Automatic optimization of helix mixer using pSeven and FlowVision

About DATADVANCE

DATADVANCE is a software vendor specialized in development of design process automation, predictive modeling and multidisciplinary design optimization software.

DATADVANCE has been incorporated in 2010 as a result of a collaborative research program by:

Institute for Information Transmission Problems of the Russian Academy of Sciences – one of the leading mathematical centers in Russia with three Fields prize winners on the staff

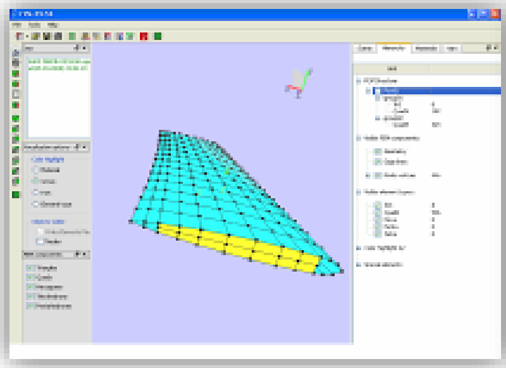
Airbus Group (formerly EADS) – a global leader in aerospace and defense industry.

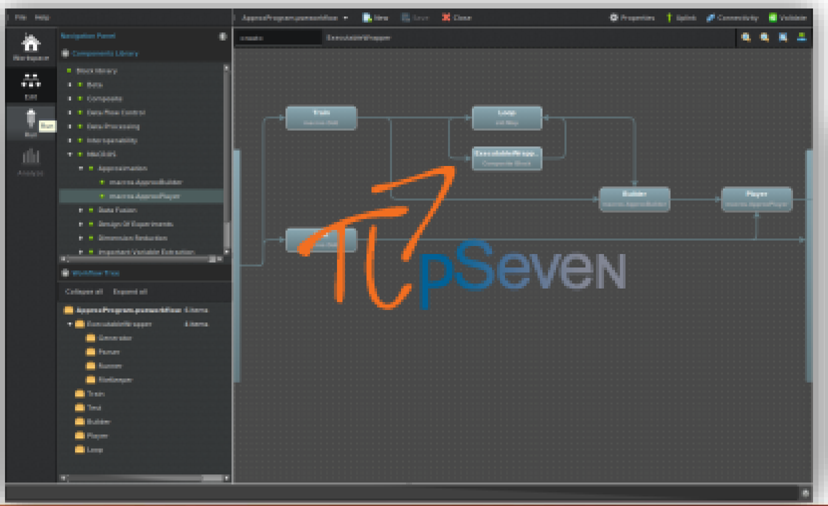
DATADVANCE offering

- **pSeven powered by MACROS technology** is a software for process integration, data mining and multidisciplinary optimization
  - helps to **reduce design time and cost**
  - improves the **quality and performance** of the product

- **Engineering Services -** solution of complex engineering problems.

- **Research and development** on specific customer's requirements.





Contents

Problem definition and optimization scheme

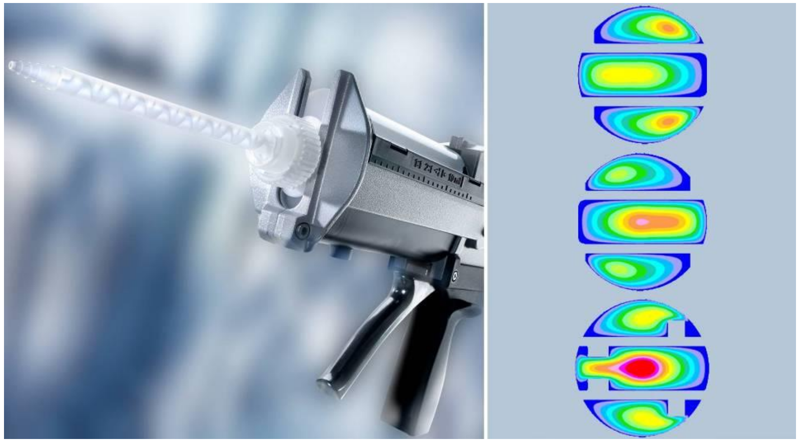
Aim: Find optimal geometry of static helix mixer

Customer: Sulzer Mixpac

Customer expectations: “ Improve mixer design “

➘ **Pressure loss to be minimized** ➚ **Mixing quality to be maximized**

SULZER



Challenges

- Huge CPU time
- Multi-objective problem
- Time limit

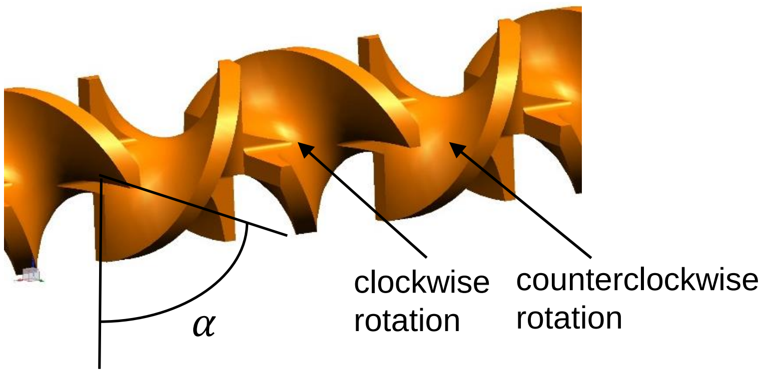
Geometry to optimize

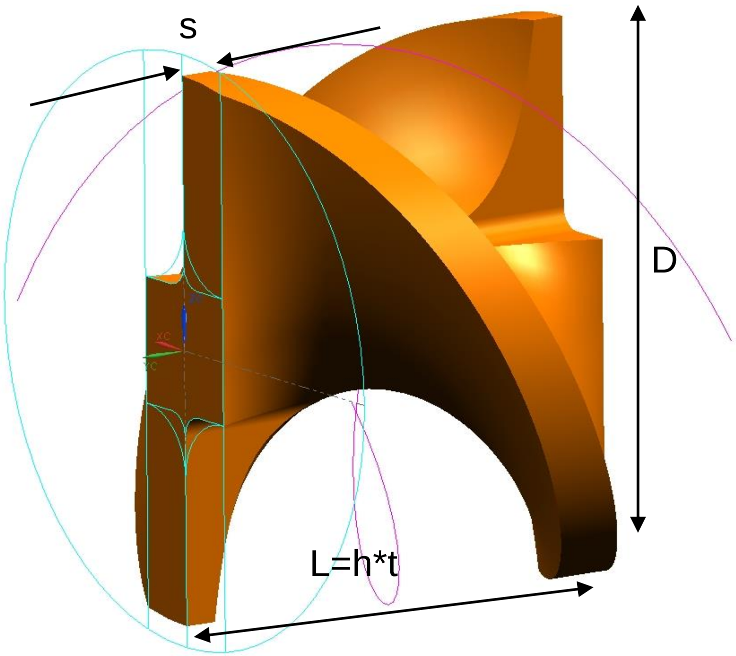
Static Helix Mixer elements

- Mixing element constructed by sweeping the profile along the spiral
- Dividing the flow at each mixing element

Geometry is controlled by

- Convolution fraction t
- Length of one total rotation (pitch) h
- Element thickness s
- Angle of two elements to each other α

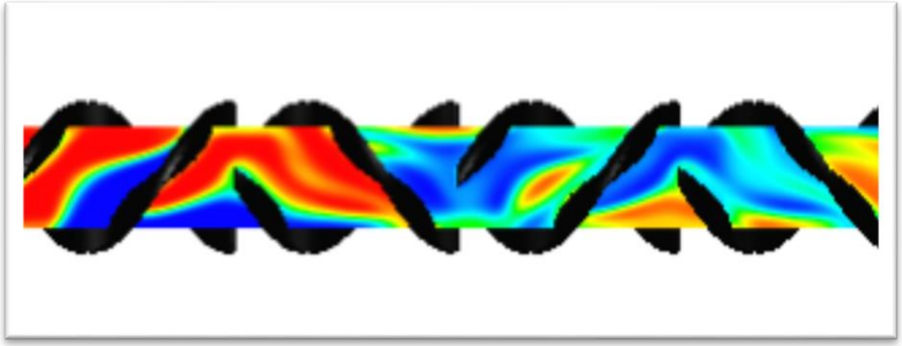




Parameters and constraints

Geometry constraints

- Convolution fraction $t \in [0.25, 0.75]$
- Pitch (length of one total rotation) $h \in [14\text{ mm}, 26\text{ mm}]$
- Element thickness $s \in [0.7\text{ mm}, 1\text{ mm}]$
- Angle of two elements to each other $\alpha \in [60°, 120°]$



