

# Calibration Kit User Guide

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**SYNOPSYS®**

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# About This Guide

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The Calibration Kit is the calibration environment that is part of Synopsys Sentaurus™ Workbench Advanced. The Calibration Kit is the interface to the calibration libraries and calibration files.

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## Related Publications

For additional information, see:

- The documentation installed with the Calibration Kit software package and available from the **Help** menu of the Calibration Kit.
  - The TCAD Sentaurus release notes, available on the Synopsys SolvNet® support site (see [Accessing SolvNet on page vi](#)).
  - Documentation available on SolvNet at <https://solvnet.synopsys.com/DocsOnWeb>.
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## Conventions

The following conventions are used in Synopsys documentation.

Convention	Description
<a href="#">Blue text</a>	Identifies a cross-reference (only on the screen).
<b>Bold text</b>	Identifies a selectable icon, button, menu, or tab. It also indicates the name of a field or an option.
Courier font	Identifies text that is displayed on the screen or that the user must type. It identifies the names of files, directories, paths, parameters, keywords, and variables.
<i>Italicized text</i>	Used for emphasis, the titles of books and journals, and non-English words. It also identifies components of an equation or a formula, a placeholder, or an identifier.
<b>Menu &gt; Command</b>	Indicates a menu command, for example, <b>File &gt; New</b> (from the <b>File</b> menu, select <b>New</b> ).

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## Customer Support

Customer support is available through the Synopsys SolvNet customer support website and by contacting the Synopsys support center.

## Accessing SolvNet

The SolvNet support site includes an electronic knowledge base of technical articles and answers to frequently asked questions about Synopsys tools. The site also gives you access to a wide range of Synopsys online services, which include downloading software, viewing documentation, and entering a call to the Support Center.

To access the SolvNet site:

1. Go to the web page at <https://solvnet.synopsys.com>.
2. If prompted, enter your user name and password. (If you do not have a Synopsys user name and password, follow the instructions to register.)

If you need help using the site, click **Help** on the menu bar.

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## Contacting Synopsys Support

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- Go to the Synopsys [Global Support Centers](#) site on [synopsys.com](http://synopsys.com). There you can find e-mail addresses and telephone numbers for Synopsys support centers throughout the world.
  - Go to either the Synopsys SolvNet site or the Synopsys Global Support Centers site and [open a case online](#) (Synopsys user name and password required).
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## Contacting Your Local TCAD Support Team Directly

Send an e-mail message to:

- [support-tcad-us@synopsys.com](mailto:support-tcad-us@synopsys.com) from within North America and South America.
- [support-tcad-eu@synopsys.com](mailto:support-tcad-eu@synopsys.com) from within Europe.
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- [support-tcad-kr@synopsys.com](mailto:support-tcad-kr@synopsys.com) from Korea.
- [support-tcad-jp@synopsys.com](mailto:support-tcad-jp@synopsys.com) from Japan.

*This chapter presents an overview of the Calibration Kit.*

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## Functionality of the Calibration Kit

The Calibration Kit extends the functionality of Sentaurus Workbench, assisting you to perform efficient 1D calibrations of the Synopsys process simulators Sentaurus Process and Sentaurus Process Kinetic Monte Carlo.

Sentaurus Workbench is the primary graphical front end of TCAD Sentaurus that integrates the simulation tools into one environment (see the *Sentaurus™ Workbench User Guide*). The Sentaurus Workbench Advanced mode provides customized viewers and wizards for calibration. The **Calibration** menu of Sentaurus Workbench provides wizards for the manipulation of the simulation flow and report generation (see [Chapter 2 on page 9](#)).

In combination with the calibration libraries containing secondary ion mass spectrometry (SIMS) data, the Calibration Kit provides a fast, accurate, and reliable method of evaluating and optimizing process conditions. It allows a predictive analysis of the influence of process equipment parameters on electrical device data. In addition, the Calibration Kit helps you to understand the sensitivity of processes to various control parameters, enabling you to optimize equipment operation quickly.

The Calibration Kit is the calibration environment in Sentaurus Workbench Advanced. It serves as a database browser, and a simulation and project manager.

The software package Optimizer, which is integrated in Sentaurus Workbench Advanced, is used for the automatic analysis and optimization of process and calibration parameters (see the *Optimizer User Guide*).

In addition to the analytic extraction in the process simulators, Sentaurus Device can be integrated for electrical parameter extraction, preceded by Sentaurus Mesh for mesh generation.

For visualization, Inspect and Sentaurus Visual are integrated into the Calibration Kit.

## Input Modules

Process descriptions and data, which are calibration libraries such as the Calibration Library, as well as simulator calibration files such as Advanced Calibration are used as input to the Calibration Kit.

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### Calibration Libraries

The calibration libraries are experiment databases consisting of the following directories:

- `processes_*`
- `experiments`
- `preferences`

You can add your own experimental data to the measurement database or create your own database. In the latter case, it is recommended to keep the same directory structure, with process files, profile files, and preference files in three directories (see [Defining the Calibration Library on page 29](#)).

The process recipes can use Ligament SPR syntax or Sentaurus Process syntax, with specific restrictions for the Calibration Kit (see [Process File Syntax on page 29](#)). The directory `experiments` can contain SIMS profiles and spreading resistance profiles.

### Process Directory

In the process directory `processes_*`, each process file contains a recipe for wafer processing and a reference to the corresponding SIMS measurements. By default, these recipes are written in the simple process representation (SPR) syntax of Ligament and do not contain any simulator models or parameters. In this case, the directory is called `processes_lig`.

The file name of the process is the same as the name of the process. The input files of Sentaurus Process are created automatically before simulation by translating Ligament SPR syntax to Sentaurus Process syntax, and by calibrating the pure recipes with simulation models. For Sentaurus Process, the calibration parameters and models are sourced before a process recipe is applied.

In the process files, the SIMS measurements are represented by `insert` statements. The `insert` statement is translated to the Calibration Kit-specific `SetPltList` statement for Sentaurus Process. In each `SetPltList` statement, the measured chemical dopant species and the file name of the SIMS profile are specified. A process file can have several `SetPltList` statements, which correspond to several SIMS profiles.



In a Sentaurus Workbench project generated by the Calibration Kit, the file names of the process flows are changed to `b@node@_fps.cmd`, where `@node@` is the number of a project node of Sentaurus Workbench. For details, see [Structure of Calibration Kit Projects on page 5](#).

## Experiment Directory

The experiment directory `experiments` contains the measured SIMS profiles in `xy` format. The first column is the depth [nm] and the second column is the concentration of the chemical dopant [ $\text{cm}^{-3}$ ]. The file names match exactly the names specified in the `1D` commands of the recipe files.

In a Sentaurus Workbench project generated by the Calibration Kit, the SIMS profiles are named `b@node@[profile].plx`, where `@node@` is the number of a project node of Sentaurus Workbench. For details, see [Structure of Calibration Kit Projects on page 5](#).

## Preference Directory

The preference directory `preferences` contains additional information. For each SIMS profile `name.sims` in the `experiments` directory, there is one preference file `name_sims.prf` in the `preferences` directory that specifies the following (Tcl) variables:

- `sims_xmin` and `sims_xmax` give the depth [nm] range for which the SIMS profile should be compared to the simulation results.
- `vis_xmin` and `vis_xmax` are the preferred minimal depth [nm] and maximal depth [nm], respectively, to be shown in a graphical representation of the profile.
- `vis_ymin` and `vis_ymax` are the preferred minimal concentration [ $\text{cm}^{-3}$ ] and maximal concentration [ $\text{cm}^{-3}$ ], respectively, to be shown in a graphical representation of the profile.
- `probe_xmax` gives the depth [nm] of the contact for device simulation to calculate the sheet resistance.

In a Sentaurus Workbench project generated by the Calibration Kit, all preference files are named `b@node@[profile].prf`, where `@node@` is the number of a project node of Sentaurus Workbench. For details, see [Structure of Calibration Kit Projects on page 5](#).

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## Calibration Files

The directory `$STROOT/tcad/$STRELEASE/lib/fabpackagelib` contains calibration (text) files with physical models and parameters for Sentaurus Process and Sentaurus Process Kinetic Monte Carlo.

## Advanced Calibration for Sentaurus Process

Two files in the `fabpackagelib` directory are used for calibrated 1D simulations of Sentaurus Process with the Calibration Kit: `AdvCal_2017.09.fps` and `calib_1d_2017.09.fps`.

The file `AdvCal_2017.09.fps` is the latest version of Advanced Calibration for Sentaurus Process. It contains a selection of physical models and parameters that are calibrated for deep-submicron technology. This file is identical to the `AdvCal_2017.09.fps` file in the directory `$(STROOT)/tcad/$(STRELEASE)/lib/sprocess/TclLib/AdvCal`.

**NOTE** When improvements to the model calibration are made, between feature releases, the file in the `fabpackagelib` directory will contain the latest version. The contents of the `AdvCal_2017.09.fps` file are explained in the *Advanced Calibration for Process Simulation User Guide*, which can be accessed from Sentaurus Workbench (**Help > Manuals**).

The file `calib_1d_2017.09.fps` contains information needed for simulations, which does not belong to the process flow or the physical models, and includes:

- The creation of a 1D simulation mesh, which is optimized for accurate 1D simulations.
- A procedure (`writePlt`) definition for writing 1D profiles in `.plt` format.
- A procedure (`OxideThickness`) definition for extracting the cap-oxide thickness.
- A selection of meshing parameters.

The last lines of the `calib_1d_2017.09.fps` file create a 1D mesh and source the file `AdvCal_2017.09.fps`, which contains the physical models.

