# A User's Perspective on Simulator Calibration

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One of the most difficult yet important aspects of TCAD simulation is proper calibration. The difficulty arises from the large number of variables that can be adjusted. In this article, some basic guidelines will be presented for obtaining better agreement between simulation and measurements. Historical note: it was Carnegie Mellon University that first advocated the tuning of simulators, an idea which has recently gained more acceptance.

There are two main points to realize when calibrating simulators:

(1) the source of the discrepancy may be in the measurement

(2) many discrepancies can be resolved by proper understanding of the limitations of the simulators. In particular, the grid, boundary conditions, and the various models, all of which are user-selectable, can have a dramatic impact on the simulation results. In addition, the simulation user should know which of the default coefficients are least well known by the TCAD community so that intelligent choices can be made during a calibration.

## Measurement Errors

When there is disagreement between simulation and measurements, it is generally assumed that the simulation is in error. It is more fair (and scientific) to consider that the difference may be due to measurement error. A further refinement would be to divide the error equally between the simulator, the measurement, and "operator error".

There is uncertainty associated with every measurement, and this must be considered during calibration. Even in the absence of error, it is important to understand what is being measured. For example, spreading resistance profiles (SRP) typically measure the electrical, and not the chemical, doping concentrations. For lightly doped material, the SRP junction can easily be several tenths of a micron shallower than the SIMS result. Commercial versions of SUPREM-3 and SUPREM-4 provide the ability to calculate both types of profiles (Figure 1). SRP measurement providers have techniques for correcting for this, but the simulation user should carefully investigate these before changing a default diffusion coefficient or assuming the simulator is wrong. A less well known problem can occur during SIMS profiling. A heavy or high energy primary ion can knock-on the dopant atoms, resulting in a false tail or a reduced peak in the dopant profile.

A simulation typically provides a single result, whereas measurements produce a range of results. A simulated oxide thickness should be compared to the range of measured oxide thicknesses, not to the "spec" or to a single measurement. A range of results can be obtained through a series of simulations by slightly varying time, temperature and pressure using DOE/RSM tools.

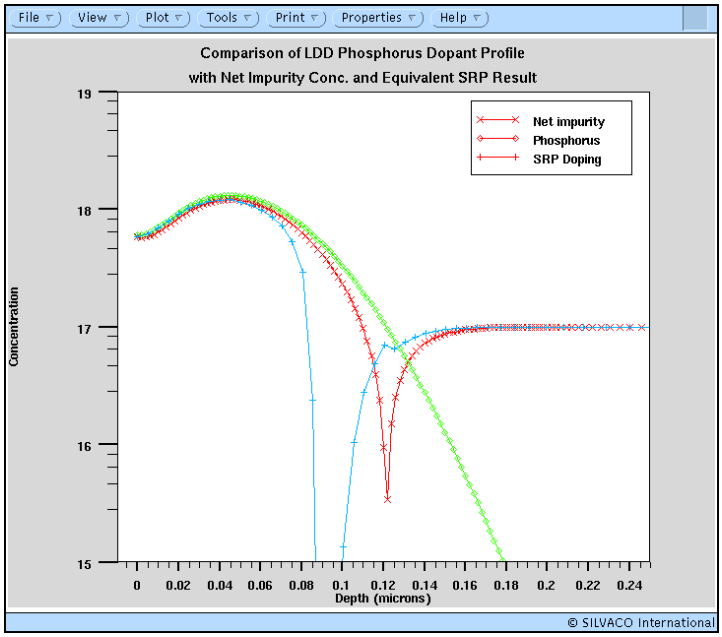


Figure 1. Comparison of SRP results to net doping. Process simulators are able to account for the differences.

## Grid Selection

The second major point is the importance of grid, boundary conditions, model selection, and model coefficients on the results. It is well known that simulation results are grid dependent, but this is often overlooked. Even in 1D mode, where there are few CPU limitations to using dense grid, simulation results may suffer from insufficient grid density in key areas. The most likely place for this to occur is in a gate oxide, where there may be only one or two grid points within the oxide. Meanwhile, the TCAD user is trying to accurately simulate the diffusion of the gate dopant through this oxide layer. In early versions of SUPREM-4, the amount of dopant implanted into a layer was extremely sensitive to the grid density. The integrated dopant concentration in the simulation could be significantly higher or lower than the implanted dose. Although enhancements to SUPREM-4 have removed the earlier problems, it is a good idea to monitor the integrated doses

throughout a process simulation and to note when sudden changes occur. This is both a check of the simulation and provides insight into the process flow. Grid choice is equally important in device simulators. A lot of progress has been made in griding, with the availability of graphical grid editors that produce grids with no obtuse triangles. Even with this capability, simulations should be run with several different grids to test the sensitivity of the results. When changes in the grid produce only small changes in the simulation results, your grid is probably fine enough. Grid density should be highest where the quantity of interest is changing rapidly (e.g., bipolar base regions and MOSFET inversion layers).