Global parameters

- Pipe with 5 mixing elements
- Pipe diameter D=10 mm
- Mixing ratio of two fluids is 1:1
- Fluid properties: $\mu = 10\ Pa \cdot s,\ \rho = 1000 \frac{kg}{m^3}$
- Inlet velocity $U_{1,2} = 0.01$ m/s
- Reynolds number $Re = 0.01$

General approach

Definitions of objective functions

- Mixing quality measured by flow dispersion of fluid concentration (the less the better)

Flow dispersion $\mathrm{DF} = \sqrt{\dfrac{\iint (C - \langle C \rangle)^2 \rho V_n dS}{\iint \rho V_n dS}}$ calculated at the 5th element

- Pressure drop dP is a pressure difference at the end of the 1st mixing element

Software used

pSeven powered by MACROS technology

Data Analysis | Design optimization
Uncertainty management | Process integration

Faster	•Save time in development cycle and reduce simulation costs •Faster simulations thanks to surrogate models •Faster optimization due to reduced number of iterations •High Performance Computing capabilities
Stronger	•Get stronger than your competitors with optimized designs •Robust methods with a high convergence rate
Smarter	•Discover *Smart Selection* feature to pick the most suitable algorithm automatically - expert level for engineers! •Understand correlations between different parameters
Higher	•Obtain higher degree of automation •Use more data samples •Get more accurate model •Get value from your test database

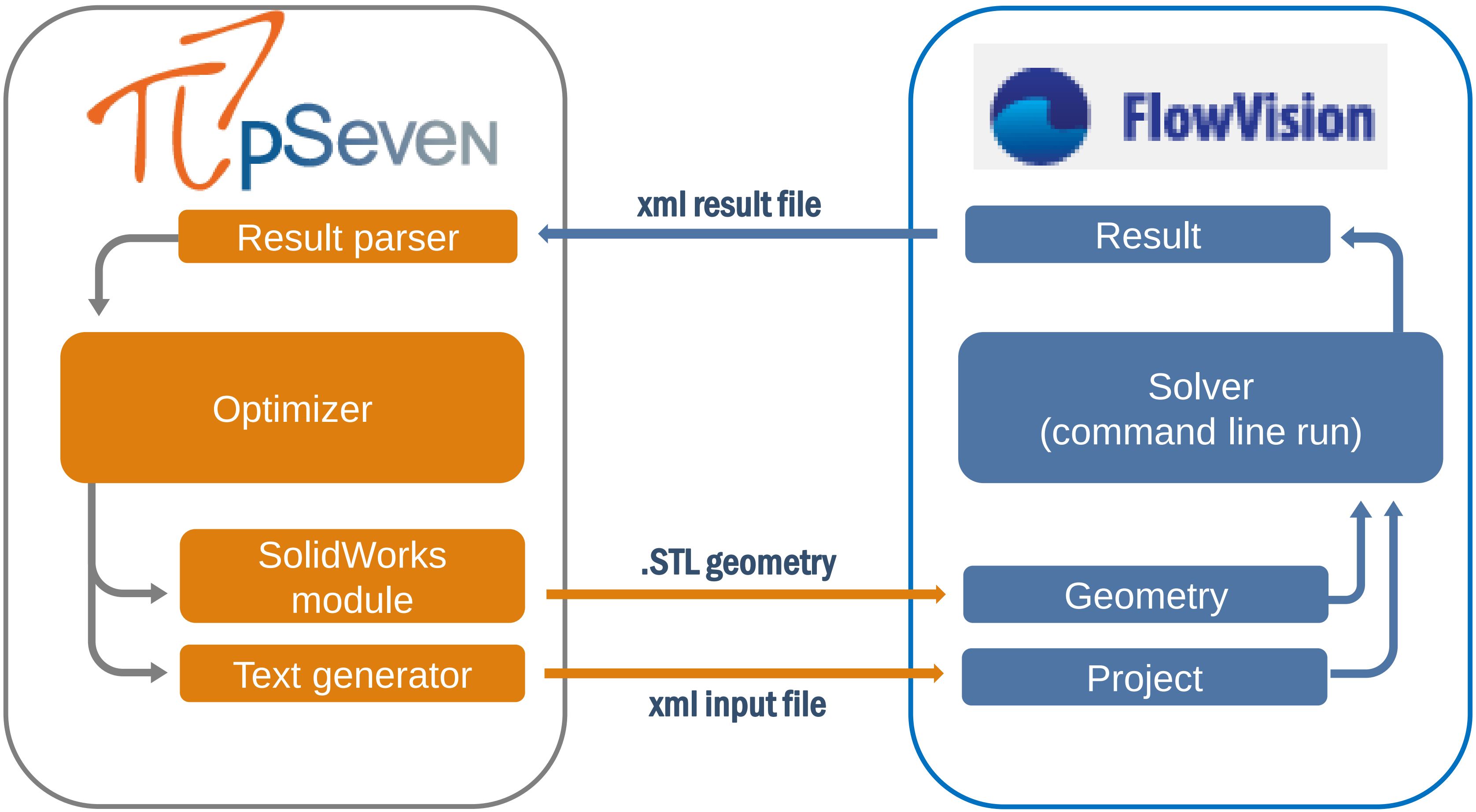
FlowVision CFD solver

Developed by TESIS company (Russia)

FlowVision main features

- 3D steady and unsteady flows of incompressible or compressible fluid
- Adaptive grid generation: geometry fitted sub-grid-resolution
- Natural linking with CAD geometry
- Gas/fluid flows in rotating systems with 'Moving body' technology
- Multi-fluid mixing and chemical processing
- Heat transfer

Process Integration and Optimization scheme



Contents

- Problem definition and optimization scheme
- **Single calculation with FlowVision solver**
- Workflow automation in pSeven
- Optimization problem definition
- Results and conclusion

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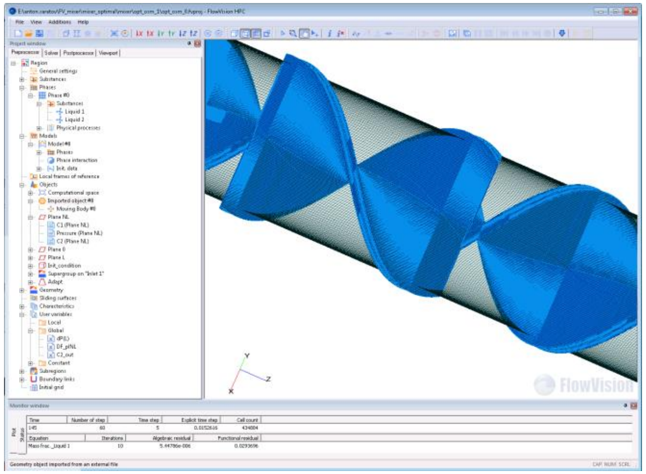
FlowVision calculation

FlowVision project contains

- Model for calculation
- Initial conditions
- Computation space parameters
- “Moving body” geometry
- Mesh settings
- Solver settings
- Coordinates of inlet/outlet planes (for post-processing)



to be updated at each step

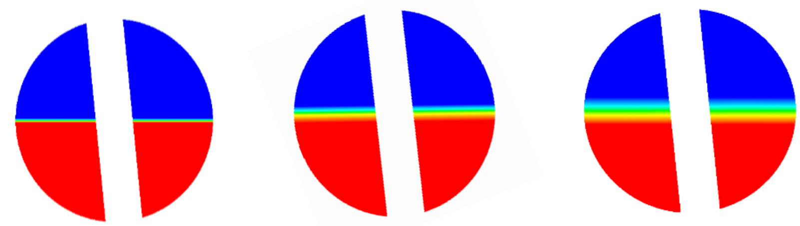
Mixer geometry to be changed during optimization

Update in SolidWorks → Export to STL format, XML file with inlet and outlet planes → Reset mesh and run solver → Resulting XML file with variables

FlowVision calculation: mesh study

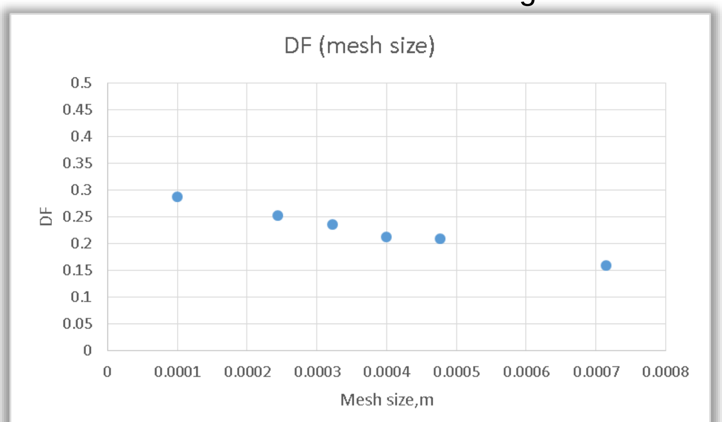
- Mesh size is a crucial parameter for CFD calculation.
- It is especially important in mixing simulations due to numerical diffusion.
- This effect can significantly change the value of dispersion [2,3].