**NOTE** Older versions of the calibration files are available in the directory `$(STROOT)/tcad/$(STRELEASE)/lib/fabpackagelib` and can be used with the latest release of Sentaurus Process.

## Advanced Calibration for Sentaurus Process Kinetic Monte Carlo

Two files in the `fabpackagelib` directory are used for calibrated pseudo-1D simulations of Sentaurus Process Kinetic Monte Carlo (Sentaurus Process KMC) with the Calibration Kit: `AdvCal_KMC_2017.09.fps` and `calib_KMC_2017.09.fps`.

The file `AdvCal_KMC_2017.09.fps` is the latest version of Advanced Calibration for Sentaurus Process KMC. It contains a selection of physical models and parameters that are calibrated for deep-submicron technology. This file is identical to the `AdvCal_KMC_2017.09.fps` file in the directory `$(STROOT)/tcad/$(STRELEASE)/lib/sprocess/TclLib/AdvCal`.

The file `calib_KMC_2017.09.fps` contains information needed for simulations, which does not belong to the process flow or the physical models, and includes:

- The creation of a 3D atomistic simulation cell and a 1D projection mesh, which is optimized for accurate pseudo-1D simulations.
- A procedure (`writePlt`) definition for writing 1D profiles in `.plt` format and for logging the thickness of the amorphous layer.
- A selection of recording options for atomistic data.
- A selection of atomistic parameters.

The last lines of the `calib_KMC_2017.09.fps` file create the simulation cell, select the atomistic mode, and source the file `AdvCal_KMC_2017.09.fps`, which contains the physical models.

## Structure of Calibration Kit Projects

A Calibration Kit project is a special type of Sentaurus Workbench project with either three or five tools, and one to seven parameters. For details about Sentaurus Workbench and its general project structure, see the *Sentaurus™ Workbench User Guide*.

Figure 1 shows an example of a Calibration Kit project. The first tool instance in the tool flow is Sentaurus Process for process simulation. Optionally, a Sentaurus Mesh tool instance can be used for mesh generation and a Sentaurus Device tool instance can be used for device simulation. The Inspect tool instance for variable value extraction is followed by Sentaurus Visual for visualization.

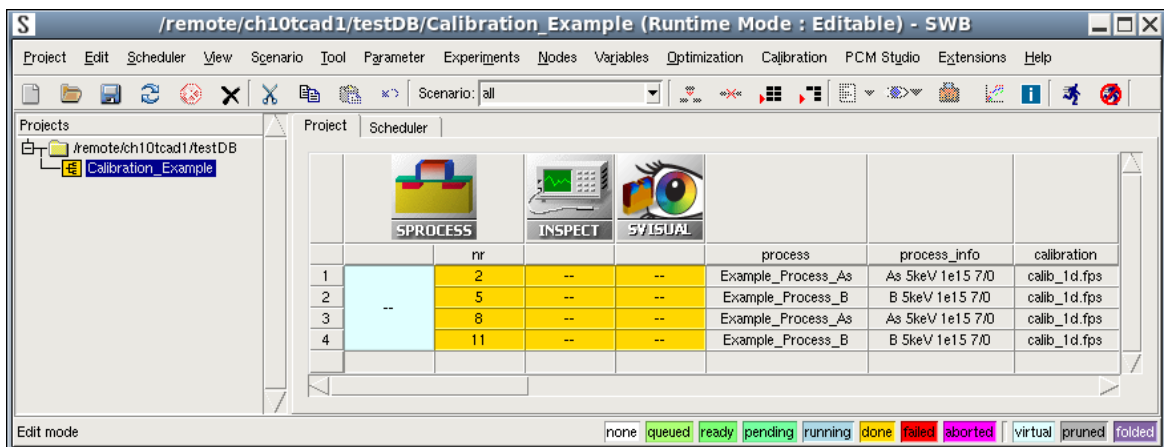


Figure 1 Calibration Kit project loaded in Sentaurus Workbench; tool flow is horizontal and experiment flow is vertical

## 1: Introduction to the Calibration Kit

### Structure of Calibration Kit Projects

The parameter `nr` of Sentauros Process represents the index of the process. Each experiment has a unique process recipe. The process file-naming convention is `b@nr@_fps.cmd` for Sentauros Process. In general, files starting with `b@nr@_*` belong to the experiment of the parameter value `@nr@`.

The Calibration Kit uses different Sentauros Workbench variables:

- `process` names the process recipe.
- `process_info` lists process information.
- `n_profile` shows the number of profiles per experiment, which are named by the variables `profile_@integer@`, where `integer` is equal to 1, 2, 3, ..., 10.

For each profile, the file `b@nr@_@{profile_@integer@}@.plx` contains the experiment data, and the file `b@nr@_@{profile_@integer@}@.prf` contains the preferences.

To identify a Sentauros Workbench project as a Calibration Kit project, an empty hidden file `.fabpackage` is included in the project directory. The `greadme.txt` file (**Project > Readme**) can be used to collect project information.

---

## Sentauros Process

The project structure is the same for Sentauros Process in continuum mode or in kinetic Monte Carlo mode. The mode is defined in the calibration files.

Sentauros Process uses the command file `n@node@_fps.cmd` as input. This command file sources the calibration file `@calibration@` of Sentauros Process, evaluates the parameter `nr` for each experiment, and sources the process recipe `b@nr@_fps.cmd`. Therefore, the parameter `nr` of Sentauros Process represents the process.

The output of the Sentauros Process tool instance is the following files:

- `b@nr@_@{profile_@integer@}@_simulation.plt` (xy plot file)
- `b@nr@_fps.tdr` (TDR file)
- `b@nr@_bnd.tdr` (TDR boundary file)

Therefore, the file name of the simulated profile (the xy plot file `b@nr@_@{profile_@integer@}@_simulation.plt`) differs only from the file name of the measured profile (the `b@nr@_@{profile_@integer@}@.plx` file) in its file extension.

The Sentauros Process tool instance defines the variables `process`, `process_info`, `calibration`, `n_profile`, and `profile_@integer@`. Sentauros Process can have a second parameter (see [Creating a New Parameterized Project on page 17](#)).

Sentaurus Process is called with the command-line option `-n` to switch off the syntax check.

Optionally, you can extract the sheet resistance analytically using the Sentaurus Process command `SheetResistance`, and the result is transferred to the Sentaurus Workbench variable `Rs_fps`.

For Sentaurus Process KMC, you can store the atomistic information using the following command:

```
kmc extract tdrWrite
```

---

## Sentaurus Mesh (Optional)

Sentaurus Mesh is used for the mesh generation of a 2D device simulation. For the calculation of sheet resistance, a 2D device is defined to represent the sheet of an ultrashallow junction of a transistor. The device definition is taken from the output files `b@nr@_fps.tdr` and `b@nr@_bnd.tdr` of Sentaurus Process.

The geometry is described by the following variables defined for Sentaurus Mesh:

- `x_sheet` defines the length [ $\mu\text{m}$ ] of the sheet (default is 20  $\mu\text{m}$ ).
- `y_sheet` defines the depth [ $\mu\text{m}$ ] of the sheet.
- `y0_sheet` defines the top position [ $\mu\text{m}$ ] of the sheet.
- `y_contact` defines the depth [ $\mu\text{m}$ ] of the contacts.
- `y0_contact` defines the top position [ $\mu\text{m}$ ] of the contacts.

The doping and grid information is stored in the `n@node@_msh.tdr` file.

---

## Sentaurus Device (Optional)

Sentaurus Device performs a 2D device simulation on the sheet defined in the `n@node|mesh@_msh.tdr` file. The voltage and the total current distribution of the sheet are computed for a voltage of 0.01 V between the left and right contacts. The results are saved in the `n@node@_des.plt` file. Sentaurus Device uses the default parameters for silicon, germanium, and SiGe from files by specifying the `DefaultParametersFromFile` flag in the global `Physics` section of the command file. The optional parameter file of Sentaurus Device is named `sdevice.par`.

## Inspect

Inspect calculates the sheet resistance and the curve differences. From the file `n@node|sdevice@_des.plt`, Inspect takes the voltage and the total current distribution, and calculates the sheet resistance. The results are stored in the Sentaurus Workbench variable `Rs_sim`. You can compare the extracted value with the experimental data for some experiments. The variable `Rs_exp`, which is defined by Sentaurus Process, retains the measured value or is set to zero if no measurement value is present.

For each profile pair, Inspect computes the difference between the measured profile and the simulated profile, that is, between `b@nr@_{profile_@integer@}.plx` and `b@nr@_{profile_@integer@}_simulation.plt`.

Different methodologies are available for this curve comparison (see [Comparing Profile Curves on page 35](#)). The variables `cv_delta_@integer@`, where `integer` is equal to 1, 2, 3, ..., 10, hold the extracted curve difference per  $\mu\text{m}$  for `profile_@integer@`.

You can view the profiles in interactive mode. If you want to save the visualization in the Inspect format, this must be performed manually.

Optionally, a spline-based curve-smoothing (a smooth, piecewise, polynomial approximation) is applied to the measured profile or the simulated profile for curve comparison.

See [Viewing Profile Files on page 27](#).

---

## Sentaurus Visual

Sentaurus Visual visualizes all measured and simulated profiles of a process in one xy plot. For each node, Sentaurus Visual takes all profiles (`b@nr@_{profile_@integer@}.plx` and `b@nr@_{profile_@integer@}_simulation.plt`), the curve comparison results (`cv_delta_@integer@`), and the preferences (`b@nr@_{profile_@integer@}.prf`), and creates a Sentaurus Visual Tcl script `n@node@_vis_out.tcl` for customized xy plot visualization.

