TLK-Thermo GmbH

Getting started with the ModelFitter for Excel

Working with the example

Guideline

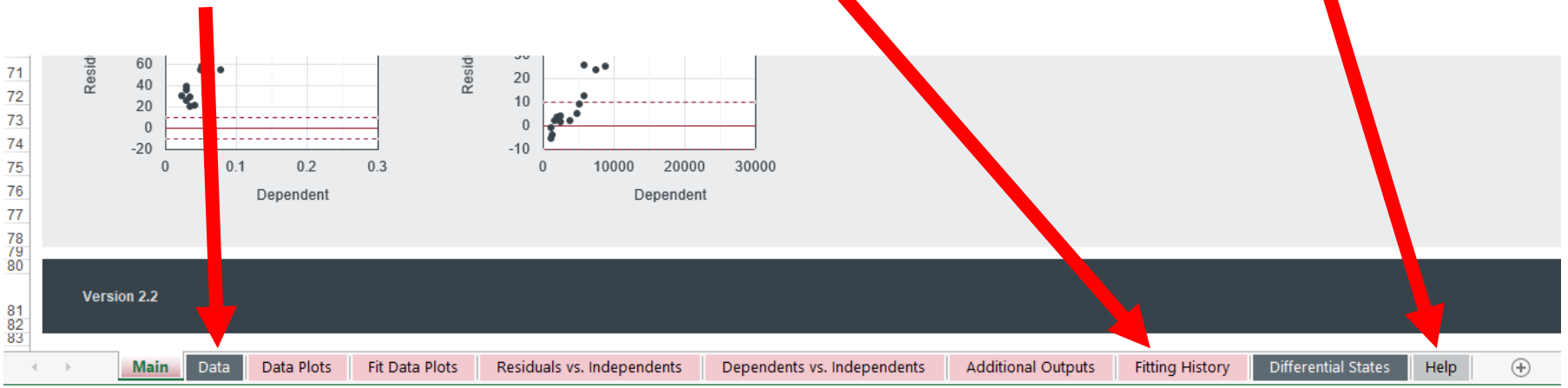
1. Overview Excel Tool
2. Help
3. Main Tab
   - Control Bar
   - Settings
   - Parameters
   - Statistics
4. Data Tab
   - Database
   - Simulation results
5. Differential State Variables
6. Plot Tabs
7. History