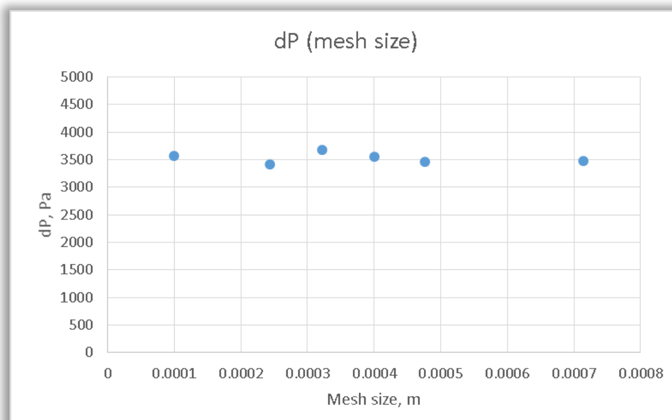
The influence of mesh resolution on numerical diffusion :



Fine mesh (0.1 mm) DF = 0.499 | Medium mesh (0.4 mm) DF = 0.486 | Coarse mesh (0.6 mm) DF = 0.477

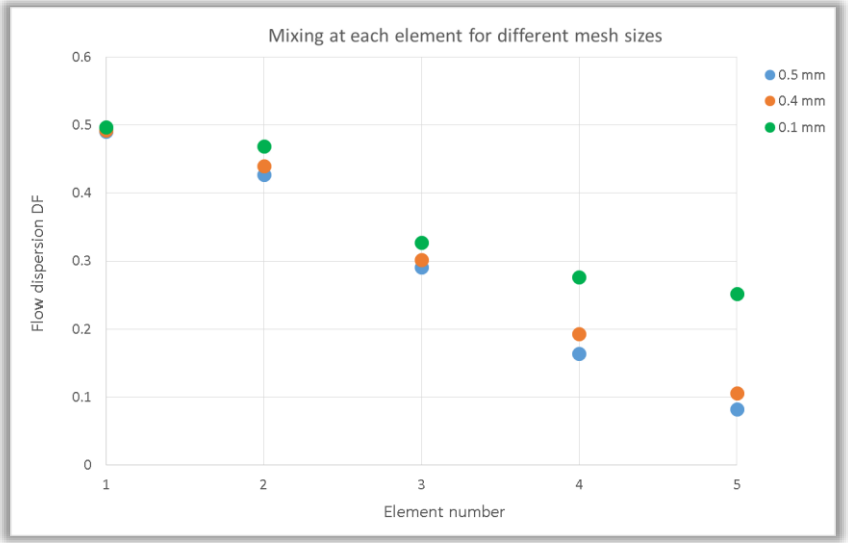
Result of single calculation on 5 elements for different mesh :



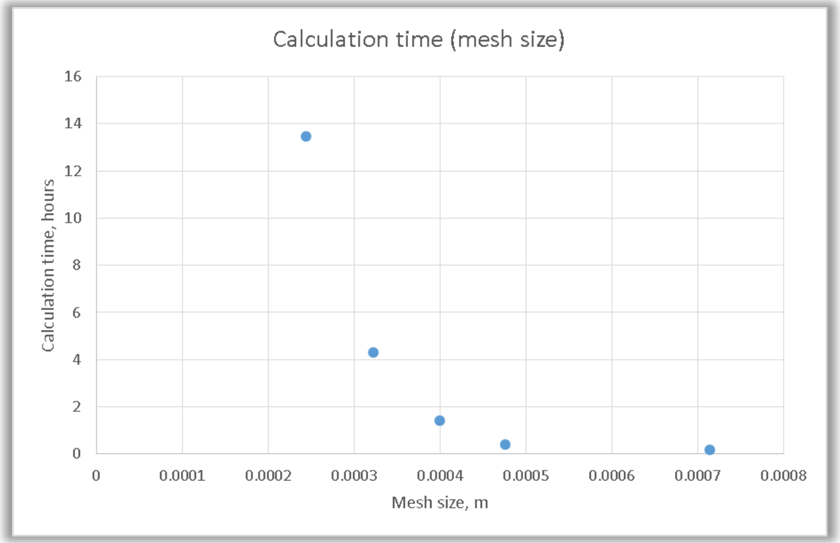


FlowVision calculation: mesh study

Mixing at different elements for different mesh size



Calculation time at single PC for different mesh size



Accuracy of fine mesh vs. calculation time – tricky choice

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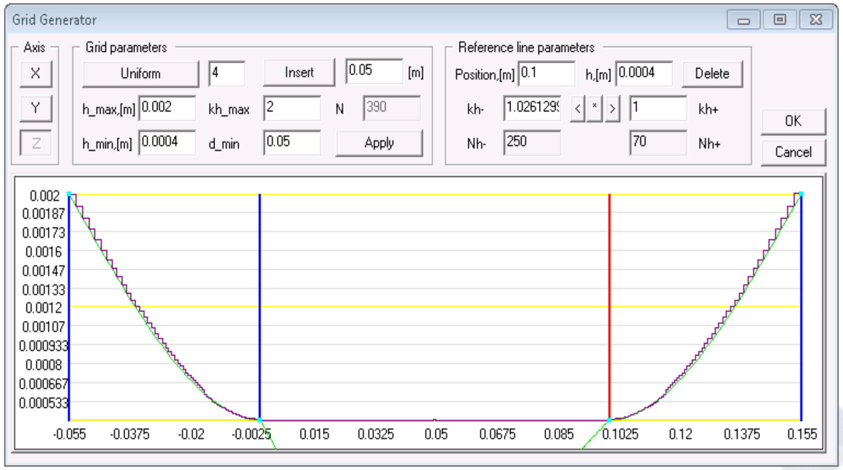
FlowVision calculation: mesh

Assumption: Relative mixing quality of different geometries can be determined with medium mesh resolution

The following mesh setup is used for optimization:

- Initial mesh: 26x26x390 cells
- Initial mesh cell size:
  - 0.4 mm in mixing area
  - 2 mm in inlet/outlet area
- Adaptive mesh refinement in mixing area with factor 2



