Rational RSM Models for Device Characteristics as Functions of Process Parameters

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ABSTRACT

Conventional polynomial Response Surface Methodology (RSM) fails to provide oscillation-free analytical models for some device data with singularity like subthreshold slope vs threshold adjustment dose, poly gate length vs stepper defocus, etc. New type of RSM model is proposed in form of rational polynomials which are generalization of the conventional polynomials. This approach delivers oscillation-free RSM surfaces and intuitive interpretation of the data.

Keywords: TCAD, RSM, device, process, optimization

INTRODUCTION

Response Surface Methodology (RSM) has been established as a powerful tool in device design [1,2], TCAD tool calibration [3], process performance optimization [4,5], and process manufacturability tuning [6,7]. Basic scenario of using RSM in conjunction with TCAD simulations consists of the following steps:

- choosing process control parameters;
- sampling control parameter space;
- simulating technological process;
- extracting device characteristics;
- choosing and fitting analytical RSM models of device characteristics as functions of process controls;
- finally analyzing/optimizing it.

Accuracy of this technique is limited by the accuracy of the involved TCAD simulations and the accuracy of the RSM model. In line with the increased predictive power of modern TCAD simulators, the requirements on the RSM model quality are toughened. To improve quality of traditional polynomial-based RSM beyond the capabilities of traditional polynomial models, several new methods have been employed involving covariance fit [8], stochastic process realization [9], and neural network representation.

In this work the rational function approximation is proposed to build simple yet robust analytical models for device characteristics.

RATIONAL POLYNOMIAL MODEL

Let D denote a device response (like a threshold voltage or current leakage) and p_i, $i = 1, \dots, n$ be process controls (oxidation time, temperature, etc.) TCAD simulation tools provide functional tabular dependence

$$D = F(p_1, \dots, p_n).$$

Let's approximate this dependence by the following rational function

$$D = \frac{M(p_1, \dots, p_n)}{R(p_1, \dots, p_n)} \qquad (1)$$

where *modulator* M and *resonator* R are polynomials of process parameters. Rational model (1) is a generalization of the conventional RSM model because the polynomial approximation is a special case of (1) when $R \equiv 1$. Model is defined in the multidimensional cubical domain

$$p_{imin} < p_i < p_{imax}, \; i = 1, \dots, n$$

Rational model covers substantially wider range of physical system behaviors than the polynomial model. While the polynomial model assumes absence of weak or strong singularity in the approximated dependence, the rational model takes them to account. This significantly improves global approximation quality because the singularity influence drops slowly with a distance.

Strong resonance $R(p_1, \dots, p_n) = 0$, or real singularity, does not take place inside the functional domain because device physical dependencies are continuous.

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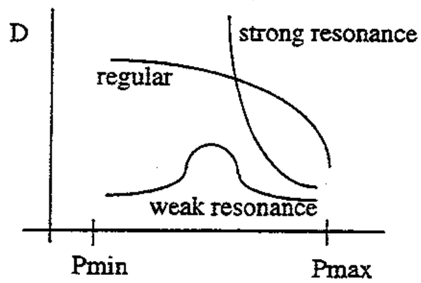

FIGURE 1. Illustration of regular, strong resonance, and weak resonance behaviors.

However, they frequently help to improve approximation characteristics when present outside of the domain boundaries.

Weak resonance points are complex roots of the $R(p_1, \ldots, p_n) = 0$ equation. Very much like summation of δ-function yields unit step function, the combination of weak singularity enable approximation of switching device behavior.

Both strong and weak resonance cases describe an important part of the device response when a device does not react to the parameter variations except for the neighborhoods of isolated parameter values.

Smooth or regular part of the device response is reflected by the numerator in (1), called the modulator. Superimposed on the resonator part of the approximation, it smooths the device dependence.

COEFFICIENT CALCULATION

Given modulator and resonator orders, the task of fitting numerical experiment data with k degrees of freedom can be reduced (by using least square minimization) to solving $M_{df} + R_{df} \equiv d \le k$ nonlinear equations for the polynomial coefficients, where M_{df} and R_{df} are modulator and resonator degrees of freedom. For each experiment point $q = 1, \ldots, Q$ residual N_q of the approximation (1) can be expressed in the form

$$N_q = D_q - \frac{M_q}{1 + R_q}$$

where $M_q = \sum_i a_i M_{iq}$; $R_q = \sum_j b_j R_{jq}$; $i = 1, \ldots, M_{df}$; $j = 1, \ldots, R_{df}$; D_q is device response in q-th experiment; a_i and b_j are polynomial coefficients of modulator and resonator respectively. We have to find a set of coefficients a_i and b_j that minimizes the residual function

$$F(a_1, \ldots, a_{mdf}, b_1, \ldots, b_{rdf}) \equiv \sum_q N_q^2 \to min$$

We use "frozen denominator" iterative procedure for $i = 1, 2, \ldots$ to minimize residual function F:

$$R_q^{(0)} = 0$$

$$\sum_q \left(\frac{D_q + D_q R_q^{(i)} - M_q^{(i)}}{1 + R_q^{(i-1)}} \right)^2 \to min$$

Necessary condition for the minimum

$$\frac{\partial F^{(i)}}{\partial a_p} = 0, p = 1, \ldots, Mdf$$

$$\frac{\partial F^{(i)}}{\partial b_p} = 0, p = 1, \ldots, Rdf$$

yields d linear equations for each step of the iteration:

$$X^{tr} \bar{a}^{(i)} X = X \bar{D}$$

where $\bar{a} = (a_1, \ldots, a_{mdf}, b_1, \ldots, b_{rdf})$ is vector of model coefficients; $\bar{D}$ is vector of device responses; X is $d \times Q$ *design matrix* with elements

$$X_{pq} = \frac{M_{pq}}{1 + R_q^{(i-1)}}, p = 1, \ldots, Mdf$$

$$X_{mdf + p, q} = \frac{(1 + R_{pq})D_q}{1 + R_q^{(i-1)}}, p = 1, \ldots, Rdf$$

$$q = 1, \ldots, Q$$

For each step of the iteration process the linear system of d equations is solved for RSM model coefficients. This process of *simple iterations* converges pretty fast in majority of considered examples. Reasonably high accuracy of the model is usually reached in 4...8 iterations.

