ABSTRACT

Title of document: FULL WAFER MAP RESPONSE SURFACE MODELS FOR COMBINATORIAL CHEMICAL VAPOR DEPOSITION REACTOR OPERATIONS

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A computational toolbox was developed to perform full wafer response surface modeling of combinatorial chemical vapor deposition wafers. It consists of a library of MATLAB object-oriented functions that are based on accurate quadrature methods. The toolbox was tested using three sets of artificially generated wafers. Once the validity of the toolbox was demonstrated, it was used to model tungsten deposition with a Spatially Programmable CVD reactor. As a result, a model of the form $T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_{14}(sqh2s1)(gap) + b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$ was considered the most appropriate fit to the data. This model takes into account the systems kinetics (it uses the square root of the hydrogen flow), the gas flows into each one of the reactor segments and the inter-segment gas diffusivity.

FULL WAFER MAP RESPONSE SURFACE MODELS FOR COMBINATORIAL CHEMICAL VAPOR DEPOSITION REACTOR OPERATIONS

by

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To my family,

for their constant support and love

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Chapter 1

Introduction

Chemical Vapor Deposition (CVD) is a materials-processing technology used for applying layers of non-volatile solids to surfaces through the decomposition of relatively high vapor pressure gases. A CVD process consists of flowing a precursor gas or gases into a deposition chamber that contains the heated object or objects to be coated. The chemical reactions that transform the gases or vapors into the solid material occur on or near the hot surfaces, resulting in the deposition of a thin film. The byproducts of the reactions and the unreacted precursor gases are then removed from the chamber.

CVD methods have been used to deposit the majority of the elements in the periodic table, some in the form of pure elements, but more often combined to form compounds. These wide variety of applications has allowed the use of CVD techniques in many different fields. For instance, chemical vapor deposition is utilized in different stages of the production of semiconductors. This process can be used to deposit thin films of the active material (e.g. silicon), the conductive interconnects (e.g. tungsten), and the insulating dielectrics (e.g. SiO_2). CVD is also widely used in the fabrication of fiberoptic cables used in communication networks. Also, more recently, this technology is being used in the production of microelectromechanical structures (MEMS).[8]

Typically chemical vapor deposition has been used because of its conformality (i.e. the ability to uniformly coat a topographycally complex substrate surface); however, in some cases a spatially non-uniform distribution may be desired (e.g. single wafer combinatorial processing used to deposit a film with properties that vary according to the location). An intentionally (and reproducibly) non-uniform film deposition may be obtained through a combinatorial approach.[1]

Joseph Hanak was one of the first to address the combinatorial approach in the 70's by stating that the research process should be capable of "synthesising, analysing, testing and evaluating . . . large parts of multicomponent systems in single steps".[5] However, a "true" combinatorial approach has only been feasible recently with the increase in computing power and the advances in automation, deposition tools and characterization techniques.[15]

Combinatorial CVD is an emerging technology that enables a faster development of new materials. The main objectives of this technology are to intentionally deposit desired non-uniformities across the substrate and to be able to get an accurate model of the system in order to obtain a correlation between processing conditions and desired film qualities.[1]

Not many CVD reactor systems have combinatorial capabilities. However, the existent ones demonstrate the ability to produce films with graded properties over a portion of the wafer's surface. A few combinatorial systems include Gladfelter's [9, 18] CVD reactor design that has three feed tubes in a triangular arrangement across the substrate, Wang's [14, 15, 16] hot-wire CVD system that features a mask and motorized shutter, a cross-flow reactor configuration where separate precursor

inlet nozzles are used presented by Hyett and Parkin [6], and Taylor and Semancik's [12] design that includes microhotplate devices to control the temperature in an array of micro-scale substrate samples.

The drawback of using CVD is that it is generally a much more complex process than, for example, physical vapor deposition (PVD). A CVD system is governed by a variety of fundamental physical and chemical principles such as mass transfer, heat transfer, thermodynamics, and kinetics. Thus, obtaining a physically-based model for the process is practically impossible.

For this reason, a computational toolbox that calculates a response surface model (up to a full second order model) for combinatorial chemical vapor deposition operations was developed. The toolbox consists on object-oriented functions develped in MATLAB for the manipulation, interpretation, and analysis of combinatorial CVD data.