Overview Excel Tool

Data
- Database
- Simulation results

History
Backup of former values

Help
Short explanations of all terms and functionalities



Main
- Fit Control
- Parameters
- Statistics
- Main plots

Plots

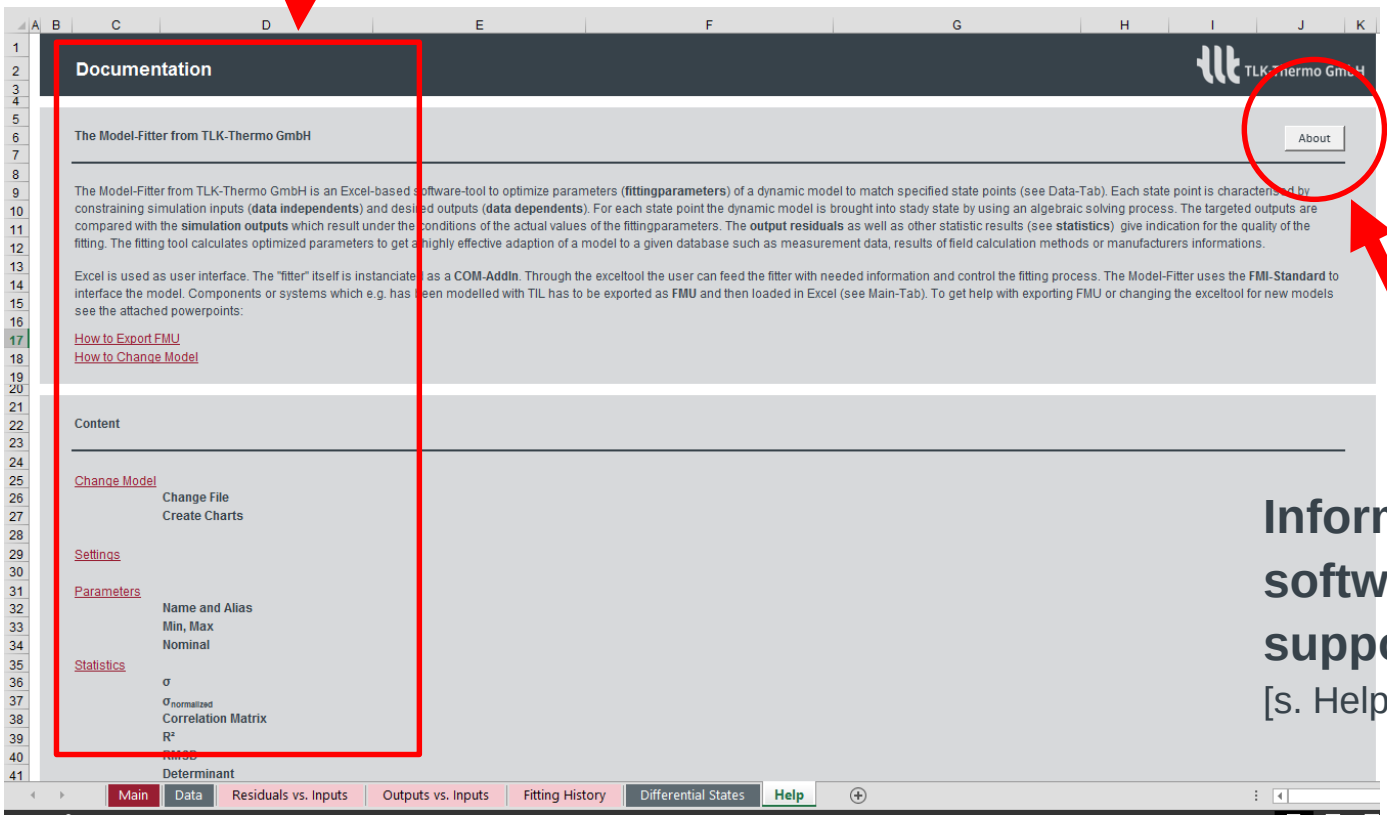
Differential States
Important user input for Differential State Variables

User defined Tabs can be added.

Help

On the Help Tab a lot of terms are explained
[s. Help Tab]

Some terms also can be easily looked up on the internet (e.g. Wikipedia, etc.)



Information about software version and support
[s. Help Tab]

