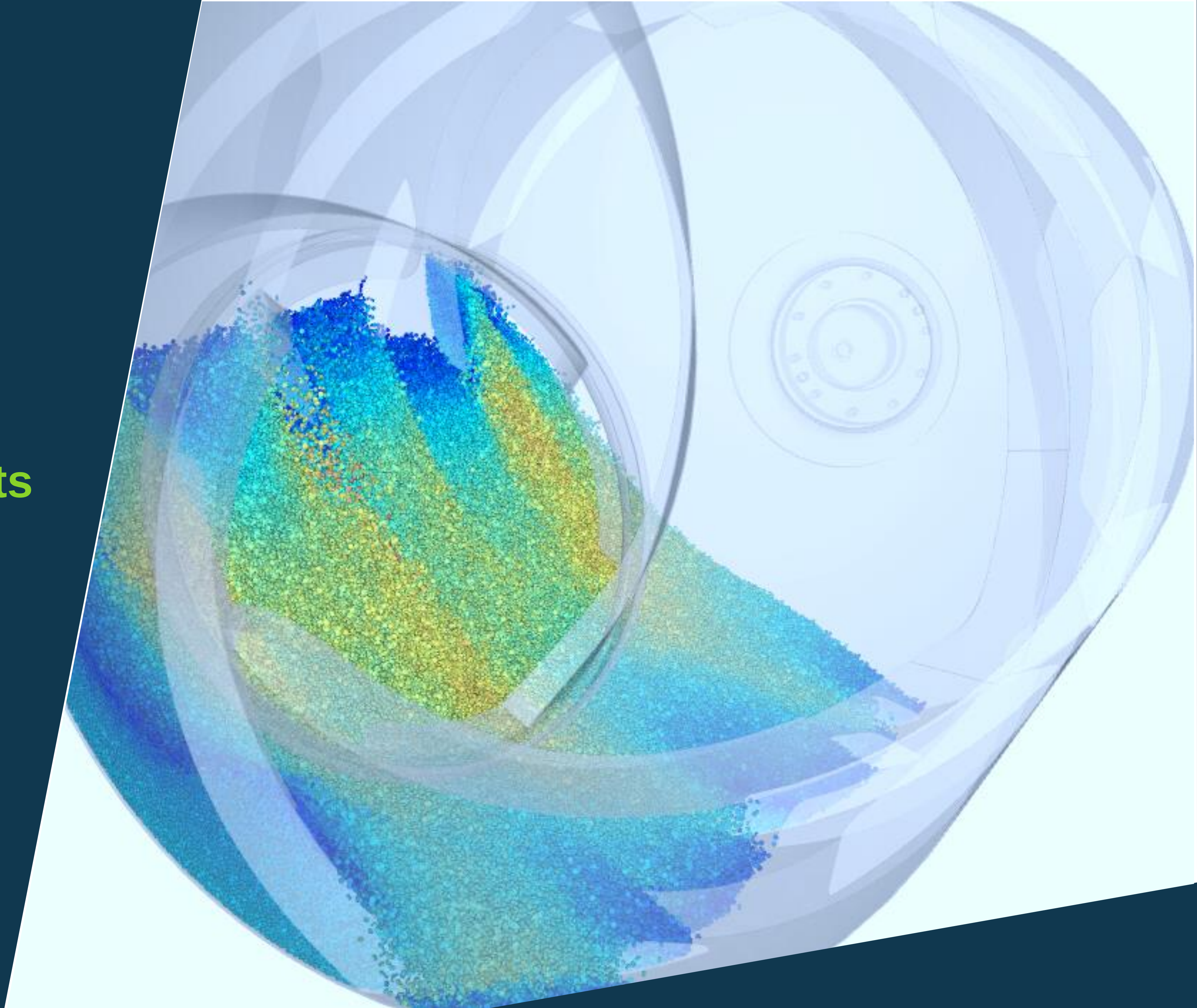
Ansys WOST Conference

Parametric geometry optimization of solids processing equipments



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Bayer AG

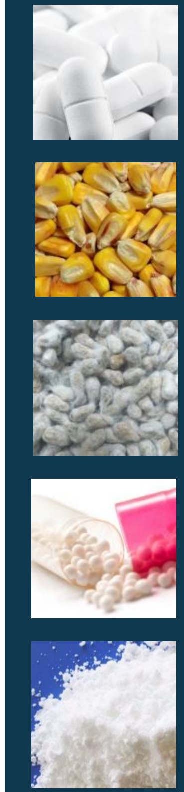
Engineering & Technology

Formulation & Processing Technologies

Motivation

Optimization of Solids Processing Equipments

Solids Processing



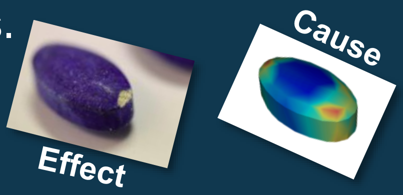
- Processes which involve handling of bulk solids (powders, seeds, tablets) ubiquitous in Life Sciences.
- Process / equipment design and optimization non-trivial.
  - Multi-factorial design space
  - Variable particle properties and bulk rheology
  - Lack of useful in-process data / sensors.