The important concepts of the response surface methodology are reviewed in Chapter 2. Then, the computational toolbox is discussed in Chapter 3 where a summary of the most relevant functions is presented. In Chapter 4 the functionality of the toolbox is tested with artificially generated wafers. After the functions are validated they are applied to the data obtained from a Spatially Programmable Chemical Vapor Depositon reactor. These results are discussed in Chapter 5. Finally, the conclusions, final remarks and suggested future work are presented in Chapter 6.

Chapter 2

Response Surfaces

The Response Surface methodology may be divided in three major steps. The first step involves the design of a series of experiments that will provide adequate and reliable measurements from which information about how the different factors (independent variables) affect the response (dependent variable) can be gathered. The second step consists in finding the "best" fit for the data by performing regression analysis (i.e. least squares method) and the pertinent hypothesis tests on the model's parameters. Finally, the objective of the last step is to find the optimal settings of the experimental factors needed to obtain a desired response.[7]

Least Squares Method

The least squares method finds the parameters for models to fit data by minimizing the sum of the square of the residuals. The residuals are defined as the difference between the observed value for the response and the predicted value obtained using the fitted model. The parameters determined by this method are normally distributed about the true parameter values with the least possible standard deviation. This statement is based upon the assumption that the uncertainties (i.e. errors) in the data are mutually independent in the statistical sense (uncorrelated) and normally distributed with zero mean and common variance.

Linear least squares problems include any model in which the p unknown parameters (β_j) are coefficients of functions of only the independent variables (x_k). In other words, the observed response Y_i is linear in β_j but not necessarily in the independent variables (x_k)

$$Y_i = \sum_{j=1}^{p} \beta_j g_j(x_{i1}, x_{i2}, \ldots, x_{im}) + \epsilon_i$$

where ϵ_i represents the random error in observation i. This can be written in matrix notation as

$$Y = X\beta + \epsilon$$

For example, if the response can be expressed by a second order model in variables x_1 and x_2

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_{11} {x_{i1}}^2 + \beta_{12} x_{i1} x_{i2} + \beta_{22} {x_{i2}}^2 + \epsilon_i$$

In matrix notation

$$Y = X\beta + \epsilon$$

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ . \\ . \\ . \\ Y_n \end{pmatrix} \quad \mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & x_{11}^2 & x_{11}x_{12} & x_{12}^2 \\ 1 & x_{21} & x_{22} & x_{21}^2 & x_{21}x_{22} & x_{22}^2 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ 1 & x_{n1} & x_{n2} & x_{n1}^2 & x_{n1}x_{n2} & x_{n2}^2 \end{pmatrix} \quad \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_{11} \\ \beta_{12} \\ \beta_{22} \end{pmatrix} \quad \epsilon = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ . \\ . \\ . \\ \epsilon_n \end{pmatrix}$$

In cases where the dependent variable Y is a scalar related to the independent variable or variables x_k and the errors in the independent variables are negligible, the function to minimize (i.e. the objective function) is the sum of squares of residuals.

$$SSE = \sum_{i=1}^{n} R_i^2 = \sum_{i=1}^{n} (Y_i - y_i)^2$$

Where

n= number of data points

Y_i= ith measured value of the dependent variable

y_i= ith predicted value of the dependent variable

R_i= ith residual (diference between the measured and predicted variables corresponding to the ith experiment)

It is important to emphasize that neither the measured value Y_i nor the predicted value y_i is exactly equal to the unknown variable of y. However, the least squares method assumes that if a sufficiently large number of measurments of Y_i are made for a single set of independent variables, the average value would approach the true value.

The goal of the least squares method is to find the parameters b_j (estimates of β_j) that minimize the objective function SSE. To accomplish this, the most common procedure is to differentiate SSE with respect to all b_j's and the resulting p expressions are set to zero generating a set of normal equations.In matrix notation the normal equations can be written as

$$X'Xb = X'Y$$

Finally, terms of the b vector (i.e. the unknown parameters b_j) are computed by

$$b = (X'X)^{-1}X'Y$$

provided that the matrix X has full column rank.