Main Tab

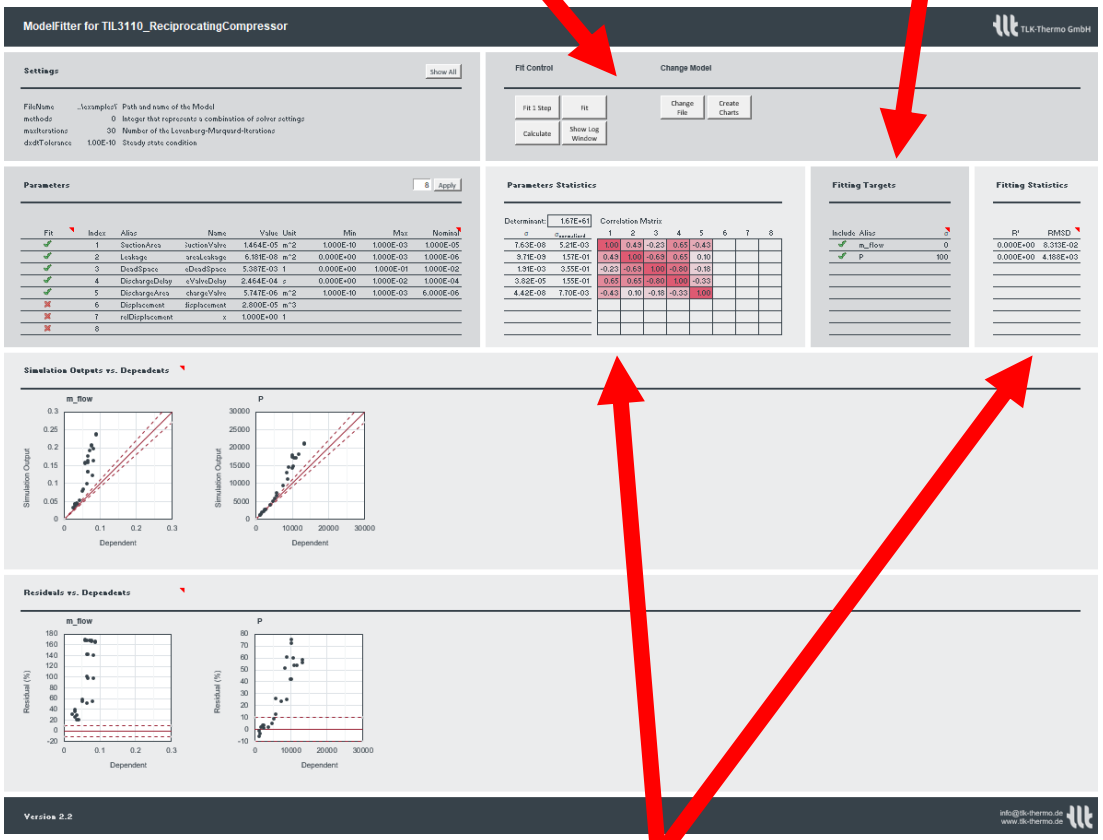
Settings for the fitting process

Control Bar

Fitting Targets

Fitting Parameters

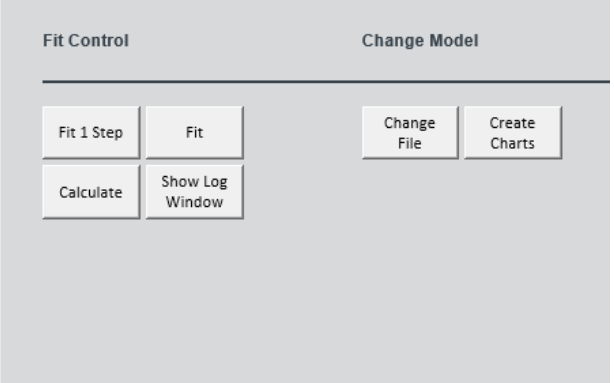
Main plots (Dependents)



Statistics

Main Tab

Control Bar



Calculate

- Calculates the included static data points [s. Data Tab]
- Outputs are simulation results and some statistics
- No fitting

Fit 1 Step

- Only 1 step
- several times Fit1Step **is not** the same as a complete fit with several steps
- New fitting parameters
- See also fitting history

Fit

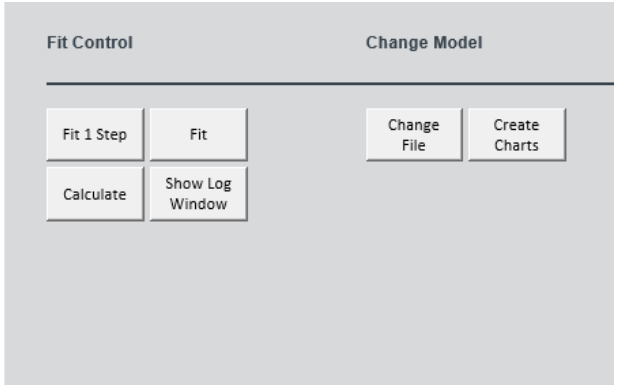
- Complete fit
- Number of steps: maxIterations [s. Settings]
- New fitting parameters
- See also fitting history

Main Tab

Control Bar

Log Window

- Shows messages from the ModelFitter
- Pops up automatically
- After closing reopen with button „Show Log Window“



Change Model

See documentation of „How to Change Model“ for changing the Exceltool to fit other models
[s. Help Tab]