All profiles of the experiment are plotted on top of each other. The curve comparison results `cv_delta_@integer@` are listed next to the curve label of the corresponding simulated profile. The borders of the curve comparison of the last profile pair are drawn in dashed style.

See [Viewing Visualization Files on page 27](#).

## CHAPTER 2 Working With Calibration Kit Projects

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*This chapter describes how to work with Calibration Kit projects.*

---

### Manipulating Calibration Kit Projects

A Calibration Kit project can be manipulated like other Sentaurus Workbench projects (for details about editing projects, see the *Sentaurus™ Workbench User Guide*). However, you can use special wizards of the Calibration Kit to guide you through project creation and extension, scenario and experiment generation, and parameterization.

It is faster and more thorough to manipulate projects using these wizards rather than the standard features of Sentaurus Workbench. The wizards are available from the **Calibration** menu of Sentaurus Workbench.

**NOTE** The **Calibration** menu is shown only in Sentaurus Workbench Advanced mode.

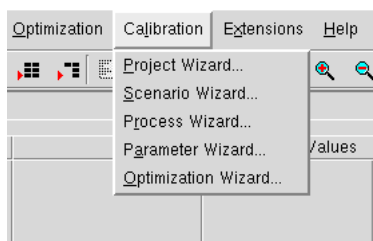


Figure 2 Wizards available from Calibration menu

**NOTE** Renumbering nodes of a Calibration Kit project can lead to a reduction of functionality. It is strongly advised *not* to renumber nodes.

---

### Creating a New Project or a New Scenario for an Existing Project

You can create a new Calibration Kit project or extend an existing project by a new scenario.

## 2: Working With Calibration Kit Projects

### Manipulating Calibration Kit Projects

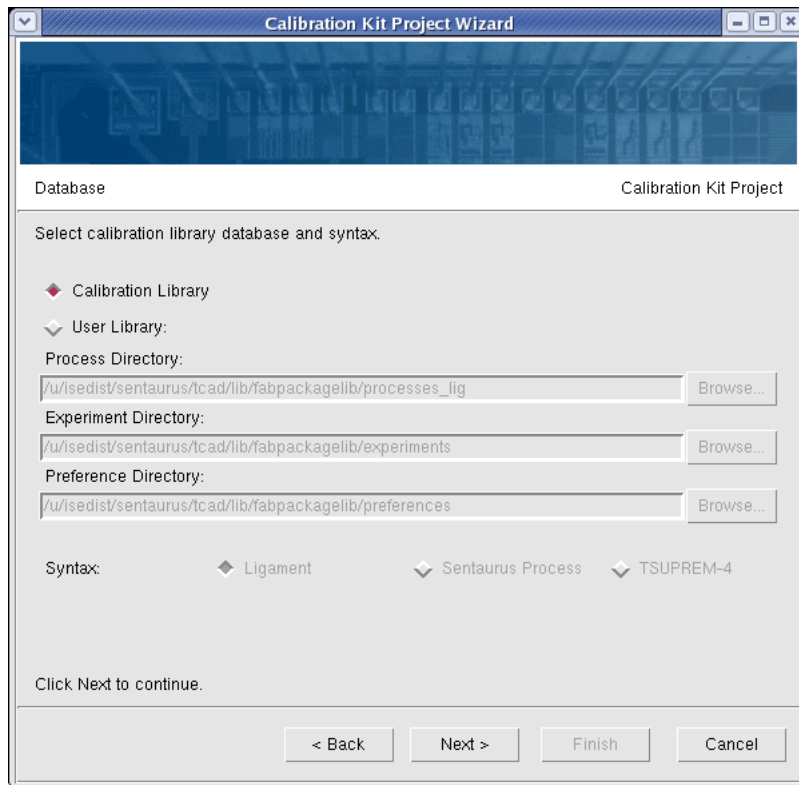
To create a new Calibration Kit project or a new scenario to an existing project:

1. Choose **Calibration > Project Wizard**.

The Project Wizard opens.

2. Click **Next** to start.
3. Select the calibration library database from either:
  - **Calibration Library**, which is the experiment database of the Calibration Library in Ligament SPR syntax.
  - **User Library**, which is a user-specified database in either Ligament SPR syntax or Sentaurus Process syntax.

If you select this option, you must specify the process directory, the experiment directory, and the preference directory, and select the syntax from either **Ligament**, **Sentaurus Process**, or **TSUPREM-4**.



4. Click **Next**.



5. Select a process list in one of the following ways:
  - Under DBPS - Database Process Search, type a search pattern in the **Process Search Pattern** field to look for processes using the DBPS in the selected database and syntax (Step 3).

Select the alphabetic order of the process list file from either **Process Names** or **Process Recipes**.

Click the **Search** button to write the results to the selected process list file (see [Database Process Search on page 32](#)).
  - Click the **Browse** button to select a list or search for a list using the DBPS. (For the syntax of a process list file `file.qps`, see [Process Searches on page 31](#).)

Click the **Edit** button to edit the selected list using the SEdit text editor.
6. Click **Next**.
7. Select the process simulator and calibration from either:
  - **Sentaurus Process** (default)

If you choose this option, under Calibration, select the implantation model, and select the diffusion model.

Select either the parameters of **Advanced Calibration** or **User Calibration**, in which case, select up to two calibration files in the Alagator (Tcl) syntax of Sentaurus Process, which usually follow the naming scheme `*.fps`.
  - **TSUPREM-4**

If you choose this option, under Calibration, select the implantation model.

Select either the parameters of **Advanced Calibration** or **User Calibration**, in which case, select the calibration files.
8. Click **Next**.
9. Select the device simulation to calculate the sheet resistance from one of the following options:
  - **Device Simulation Disabled** (default)
  - **Device Simulation Enabled**

If this option is selected, the Sentaurus Mesh and Sentaurus Device tool instances are part of the project. Click the **Browse** button to select the parameter file for Sentaurus Device. The file format usually follows the naming convention `*.par` and is named `sdevice.par` in the project. If no file is selected, Sentaurus Device uses the default parameters.
10. Click **Next**.

## 2: Working With Calibration Kit Projects

### Manipulating Calibration Kit Projects

11. Select the methodology for the simulation and the experiment profile comparison from the following options:

For numeric comparison, select one of the following options:

- **Relative Logarithmic Square Difference** (default)
- **Relative Linear Square Difference**
- **Arithmetic Mean of Relative Error**
- **Quadratic Mean of Relative Error**

The options of the **Noise Filter** field are deactivated by default. Select the options as required to activate the noise filter (spline-based curve-smoothing) for experiment data, or simulation data, or both.

Select the visualization tool. Sentaurus Visual is the default.

12. Click **Next**.

13. Select a project and scenario name from the following options:

- Select the **Create New Project** option for a new project.

Type the scenario name, and click the **Browse** button to select a project directory or type the project name.

- Select the **Add to Project** option to add a new scenario to an existing project.

Type the scenario name, and click the **Browse** button to select a project.

The new experiments will have the same structure as the rest of the project, that is, the selection of device simulation follows the existing project selection.

14. Click **Finish**.

15. If the project or scenario is created and loaded successfully, click **OK** in the Progress dialog box.

The generated project has the structure of the Calibration Kit described in [Structure of Calibration Kit Projects on page 5](#). For each process in the process list, the Project Wizard creates an experiment that follows the file-naming convention of the Calibration Kit. In the case of a database in Ligament SPR syntax, the process is translated to the syntax of the selected process simulator (see [Process File Syntax on page 29](#)). In the case of a database in Sentaurus Process syntax, the process is copied; it is not translated. For Sentaurus Process, the resulting process file is `b@nr@_fps.cmd`.

The file name of the process sets the variable `process`. The file names of the profiles set the variables `profile_@integer@`.

The variable `process_info` takes `INFO` as a value if `processinfo` appears as a remark or comment in the process file. For Ligament, this is:

```
remark (text : "processinfo 'BF2 2.5keV 1e15'");
```

For Sentaurus Process, `processinfo` is:

```
## processinfo "INFO"
```

Analogously, the variable `Rs_exp` is set to `VALUE` if `sheetresistance` appears as a remark or comment in the process file. For Ligament, this is:

```
remark (text : "sheetresistance 'VALUE'")
```

or:

```
remark (text : "sheetresistance 'Rs=VALUE'")
```

For Sentaurus Process, `sheetresistance` is:

```
## sheetresistance "VALUE"
```

or:

```
## sheetresistance "Rs=VALUE"
```

The variable `y_sheet` is set to 1.25 times the valid depth (set as `sims_xmax` in the preference file) of the deepest profile. If no preference (`sims_xmax`) is present, the default value of 50 nm is used. In addition, the variable `y_contact` is set to 0.25 times the valid depth (set as `sims_xmax` in the preference file) of the shallowest profile, unless the depth is defined explicitly (as `probe_xmax` in the preference file). If no preference (`probe_xmax` or `sims_xmax`) is present, the default value of 5 nm is used.

---

## Defining a New Scenario for a Project

To focus on a specific selection of experiments for a Calibration Kit project, a project can be split into scenarios. For example, a project can be split into scenarios of different dopant elements.