Analysis of Variance

The analysis of variance is a technique that divides the total variabily into meaningful components. For instance, the total variation in a set of data, known as the total sum of squares (SST) can be partitioned into two parts; the sum of squares explained by the fitted model (SSR), and the sum of squares unaccounted for by the fitted model (SSE).

$$SST = SSR + SSE$$

The total sum of squares is computed by summing the squares of the deviations of the observed Y_i's about their average $\overline{Y}$.

$$SST = \sum_{i=1}^{n}(Y_i - \overline{Y})^2$$

The degrees of freedom associated to SST are $n-1$, where n is the total number of observations.

The sum of squares explained by the fitted model is known as the sum of squares due to regression (SSR) and it is calculated by adding the squares of the difference between the value predicted by the fitted model and the overall average

Source of Variation	Degrees of Freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	f_0	P-value
Regression (Fitted Model)	p-1	SSR	SSR/(p-1)	MSR/MSE	
Residual (Error)	n-p	SSE	SSE/(n-p)		
Total	n-1	SST			

of the observed values.

$$SSR = \sum_{i=1}^{n} (y_i - \overline{Y})^2$$

The degrees of freedom associated to SSR are $p - 1$, where p is the number of parameters in the fitted model.

The sum of squares unaccounted for by the fitted model is also known as the sum of squares residuals (SSE).

$$SSE = \sum_{i=1}^{n} (Y_i - y_i)^2$$

The degrees of freedom associated to SSE are $n - p$.

This information is usually summarized in a table known as the Analysis of Variance Table or ANOVA Table that also has the value for f_0 and the *P-value* that are measurements of the model adequacy. These values are explained later in the *Model Comparison* section.

Adequacy of the Model

A common criterion to determine the adequacy of a model is the *coefficient of determination* R^2 that gives the proportion of variability in the data set that is

accounted for by the fitted model.

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

If the model is "perfect" the value for R^2 is 1, whereas if it is useless this value will be closer to zero.

Another way to check the adequacy of the model is by performing tests of significance that are discussed in the Model Comparison section.

Test of Hypothesis Concerning Individual Parameters

The estimators b_j are assumed to be normally distributed with mean β_j and variance σ^2_{bj}. The estimates of the variances of the parameters are obtained through the elements of the inverse of the matrix $X'X$ and the model variance σ^2. The diagonal elements of the matrix $[X'X]^{-1}\sigma^2$ estimate the variance of b_j's, and the off-diagonal elements estimate the covariances of the parameters. The value for σ^2 is estimated by

$$\sigma^2 \approx s^2 = \frac{SSE}{(n-p)}$$

Having knowledge of the distribution of the parameters makes it possible to test hypothesis about them. For example, it can be tested whether or not β_j equals a set value β_{jo} using a t-test.

$$t = \frac{b_j - \beta_{jo}}{s_{bj}}$$

where s_{bj} is the estimate of the standard deviation for parameter b_j and is calculated by taking the square root of the variance of b_j.

$$\sigma_{bj} \approx s_{bj} = \sqrt{[X'X]^{-1}_{jj}\sigma^2}$$

If $-t_{\alpha/2,dof} < t < t_{\alpha/2,dof}$ the null hypothesis ($H_0 : b_j = \beta_{jo}$) is accepted, otherwise it is rejected. The value $t_{\alpha/2,dof}$ may be obtained from tables (or computations with an adequate software) and depends on the significance level α (that gives a $100(1-\alpha)\%$ confidence in the test) and the degrees of freedom of the residuals ($dof = n - p$).

The example developed later in this chapter demonstrates how this hypothesis test is carried out.

Model Comparison

More than one model can be fitted to the same set of data and it is important to compare these models in order to determine the one that represents the data most accurately. Different criteria can be used to determine which model is the "best". For instance the decision may be based on which model produces a better R^2. However, R^2 is a weak test and other methods should be used. One if these methods is based on the *F distribution*.