Main Tab

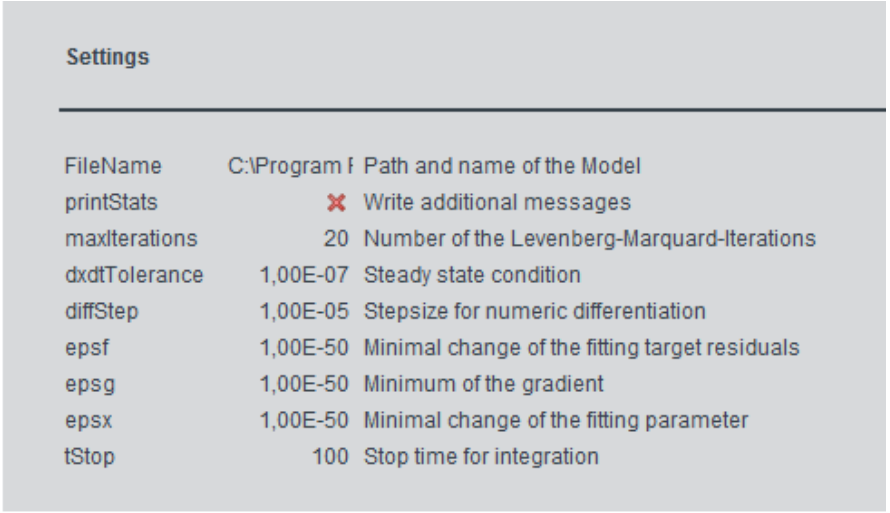
Settings

Most important settings

- **printStats**:
  Additional information about the performance of the fitting process are written into the log window
- **maxIterations**:
  Maxmimum number of steps the ModelFitter does to improve the fitting parameters
- **dxdtTolerance**:
  Global tolerance for the change of differential state variables during steady state

Only if problems occur consider to adjust the settings

[s. Help Tab]



Settings

FileName	C:\Program F	Path and name of the Model
printStats	✖	Write additional messages
maxIterations	20	Number of the Levenberg-Marquard-Iterations
dxdtTolerance	1,00E-07	Steady state condition
diffStep	1,00E-05	Stepsize for numeric differentiation
epsf	1,00E-50	Minimal change of the fitting target residuals
epsg	1,00E-50	Minimum of the gradient
epsx	1,00E-50	Minimal change of the fitting parameter
tStop	100	Stop time for integration

Main Tab

Parameters

Fitting parameters [s. Main Tab]

- Have to be marked as such
- As name the full variable path is needed, e.g. „comp.areaSuctionValve“
- Start with meaningful values

Fixed parameters [s. Main Tab]

Parameters that are marked with a red cross are assigned as fixed parameters during simulation

Parameters

9 Apply

Fit	Index	Alias	Name	Value	Unit	Min	Max	Nominal
✓	1	SuctionArea	SuctionValve	1,464E-05	m^2	1,000E-10	1,000E-03	1,000E-05
✓	2	Leakage	ıreaLeakage	6,181E-08	m^2	0,000E+00	1,000E-03	1,000E-06
✓	3	DeadSpace	ɜDeadSpace	5,387E-03	1	0,000E+00	1,000E-01	1,000E-02
✓	4	DischargeDelay	ıeValveDelay	2,464E-04	s	0,000E+00	1,000E-02	1,000E-04
✓	5	DischargeArea	ıchargeValve	5,747E-06	m^2	1,000E-10	1,000E-03	6,000E-06
✗	6	pInitialLow	InitialSuction	1,000E+06	Pa			
✗	7	pInitialHigh	ialDischarge	8,000E+06	Pa			
✗	8	x	x	1,000E+00	1			
✗	9							

Main Tab

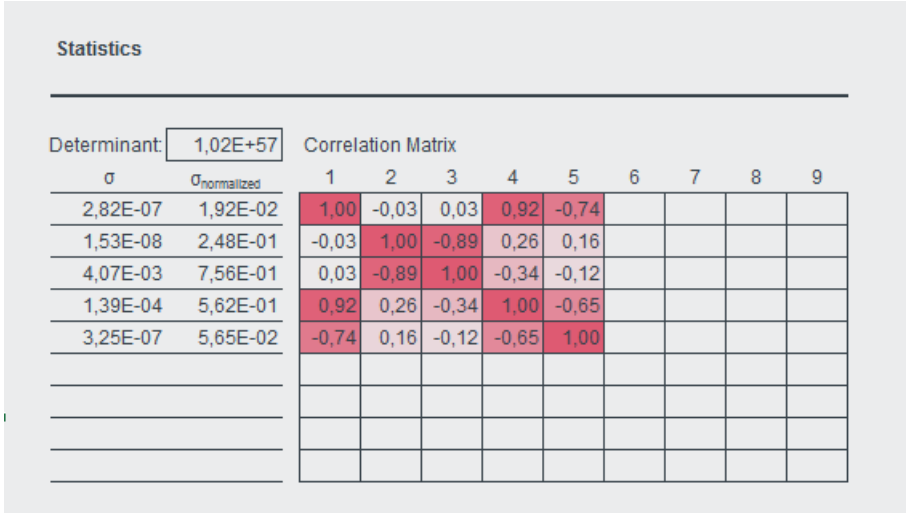
Statistics

Sigma

„How near are the current values of the fitting parameters to the optimum?“

Correlation Matrix

„How does the fitting parameters influence each other?“



Statistics

Determinant: 1,02E+57

σ	$\sigma_{normalized}$
2,82E-07	1,92E-02
1,53E-08	2,48E-01
4,07E-03	7,56E-01
1,39E-04	5,62E-01
3,25E-07	5,65E-02