Discrete Element Modeling

- Computational method to model behavior of bulk solids by computing

$$m_\mathrm{i}\, \mathbf{a}_\mathrm{i} = \sum \boldsymbol{F}_{ij} \qquad \boldsymbol{F} = f(\boldsymbol{r}_{ij}, \boldsymbol{v}_{ij}, \dots)$$

  for up to millions of particles.
- Increasing adoption to industrial scale processes due to GPU acceleration.
- Useful tool to gather process insights.



Challenge

- Process and equipment geometry optimization using DEM difficult due to computational costs for each design evaluation.
- Simulation workflows contain multiple nodes (CAD, DEM solver, post-processing)
- Potential solution with OptiSLang
  - Process automation
  - Surrogate modeling
  - Optimization using surrogate model

Project Examples

Seed Processing Equipments

Cotton Seed Reactor Process Optimization

World-scale continuous cotton seed delinting plant.

DELTAPINE® Cotton

Chemical Delinting = Removal of cellulose linters

// Optimize seed residence-time distribution in a rotating-drum reactor.

Seed Treater Design Optimization

Seed treating : Coating of seeds with layer of active ingredients and exipients to protect seed during early germination.

Lab rotary batch treater

Liquid slurry atomizer

Mixing fins

// Product build-up close to mixing fins observed for certain adhesive coatings.

// Design optimization to reduce build-up.

Modeling Pipeline and Tools

Software toolbox

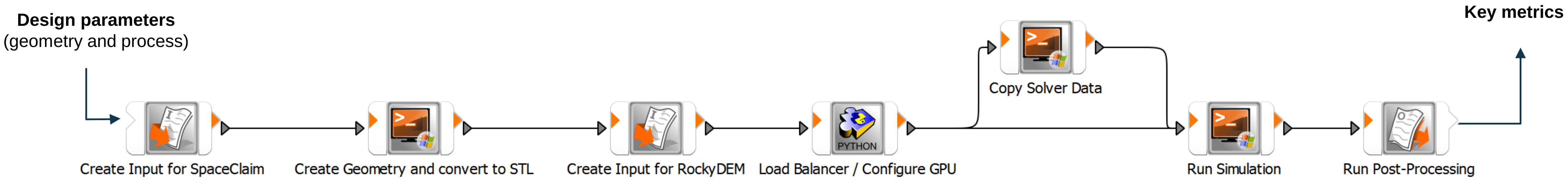
Ansys SpaceClaim
- Parametric CAD using SpaceClaim scripting.
- Geometry discretization

ROCKY
- DEM solver
- Post processing using python scripting

Ansys / DYNARDO optiSLang®
- Process automation
- Sensitivity studies
- Surrogate modeling
- Optimization

