Calibration Kit User Guide

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About This Guide

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.

For additional information, see:

- 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 SolvNetPlus support site (see Accessing SolvNetPlus on page 6)
- Documentation available on the SolvNetPlus support site

Conventions

The following conventions are used in Synopsys documentation.

Convention	Description
Bold text	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.
Italicized text	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.
Menu > **Command**	Indicates a menu command, for example, **File** > **New** (from the **File** menu, choose **New**).

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- support-tcad-kr@synopsys.com from Korea
- support-tcad-jp@synopsys.com from Japan

1

Introduction to the Calibration Kit

This chapter presents an overview of the Calibration Kit.

Functionality of the Calibration Kit

The Calibration Kit extends the functionality of Sentaurus Workbench, with which you can 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 calibration viewers and wizards. The **Calibration** menu of Sentaurus Workbench also includes wizards for manipulating simulation flows and generating reports (see Chapter 2 on page 15).

Using calibration libraries containing secondary ion mass spectrometry (SIMS) data and sheet resistance data, the Calibration Kit provides a fast and accurate 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 Optimizer tool, which is integrated in Sentaurus Workbench Advanced, can be used for the automatic analysis and optimization of process and calibration parameters.

In addition to the analytic extraction in the process simulators, Sentaurus Device can be integrated for electrical parameter extraction.

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, and simulator calibration files such as Advanced Calibration are used as input to the Calibration Kit.

Calibration Libraries

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 Experiment Database: Calibration Library on page 35).

In general, process recipes use the Sentaurus Process syntax, with specific restrictions for the Calibration Kit (see Restrictions on Sentaurus Process Syntax on page 35). The `experiments` directory can contain SIMS profiles and spreading resistance profiles.

Process Directory

In the `processes_*` directory, each process file contains a recipe for wafer processing and a reference to the corresponding SIMS measurements. By default, these recipes are written in Sentaurus Process syntax. In this case, the directory is called `processes_sp`.

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 copying the recipes and by extending the pure recipes with simulation models. For Sentaurus Process, calibration parameters and models are sourced before a process recipe is applied.

In the process files, SIMS measurements are represented by `insert` statements. The `insert` statement is translated to the Calibration Kit–specific `SetPltList` statement for Sentaurus Process. Each `SetPltList` statement specifies the measured chemical dopant species and the file name of the SIMS profile. 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 process flows change to `b@node@_fps.cmd`, where `@node@` is the number of a project node of Sentaurus Workbench. See Structure of Calibration Kit Projects on page 11.

Experiment Directory

The `experiments` directory 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 [cm^{-3}]. File names match the names specified in the `1D` commands of the recipe files.

In a Sentaurus Workbench project generated by the Calibration Kit, SIMS profiles are named `b@node@_[profile].plx`, where `@node@` is the number of a project node of Sentaurus Workbench. See Structure of Calibration Kit Projects on page 11.

Preference Directory

The `preferences` directory 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 [cm^{-3}] and maximal concentration [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. See Structure of Calibration Kit Projects on page 11.

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_2022.03.fps` and `calib_1d_2022.03.fps`.

The file `AdvCal_2022.03.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_2022.03.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_2022.03.fps` file are explained in the *Advanced Calibration for Process Simulation User Guide*, which can be accessed from Sentaurus Workbench (choose **Help** > **Manuals**).

The file `calib_1d_2022.03.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_2022.03.fps` file create a 1D mesh and source the file `AdvCal_2022.03.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_2022.03.fps` and `calib_KMC_2022.03.fps`.

The file `AdvCal_KMC_2022.03.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_2022.03.fps` file in the directory `$STROOT/tcad/$STRELEASE/lib/sprocess/TclLib/AdvCal`.

The file `calib_KMC_2022.03.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

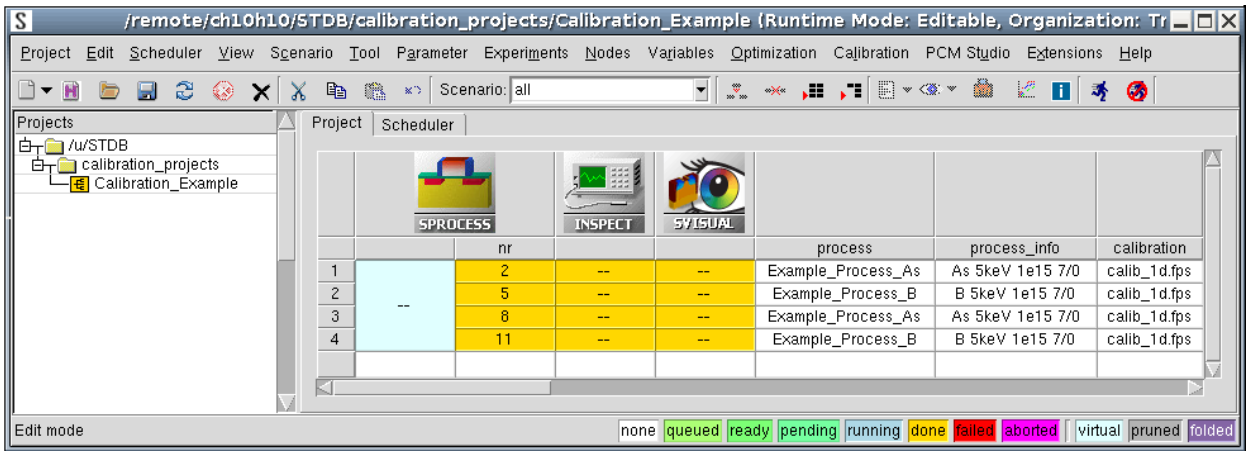
The last lines of the `calib_KMC_2022.03.fps` file create the simulation cell, select the atomistic mode, and source the file `AdvCal_KMC_2022.03.fps`, which contains the physical models.