## Boundary Conditions

Improper boundary conditions are usually the result of making the simulation structure too small. This often occurs in process simulation. The reflecting boundary condition at the bottom surface causes any dopant that diffuses to the bottom to be reflected back towards the surface. In SUPREM-4, the same is true for point defects, and these can diffuse many microns into the substrate. Consequently, SUPREM-4 structures should be much deeper than any junction depth, and the final profile of the point defects should be checked to see that the point defects have not diffused to the bottom of the structure (see Figure 2 for an example).

Improper boundary conditions occur in device simulation as well. Check that the depletion layer does not extend to the bottom or far side of the simulation structure. If this occurs, the depletion layer spreading is being artificially constrained by the problem definition, and you are trying to solve a different problem that what you intended (and the simulator may not like it). In PISCES, there is an assumption that the normal component of the electric field along the edges of the simulation structure is zero. This can be restated as the potential contours are perpendicular to the edges. If the potential contours bend near the edges, make the structure wider.

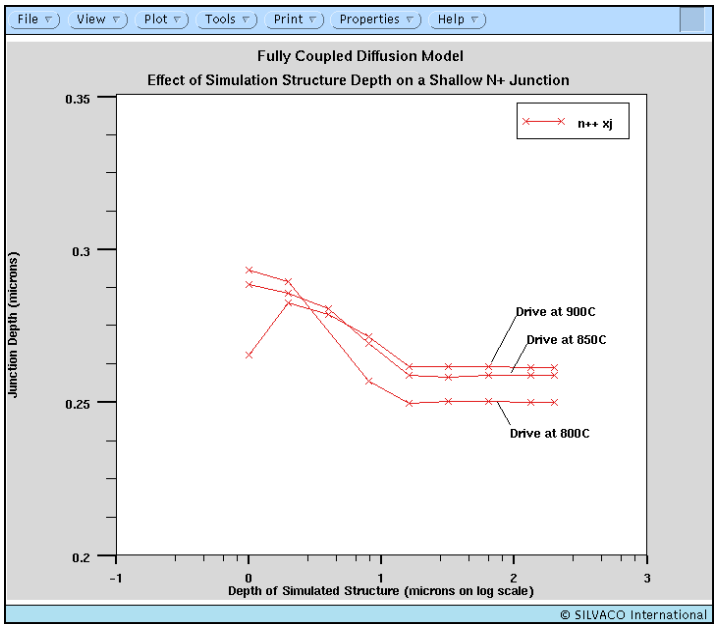


Figure 2. Example of errors possible in process simulations using point defect diffusion models. For this process a simulation must be >30 microns to give a consistent junction depth for a heavy arsenic implant.

## Model Selection

Model selection is as important as any other factor in obtaining good results. This requires knowledge of each model and its limitations. The default model is often a simple one. In some versions of SUPREM-4, oxidation enhanced diffusion is not simulated with the default diffusion model. The default oxidation model may not be suitable for trench or poly oxidations. In device simulators, the default lifetime values are likely to need adjustment for your process. Also, a mobility model must be chosen that accounts for surface field reduction for reasonable MOSFET results. It is important to know the range of validity of each model as well. A particular mobility model may not be valid in the doping range of interest. This is a complex subject, and a good opportunity to consult with your TCAD applications engineer.

## Tuning Model Coefficients

Some model coefficients are less well known than others, but an engineer tuning a simulator is likely to modify the coefficients they are most familiar with. Diffusion coefficients are fairly well known, although less so for oxidation enhanced diffusion (OED) and transient enhanced diffusion (TED). An engineer may adjust diffusion coefficients to get better agreement between simulated and measured threshold voltages, but it is more likely that the segregation coefficient should be calibrated. The default value may be an average of reported values, whereas you are mainly interested in low temperature values. Check the literature for values that may better apply to your particular situation. It is even more likely that the work-function needs to be calibrated.

## Summary

In brief, begin a calibration with a well characterized process. Check the basic parameters first, being aware of the measurement limitations and knowing the typical range of measured values. Compare large area devices before the small ones. Use the same electrical definitions in the simulations as in the measurements. Understand your model selection and any model limitations. Remember to modify the grid and structure size. Try to adjust as few coefficients as possible, and understand why you have chosen certain parameters to calibrate. An optimizer can be valuable here. Consider whether highly accurate simulations (5%) are worth the extra effort over 10-20% agreement. Finally, consult with your applications engineer. The time invested will be well worth it.