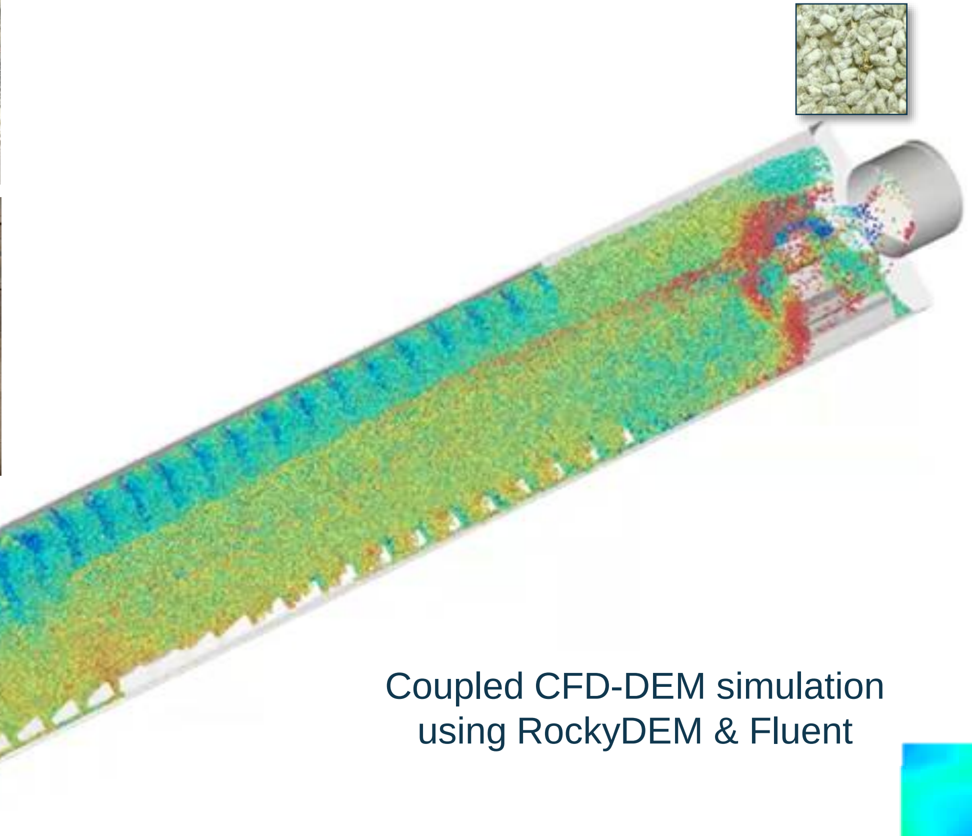
Process automation

(OptiSLang parametric system)



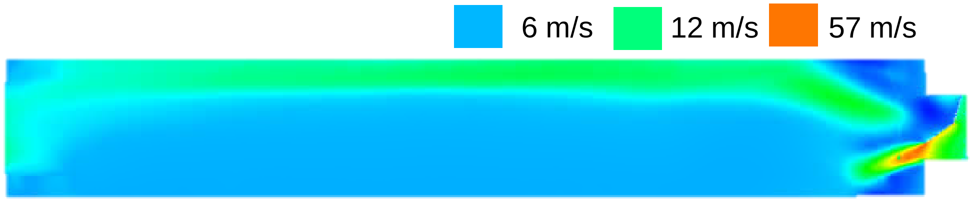
Cotton Seed Delinting

Optimization of Residence Time Distribution in Rotating Drum Reactor



- 10 t/h seed throughput with heated air for drying / reaction enthalpy.
- Residence time distribution (RTD) depends on large set of factors, e.g. throughput, rotation speed, air flow rate, …
- Desirable mean residence known.
  Minimization of sd(RTD) goal.
- Operational plant. Interest to minimize downtime for testing.

Coupled CFD-DEM simulation using RockyDEM & Fluent



Cross-section Velocity distribution

Optimization Problem

- CFD-DEM provides good prediction for residence time distribution (RTD). Mean residence time typically in the order of 30 – 60 mins.

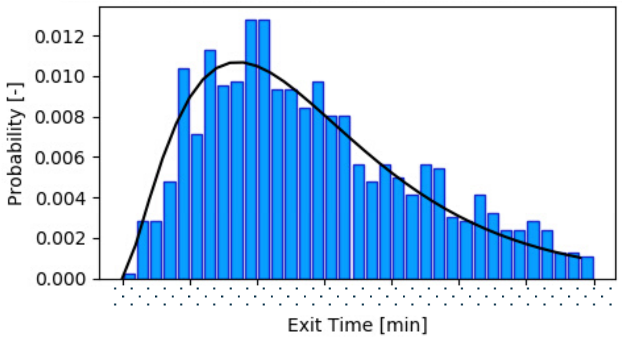


Fig.: Base line RTD

- Regression using nCSTR model possible

$$E(t) = \frac{1}{\tau}\left(\frac{t}{\tau}\right)^{n-1} \frac{n^n}{(n-1)!} \exp\left[\frac{-nt}{\tau}\right]$$

τ ... Mean residence time
n ... Tanks in series

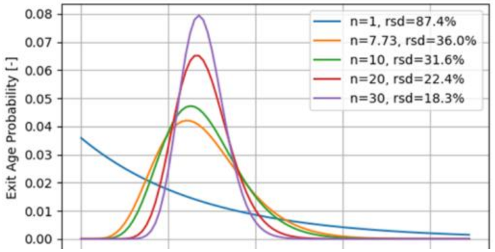


Fig.: Effect of increasing n

- Optimization problem: Find design with narrow RTD (maximize n) and desired mean residence time.