Correlation Matrix

1	2	3	4	5	6	7	8	9
1,00	-0,03	0,03	0,92	-0,74				
-0,03	1,00	-0,89	0,26	0,16				
0,03	-0,89	1,00	-0,34	-0,12				
0,92	0,26	-0,34	1,00	-0,65				
-0,74	0,16	-0,12	-0,65	1,00				

Determinant

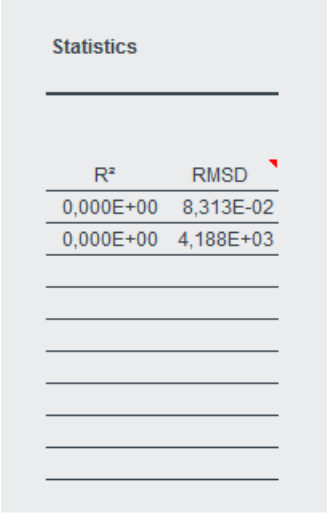
„How well does the database (e.g. measurement plan) fit to the model compared to other databases?“

Main Tab

Statistics

R^2

„How well does the fitting parameters hit the database?“



RMSD

„How big is the variation of the residuals?“

(residuals = dependent – simulation output)

Data Tab

Database

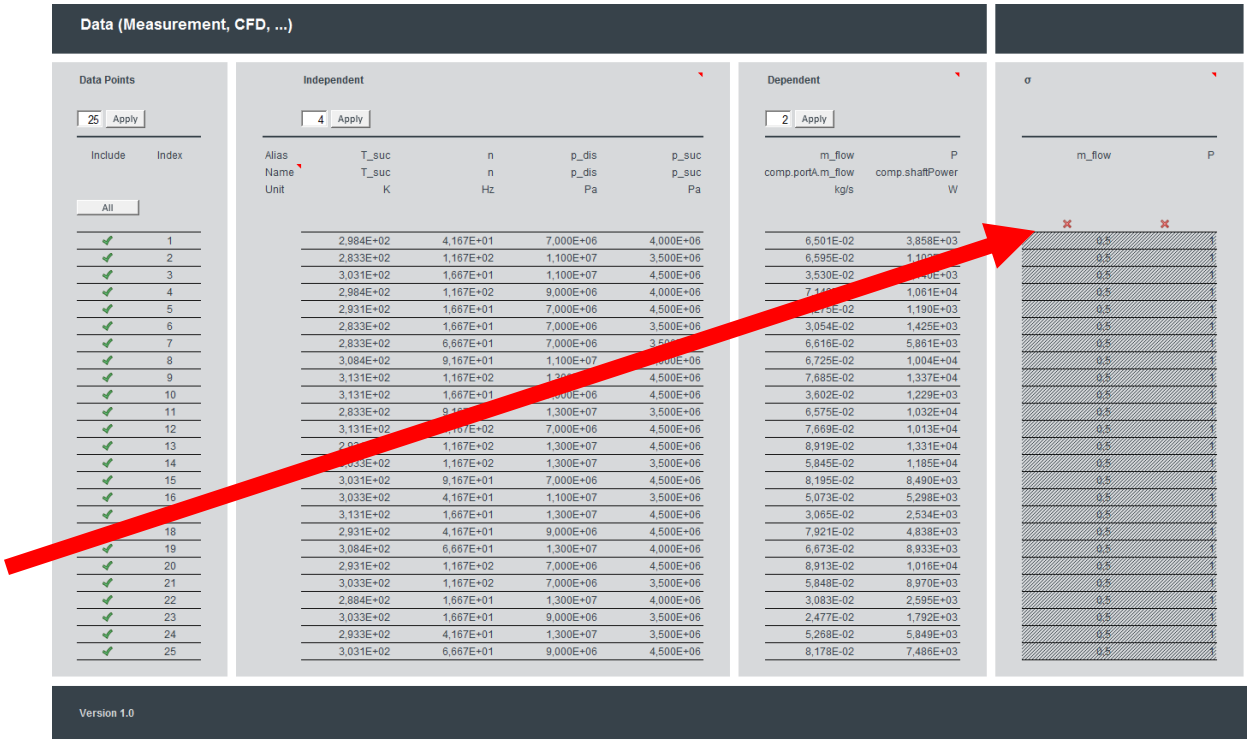
The Database contains [s. Data on Data Tab]