"The *F distribution* is defined as the ratio of two χ^2 distributions divided by their degrees of freedom"[17]. Values for F are tabulated depending on the confidence level (α) and the degrees of freedom of the numerator (ν_1) and the denominator(ν_2).

$$F(\alpha, \nu_1, \nu_2) = \frac{\chi^2(\nu_1)/\nu_1}{\chi^2(\nu_2)/\nu_2}$$

The $\chi^2(\nu)$ distribution is defined as the distribution of the sum of squared normal distributed variables.

$$\chi^2(\nu) = \sum_{i=1}^{\nu} u_i^2$$

where ν represents the degrees of freedom and u is normally distributed with a mean of 0 and a standard deviation of 1.

The SSE (the sum of the square residuals) follows a χ^2 distribution with $n-p$ degrees of freedom and the difference of SSE between two models follows the same distribution with $p_1 - p_2$ degrees of freedom (model 1 - model 2). Therefore, the following ratio should follow the *F distribution*

$$F(\alpha, p_1 - p_2, n - p_1) = \frac{(SSE_{p2} - SSE_{p1})/(p_1 - p_2)}{SSE_{p1}/(n - p_1)}$$

where subscript 1 refers to the model with a larger number of parameters. Rearranging to obtain a ratio between SSE_{p2} and SSE_{p1}

$$\frac{SSE_{p2}}{SSE_{p1}} = (p1 - p2)\frac{F(\alpha, p_1 - p_2, n - p_1)}{n - p_1} + 1$$

If this ratio is larger than the actual ratio between SSE_{p2} and SSE_{p1}, it can be said with a $100(1-\alpha)\%$ of confidence that adding the the extra $p_1 - p_2$ terms to the model with larger number of parameters does not improve significantly from the model with less parameters.

In the event that the two models being compared have the same number of

parameters this procedure cannot be applied. However, in this case the sum of square of the residuals is a good representative as to which model is "better".

A special case of model comparison is the test of significance for a model. This test gives an idea of model adequacy. The usual test of significance compares a "fake" model that only includes β_0 (i.e. all other β_j are zero) to the model of interest. The sum of residuals of the "fake" model is the total sum of residuals SST with $n-1$ degrees of freedom, and the sum of residuals of the "actual" model is SSE with $n-p$ degrees of freedom. Thus,

$$f_0 = \frac{(SST - SSE)/((n-p)-(n-1))}{SSE/(n-p)} = \frac{SSR/(p-1)}{SSE/(n-p)} = \frac{Mean\ Square\ Regression}{Mean\ Square\ Residual}$$

Therefore, the value of f_0 is compared to a tabulated value $F_{\alpha,p-1,n-p}$ that represents the upper 100α % of the F-distribution. If f_0 is greater than $F_{\alpha,p-1,n-p}$ then the "fake" model is rejected at the α level of significance (the variation accounted by the model is significantly greater than the unexplained variation). However, the possibility that another model is a better fit to the data is not rejected. A "better" model may include other variables or the deletion of one or more of the variables considered in the model.

The strength of the conclusion of a statisical test can be determined from the *P-value* that represents the lowest level of significance at which a null hypothesis is rejected.

Table 2.1: Example data

x_1	x_2	y_{data}	y_{true}
0	1	5.94	6.00
0	2	8.75	9.00
0	3	14.02	14.00
0	4	21.01	21.00
0.5	1	1.58	1.75
0.5	2	5.68	5.50
0.5	3	11.43	11.25
0.5	4	18.99	19.00
1	1	-4.45	-4.50
1	2	0.03	0.00
1	3	6.47	6.50
1	4	15.11	15.00

Example

Consider the case where there are two independent variables: x_1 that takes values from 0 to 1, and x_2 that takes 1, 2, 3, or 4 as values. The "true" response follows a second order polynomial $y_{true} = 5 - 8x_1 - 4x_1^2 + 1.5x_1x_2 + x_2^2$ (i.e. $b_0 = 5$, $b_1 = -8$, $b_2 = 0$, $b_{11} = -4$, $b_{12} = 1.5$, $b_{22} = 1$). The data generated using a full factorial design of experiment with a noise of 1.5% is presented in Table 2.1.