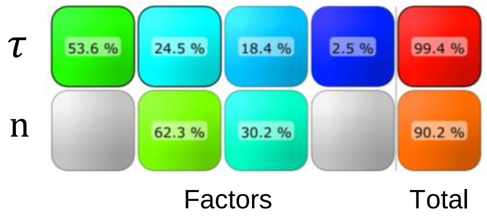
$$\min_{D}\left[\frac{1}{n}, (\tau - \tau_{Set})^2\right]$$

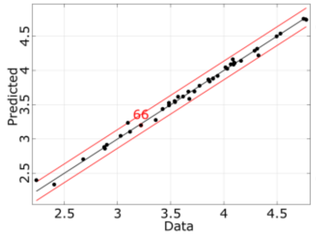
- Given significant cost of model evaluation process automation and surrogate modeling necessary.

- Optimization problem solved using OptiSLang
  - Latin hypercube sampling to explore design space (7 dim.)
  - Surrogate modeling using Kriging kernel functions
  - Global optimization using particle swarm optimizer

Results

// Surrogate model provides predictions comparable to mechanistic model. and relative importance of factors (Coefficient of prognosis matrix)





// Multi-objective particle swarm optimization provides a Pareto front along which at least one objective is minimal.

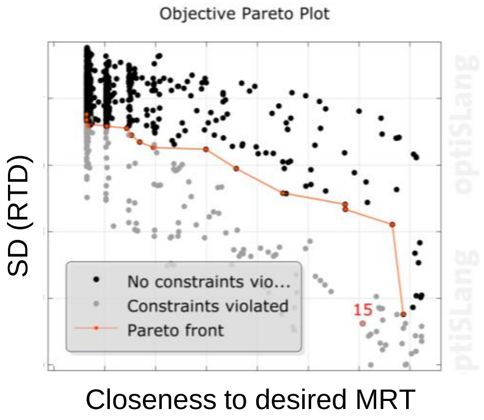


Fig.: Pareto frontier

// RTD comparison of predicted baseline and selected Pareto optium.

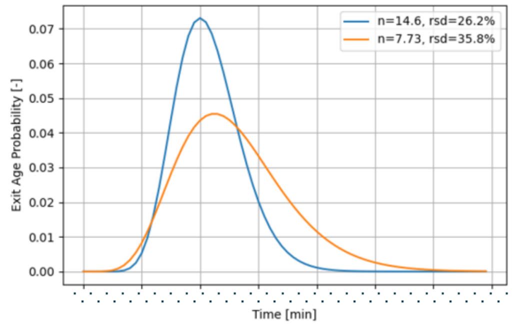


Fig.: Baseline vs. Selected

// Major learning on design limits: No narrower RTD possible without significantly reducing MRT.

// Model predictions validated on production scale.

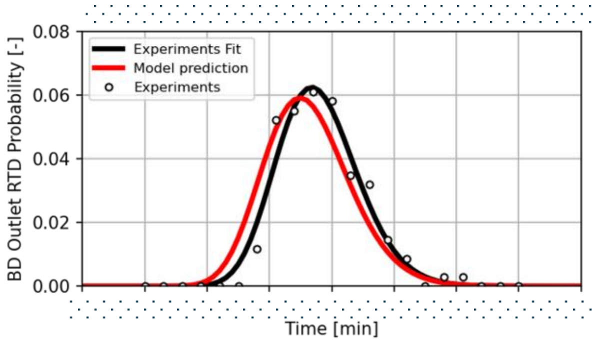


Fig.: Production scale validation

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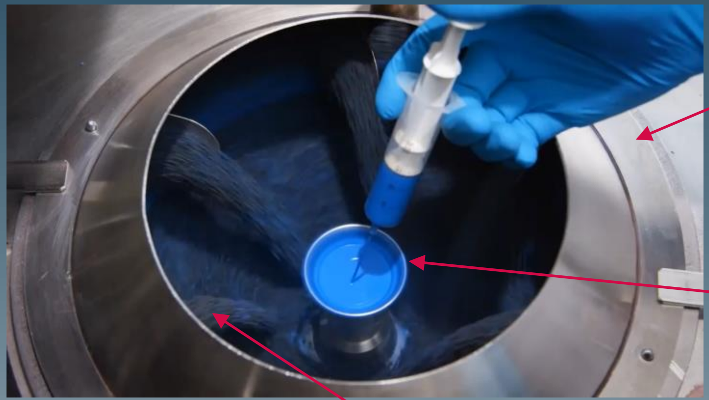

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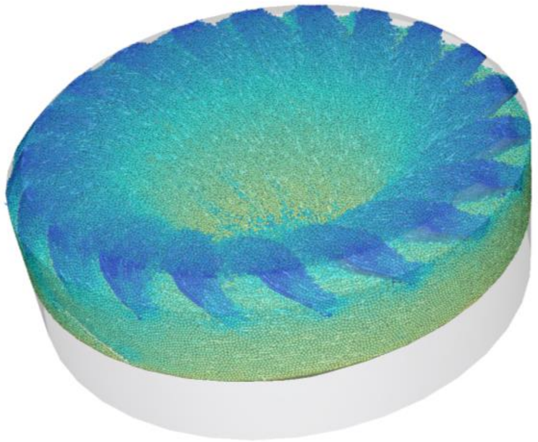
Seed Treater Design Optimization