- Static points (Data Points) of
- Simulation inputs (Independents),
- Desired outputs (Dependents) and
- Standard Deviation (sigma)

Sigma is also used for weighting the dependents to each other

Here a global sigma for every dependent is entered on the Main Tab

[s. Targets on Main Tab]



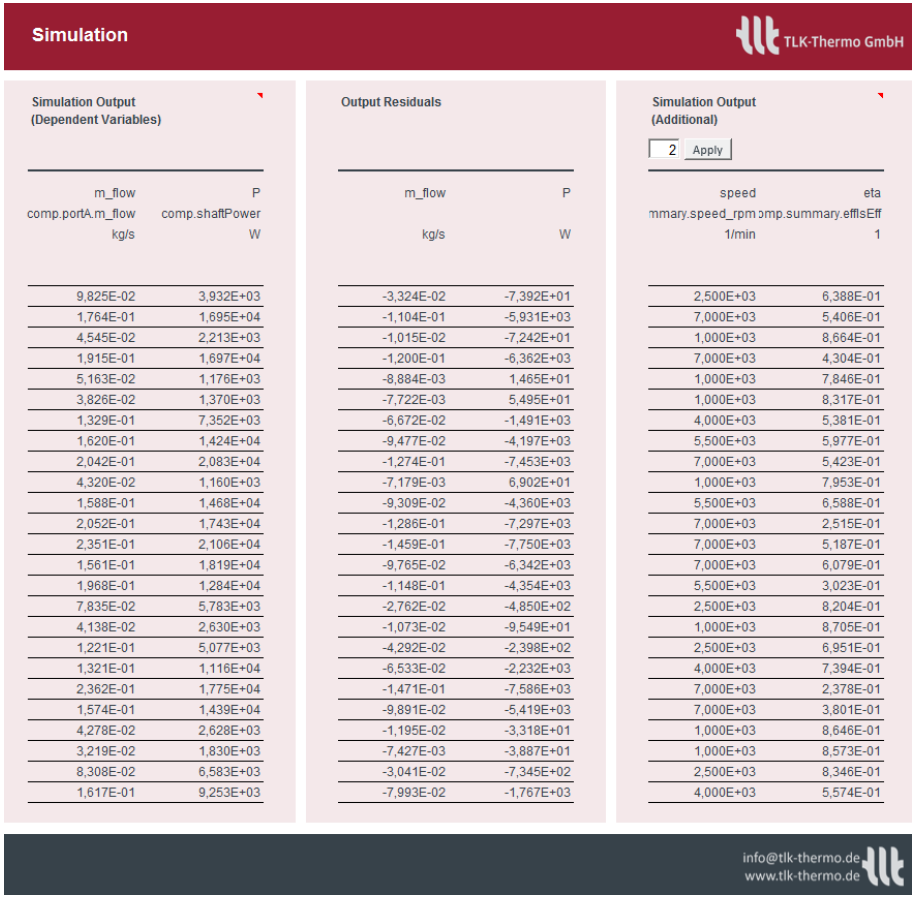
Data Tab

Simulation results

Beside the Database simulation results are shown
[s. Simulation on Data Tab]

- Simulation output
- Calculated residuum between simulation output and dependents
- Possible additional ouputs

Data Points
[s. Database]



Differential State Variables

The steady state definition is mainly influenced by the values given here

Cumulating and effectless differential state variables are marked with a cross
[s. Differential State Tab]

Differential State Variables — TLK-Thermo GmbH

Differential State Variables — Autodetect | Reset

Of some specific differential state variables the differentiation cannot be brought to zero ("**cumulating Variables**"). In this case, those variables has to be marked for being ignored while the fitter tries to bring the rest of the differential states to zero. Otherwise the fitter could not come to stady state.
Autodetect is a function to detect recommended nominal values of the differential state variables. Additionally, the exclusion of the state variables that should be ignored is automatically executed.