Structure of Calibration Kit Projects

A Calibration Kit project is a special type of Sentaurus Workbench project with either three or four tools, and one to seven parameters. Both traditional and hierarchical project organizations are supported. 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 Device tool instance can be used for device simulation. The Inspect tool instance for curve comparison 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



The nr parameter of Sentaurus 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 Sentaurus Process. In general, files starting with b@nr@_* belong to the experiment of the parameter value @nr@.

The Calibration Kit uses different Sentaurus 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 Sentaurus Workbench project as a Calibration Kit project, an empty hidden file .fabpackage is included in the project directory. You can use the greadme.txt file (choose **Project** > **Readme**) to collect project information.

Sentaurus Process

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

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

The output of the Sentaurus 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 Sentaurus Process tool instance defines the variables process, process_info, calibration, n_profile, and profile_@integer@. Sentaurus Process can also have a second parameter (see Creating a New Parameterized Project on page 23).

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 atomistic information using the following command:

```
kmc extract tdrWrite
```

Sentaurus Device (Optional)

The Sentaurus Device PMI `sheetresistance` is used for sheet resistance calculation. In this approach, Sentaurus Device solves the Poisson equation or the complete set of drift-diffusion equations by using the doping profile from Sentaurus Process as input.

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`.

The Sentaurus Workbench variable `Rs_sim` stores the results of the sheet resistance calculations. You can compare the extracted value with experimental data for some experiments. The variable `Rs_exp`, which Sentaurus Process defines, retains the measured value or is set to zero if no measurement value is present.

Inspect

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

Different methodologies are available for this curve comparison (see Comparing Profile Curves on page 40). The variables `cv_delta_@integer@`, where `integer` is equal to `1`, `2`, `3`, …, `10`, hold the extracted curve difference per µm for `profile_@integer@`.

You can view 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 32.

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 33.

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Working With Calibration Kit Projects

This chapter describes how to work with Calibration Kit projects.

Manipulating Calibration Kit Projects

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

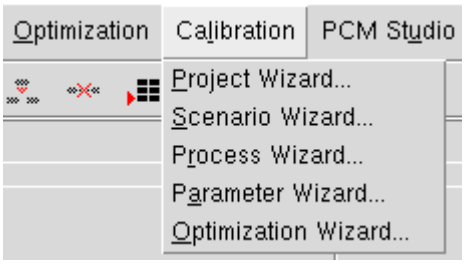
It is faster and more thorough to manipulate projects using these wizards rather than the standard features of Sentaurus Workbench. The wizards are available from the **Calibration** menu of Sentaurus Workbench.

Note:

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

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

Figure 2 Wizards available from the Calibration menu



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 adding a new scenario.

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

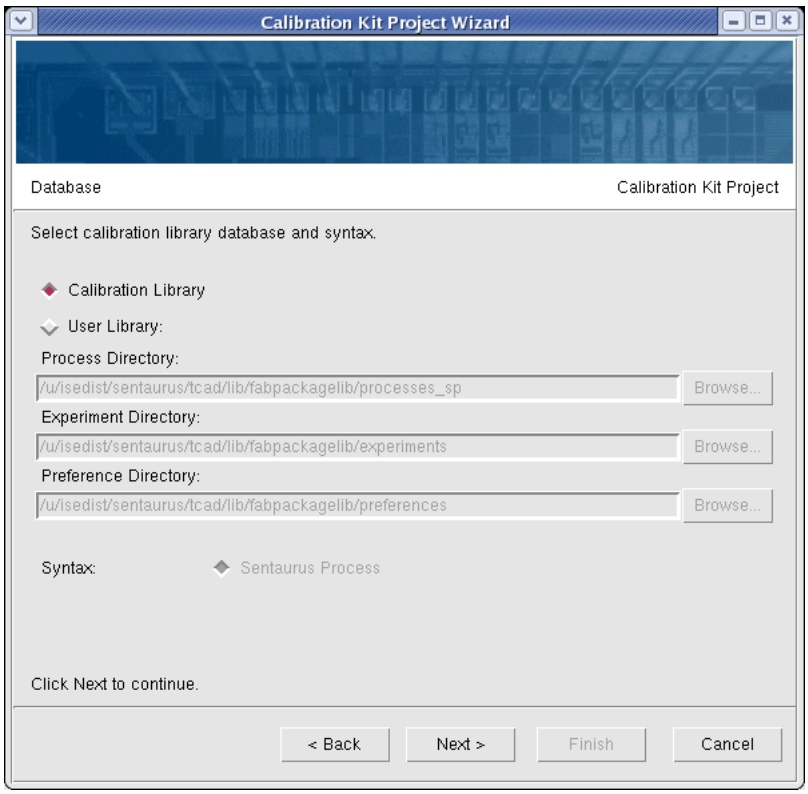
1. Choose **Calibration** > **Project Wizard**.