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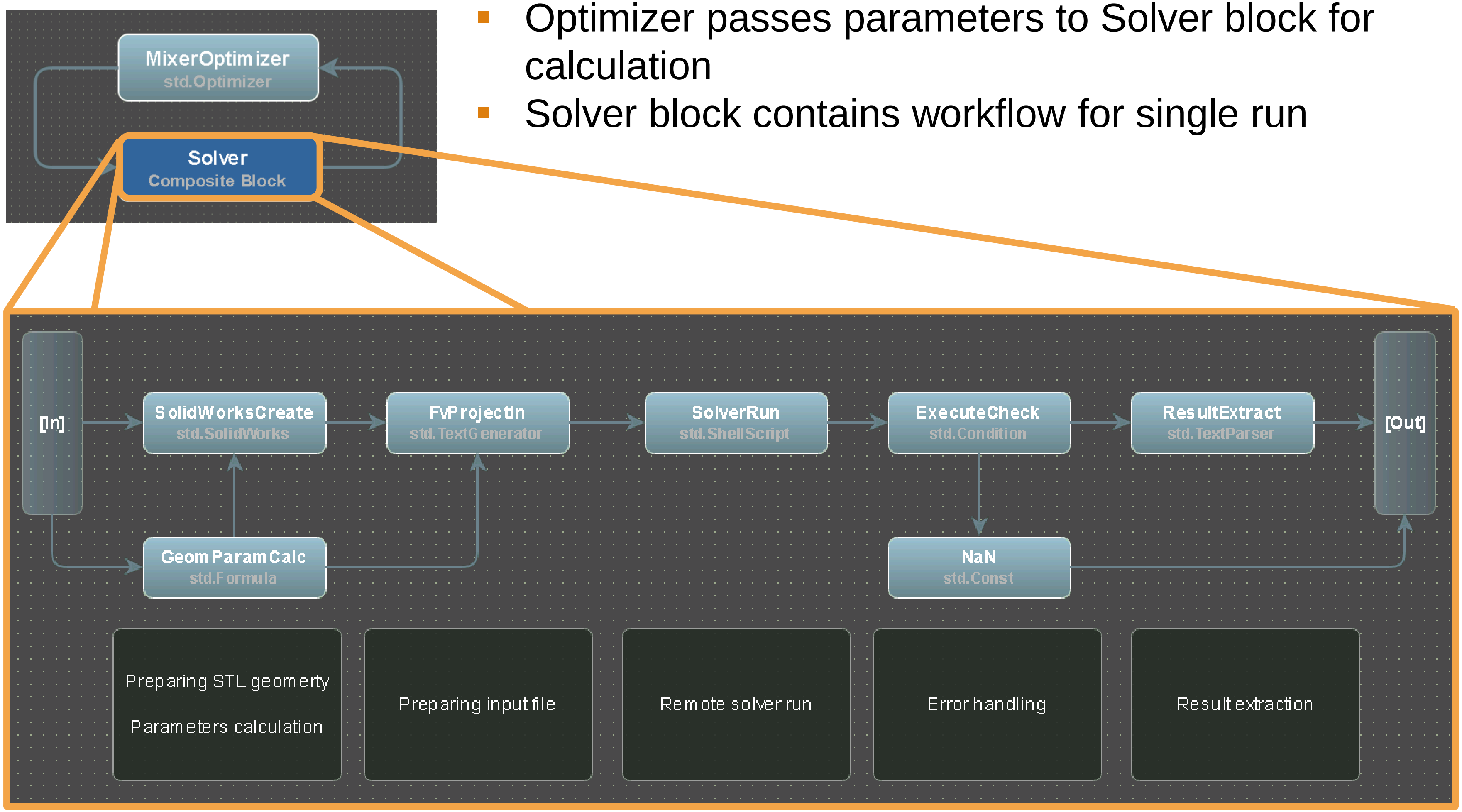
Contents

pSeven workflow

- Optimizer passes parameters to Solver block for calculation
- Solver block contains workflow for single run



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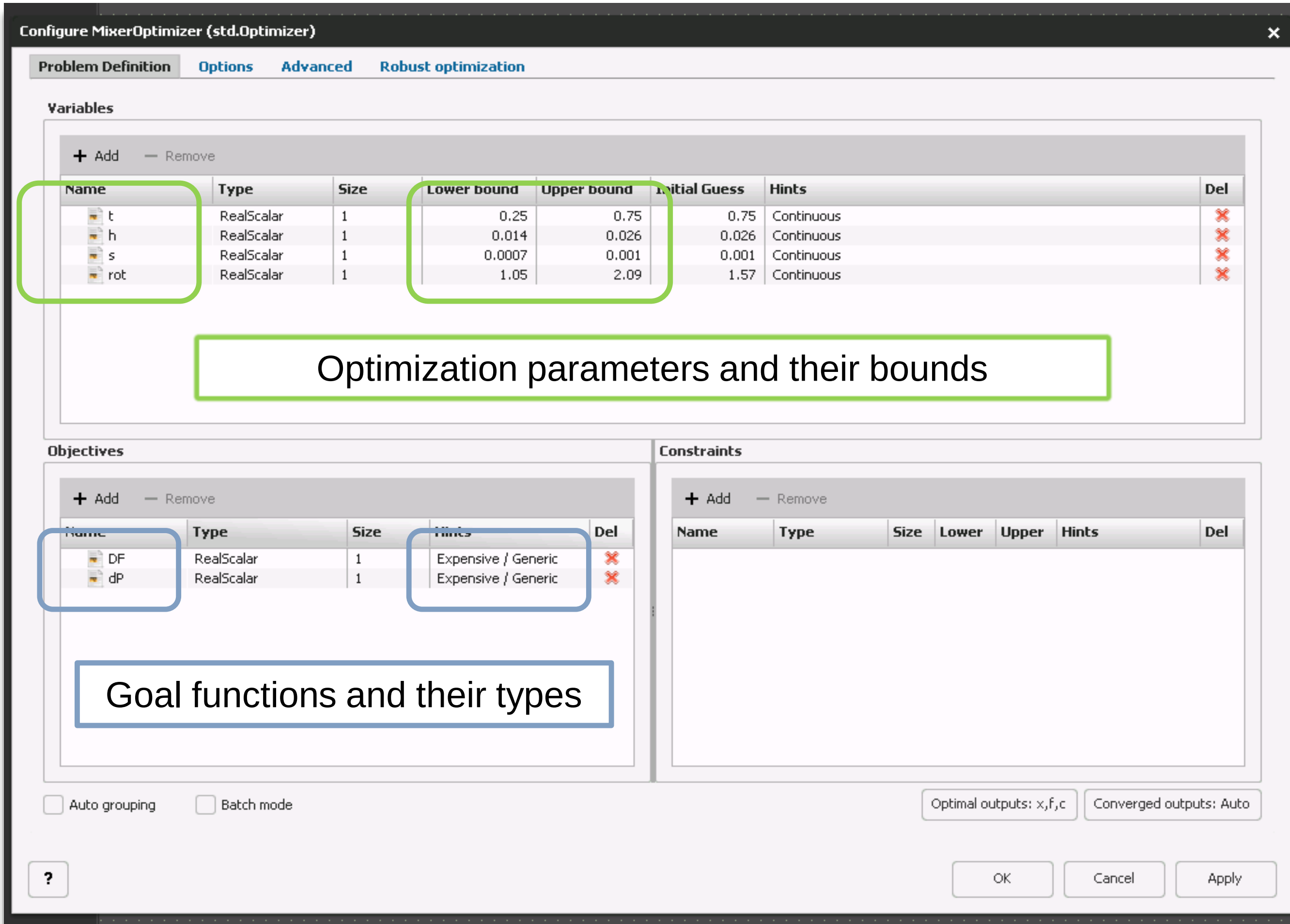
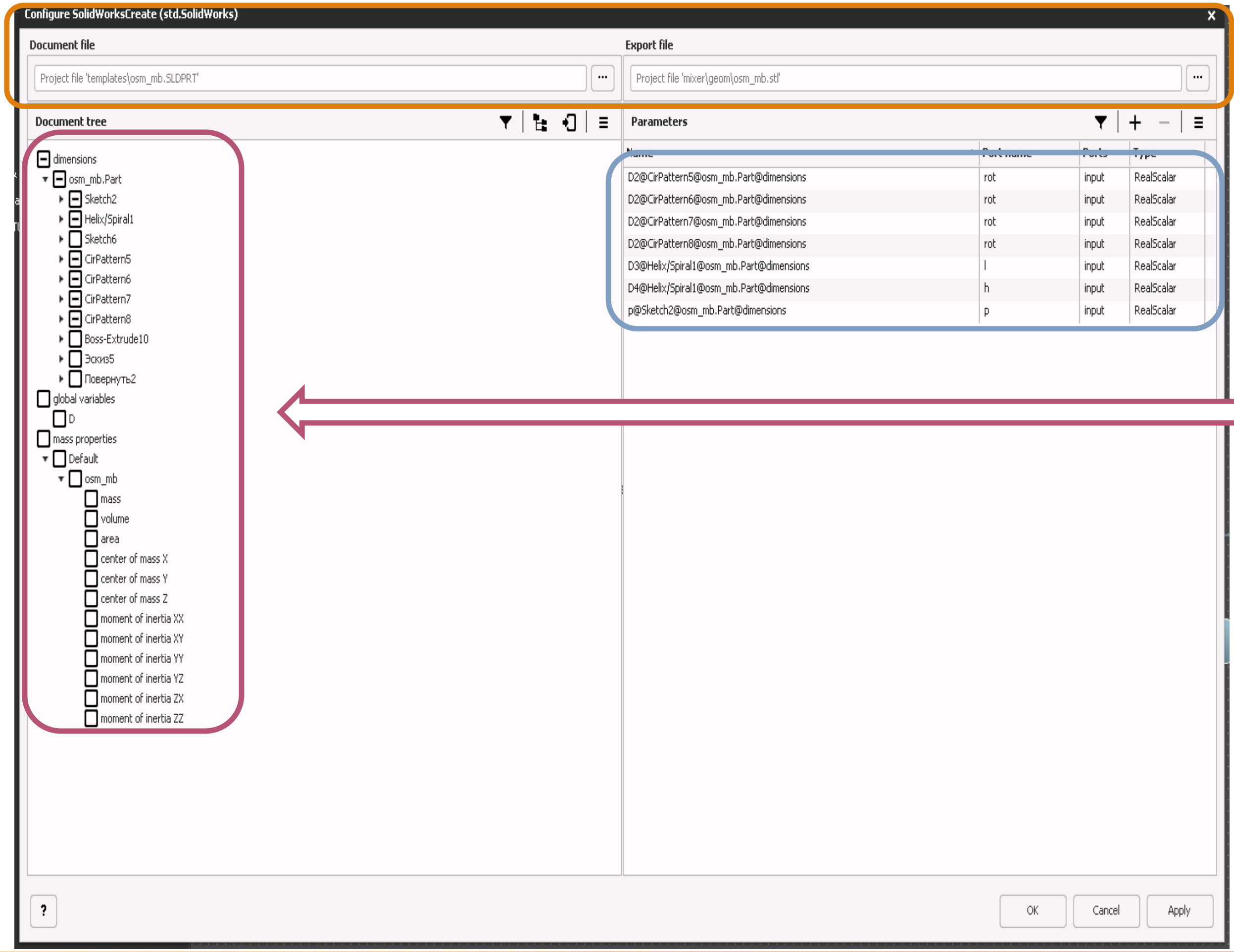
pSeven workflow: Optimizer