Use as State Variable	Name	Unit	Min	Max	Nominal
✓	comp.suctionChamberVLEFluid.p		0,00E+00	1,00E+300	1,00E+06
✓	comp.dischargeChamberVLEFluid.p		0,00E+00	1,00E+300	7,99E+06
✓	comp.portA.h_outflow		-1,00E+300	1,00E+300	3,50E+05
✓	comp.portB.h_outflow		-1,00E+300	1,00E+300	3,50E+05
✗	comp.getInputsRotary.rotatoryFlange.phi		-1,00E+300	1,00E+300	1,00E-03

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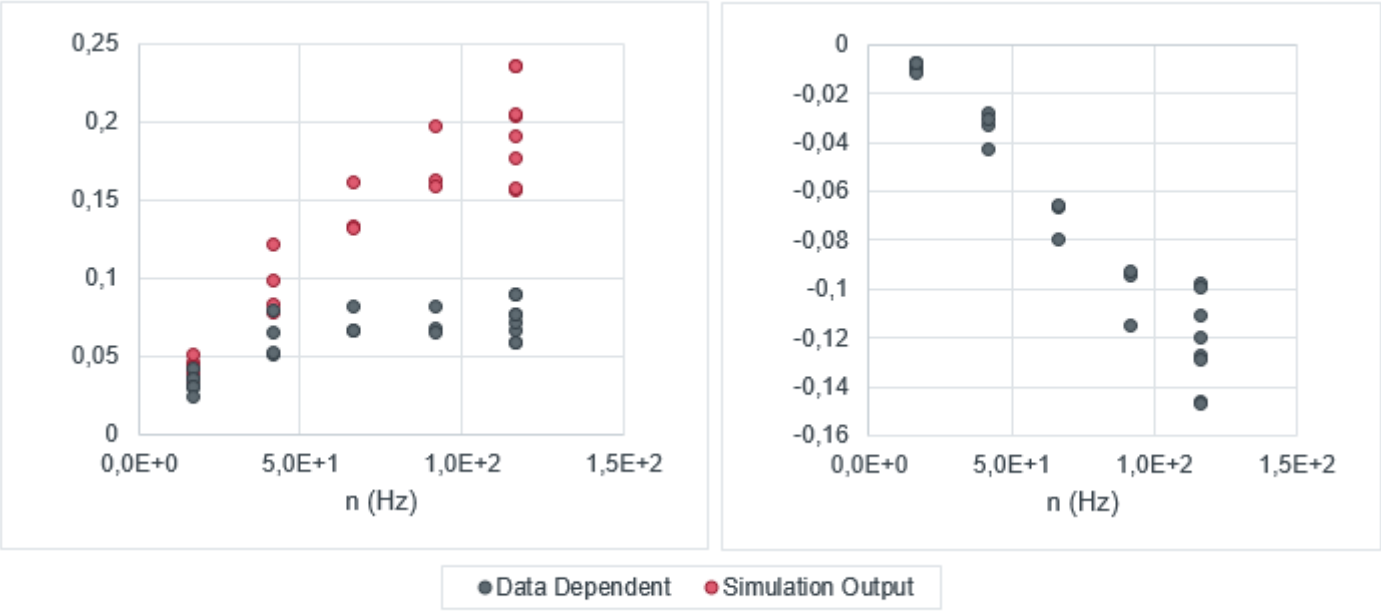
Plot Tabs

Dependents vs. Independents
Here the mass flow rate in the simulation rises too high compared with the dependent with respect to the speed (independent)
[s. Outputs vs. Inputs Tab]