To create a new scenario for a Calibration Kit project:

1. Open a Calibration Kit project.
2. Choose **Calibration > Scenario Wizard**.

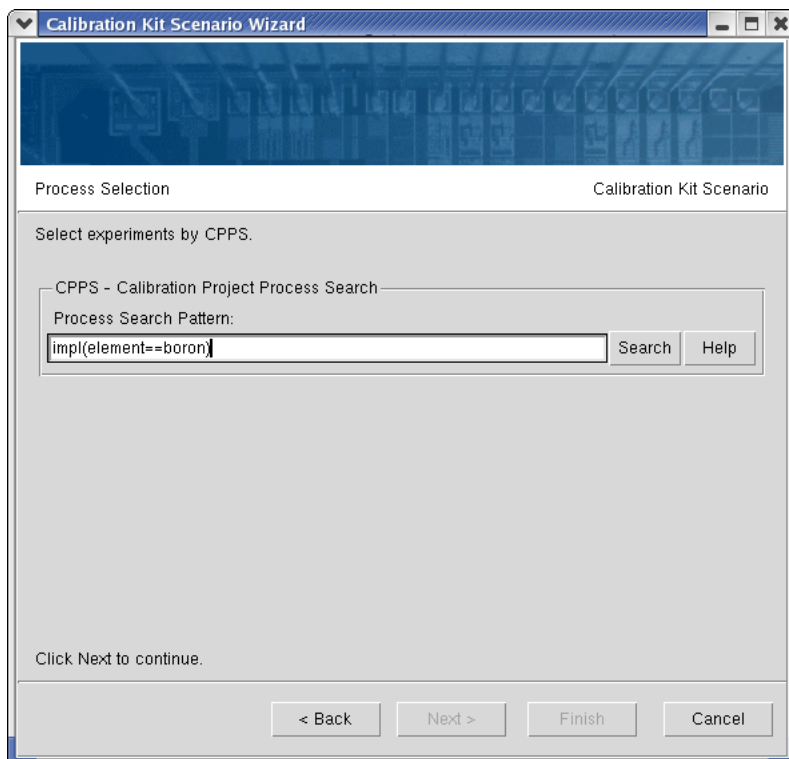
The Scenario Wizard opens.

3. Click **Next** to start.

## 2: Working With Calibration Kit Projects

### Manipulating Calibration Kit Projects

4. Under CPPS - Calibration Project Process Search, type a search pattern in the **Process Search Pattern** field to select experiments, and click **Search** (see [Calibration Project Process Search on page 33](#)).



5. Click **Next**.
6. Type the name of the new scenario in the **Scenario Name** field.
7. Click **Finish**.
8. If the scenario is created and loaded successfully, click **OK** in the Progress dialog box.

The structure of the Calibration Kit project is unchanged by the creation of a new scenario.

---

## Creating a New Short Loop Experiment

You can add a new short loop experiment (in Ligament SPR syntax or Sentaurus Process syntax) to a database or add a new experiment to a Calibration Kit project.

To create a new short loop experiment for a Calibration Kit project:

1. Open a Calibration Kit project.

2. Choose **Calibration > Process Wizard**.

The Process Wizard opens.

3. Click **Next** to start.

4. Select the substrate and oxide properties.

If the oxide thickness is 0, the oxide deposition step is omitted.

5. Click **Next**.

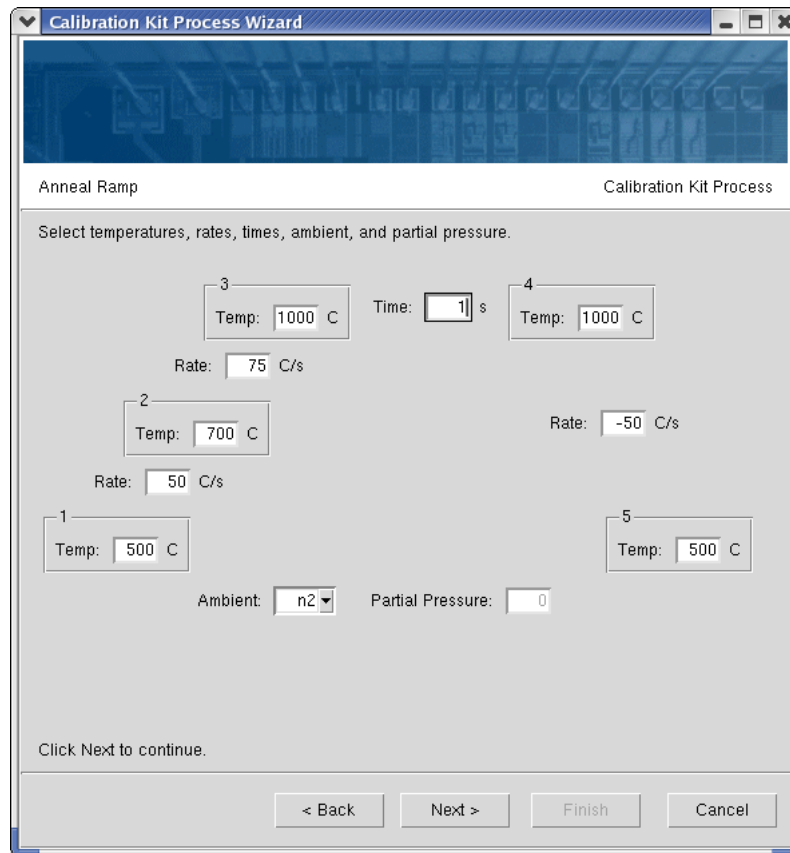
6. Select the implantation properties of the first and second implantations.

If the **Element** field is set to 0, the corresponding implantation step is omitted.

7. Click **Next**.

8. Select the anneal ramp properties.

If the **Rate** or **Time** fields are set to 0, the corresponding diffusion step is omitted.



## 2: Working With Calibration Kit Projects

### Manipulating Calibration Kit Projects

9. Click **Next**.

10. Select the properties for the first and second measurements:

- If the **Element** field is set to 0, the corresponding measurement step is omitted.
- For the **Experiment Data** field, click **Browse** to select the experimental measurement data (SIMS).

Click **View** to view the selected SIMS using Inspect.

- Select the depth scale of the selected SIMS.
- For the **Preferences** field, click **Browse** to select the preferences.

Click **Create** to create new preferences and to edit them with the SEdit text editor.

11. Click **Next**.

12. Select a process name and syntax:

- Type the name of a process in the **Name** field.
- From the **Syntax** field, select the required option.
- Click the **Edit** button to edit the flow if required.

If Ligament SPR syntax is selected, the flow is loaded into the Ligament Flow Editor.  
If Sentaurus Process syntax is selected, the flow is loaded into a text editor.

If needed, the flow can be further modified beyond the guidelines of the previous wizard pages.

When **Edit** is clicked, the current values of the process steps defined in the previous steps are considered. Further changes to the process through the previous wizard pages no longer affect the flow, unless **Edit** is clicked again.

If **Edit** is clicked again, the current values of the process steps defined in the previous wizard steps are reconsidered, and the previous changes of the flow in the editor are deleted.

13. Click **Next**.

14. Select whether the process is added to a database or the currently loaded project:

- Select the **Add to Project** option to add a new experiment with the created process flow to the currently loaded Calibration Kit project.

This option is available only if the currently loaded project is a Calibration Kit project and contains the same simulator that was previously selected as the process syntax.

- Select the **Add to User Library** option to add the process flow permanently to a database. Select the process directory for the process recipes, the experiment directory for the measurement data, and the preference directory for the preferences.

15. Click **Finish**.

16. If the experiment is created successfully, click **OK** in the Progress dialog box.

If added to a database, the process recipe is stored in the same format as those in the calibration libraries (see [Process File Syntax on page 29](#)). The process flow includes the correlated profile and `process_info` information.

If added to a project, the experiment has the same structure as the other experiments of the project. The variable `process` is defined by the process name. If an experiment profile is referenced, the variable `profile_@integer@` is defined by the name of the experiment profile. If no experiment profile is referenced, the variable `profile_@integer@` is defined by `@process-name@_@integer@`. Depending on the declared implantation and diffusion steps, the variable `process_info` is set.

The variable `y_sheet` is set to 1.25 times the valid depth (set as `sims_xmax` in the preference file) of the deepest profile. If no preference (`sims_xmax`) is present, the default value of 50 nm is used. In addition, the variable `y_contact` is set to 0.25 times the valid depth (set as `sims_xmax` in the preference file) of the shallowest profile, unless the depth is defined explicitly (as `probe_xmax` in the preference file). If no preference (`probe_xmax` or `sims_xmax`) is present, the default value of 5 nm is used.

**NOTE** If the process flow is edited further after the wizard generation, you must ensure that the variable values (such as the number of profiles `n_profile`) are correct.

---

## Creating a New Parameterized Project

You can create a new Calibration Kit project with new physical Sentaurus Process parameters, and an optional command file for the Optimizer tool.

To create a new Calibration Kit project with new physical Sentaurus Process parameters:

1. Open a Calibration Kit project and select an experiment.
2. Choose **Calibration > Parameter Wizard**.  
The Parameter Wizard opens.
3. Click **Next** to start.
4. Parameterize the selected process (the name and simulator syntax of the selected process is displayed):
  - a) Select up to six parameter names for `parameter` (for example, `energy`).

## 2: Working With Calibration Kit Projects

### Manipulating Calibration Kit Projects

- b) Select to either **Include** or **Exclude** the experiment data.

If experiment data is included, the experiments of the resulting project contain the experiment profiles (SIMS) of the selected experiment.

- c) Click **Edit** to load the flow is loaded into an editor.