“Smart Selection” makes it easy-to-use: All you have to provide is a few parameters



pSeven workflow: SolidWorks block

- Easy access to the model tree through CAD API
- Smooth integration of model parameters to the block ports



Initial model and export file

Geometry parameters

Model parameters tree

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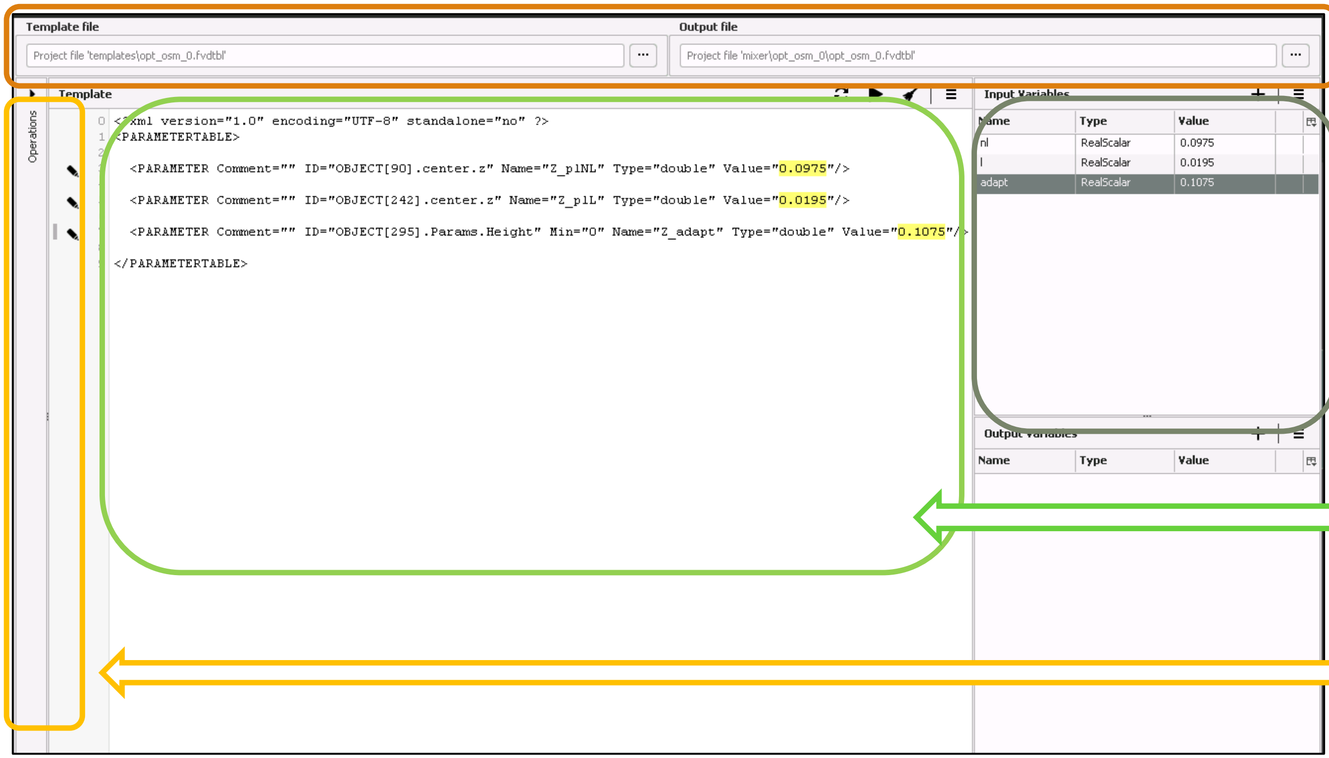
pSeven workflow: creating the input text file

Create the rule for variables substitution in one click!



Template and result files

Input parameters

Compose/preview area

Text operations (generated automatically)

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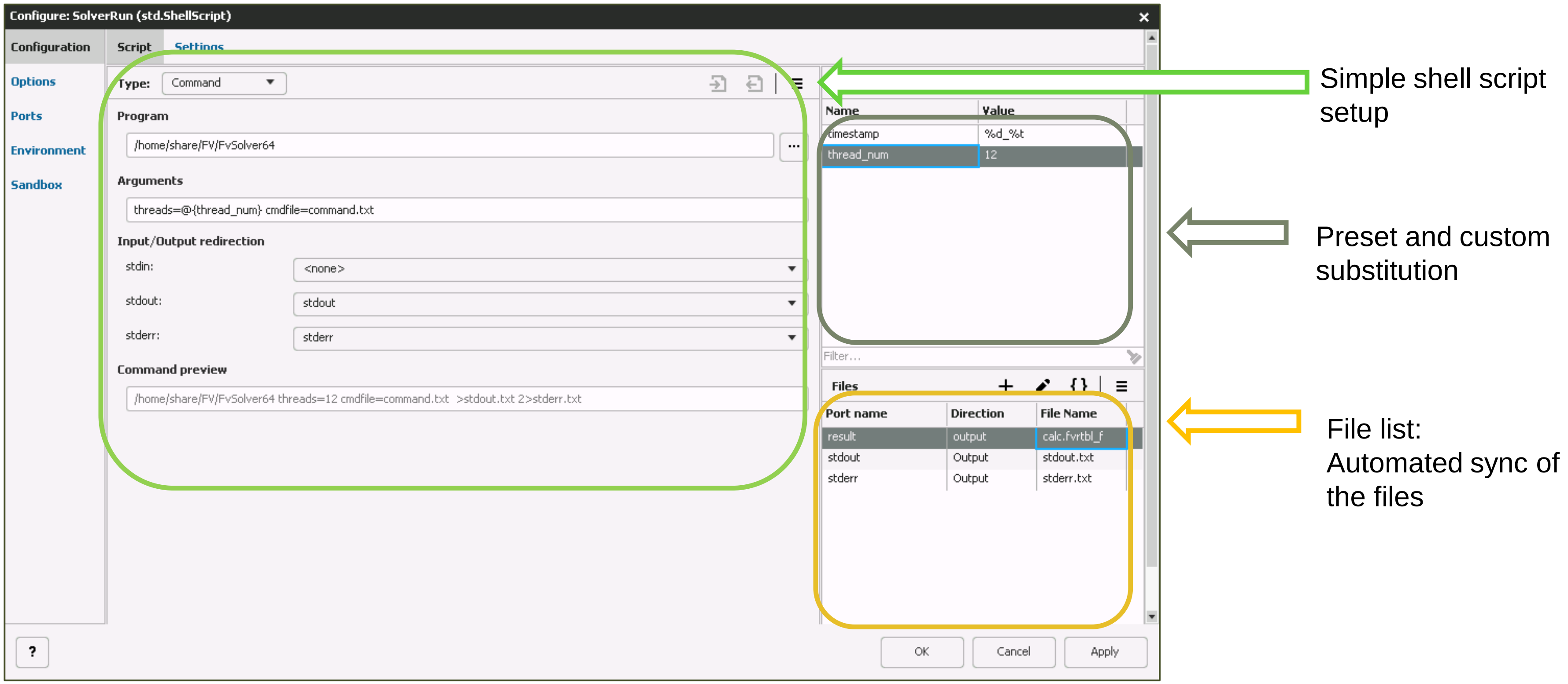
pSeven workflow: integrating executable file