A second order polynomial is fitted using the least squares method. For this, the matrix X is constructed and the vector b that holds the estimated parameters is calculated.

$$\mathbf{X} = \begin{array}{c} \begin{array}{cccccc} 1 & x_1 & x_2 & x_1^2 & x_1x_2 & x_2^2 \end{array} \\ \begin{pmatrix} 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 2 & 0 & 0 & 4 \\ 1 & 0 & 3 & 0 & 0 & 9 \\ 1 & 0 & 4 & 0 & 0 & 16 \\ 1 & 0.5 & 1 & 0.25 & 0.5 & 1 \\ 1 & 0.5 & 2 & 0.25 & 1 & 4 \\ 1 & 0.5 & 3 & 0.25 & 1.5 & 9 \\ 1 & 0.5 & 4 & 0.25 & 2 & 16 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & 1 & 2 & 4 \\ 1 & 1 & 3 & 1 & 3 & 9 \\ 1 & 1 & 4 & 1 & 4 & 16 \end{pmatrix} \end{array}$$

$$b = [X'X]^{-1}X'ydata$$

$$b' = [4.7080 \quad -7.5532 \quad 0.1329 \quad -4.2277 \quad 1.4532 \quad 0.9862]$$

Then, the total sum of squares, sum of squares due to regression, and the sum of squares of residuals are calculated in order to perform an Analysis of Variance.

$$SST = \sum_{i=1}^{n}(Y_i - \overline{Y})^2 = 655.775$$

$$SSR = \sum_{i=1}^{n}(y_i - \overline{Y})^2 = 655.660$$

$$SSE = \sum_{i=1}^{n}(Y_i - y_i)^2 = 0.115$$

Table 2.2: ANOVA Table 2^{nd} order model

Source of Variation	Degrees of Freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	f_0	P-value
Regression (Fitted Model)	5	655.660	131.132	6830	3.56×10^{-11}
Residual (Error)	6	0.115	0.0192		
Total	11	655.775			

The results are summarized in an ANOVA Table in Table 2.2. The coefficient of determination R^2 for this model is 0.99982.

After obtaining the vector b using the Least Squares method, a test of significance is perfomed on the model to determine its adequacy. In order to do this, the model is compared to a "fake" model that only contains the b_0 coefficient.

$$f_0 = \frac{SSR/(p-1)}{SSE/(n-p)} = \frac{655.660/5}{0.115/6} = 6829.79$$

When this value is compared to the tabulated value for $F_{0.05,5,6} = 4.3874$ (95% confidence) it is clear that the second order model is a much better approximation to the data than the "fake" model. The *P-value* is close to zero indicating that the second order model is prefered over the "fake" model regardless of the confidence level.

Once it has been determined that the model is in fact an improvement over the "fake" model, the significance of each parameter is checked by using a *t-test* to determine if its value is zero.

$$t = \frac{b_j - 0}{s_{bj}} = \frac{b_j}{s_{bj}}$$

The standard deviation of each parameter is calculated by

$$s_{bj} = \sqrt{[X'X]^{-1}_{jj}\sigma^2}$$

where

$$\sigma^2 \approx \frac{SSE}{n-p} = 0.0192$$

Thus,

$$s_{b0} = \sqrt{3.375 \times 0.0192} = 0.255$$

$$s_{b1} = \sqrt{9 \times 0.0192} = 0.416$$

$$s_{b2} = \sqrt{2.25 \times 0.0192} = 0.208$$

$$s_{b11} = \sqrt{6 \times 0.0192} = 0.339$$

$$s_{b12} = \sqrt{0.4 \times 0.0192} = 0.088$$

$$s_{b22} = \sqrt{0.0833 \times 0.0192} = 0.040$$

And

$$t_{b0} = \frac{4.7080}{0.255} = 18.5$$

$$t_{b1} = \frac{-7.5532}{0.416} = -18.2$$

$$t_{b2} = \frac{0.1329}{0.208} = 0.639$$

$$t_{b11} = \frac{-4.2277}{0.339} = -12.5$$

$$t_{b12} = \frac{1.4532}{0.088} = 16.5$$

$$t_{b22} = \frac{0.9862}{0.040} = 24.6$$

Table 2.3: ANOVA Table updated 2^{nd} order model

Source of Variation	Degrees of Freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	f_0	P-value
Regression (Fitted Model)	4	655.652	163.91	9313	4.09×10^{-13}
Residual (Error)	7	0.123	0.0176		
Total	11	655.775			

For a 95% level of confidence, the critical value to which all t's are compared to is $t_{0.025,6} = 2.4469$. The value corresponding to b_2 is the only one that falls in the acceptance interval, therefore b_2 is set to zero and the model recalculated following the same procedure.

