quickly learned that current ingredient inventory was not sufficient to achieve all the performance targets simultaneously, which focused their efforts on which new ingredients to source.

Additionally, the customer team is now fully up to speed with the AI-driven product development methodology, they have a scalable data structure for chemical data, and a clear understanding of candidate selection strategies for data-driven R&D projects.

Next Steps



Summary

With an AI-driven approach to product development, companies can quickly gain valuable insights in a short time frame, even on cold start projects with zero historical data. This approach requires fewer experiments than a traditional design of experiment matrix and produces more valuable results than relying on scientific intuition alone.

Citrine's global team were able to support the customer team as they started using the Citrine Platform virtually, using synchronous and asynchronous tools. Insights gained during the project are now being used to guide future research directions.

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