   The Project Wizard opens.

2. Click **Next** to start.

3. Select the calibration library database from the following options:

   - **Calibration Library** is the default experiment database of the Calibration Kit.
   - **User Library** is a user-specified database in Sentaurus Process syntax. If you select this option, you must specify the process, experiment, and preference directories.



4. Click **Next**.

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

   - Enter a search pattern in the **Process Search Pattern** box to look for processes using the Database Process Search (DBPS) module in the selected database and syntax (Step 3).

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

Click **Search** to write the results to the selected process list file (see Database Process Search on page 37).

- Click **Browse** 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 36.)

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

6. Click **Next**.
7. Select the Sentaurus Process model and calibration from the following options:
   - Select an implantation model and a diffusion model.
   - Select the parameters of either **Advanced Calibration** or **User Calibration**. If you select **User Calibration**, then select up to two calibration files in the Alagator (Tcl) syntax of Sentaurus Process, which usually follow the naming scheme `*.fps`.
8. Click **Next**.
9. Select the device simulation to calculate the sheet resistance from the following options:
   - **Device Simulation Disabled** (default)
   - **Device Simulation Enabled**: If you select this option, then the Sentaurus Device tool instance is part of the project. Click **Browse** 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**.
11. Select the methodology for the simulation and the experiment profile comparison.

    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 **Noise Filter** options are deactivated by default. Select to activate the noise filter (spline-based curve-smoothing) for **Experiment Data**, **Simulation Data**, or both.

    Select the visualization tool. **Sentaurus Visual** is the default.
12. Click **Next**.

13. Select a project and scenario name in one of the following ways:
    - Enter the scenario name, and select **Create New Project** for a new project.

      Click **Browse** to select a project directory, or enter the project name.
    - Enter the scenario name, and select **Add to Project** to add a new scenario to an existing project.

      Click **Browse** to select a project directory.

      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, then click **OK** in the Progress dialog box.

The generated project has the structure described in Structure of Calibration Kit Projects on page 11. 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 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 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 Sentaurus Process, `sheetresistance` is one of the following:

```
## sheetresistance "VALUE"

## sheetresistance "Rs=VALUE"
```

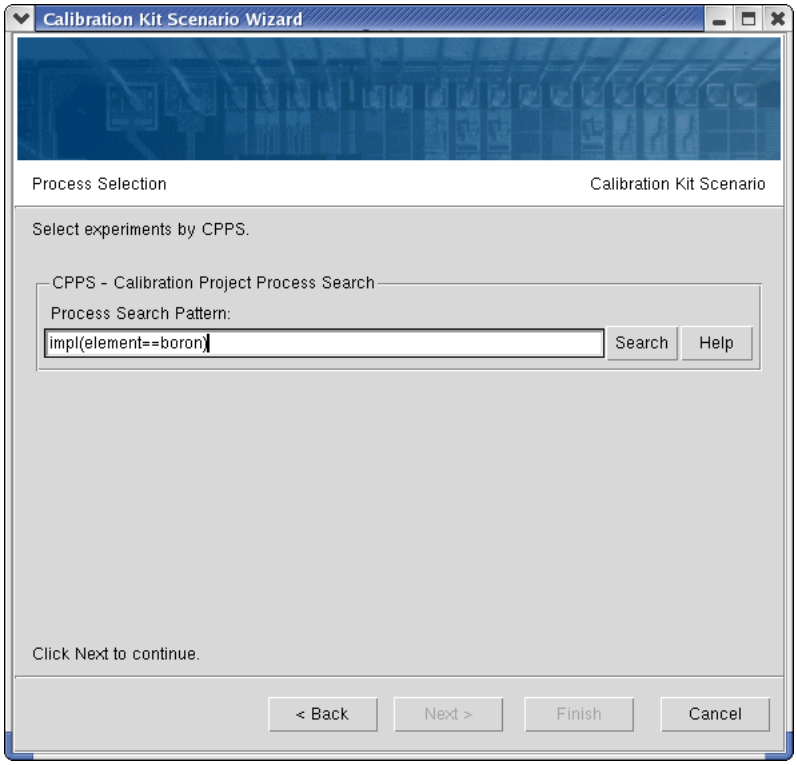
Creating a New Scenario for a Project

To focus on a specific selection of experiments for a Calibration Kit project, you can split a project into scenarios. For example, you can split a project 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.
4. Enter a search pattern in the **Process Search Pattern** box to select experiments, and click **Search** (see Calibration Project Process Search on page 38).