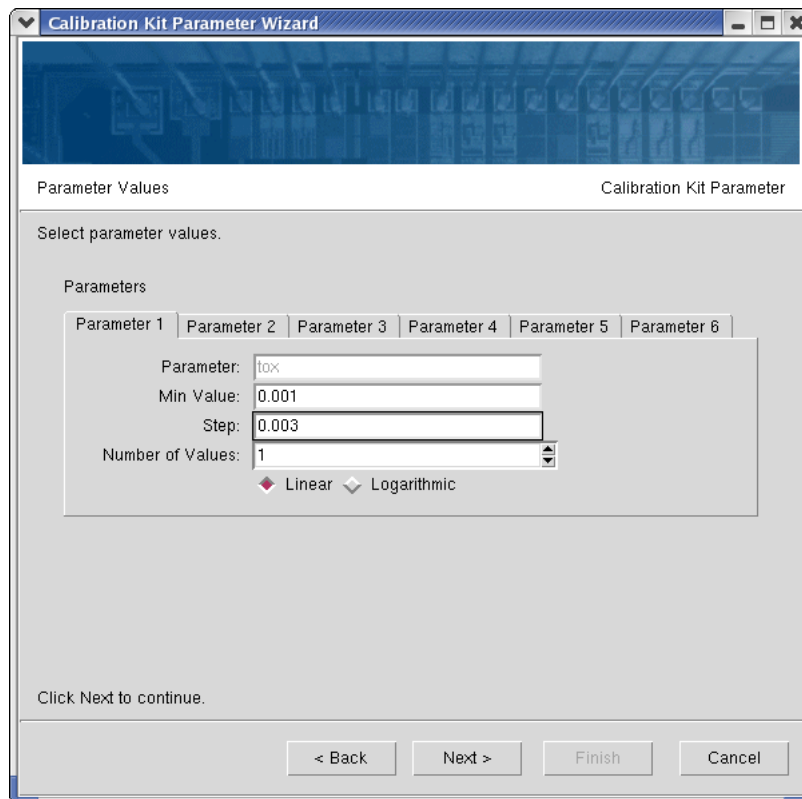
Edit the flow by replacing the argument values to be parameterized with @parameter@. For example, for the parameter energy and Sentaurus Process syntax, type:

```
implant Arsenic dose=1e+15 energy=@energy@ tilt=0 rot=0
```

Save the file.

5. Click **Next**.

6. Specify the parameter values of each parameter on the respective tabs:



- a) Select the minimal value of the parameter.
- b) Select the iteration step between parameter values.
- c) Select the number of parameter values.



- d) If the **Linear** option is selected, the difference between the values is equal to the iteration step. If the **Log** option is selected, the value of each step is equal to the value of the previous step multiplied by the value of the iteration step.
7. Click **Next**.
  8. Select a calibration parameter file for the process simulator of the parameterized process file:
    - Under Calibration, select the implantation model, and select the diffusion model.
    - Select either the parameters of **Advanced Calibration** or **User Calibration**, in which case, select up to two calibration files in the Alagator (Tcl) syntax of Sentaurus Process, which usually follow the naming scheme \*.fps.
  9. Click **Next**.
  10. Select the device simulation to calculate the sheet resistance from one of the following options:
    - **Device Simulation Disabled** (default)
    - **Device Simulation Enabled**

If this option is selected, the Sentaurus Mesh and Sentaurus Device tool instances are part of the project. Click the **Browse** button to select the parameter file for Sentaurus Device. The file format usually follows the naming convention \*.par and is named sdevice.par in the project. If no file is selected, Sentaurus Device uses the default parameters.
  11. Click **Next**.
  12. Select an Optimizer task and the corresponding task conditions, if required, from the following options:
    - **None**
    - **Sentaurus PCM Studio**
    - **Screening**
    - **Optimization**
    - **Iterative Optimization**
    - **Generic Optimization**
  13. Click **Next**.
  14. Select the methodology for the simulation and the experiment profile comparison from the following options.

## 2: Working With Calibration Kit Projects

### Manipulating Calibration Kit Projects

For numeric comparison, select one of the following options:

- **Relative Logarithmic Square Difference** (default)
- **Relative Linear Square Difference**
- **Arithmetic Mean of Relative Error**
- **Quadratic Mean of Relative Error**

The options of the **Noise Filter** field are deactivated by default. Select the options as required to activate the noise filter (spline-based curve-smoothing) for experiment data, or simulation data, or both.

Select the visualization tool. Sentaurus Visual is the default.

15. Click **Next**.

16. Select a project and scenario name:

- a) Type a scenario name.
- b) Click **Browse** to select a project directory, or type the project name.

17. Click **Finish**.

18. If the project is created and loaded successfully, click **OK** in the Progress dialog box.

If no Optimizer task is selected (**Task Type** is set to **None**), the new project has the structure of a Calibration Kit project with two to seven parameters, that is, the parameter `nr` and the selected parameters. The variable `process` is the selected process name combined with the parameter value. The variable `process_info` contains the parameter name and value. The values of the variables `profile_@integer@` consist of the process name `process` and sequential numbering, for example, `<process>_1`.

The project contains as many experiments as there are possible combinations of parameter values.

If an Optimizer task is selected, the new project has the structure of a Calibration Kit project with two to seven parameters, that is, the parameter `nr` is a user-defined Optimizer parameter and the selected parameters are design-of-experiments (DoE) Optimizer parameters.

The only available variables are the process name `process`, the calibration file `calibration`, and the number of profiles per process `n_profile`. The project contains only one experiment with the mean parameter values. For each pair of profiles, a unique curve comparison variable `cv_delta_@integer@_@integer@` is evaluated and is used as a response for the Optimizer tool. The corresponding command file of Optimizer is included in the project.

For information about the Optimizer tool, see the *Optimizer User Guide*.

---

## Creating a New Project for Optimization

You can create a new Calibration Kit project with new calibration parameters of Sentaurus Process, and an optional command file of the Optimizer tool.

To create a new Calibration Kit project with new calibration parameters of Sentaurus Process:

1. Choose **Calibration > Optimization Wizard**.

The Optimization Wizard opens.

2. Click **Next** to start.

3. Select the calibration library database from either:

- **Calibration Library**, which is the experiment database of the Calibration Library in Ligament SPR syntax.
- **User Library**, which is a user-specified database in either Ligament SPR syntax or Sentaurus Process syntax.

If you select this option, you must specify the process directory, the experiment directory, and the preference directory, and select the syntax from either **Ligament**, **Sentaurus Process**, or **TSUPREM-4**.

4. Click **Next**.

5. Select a process list in one of the following ways:

- Under DBPS - Database Process Search, type a search pattern in the **Process Search Pattern** field to look for processes using the DBPS in the selected database and syntax (Step 3).

Select the alphabetic order of the process list file from either **Process Names** or **Process Recipes**.

Click the **Search** button to write the results to the selected process list file (see [Database Process Search on page 32](#)).

- Click the **Browse** button to select a list or search for a list using the DBPS. (For the syntax of a process list file `file.qps`, see [Process Searches on page 31](#).)

Click the **Edit** button to edit the selected list using the SEdit text editor.

6. Click **Next**.

7. Select the process simulator and calibration from either:

- **Sentaurus Process** (default)

If you choose this option, under Calibration, select the implantation model, and select the diffusion model.

## 2: Working With Calibration Kit Projects

### Manipulating Calibration Kit Projects

Select either the parameters of **Advanced Calibration** or **User Calibration**, in which case, select up to two calibration files in the Alagator (Tcl) syntax of Sentaurus Process, which usually follow the naming scheme \*.fps.

- **TSUPREM-4**

If you choose this option, under Calibration, select the implantation model.

Select either the parameters of **Advanced Calibration** or **User Calibration**, in which case, select the calibration files.

8. Click **Next**.

9. Parameterize the selected calibration file by entering the values of the fields for the parameters:

**NOTE** For Sentaurus Process, only the second selected calibration file can be parameterized.

- a) Select up to four parameter names for `parameter` (for example, `ifactor`).
- b) Select the minimal value and the maximal value of a parameter.
- c) Select either the **Linear** option or the **Logarithmic** option.
- d) Click **Edit** to load the calibration file into an editor.

Edit the file by replacing the calibration parameter values to be parameterized with Sentaurus Workbench parameter calls `@parameter@`. (This calibration file will be preprocessed by Sentaurus Workbench as well.)

Save the file.

10. Click **Next**.

11. Select an Optimizer task and the corresponding task conditions, if required, from the following options:

- **None**

If this option is selected, no Optimizer task is used, but you must select the number of different parameter values for each parameter.

- **Sentaurus PCM Studio**

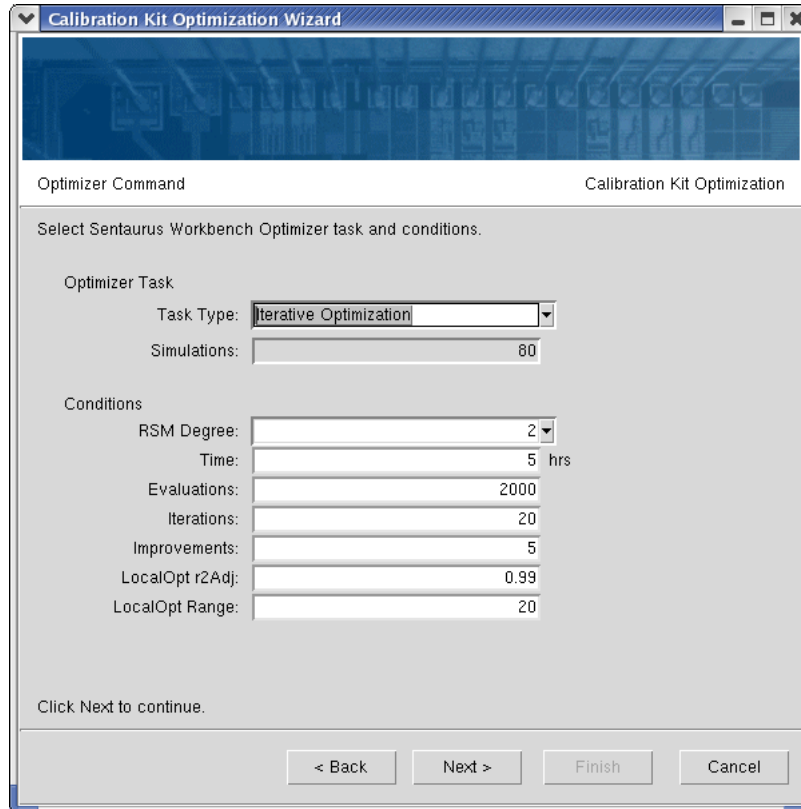
If this option is selected, no Optimizer task is used, but you can add more parameter values after the creation of the project.

