From research to business value

EVONIK

CASE STUDY

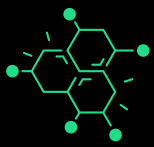
Optimization of chemical mixers design via tensor trains and quantum computing with Evonik

Efficiently designing optimal chemical mixers and reactors is critical for improving manufacturing processes across many industries like pharmaceuticals, agriculture, and more. Better mixer designs directly enable higher product quality, increased yields, reduced costs, and decreased environmental impacts. However, identifying the ideal mixer shape to maximize mixing performance is incredibly challenging. Testing physical prototype after prototype is slow and costly. Computational modeling and simulation helps, but evaluating different designs is still computationally intensive. New optimization methods are required to make this process faster, cheaper, and more effective so we can accelerate chemical innovation.

Key Takeaway

Using a proprietary tensor train-based optimization approach, Terra Quantum's TetraOpt algorithm achieved a 2.3x lower cost function versus standard Bayesian methods for optimizing the geometry of a chemical mixer, enabling significantly improved mixing efficiency. By leveraging parallelization and more global search, TetraOpt reduces the time and computational effort required to identify optimal mixer designs. These results showcase the potential of quantum-inspired algorithms to accelerate and enhance chemical engineering design processes.

The Problem



The goal is to optimize the geometry of a Y-shaped fluid mixer to maximize mixing quality. Mixing is evaluated computationally by a coefficient of variation (CoV) metric. The challenge lies in minimizing the CoV by tweaking geometry parameters.

Results

2.3x **Lower average CoV versus Bayesian optimization.**

2.2x **Lower best CoV versus Bayesian optimization.**

35% **Decrease in runtime versus the existing Bayesian optimization approach.**

Access our publication for more: Optimization of chemical mixers design via tensor trains and quantum computing

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The Approach

Terra Quantum's optimization team knew that optimizing the complex mixer geometry would require testing a massive number of potential designs, however exhaustive testing was impossible - they needed a smarter approach, which is why they used TetraOpt.

- TetraOpt breaks the problem into parallel pieces using tensor train decomposition.
- It chooses new candidate designs dynamically based on past results.
- Parallel exploration allows it to find improved solutions faster.

While there is room for more innovation with quantum computing, this demonstrates the power of quantum-inspired algorithms.

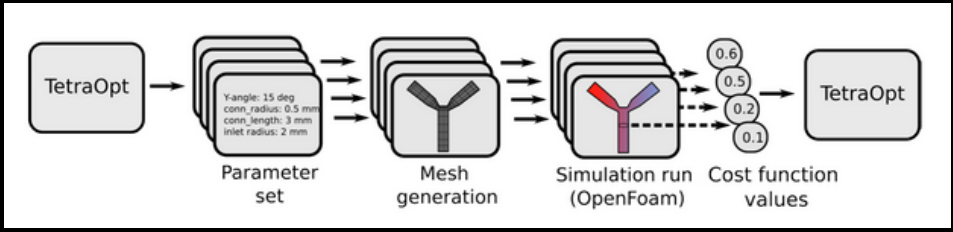

Fig. 18: Visualisation of the TetraOpt generalised black-box optimizer

Tensor Trains

Tensor Networks are a new approach to linear algebra emerging from quantum physics for very efficient solutions to high-dimensional problems, relying on decomposing a huge tensor into a product of smaller ones. Tensor trains are a type of tensor network that have a simple, linear structure. They are the most well-studied of all tensor networks.

Conclusion

For optimizing mixer geometry, TetraOpt significantly outperformed standard Bayesian optimization. The highly parallelizable approach shows great promise for accelerating and improving chemical engineering design.

> The cooperation with Terra Quantum has allowed us to understand the potential current and future benefit of Quantum Computing for a specific class of Evonik use cases. The software prototype that has now been developed is promising with not only faster but also better results. We are now exploring how we could work towards realizing the business benefits of these efforts for multiple use cases.
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> - Henrik Hahn, Chief Digital Officer, Evonik Industries