5. Click **Next**.
6. Enter the name of the new scenario in the **Scenario Name** box.
7. Click **Finish**.
8. If the scenario is created and loaded successfully, then 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 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:

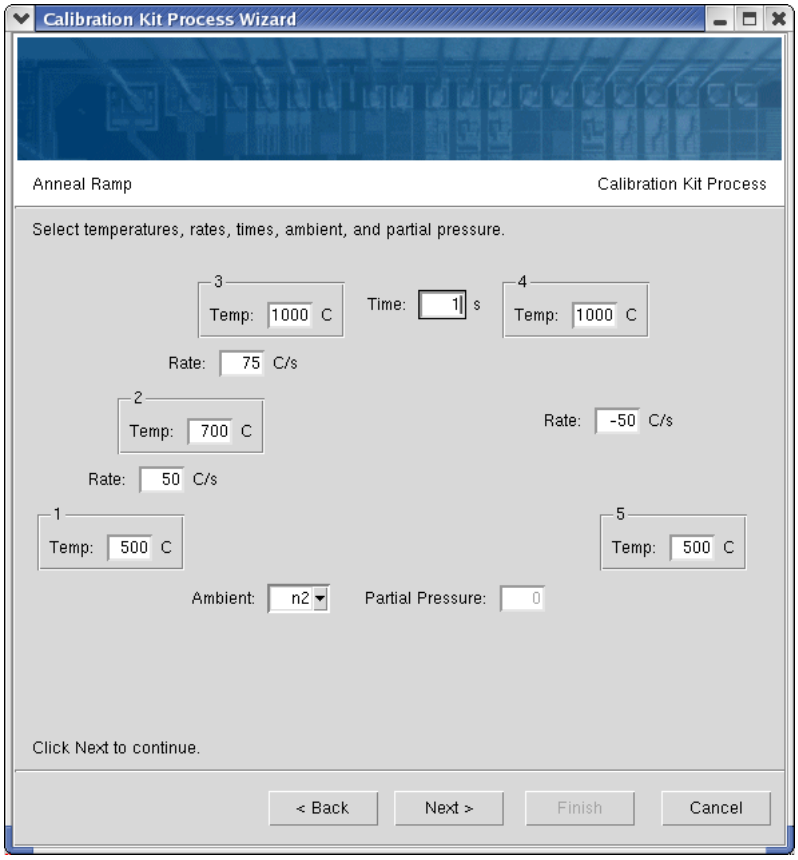
1. Open a Calibration Kit project.
2. Choose **Calibration** > **Process Wizard**.

   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**, then the corresponding implantation step is omitted.
7. Click **Next**.
8. Select the anneal ramp properties.

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



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:
    - Enter the name of a process in the **Name** box.
    - Click **Edit** to edit the flow in Sentaurus Process syntax if required.

      The flow loads into a text editor.

      If needed, you can further modify the flow beyond the guidelines of the previous steps.

      When you click **Edit**, the current values of the process steps defined earlier are considered. Further changes to the process in the previous steps no longer affect the flow, unless you click **Edit** again.

      If you click **Edit** again, then the current values of the process steps defined in the previous steps are reconsidered, and the previous changes to 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 **Add to Project** 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 **Add to User Library** 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, then click **OK** in the Progress dialog box.

If the process recipe is added to a database, it is stored in the same format as those in the calibration libraries (see Process File Syntax on page 35). The process flow includes the correlated profile and `process_info` information.

If the experiment is added to a project, it has the same structure as 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.

Note:

If you edit the process flow further after it is generated, then 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`).
   b. Select to either **Include** or **Exclude** the experiment data.

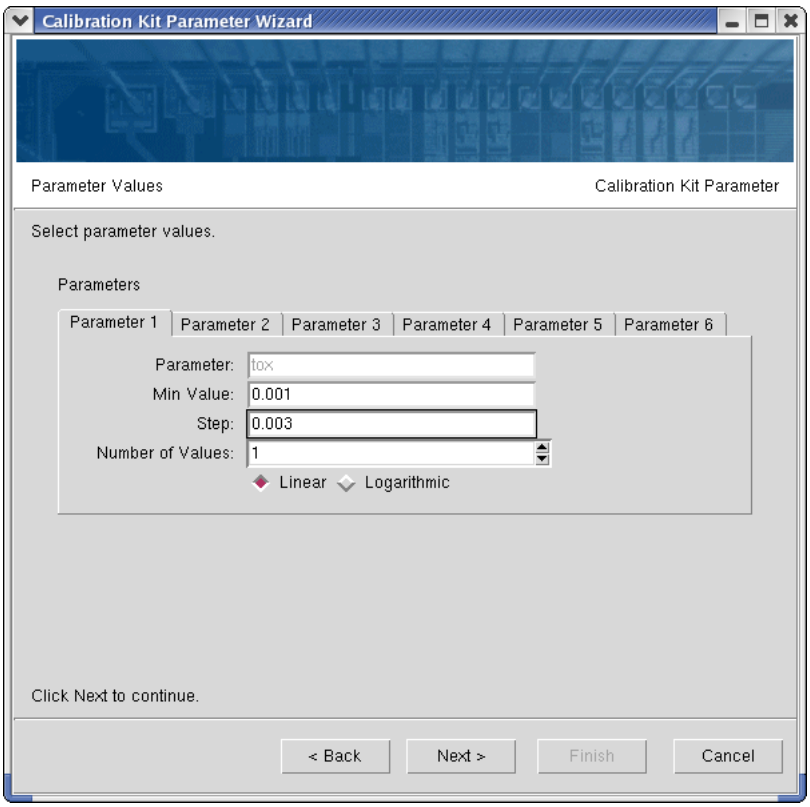
      If you include experiment data, the experiments of the resulting project contain the experiment profiles (SIMS) of the selected experiment.
   c. Click **Edit** to load the flow into an editor.