- **Screening**

- **Optimization**

- **Iterative Optimization**
- **Generic Optimization**

In addition, the project has a convenient structure for exporting the project view and profiles to Sentaurus PCM Studio. For all other task types, a project with the corresponding Optimizer command file is generated. (For information about Optimizer tasks, see the *Optimizer User Guide*.)



12. Click **Next**.
13. Select the device simulation to calculate the sheet resistance from one of the following options:
  - **Device Simulation Disabled** (default)
  - **Device Simulation Enabled**

If this option is selected, the Sentaurus Mesh and Sentaurus Device tool instances are part of the project. Click the **Browse** button to select the parameter file for Sentaurus Device. The file format usually follows the naming convention \*.par and is named sdevice.par in the project. If no file is selected, Sentaurus Device uses the default parameters.

## 2: Working With Calibration Kit Projects

### Manipulating Calibration Kit Projects

14. Click **Next**.

15. Select the methodology for the simulation and the experiment profile comparison from the following options:

For numeric comparison, select one of the following options:

- **Relative Logarithmic Square Difference** (default)
- **Relative Linear Square Difference**
- **Arithmetic Mean of Relative Error**
- **Quadratic Mean of Relative Error**

The options of the **Noise Filter** field are deactivated by default. Select the options as required to activate the noise filter (spline-based curve-smoothing) for experiment data, or simulation data, or both.

Select the visualization tool. Sentaurus Visual is the default.

16. Click **Next**.

17. Select a project and scenario name:

- a) Type a scenario name.
- b) Click **Browse** to select a project directory, or type the project name.

18. Click **Finish**.

19. If the project is created and loaded successfully, click **OK** in the Progress dialog box.

If no Optimizer task is selected (**Task Type** is set to **None**), the new project has the structure of a Calibration Kit project with two to seven parameters, that is, the parameter `nr` and the selected parameters. For each process in the process list and each parameter value combination, the Optimization Wizard creates an experiment that follows the file-naming convention of the Calibration Kit.

In the case of a database in Ligament SPR syntax, the process is translated to the selected process simulator syntax (see [Process File Syntax on page 29](#)). In the case of a database in Sentaurus Process syntax, the process is copied; it is not translated. For Sentaurus Process, the resulting process file is `b@nr@_fps.cmd`.

If an Optimizer task is selected, the new project has the structure of a Calibration Kit project with two to seven parameters, that is, the parameter `nr` is a user-defined Optimizer parameter and the selected parameters are DoE Optimizer parameters.

The only available variables are the process name `process`, the calibration file `calibration`, and the number of profiles per process `n_profile`. The project contains only one experiment per process in the process list with mean parameter values. For each pair of

profiles, a unique curve comparison variable `cv_delta_@integer@_@integer@` is evaluated and is used as a response for Optimizer. The corresponding command file of Optimizer is included in the project.

For information about the Optimizer tool, see the *Optimizer User Guide*.

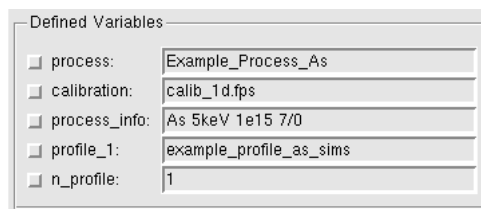
---

## Editing Variables

You can change the variable values of a Calibration Kit experiment using Sentaurus Workbench.

To edit a variable:

1. Select the corresponding node:
  - This is the second Sentaurus Process node for the variables `process`, `calibration`, `process_info`, `Rs_exp`, `n_profile`, and `profile_@integer@` (where `integer` is equal to 1, 2, 3, ..., 10).
  - This is the Sentaurus Mesh node for the variables `*_contact` and `*_sheet`.
2. Edit the variable values in one of the following ways:
  - Choose **Nodes > Set Variable Value**.  
The Add Variable to Node dialog box is displayed.  
Enter the name and the value of the variable, and click **OK**.
  - Choose **Nodes > Edit Properties**.  
The Node information dialog box is displayed.  
Under Defined Variables, edit the definition of the variable (as shown in the following example), and click **OK**.



---

## Visualizing Project Files

Each Calibration Kit project has dedicated viewers that are defined in the project tool database (`gtoolddb.tcl`) of Sentaurus Workbench. These viewers are specifically for the files of Calibration Kit projects.

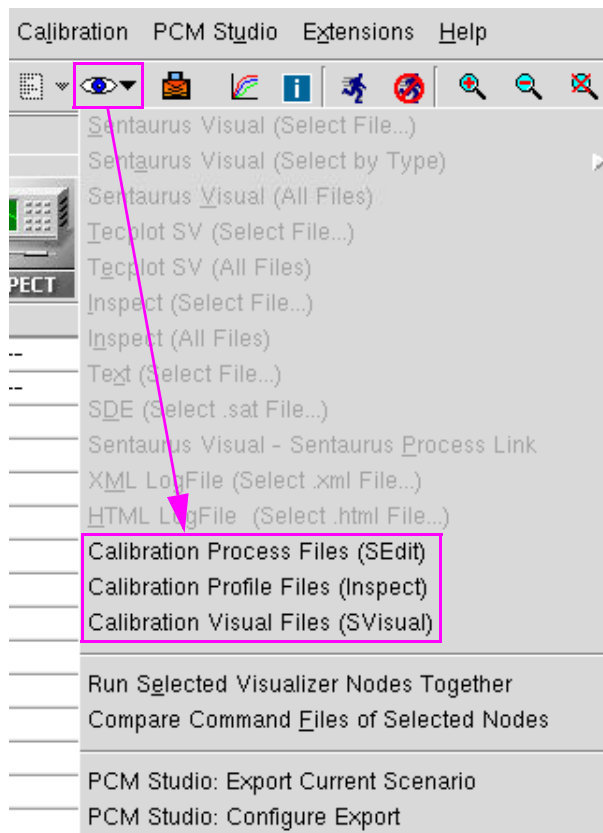


Figure 3 Specific viewers of files of Calibration Kit projects available from the visualization toolbar button

---

## Viewing Process Files

To view process files:

- Choose the  button > **Calibration Process Files (SEdit)**.

These files open in the SEdit text editor. For Sentaurus Process, the process files are the Sentaurus Process command files (`b@node@_fps.cmd` or `pp@node@_fps.cmd`) and general files (`*.fps`). The selection is restricted to the `nr` nodes of Sentaurus Process.



## Viewing Profile Files

To view profile files:

- Choose the  button > **Calibration Profile Files (Inspect)**.

The selected measured profiles (b@node@\_\*.plx) and simulated profiles (b@node@\_\*.plt) open in Inspect. All of the selected profiles are loaded into one xy plot. The selection is restricted to the nr nodes of Sentaurus Process.

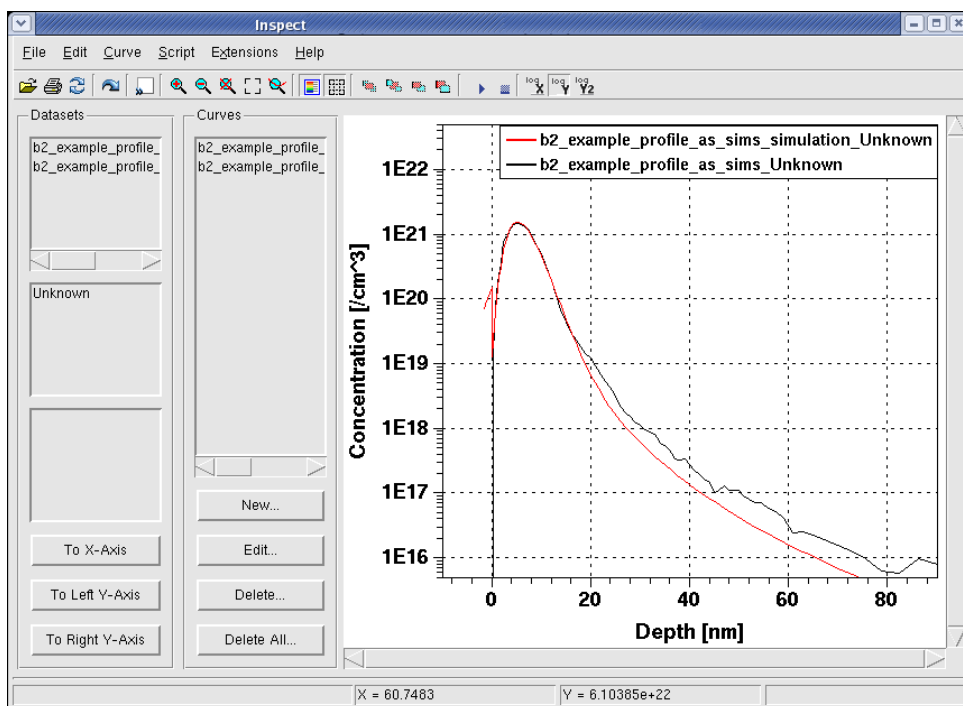


Figure 4 An experiment visualized in Inspect

## Viewing Visualization Files

To view visualization files:

- Choose the  button > **Calibration Visual Files (SVisual)**.