- Running any program from shell
- Running processes on remote computer via SSH
- HPC compatibility, Batch systems support



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Contents

Optimization problem definition

- 4 parameters

Parameter	Name	Min. value	Max.value
Pitch	h	14 mm	26 mm
Convolution	t	0.25	0.75
Rotation	α	60°	120°
Thickness	s	0.7 mm	1 mm

- Additional parameters and constraints: none
- 2 objective functions

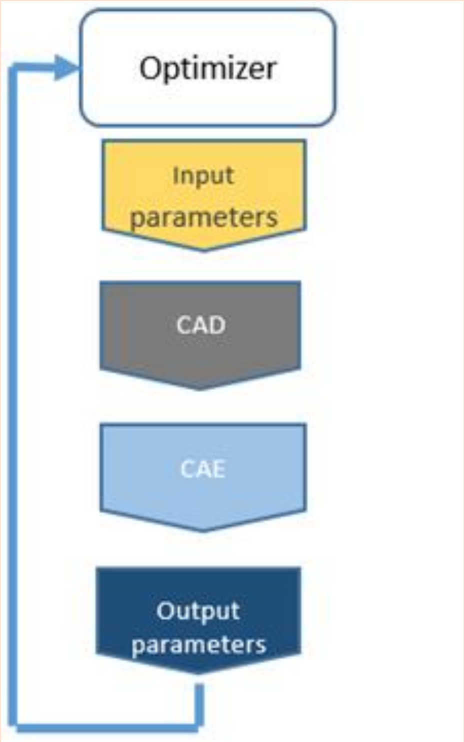
Function	Name	Optimal	Type	Cost
Flow dispersion	DF	Minimum	Generic	Expensive*
Pressure drop	dP	Minimum	Generic	Expensive*

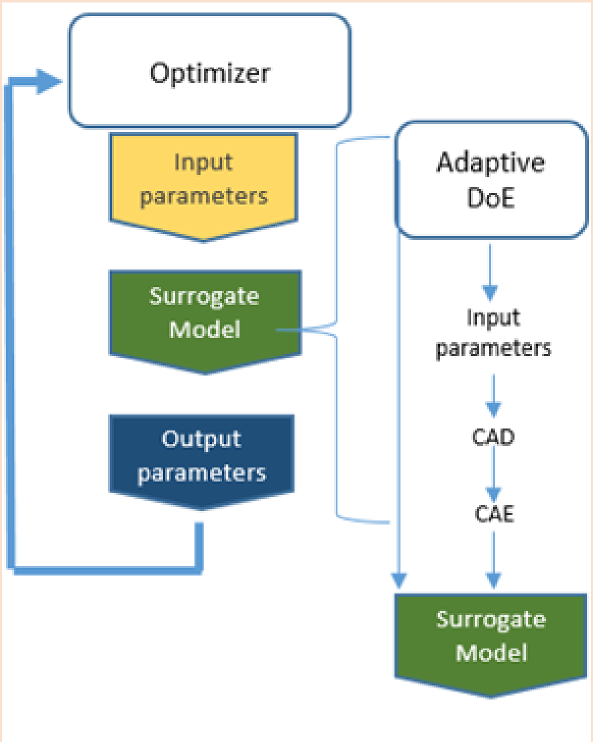
Two objective optimization problem with computationally expensive* objectives to solve

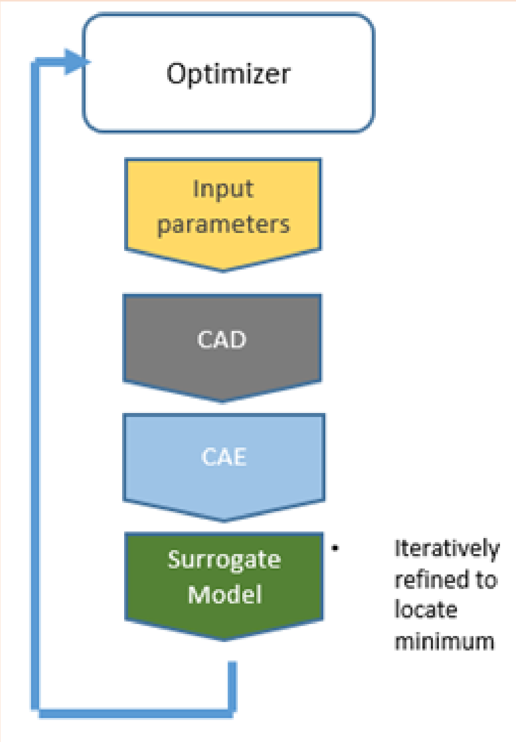
* Expensive means time-consuming in evaluation. *Smart Selection* technique uses this parameter for automated optimization method selection

Different optimization strategies in pSeven

Direct optimization	Optimization using Surrogate Model	Surrogate-Based Optimization







ADVANTAGES

Direct optimization	Optimization using Surrogate Model	Surrogate-Based Optimization
Use your favorite software tools and familiar familiar processes: SolidWorks ®, CATIA®, NX™, Creo®, KOMPAS-KOMPAS-3D; CAE solvers and other engineering engineering tools)	• Invest time to build a surrogate model only once model only once • Extremely fast calculations • Get trade-offs among the objectives	• Minimize sample size to build surrogate models surrogate models • Iterative surrogate model construction construction • Ideal for expensive CAE simulations

Optimization algorithm and parameters

- Two objective optimization functions with computationally expensive* simulations

  Method applied – **Multi-Objective Surrogate-Based Optimization (MOSBO)**

MOSBO main features

- Minimization of a number of evaluations of expensive models
- Global minima localization
- Stability to the model noise
- Errors (NaN) handling
- User defined calculations budget

Total number of calculations (budget) set to 110.

Budget was assigned based on total optimization time limit (3 days)

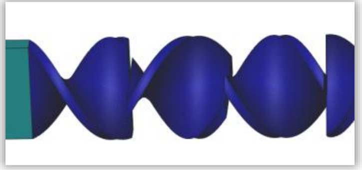
* Expensive means time-consuming in evaluation. This parameter is used for automated optimization method selection

Contents

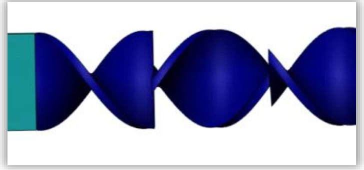
Results: Pareto-frontier

Initial geometry can be significantly improved!

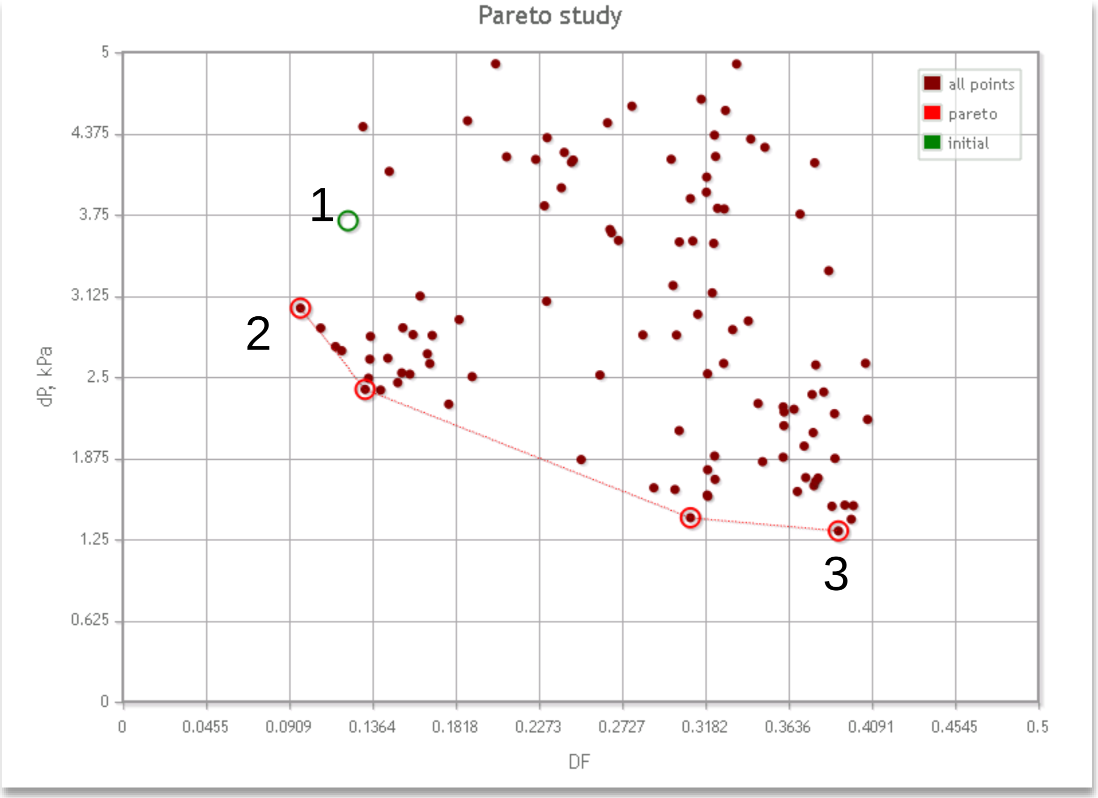
1. Initial geometry:
DF = 0.123, dP = 3704 Pa
h = 20 mm
t = 0.5
α = 90^0
s = 1 mm