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

      ```
      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 you select **Linear**, then the difference between values is equal to the iteration step.

      If you select **Log**, then 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:
   - Select an implantation model and a diffusion model.
   - Select the parameters of either **Advanced Calibration** or **User Calibration**. If you select **User Calibration**, then 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 the following options:
    - **Device Simulation Disabled** (default)
    - **Device Simulation Enabled**: If you select this option, the Sentaurus Device tool instance is part of the project. Click **Browse** 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.

    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 **Noise Filter** options are deactivated by default. Select to activate the noise filter (spline-based curve-smoothing) for **Experiment Data**, **Simulation Data**, or both.

    Select the visualization tool. **Sentaurus Visual** is the default.
15. Click **Next**.
16. Select a project and scenario name:
    a. Enter a scenario name.
    b. Click **Browse** to select a project directory, or enter the project name.
17. Click **Finish**.
18. If the project is created and loaded successfully, then click **OK** in the Progress dialog box.

If no Optimizer task is selected (**Task Type** is **None**), then the new project has the structure of a Calibration Kit project with two to seven parameters: the `nr` parameter 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: the `nr` parameter 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.

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 the following options:

   - **Calibration Library** is the default experiment database of the Calibration Kit.
   - **User Library** is a user-specified database in Sentaurus Process syntax. If you select this option, you must specify the process, experiment, and preference directories.

4. Click **Next**.

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

   - Enter a search pattern in the **Process Search Pattern** box to look for processes using the DBPS in the selected database and syntax (Step 3).

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

Click **Search** to write the results to the selected process list file (see Database Process Search on page 37).

- Click **Browse** 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 36.)

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

6. Click **Next**.
7. Select the Sentaurus Process model and calibration from the following options:
   - Select an implantation model and a diffusion model.
   - Select the parameters of either **Advanced Calibration** or **User Calibration**. If you select **User Calibration**, select up to two calibration files in the Alagator (Tcl) syntax of Sentaurus Process, which usually follow the naming scheme `*.fps`.
8. Click **Next**.
9. Parameterize the selected calibration file by entering the values of the fields for the parameters:
   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 **Linear** or **Logarithmic**.
   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 is preprocessed by Sentaurus Workbench as well.)

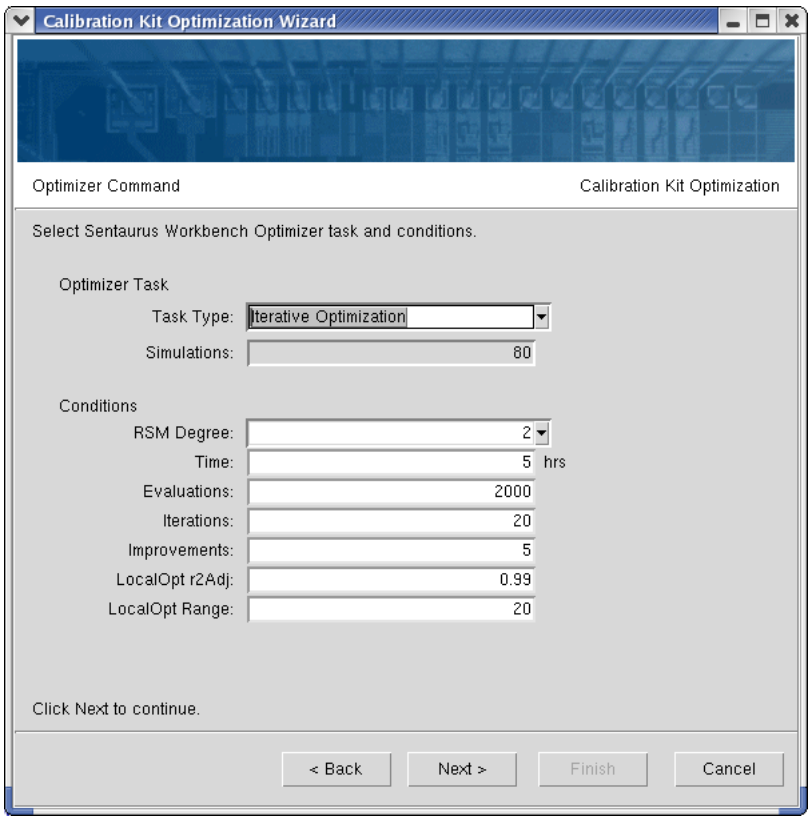
      Save the file.