The selected measured profiles (b@node@\_\*.plx) and the simulated profiles (b@node@\_\*.plt) open in Sentaurus Visual. All of the selected xy plot visualization scripts (n@node@\_vis\_out.tcl) are loaded and arranged next to each other. The selection is restricted to Sentaurus Visual nodes. For more information, see the *Sentaurus™ Visual User Guide*.

## 2: Working With Calibration Kit Projects

Confidentiality Warning

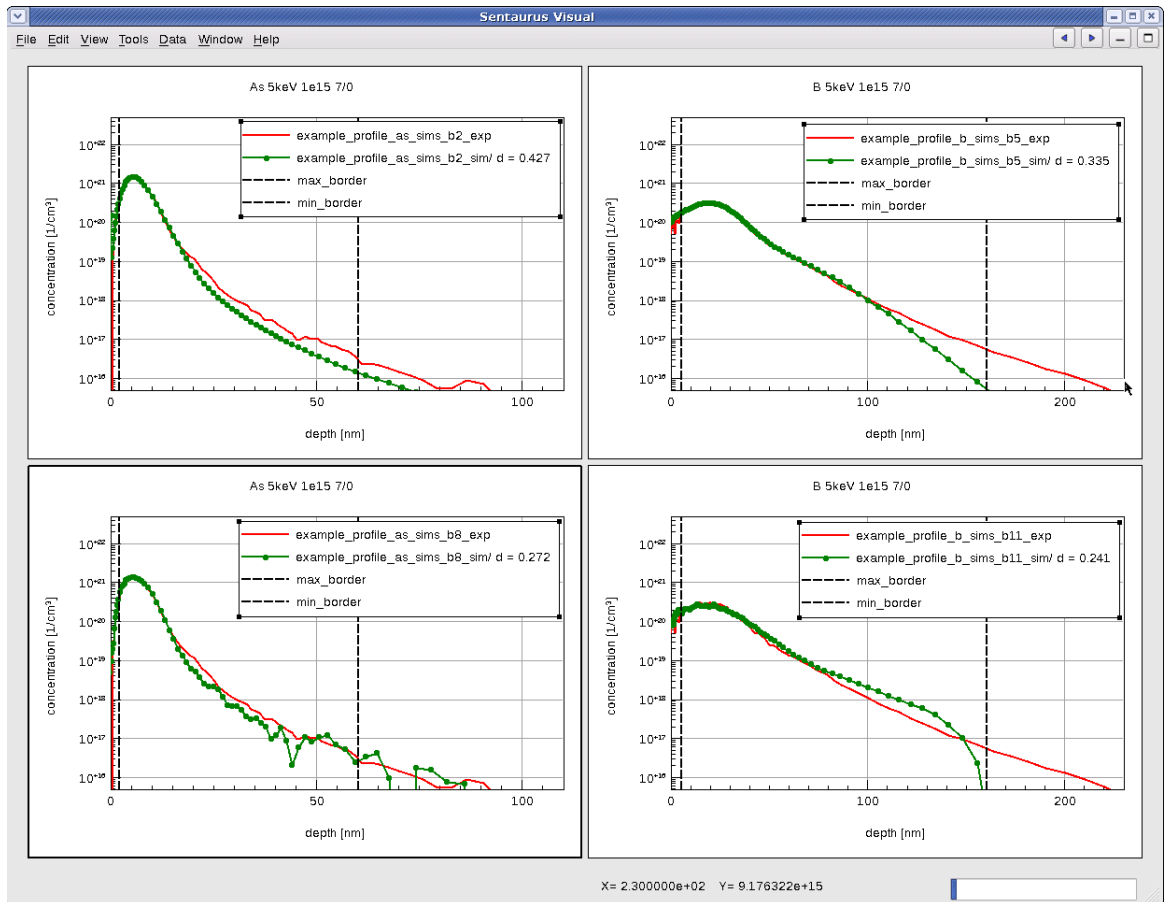


Figure 5 Four experiments visualized in Sentaurus Visual

---

## Confidentiality Warning

The file `$$STROOT/tcad/$$STRELEASE/lib/fabpackagelib/confidentwarning.txt` contains the text for the confidentiality warning that appears on the first page of the Project Wizard, Scenario Wizard, and Optimization Wizard. If the file is empty or does not exist, no confidentiality warning is displayed.

The file `$$STCALIB/confident.txt` contains the text for the confidentiality warning that appears in a separate dialog box when the third page of the Project Wizard and Optimization Wizard is displayed. If the file is empty or does not exist, no confidentiality warning is displayed.

## CHAPTER 3 Calibration Library, Process Searches, and Profiles

---

*This chapter provides details about the Calibration Library, process searches, and working with profiles.*

---

### Experiment Database: Calibration Library

This section describes the Calibration Library of the Calibration Kit.

---

#### Defining the Calibration Library

The default experiment database of the Calibration Kit – the Calibration Library – is defined using the system environment variable `STCALIB`. By default, `STCALIB` is set to the directory `$(STROOT_LIB)/fabpackage.lib`, which contains a database including process examples for demonstration purpose only and without any real experimental relevance.

The `STCALIB` databases (such as the Calibration Library or user databases) include three directories:

- The process directory, which is either `processes_lig` containing the process files in Ligament SPR syntax, or `processes_sprocess` containing the process files in Sentaurus Process syntax.
- The experiment directory `experiments` contains the SIMS profile files in xy plot format.
- The preference directory `preferences` contains the preference files (see [Profiles on page 34](#)).

---

#### Process File Syntax

In general, the Calibration Kit uses databases of process recipes in Ligament SPR syntax and Sentaurus Process syntax as input. However, the process recipes of the Calibration Library are delivered in Ligament SPR syntax and are translated to Sentaurus Process syntax before simulation.

### 3: Calibration Library, Process Searches, and Profiles

Experiment Database: Calibration Library

For the Calibration Library (as well as other user databases) to be input to the Calibration Kit, the general Ligament SPR syntax and Sentaurus Process syntax are subject to restrictions.

## Restrictions on Ligament SPR Syntax

During the creation of a Calibration Kit project, the process recipes in Ligament SPR syntax are translated to Sentaurus Process syntax. First, the translator of the Calibration Kit uses the Ligament Translator. Then, some process flow translations specific to the Calibration Kit are applied (see [Restrictions on Sentaurus Process Syntax](#)).

In Ligament process flows, the arguments `save`, `grid`, `debug`, and `check1d` of the `environment` statement must all be set to `false`. The arguments `title`, `region`, and `*_grid_*` of the `environment` statement are irrelevant, since they are ignored during translation.

The 1D measurements are stated in an `insert` statement.

For Sentaurus Process, the 1D measurement statement is specified by the `SetPltList` statement, which is defined in `calib_1d_*.fps`. The `SetPltList` statement must only contain the `species` variable and a comment of the corresponding SIMS profile at the end of the same line (see [Restrictions on Sentaurus Process Syntax](#)).

For Sentaurus Process, the 1D profile load statement is specified by the `profile` statement, which must only contain the `species` variable and a comment of the corresponding profile at the end of the same line (see [Restrictions on Sentaurus Process Syntax](#)).

The process information `<INFO>` can be declared in a `remark` statement with `processinfo` `'<INFO>'` as text.

The measured sheet resistance value `<VALUE>` can be declared in a `remark` statement with `sheetresistance` `'Rs=<VALUE>'` as text.

The measured cap-oxide thickness value `<VALUE>` in [nm] can be declared in a `remark` statement with `OxideThickness` `<VALUE>` as text.

## Restrictions on Sentaurus Process Syntax

The process recipes in Sentaurus Process syntax in the database must include only process physics parameters. However, if you include simulator or model parameters in the process recipe files, the reliability of the simulation might be reduced.

The Sentaurus Process recipes must not contain `line` statements or `region` statements (the sourced file `calib_1d_2017.09.fps` or `calib_KMC_2017.09.fps` places these

statements in the input files of Sentaurus Process). During translation from Ligament SPR syntax to Sentaurus Process syntax, all statements preceding the first `init` statement are removed.

The 1D measurement statement is specified by the `SetPltList` statement, which is defined in `calib_1d_2017.09.fps` or `calib_KMC_2017.09.fps`. The `SetPltList` statement must contain only the `species` variable and a comment of the corresponding SIMS profile at the end of the same line, for example:

```
SetPltList BTotal ; # B_sims_profile.sims
```

The 1D profile load statement is specified by the `profile` statement, which must contain only the `species` variable and a comment of the corresponding profile at the end of the same line, for example:

```
profile name=Boron ; # B_sims_profile.sims
```

The process information `<INFO>` can be declared in a comment line with `processinfo "<INFO>"` as comment, for example:

```
## processinfo "B 0.5keV 1e15"
```

The measured sheet resistance value `<VALUE>` can be declared in a comment line with `sheetresistance "Rs=<VALUE>"` as a comment, for example:

```
## sheetresistance "Rs=491"
```

The measured cap-oxide thickness value `<VALUE>` in [nm] can be declared in a comment line with `OxideThickness <VALUE>` as comment.

---

## Process Searches

The module Quick Process Search (QPS) provides basic functionality for the process search in the process directory of the database. The Database Process Search (DBPS) module and the Calibration Project Process Search (CPPS) module are based on QPS.