Implementation of this algorithm in TMA Work-Bench framework [10] uses three following criteria of the covergence: coefficient of determination R^2, adjusted coefficient of determination $R^2{}_{adj}$, and predictive sum of squares $R^2{}_{press}$.

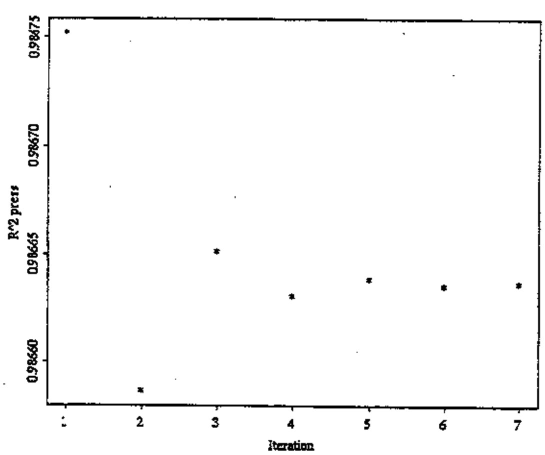

FIGURE 2. $R^2{}_{press}$ vs iteration count for subthreshold slope RSM model.

EXAMPLES

The proposed approach substantially improves RSM model quality for a number of device characteristics with singularity, including:

- subthreshold slope as a function of threshold adjustment dose and LDD dose;
- junction leakage as a function of oxidation time and implant dose.

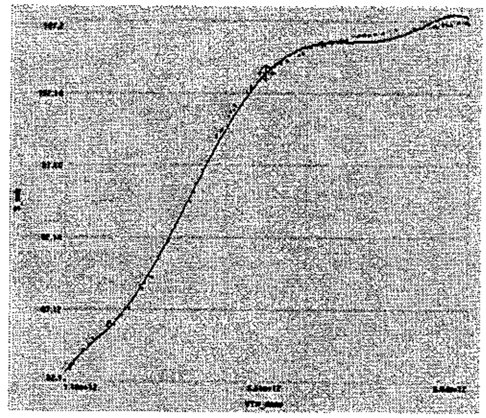

FIGURE 3. Six order polynomial approximation for subthreshold slope vs. threshold adjustment dose exhibits artificial oscillations.

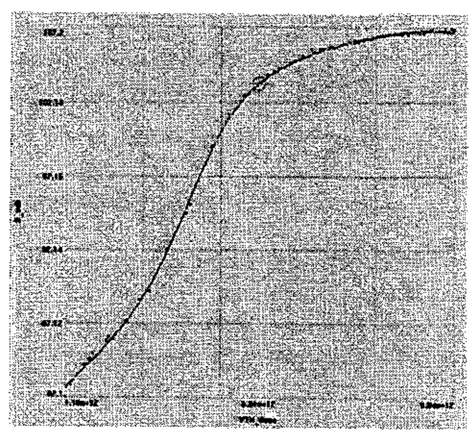

FIGURE 4. Sixth order rational model (second order modulator and forth order resonator) for the same data provides smooth approximation.

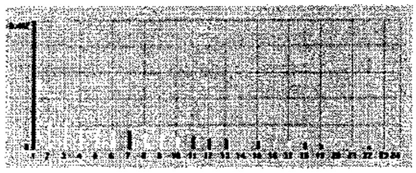

FIGURE 5. A high quality polynomial gate length model has 23 degrees of freedom. The figure displays absolute values of coefficients (model spectrum). Interactive coefficients (shown in white) dominate spectrum.

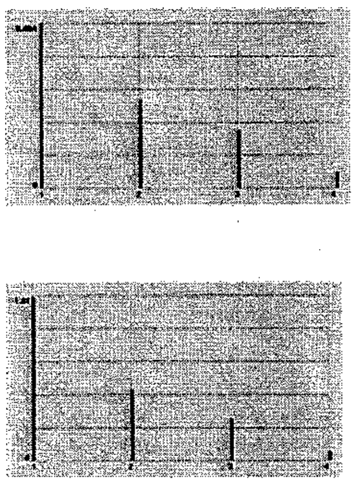

FIGURE 6. Rational gate length model of the same quality has only 6 degrees of freedom. Three bars of the top figure represent numerator coefficients and three bars of the bottom figure represent denominator coefficients. The model does not have any interaction terms.

CONCLUSION

Conventional RSM polynomial models explains three fundamental types of physical system responses: constant, linear, and regular nonlinear. An important type of a resonance (singular nonlinear) response can be explained only by engaging the rational approximation (1). Factorization of the response function on modulator (numerator) and resonator (denominator) delivers oscillation-free smooth RSM surfaces with significantly lower than polynomial model degrees of freedom. This provides an intuitive interpretation of the data and removes artificial extrema in RSM-based optimization.

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