   Note:
   For Sentaurus Process, only the second selected calibration file can be parameterized.

10. Click **Next**.
11. Select an Optimizer task and the corresponding task conditions, if required, from the following options:
    - **None**: If you select this option, no Optimizer task is used, but you must select the number of different parameter values for each parameter.
    - **Sentaurus PCM Studio**: If you select this option, 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.



12. Click **Next**.
13. Select the device simulation to calculate the sheet resistance from the following options:
    - **Device Simulation Disabled** (default)
    - **Device Simulation Enabled**: If you select this option, then the Sentaurus Device tool instance is part of the project. Click **Browse** 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.

14. Click **Next**.
15. Select the methodology for the simulation and the experiment profile comparison.

    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 **Noise Filter** options are deactivated by default. Select to activate the noise filter (spline-based curve-smoothing) for **Experiment Data**, **Simulation Data**, or both.

    Select the visualization tool. **Sentaurus Visual** is the default.
16. Click **Next**.
17. Select a project and scenario name:
    a. Enter a scenario name.
    b. Click **Browse** to select a project directory, or enter the project name.
18. Click **Finish**.
19. If the project is created and loaded successfully, then click **OK** in the Progress dialog box.

If no Optimizer task is selected (**Task Type** is **None**), the new project has the structure of a Calibration Kit project with two to seven parameters: the `nr` parameter 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 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: the `nr` parameter 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 the Optimizer tool. The corresponding command file of Optimizer is included in the project.

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`).

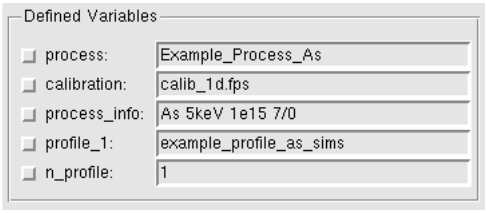
2. Edit the variable values in one of the following ways:

   - Choose **Nodes** > **Set Variable Value**.

     In the Add Variable to Node dialog box, enter the name and the value of the variable, and click **OK**.

   - Choose **Nodes** > **Edit Properties**.

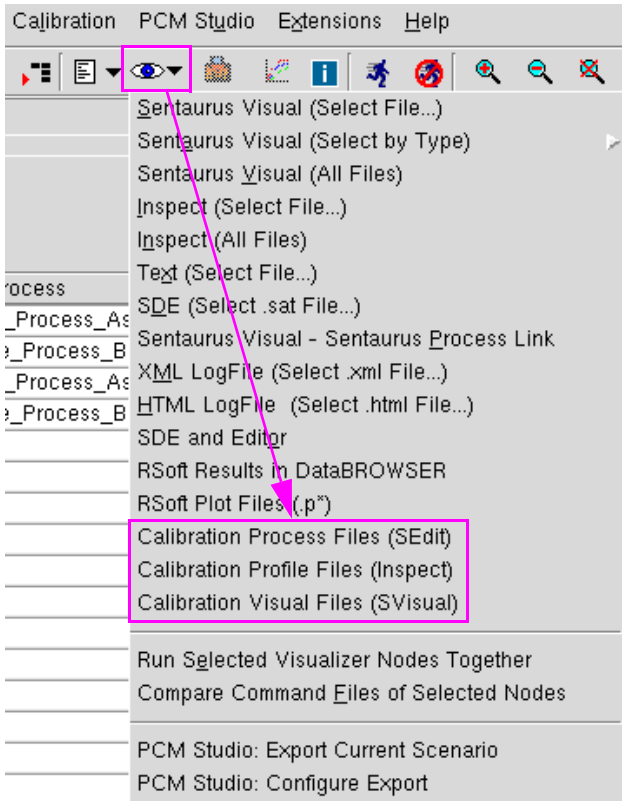
     In the Node information dialog box, edit the definition of the variable (as shown in the following example), and click **OK**.



Visualizing Project Files

Each Calibration Kit project has dedicated viewers that are defined in the project tool database (`gtooldb.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.