---

## Syntax of the QPS List File

The results of DBPS and CPPS as well as the input process list to the Calibration Kit project and the scenario wizards are QPS files `file.qps`. The file contains a header line and a process list.

### 3: Calibration Library, Process Searches, and Profiles

#### Process Searches

The syntax is:

```
Processes  Profiles      Processinfo  R_sheet
<process> <profile_1>  <info>      <r_sheet>
           <profile_2>
```

---

## Database Process Search

The Database Process Search (DBPS) looks for process flows written in the syntax of Ligament or Sentauros Process in a directory (such as \$STCALIB/processes\_\*). The processes that match the search criterion are listed in the process list file.

The search criterion – the process search pattern – consists of *conditions* connected by logical *operators* &&, ||, !, and grouped by parentheses. The operator && means *and*, || means *or*, and ! means *not*. The conditions consist of a *keyword* and *arguments*, for example, impl(element==As) or nimpl>0.

In general, the keyword takes only one argument. Only the impl() and diff() keywords can have more than one argument that are connected by logical operators. Some arguments consist of an argument type and a value connected by *comparators*: ==, <=, >=, <, >, or !=. Some arguments do not have comparators or argument types.

Table 1 lists the DBPS process flow keywords and their syntax, which are allowed in the DBPS criterion.

Table 1 DBPS keywords and syntax

Keyword	Meaning	Argument	Example
impl()	Implantation statement scan, true if (1)	element, elem energy, en dose tilt rotation, rot	impl(elem==as) impl(en>0 && en<100) impl(dose>=1e12) impl(tilt!=0) impl(rot<1)
diff()	Diffusion statement scan, true if (1)	maxT (maximum temperature) totaltime peakttime (time at maximum temperature) pn2 (partial pressure for N <sub>2</sub> ) po2 (partial pressure for O <sub>2</sub> ) ph2o (partial pressure for H <sub>2</sub> O)	diff(maxT==1000) diff(totaltime>5) diff(peakttime!=0)  diff(pn2==1) diff(po2>0 && po2<1) diff(ph2o!=0)
plot()	Plot statement scan, true if (2)	X, Xtot, Xtotal, Xactive (where X is one of as, p, b, in, ge, sb, ga, al, n)	plot(bactive)
nimpl	Number of implantation statements scan, true if (3)	–	nimpl==1

Table 1 DBPS keywords and syntax

Keyword	Meaning	Argument	Example
ndiff	Number of diffusion statement scan, true if (3)	–	ndiff>0
file()	File name scan, true if (2)	<string>	file(USJ)
grep()	Process file scan, true if (2)	<string>	grep(comment)

(1) At least one statement exists in the process file, for which the arguments are evaluated as true.  
(2) At least one statement exists in the process file, for which the argument is evaluated as true.  
(3) Comparison is evaluated as true.

## Calibration Project Process Search

The Calibration Project Process Search (CPPS) looks for experiments in a calibration project of Sentaurus Workbench. The tool scans process flows written in the syntax of Sentaurus Process in the same way as DBPS. However, CPPS scans variables of the Sentaurus Workbench. The experiments that match the search criterion are listed in the process list file.

The search criterion – the process search pattern – consists of *conditions* connected by logical *operators* &&, ||, !, and grouped by parentheses. The operator && means *and*, || means *or*, and ! means *not*. The conditions consist of a *keyword* and *arguments*, for example, `impl(element==As)` or `nimpl>0`.

In general, the keyword takes only one argument. Only the `impl()` and `diff()` keywords can have more than one argument that are connected by logical operators. Some arguments consist of an argument type and a value connected by *comparators*: ==, <=, >=, <, >, or !=. Some arguments do not have comparators or argument types.

Table 2 lists the DBPS process flow keywords and their syntax, which are allowed in the CPPS criterion.

Table 2 Keywords and syntax for CPPS of DBPS

Keyword	Meaning	Argument	Example
impl()	Implantation statement scan, true if (1)	element, elem energy, en dose tilt rotation, rot	impl(elem==as) impl(en>0 && en<100) impl(dose>=1e12) impl(tilt!=0) impl(rot<1)

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#### Profiles

Table 2 Keywords and syntax for CPPS of DBPS

Keyword	Meaning	Argument	Example
diff()	Diffusion statement scan, true if (1)	maxT (maximum temperature) totaltime peakttime (time at maximum temperature) pn2 (partial pressure for N <sub>2</sub> ) po2 (partial pressure for O <sub>2</sub> ) ph2o (partial pressure for H <sub>2</sub> O)	diff(maxT==1000) diff(totaltime>5) diff(peakttime!=0)  diff(pn2==1) diff(po2>0 && po2<1) diff(ph2o!=0)
plot()	Plot statement scan, true if (2)	X, Xtot, Xtotal, Xactive (where X is one of as, p, b, in, ge, sb, ga, al, n)	plot(bactive)
nimpl	Number of implantation statements scan, true if (3)	–	nimpl==1
ndiff	Number of diffusion statement scan, true if (3)	–	ndiff>0
grep()	Process file scan, true if (2)	<string>	grep(comment)
(1) At least one statement exists in the process file, for which the arguments are evaluated as true. (2) At least one statement exists in the process file, for which the argument is evaluated as true. (3) Comparison is evaluated as true.			

Table 3 lists the Sentaurus Workbench variable keyword and its syntax, which is allowed in the search criterion.

Table 3 Keywords and syntax for CPPS of Sentaurus Workbench variable

Keyword	Meaning	Argument	Example
process()	Process variable scan, true if at least one statement exists in the process file, for which the arguments are evaluated as true	<string>	process(USJ)

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## Profiles

This section discusses different aspects of profiles.

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### Visualizing Profiles

The visualization limits of each profile can be set in the preference file. The depth [nm] is set by:

```
set vis_xmin [integer]
set vis_xmax [integer]
```



The concentration [ $\text{cm}^{-3}$ ] is set by:

```
set vis_ymin [integer]
set vis_ymax [integer]
```

These values are the lower and upper limits of the visualization to be shown. A limit is evaluated by the visualization tool if the corresponding limit is not present in the preference file.

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## Comparing Profile Curves

Inspect calculates the differences of the measured and computed profile curves, which can be viewed in the Inspect log file. Optionally, the noise of the profile curves can be filtered by spline-based curve-smoothing. The difference is processed as the variable `cv_delta_@integer@` of Sentaurus Workbench for each profile pair.

The quality limits of each profile can be set in the preference file. The depth [nm] is set by:

```
set sims_xmin [integer]
set sims_xmax [integer]
```

These values are the lower and upper limits of the profile curve comparison. The default limits are used as borders if the above limits are not defined. The default values are:

```
set sims_xmin 5
set sims_xmax 50
```

The minimal and maximal concentrations [ $\text{cm}^{-3}$ ] are set by:

```
set sims_ymin [double]
set sims_ymax [double]
```

Concentrations outside of this range are set to the corresponding border value of the profile curve comparison. The default limits are used as borders if the above limits are not defined. By default, `sims_ymin` is half the concentration of the smoothed experiment profile curve at the depth `sims_xmax`, while the default for `sims_ymax` is `1e23`.

**NOTE** If several profile pairs are visualized in one plot, only the comparison borders of the last profile pair are shown.

The profile curve comparison can be performed using different methodologies:

- Relative logarithmic square difference
- Relative linear square difference
- Arithmetic mean of relative error
- Quadratic mean of relative error

## Relative Logarithmic Square Difference

The formula for the relative logarithmic square difference for the experiment profile curve  $fe$  and the simulated profile curve  $fs$  is:

$$\int_{xmin}^{xmax} (\log(fe(x)) - \log(fs(x)))^2 dx \quad (1)$$

where the borders of integration  $xmin$  and  $xmax$  are the lower and upper limits of the profile curve comparison, respectively. The relative logarithmic square difference is set per depth [ $\mu\text{m}^{-1}$ ].

## Relative Linear Square Difference

The formula for the relative linear square difference for the experiment profile curve  $fe$  and the simulated profile curve  $fs$  is:

$$\int_{xmin}^{xmax} (fe(x) - fs(x))^2 dx \quad (2)$$

where the borders of integration  $xmin$  and  $xmax$  are the lower and upper limits of the profile curve comparison, respectively. The relative linear square difference is set per depth [ $\mu\text{m}^{-1}$ ].

## Arithmetic Mean of Relative Error

The formula for the arithmetic mean of the relative error for the experiment profile curve  $fe$  and the simulated profile curve  $fs$  is:

$$\frac{\int_{xmin}^{xmax} P(x) \left| \frac{fe(x) - fs(x)}{fe(x)} \right| dx}{\int_{xmin}^{xmax} P(x) dx} \quad (3)$$

where the borders of integration  $xmin$  and  $xmax$  are the lower and upper limits of the profile curve comparison, respectively. For each measurement point,  $P(x)$  results in 1, or else in 0.

## Quadratic Mean of Relative Error

The formula for the quadratic mean (or root-mean-square) of the relative error for the experiment profile curve  $fe$  and the simulated profile curve  $fs$  is:

$$\sqrt{\frac{\int_{xmin}^{xmax} P(x) \left| \frac{fe(x) - fs(x)}{fe(x)} \right|^2 dx}{\int_{xmin}^{xmax} P(x) dx}} \quad (4)$$

where the borders of integration  $xmin$  and  $xmax$  are the lower and upper limits of the profile curve comparison, respectively. For each measurement point,  $P(x)$  results in 1, or else in 0.

### **3: Calibration Library, Process Searches, and Profiles**

Profiles