2. Best mixing:
DF = 0.097, dP = 3030 Pa
h = 26 mm
t = 0.517
α = 91.7^0
s = 0.9 mm



3. Lowest pressure drop:
DF = 0.391, dP = 1315 Pa
h = 26 mm
t = 0.266
α = 60.2^0
s = 0.8 mm



Initial geometry refers to sample values from presentation: h=20mm, t=0.5, α=90^0, s=1mm.

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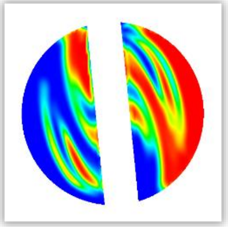
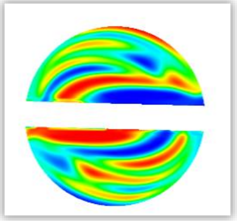
Results: fine mesh calculations

Mesh

- Medium (554 000 cells) used for optimization to reduce simulation time
- Fine (4 200 000 cells) used for initial and best mixing geometry simulation to provide more reliable values of objectives

	Fine mesh	Coarse mesh	Result (fine mesh)
Initial geometry	DF = 0.374 dP = 3985 Pa	DF = 0.123 dP = 3704 Pa	 After 5 elements
Best mixing geometry	DF = 0.289 dP = 3105 Pa	DF = 0.097 dP = 3030 Pa	 After 5 elements

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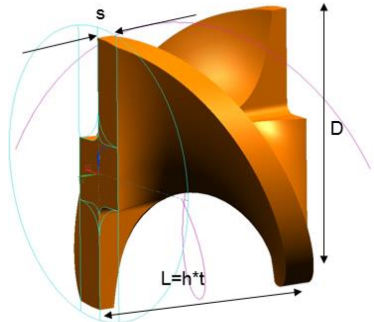
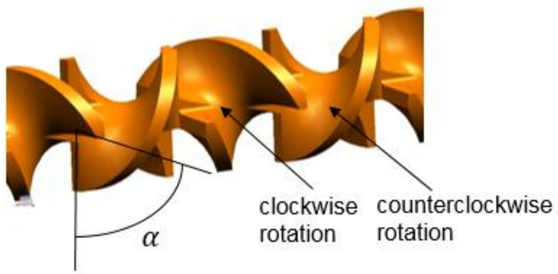
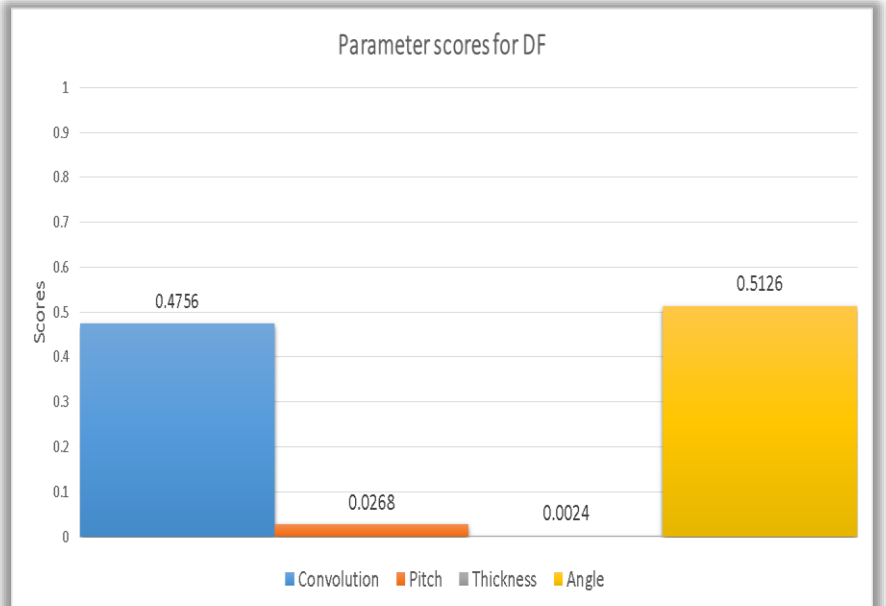
Results: parameters sensitivity study

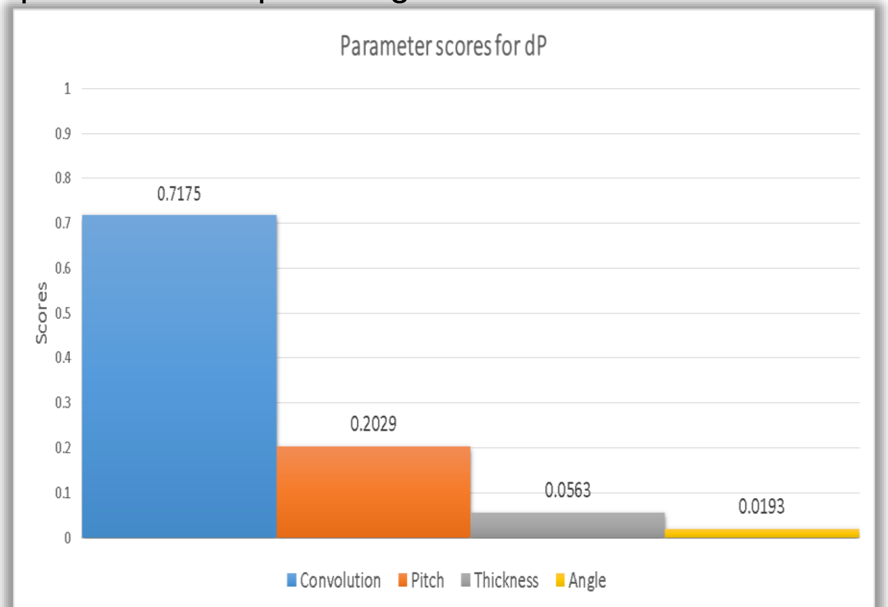
Sensitivity analysis allows estimating the importance of input parameters to the function outputs