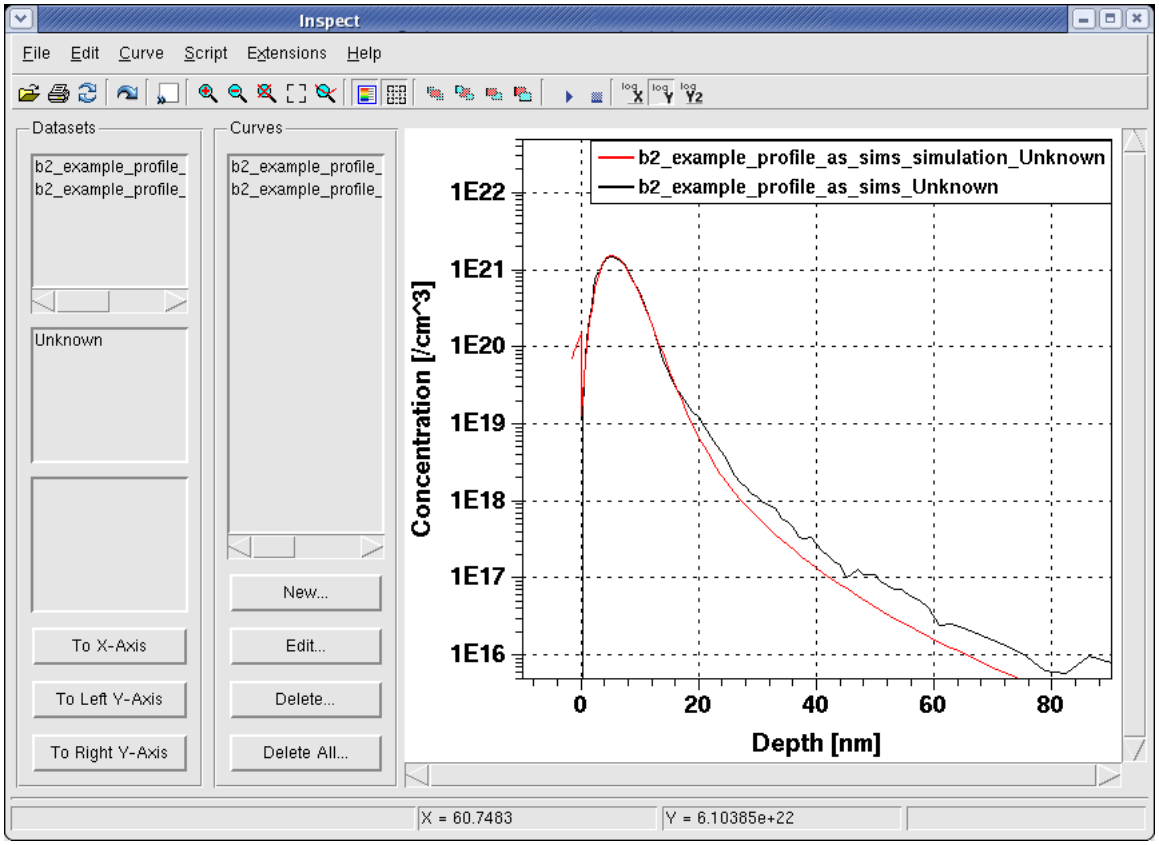
Viewing Profile Files

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 the Inspect tool. 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 the Inspect tool