Root Cause Analysis



Low Shear Zones

Optimization Problem

$$\min_{D} \left[\text{Low Shear Zones}, \quad \frac{1}{\text{Lacey Mixing Index}}, \quad t_{\text{Discharge}} \right]$$

Design Optimization

Automated Screening of parametric SpaceClaim CADs

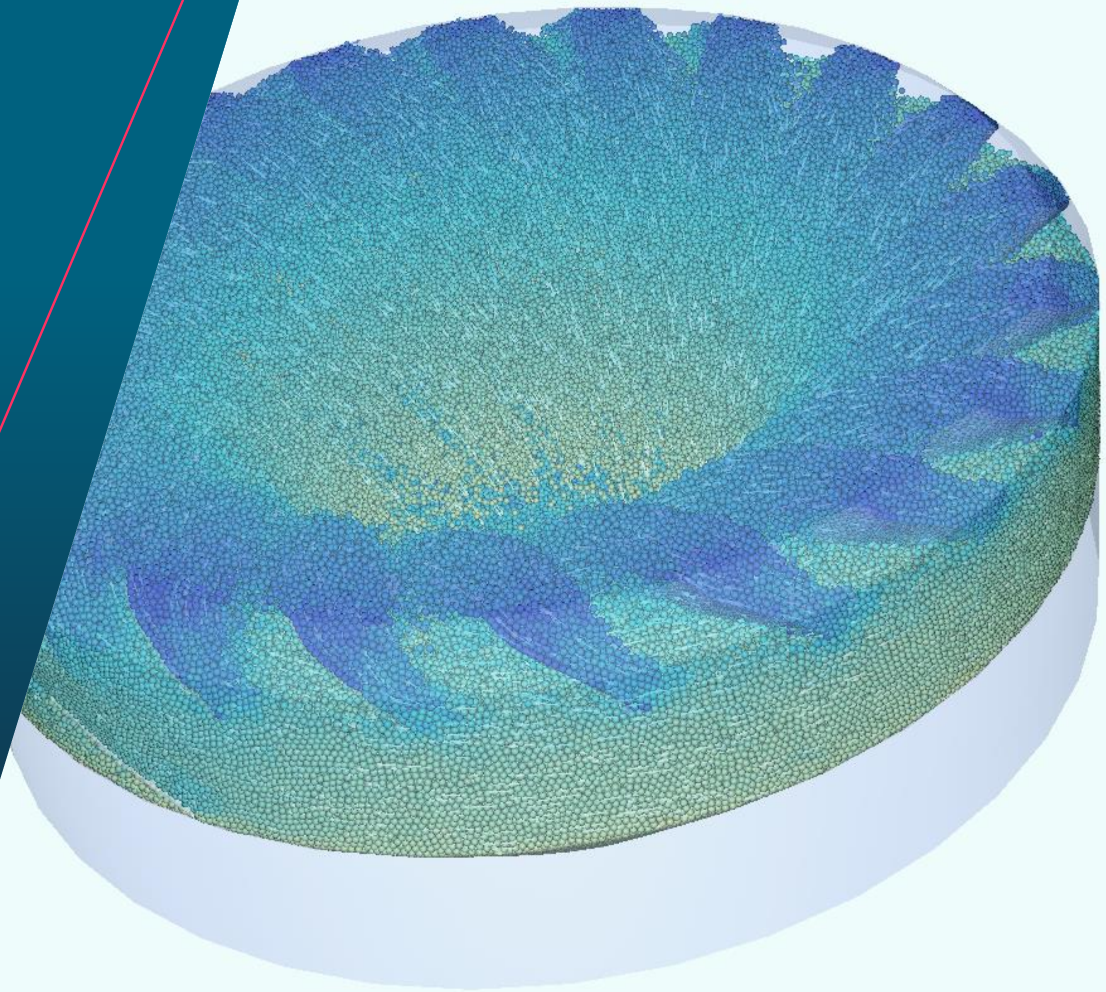
Selected Design

Before

After

Summary

- DEM able to provide insights into „black-box“ solids processes.
- Process automation and surrogate modeling using OptiSLang a feasible approach to solve optimization problems in solids processing.
- Significant time and cost savings compared to physical trial-and-error experimentation.



Thank you ! Questions ?

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