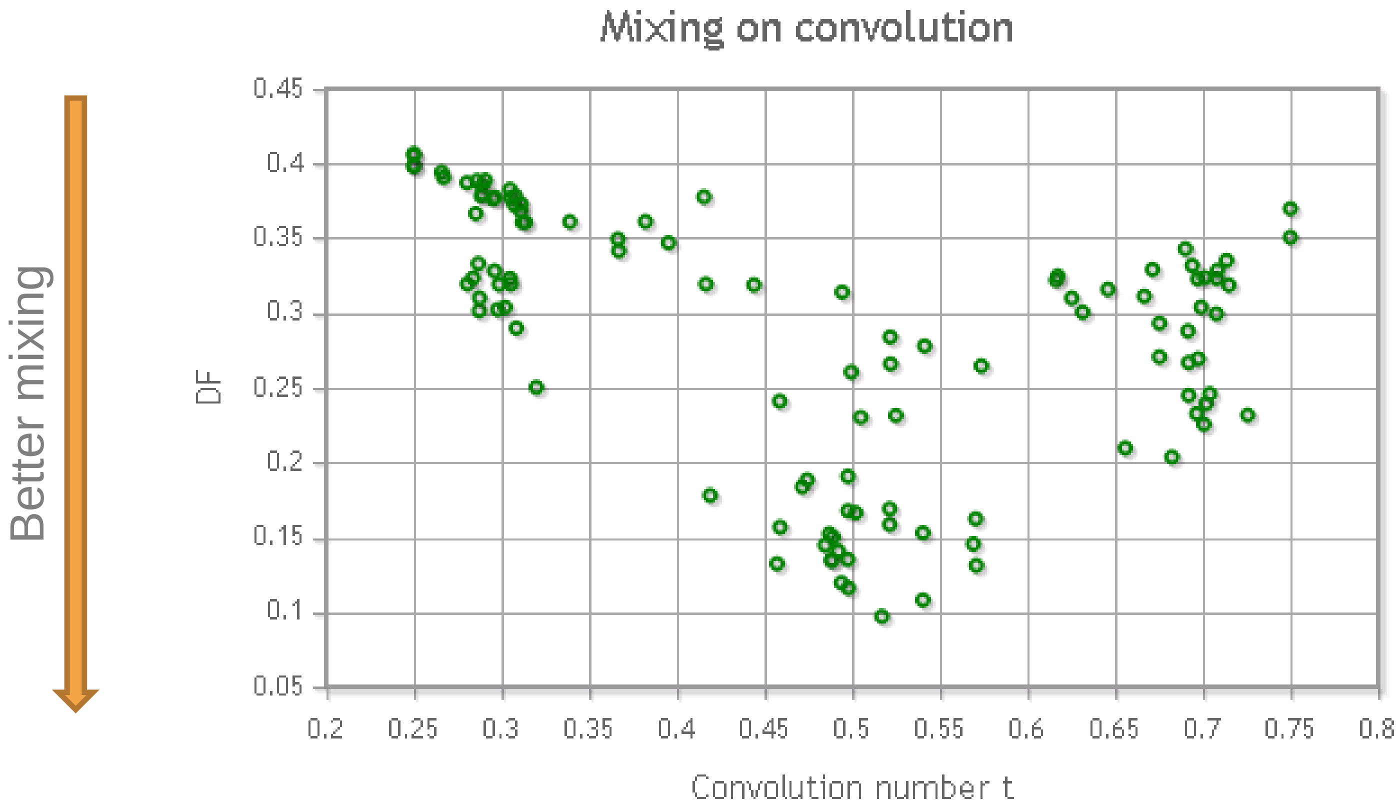
Histograms show the normalized scores* of parameters impact on goal functions





Results: mixing vs. convolution

All points at “mixing quality – convolution” plane
Best mixing corresponds to t = 0.5



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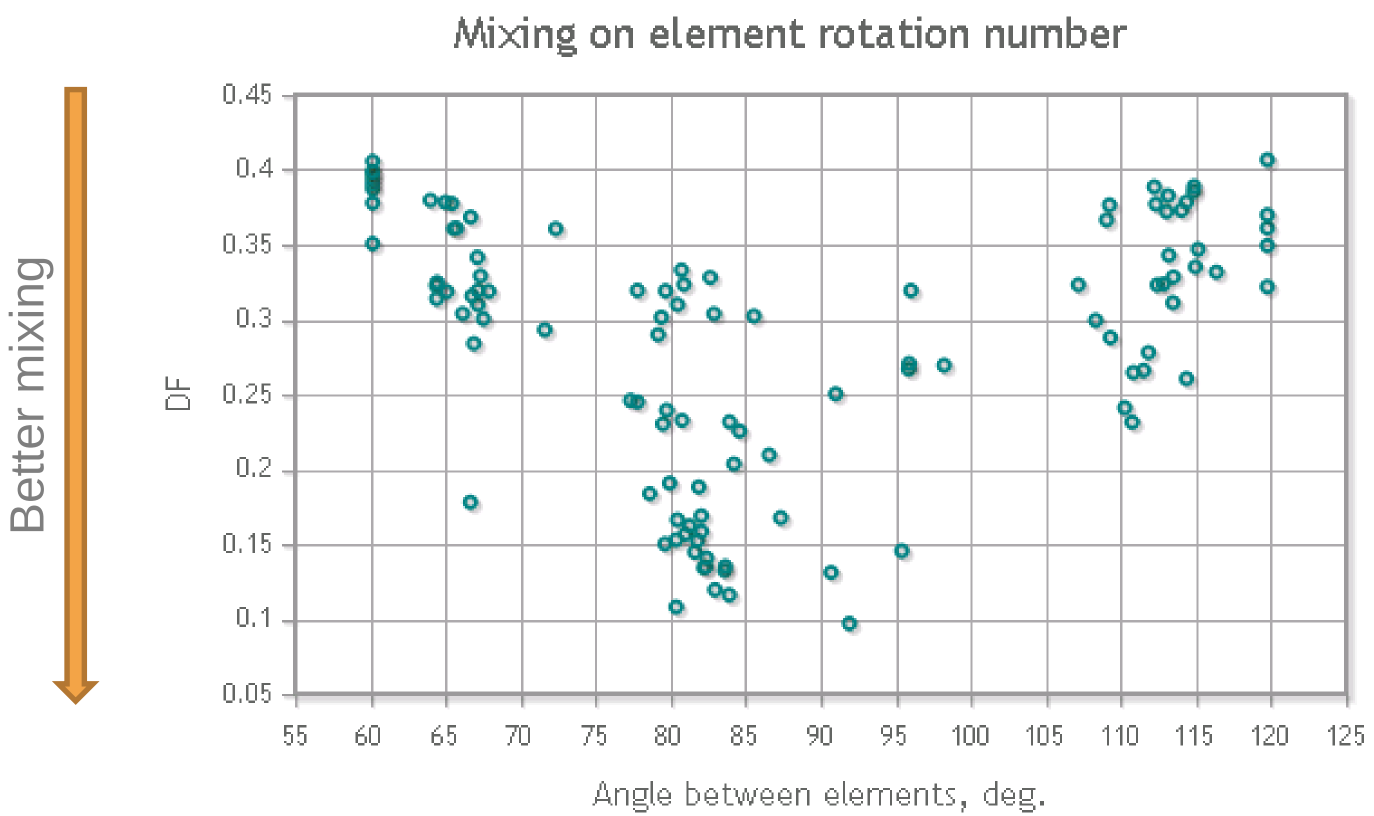
Results: mixing vs. element rotation angle

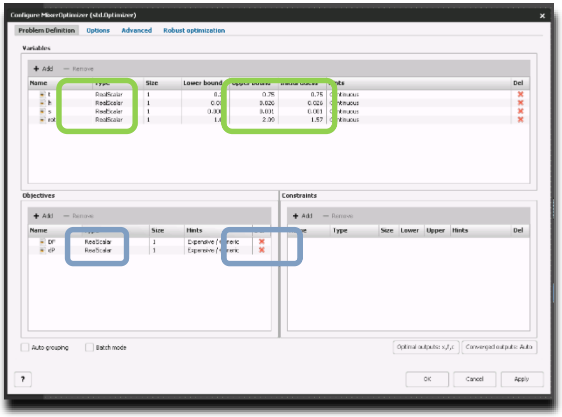
Best Mixing corresponds to ~ 90º



Conclusion

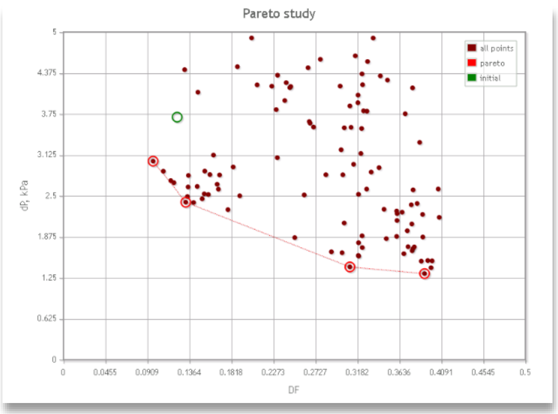
pSeven powered by MACROS technology ensured:

- Automatically selecting the best suitable optimization method – MOSBO - thanks to ***Smart Selection* technique**
- Solving a challenging customer problem of multi-objective helix optimization problem successfully with **just 110 evaluations of computationally expensive CFD model**



Pareto frontier (mixing quality vs pressure drop) discovered

- **Pressure drop could be decreased by 1.5** at the same mixing quality vs. initial configuration
- **Mixing quality could be increased by at least 20%** at the same pressure drop as initial configuration



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1. Automatically Optimization of Helix Mixer, Sulzer Chemtech, 2013
2. “Laminar Flow in Static Mixers with Helical Elements”, A. Bakker, R.D. LaRoche, E.M. Marshall, The Online CFM Book, 2000, http://www.bakker.org/cfm
3. “Analysis and optimization of Kenics static mixers “, O.S. Galaktionov, P.D. Anderson, G.W.M. Peters, H.E.H. Meijer, International Polymer Processing, 18(2), 138-150, 2003

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