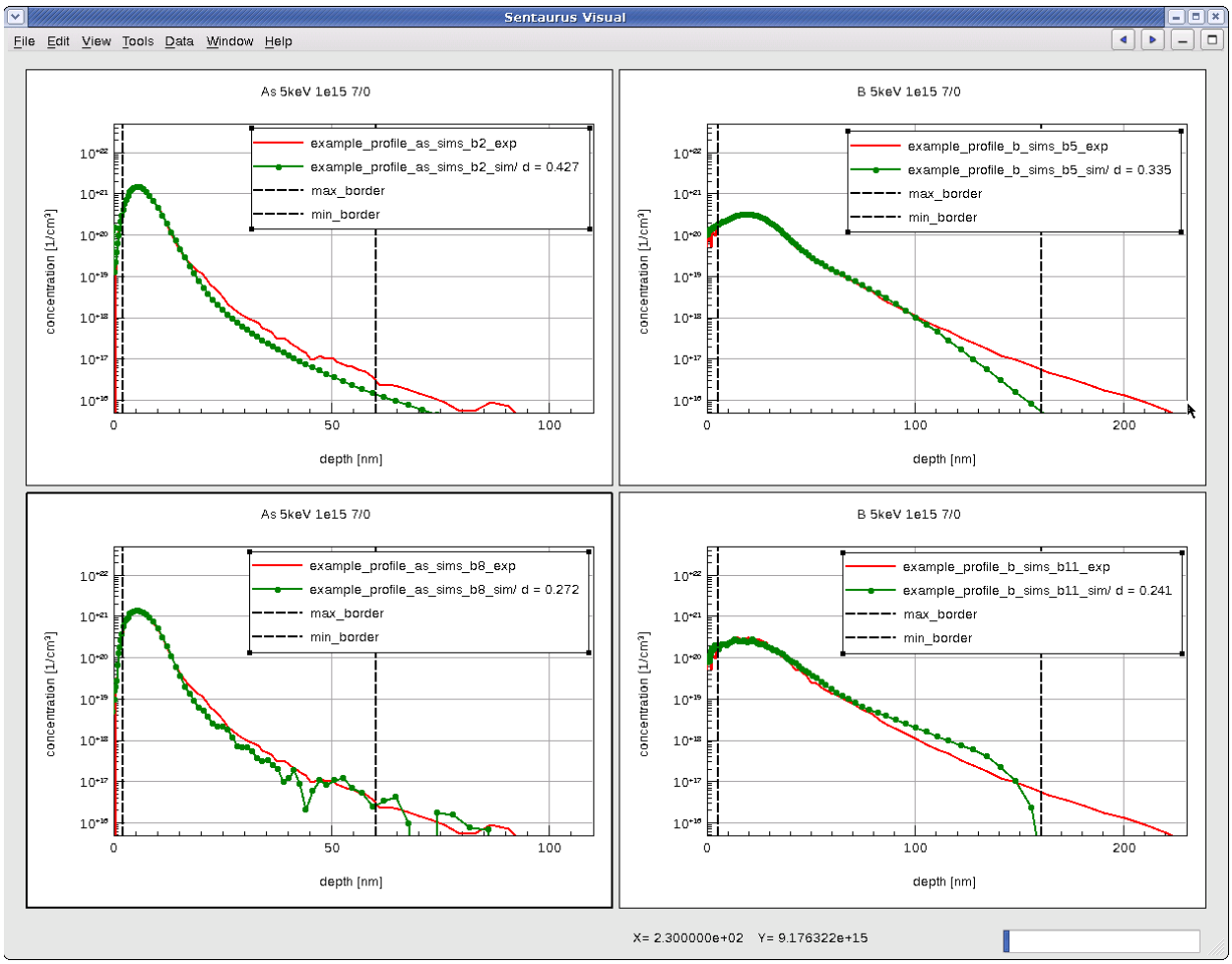
Viewing Visualization Files

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*.

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, Scenario, and Optimization wizards. 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 and Optimization wizards is displayed. If the file is empty or does not exist, no confidentiality warning is displayed.

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

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

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

- The process directory `processes_sp` contains the process files in Sentaurus Process syntax.
- The `experiments` directory contains the SIMS profile files in xy plot format.
- The `preferences` directory contains the preference files (see Profiles on page 40).

Process File Syntax

In general, the Calibration Kit uses databases of process recipes in Sentaurus Process syntax as input. For the Calibration Library and other user databases to be input to the Calibration Kit, Sentaurus Process syntax is subject to restrictions.

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_2022.03.fps` or `calib_KMC_2022.03.fps` places these statements in the input files of Sentaurus Process).

The 1D measurement statement is specified by the `SetPltList` statement, which is defined in `calib_1d_2022.03.fps` or `calib_KMC_2022.03.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 a 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 a comment.

Process Searches

The Quick Process Search (QPS) module 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. The syntax is:

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

Database Process Search

The DBPS module looks for process flows written in Sentaurus Process syntax in a directory (such as `$STCALIB/processes_*`). Processes that match the search criterion are listed in the process list file.

The search criterion is the process search pattern, which consists of *conditions* connected by logical *operators* `&&`, `||`, `!`, and grouped by parentheses. The operator `&&` means *and*, `||` means *or*, and `!` means *not*. 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 DBPS process flow keywords and syntax allowed in DBPS criterion

Keyword	Description	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`
		`peaktime` (time at maximum temperature)
		`pn2` (partial pressure for N_2)
		`po2` (partial pressure for O_2)
		`ph2o` (partial pressure for H_2O)
			`diff(maxT==1000)`
			`diff(totaltime>5)`
			`diff(peaktime!=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`

Table 1 DBPS process flow keywords and syntax allowed in DBPS criterion (Continued)

Keyword	Description	Argument	Example
`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 CPPS module looks for experiments in a calibration project of Sentaurus Workbench. It scans process flows written in Sentaurus Process syntax in the same way as DBPS. However, CPPS scans variables of Sentaurus Workbench. Experiments that match the search criterion are listed in the process list file.

The search criterion is the process search pattern, which consists of *conditions* connected by logical *operators* `&&`, `||`, `!`, and grouped by parentheses. The operator `&&` means *and*, `||` means *or*, and `!` means *not*. 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 DBPS process flow keywords and syntax allowed in CPPS criterion

Keyword	Description	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)`

Table 2 DBPS process flow keywords and syntax allowed in CPPS criterion (Continued)

Keyword	Description	Argument	Example

`diff()`	Diffusion statement scan, true if (1)	`maxT` (maximum temperature)
		`totaltime`
		`peaktime` (time at maximum temperature)
		`pn2` (partial pressure for N_2)
		`po2` (partial pressure for O_2)
		`ph2o` (partial pressure for H_2O)
			`diff(maxT==1000)`
			`diff(totaltime>5)`
			`diff(peaktime!=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 Sentaurus Workbench keyword and syntax allowed in CPPS criterion

Keyword	Description	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)`

Profiles

This section discusses different aspects of profiles.

Visualizing Profiles

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

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

The concentration [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. The visualization tool evaluates a limit if the corresponding limit is not present in the preference file.

Comparing Profile Curves

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

You can set the quality limits of each profile 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 [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`. The default for `sims_ymax` is `1e23`.

Note:

If several profile pairs are visualized in one plot, then 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:

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

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 [μm^{-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:

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

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 [μm^{-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:

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

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:

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

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.