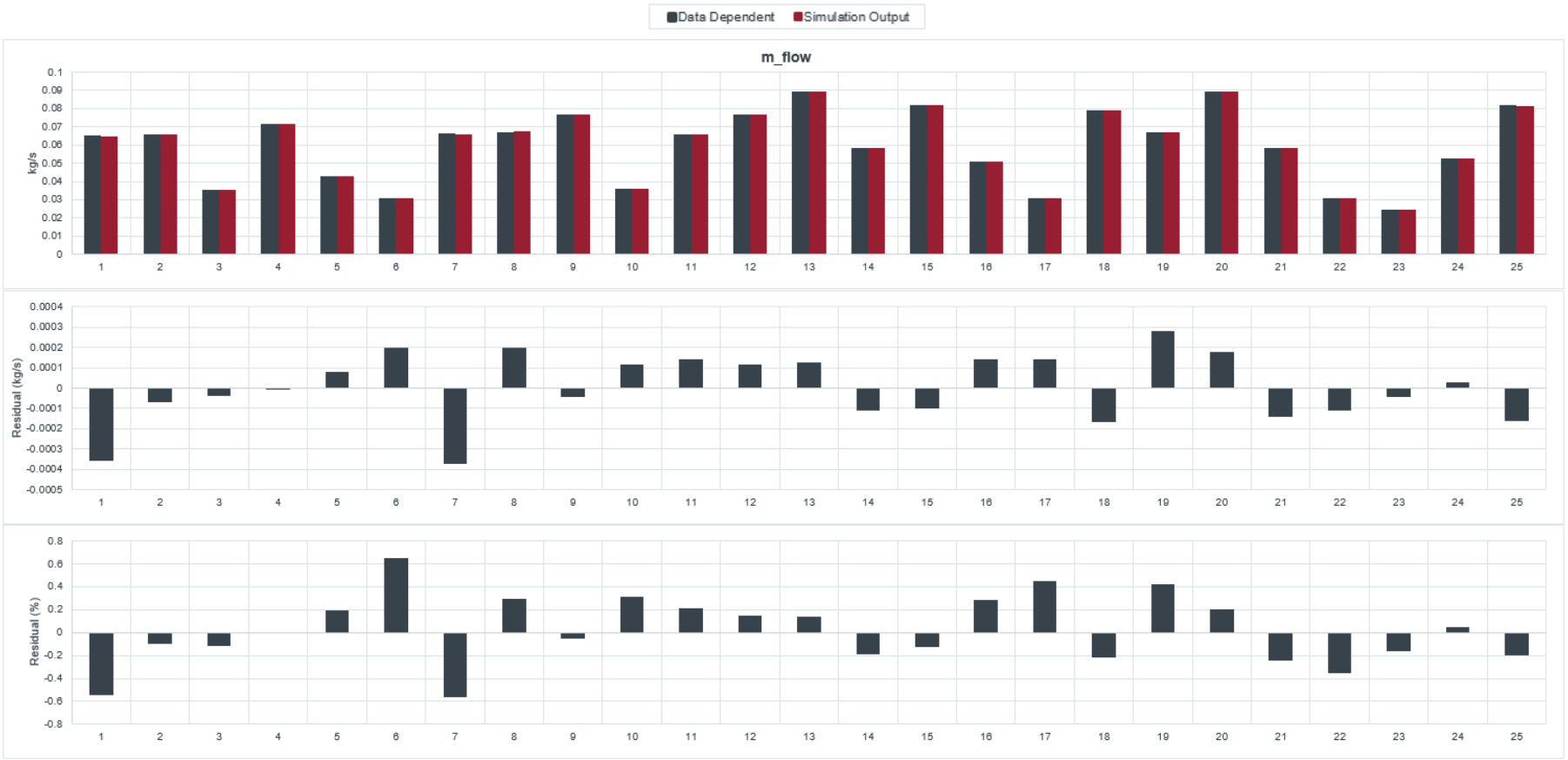
Residuals vs. Independents
Same conclusion. Residual between simulation output and dependent grows with higher speed.
[s. Residuals vs. Inputs Tab]



Plot Tabs

Via bar charts, particular data points can easily be localized.

[s. Tabs of Data Plots, Fit Data Plots, Additional Outputs]



History

In case of a Fit, a Fit1Step or essential changes of the differential state variables informations are saved in the fitting history

[s. Fitting History Tab]

History of Fitting Parameter

Clear All

Fit One Step

Time Stamp	Fit	Index	Alias	Name	Start Value	Fitted Value	Unit	$\sigma_{normalized}$	Dependents	R^2	RMSD	Target
15.06.2016 13:46:23	1	1	SuctionArea	SuctionValve	1,464E-05	7,744E-06	m^2	1,92E-02	m_flow	0,000E+00	8,313E-02	1
	1	2	Leakage	ɜreaLeakage	6,181E-08	2,383E-07	m^2	2,48E-01	P	0,000E+00	4,188E+03	1
	1	3	DeadSpace	ɜDeadSpace	5,387E-03	1,241E-02	1	7,56E-01				
	1	4	DischargeDelay	ɹeValveDelay	2,464E-04	2,449E-04	s	5,62E-01				
	1	5	DischargeArea	ɨchargeValve	5,747E-06	5,306E-06	m^2	5,65E-02				
	0	6	pInitialLow	InitialSuction	1,000E+06	1,000E+06	Pa					
	0	7	pInitialHigh	ialDischarge	8,000E+06	8,000E+06	Pa					
	0	8	x	x	1,000E+00	1,000E+00	1					

ModelFitter

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