The X matrix for the updated model does not have the x_2 column.

$$X = [1 \;\; x_1 \;\; x_1^2 \;\; x_1x_2 \;\; x_2^2]$$

where 1, x_1, x_1^2, x_1x_2 and x_2^2 represent vectors of the same length as the original data.

The estimated parameters obtained for this model are $b_0 = 4.8557$, $b_1 = -7.5827$, $b_{11} = -4.2277$, $b_{12} = 1.4651$, and $b_{22} = 1.0108$. The Analysis of Variance for the updated model is found in Table 2.3.

The R^2 for the updated model is 0.99981.

To be certain that the updated model is "better" than the original one a model comparison is performed. For this, the ratio of the sum of square of the residuals is compared to the critical value

$$(6-5)\frac{F(0.05, 6-5, 12-6)}{12-6} + 1 = 1 \times \frac{5.9874}{6} + 1 = 1.9979$$

If the actual ratio is greater than the critical value, the model with more parameters (i.e. original model) is better than the other one.

$$\frac{SSE_{updated}}{SSE_{original}} = \frac{0.123}{0.115} = 1.07$$

Because the actual ratio is smaller than the critical value it can be said that the updated model is prefered over the original one. The *P-value* for this test is 0.54, meaning that the level of significance should be 0.54 (confidence level of 46%) in order to accept the original model as the "best" fit. Notice that even though the R^2 for the second order model is greater that the R^2 for the updated second order model, the updated model is more appropriate.

In real life, the "true" form of the response is not always known. Therefore, different polynomials may be tried to fit the same data. For instance, the data may be fitted to a first order polynomial using, once again, the method of least squares with

$$X = [1 \quad x_1 \quad x_2]$$

The estimates of the parameters in this case are $b_0 = -1.6873$, $b_1 = -8.1478$, $b_2 = 5.7906$ and the model has a $R^2 = 0.96943$. The Analysis of Variance is presented in Table 2.4.

The ratio of the sum of square of the residuals for the first order model and the updated second order model is

$$\frac{SSE_{1st\ order}}{SSE_{updated}} = \frac{20.045}{0.123} = 162$$

Comparing this value to the critical ratio (2.3535) it can be stated that the

Table 2.4: ANOVA Table 1^{st} order model

Source of Variation	Degrees of Freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	f_0	P-value
Regression (Fitted Model)	2	635.730	317.86	143	1.53×10^{-7}
Residual (Error)	9	20.045	2.2272		
Total	11	655.775			

updated second order model is significantly better than the first order approximation ($P\text{-}value \approx 0$).

Chapter 3

Response Surface Model computational toolbox

The computational toolbox used to manipulate and analyze the data obtained from combinatorial CVD consists in a group of object-oriented functions written in MATLAB. The toolbox is based on a highly accurate, quadrature-based set of weighted residual methods that allows accurate wafer map representation and interpolation.[2] Most functions work with parametrized data objects that have three data fields: the data point (actual value); the data structure, which holds the parameters' information (names and values); and the data field, where the data identification (name) is stored.

The Least Squares Method developed to calculate the predictive models extracts the parameters' information and data values from the parametrized data objects and proceeds with the calculations. The use of paramatrized data objects makes it possible to calculate a complete wafer map model interpolating it to a quadrature grid. This way the model predictions may be of a single point or a full wafer map. The predicted object belongs to the same class as the data used to obtain it. In other words, if the data used was a full wafer the predicted object will belong to the wafer class, and if it was a single point the predicted object will be a single point.

rsmodel

The *rsmodel* function takes as inputs a vector of parametrized data objects that contain the data information and operation conditions (independent variables values), a cell array with the terms of the model to be fitted, and a character string with the name of the parameters.

If the name of the parameters is not specified the function uses all the parameters except those that present no variability (i.e. remain constant). If the model order is not specified the function tries to fit the highest order model possible (up to a full second order model). To determine the largest number of terms possible (i.e. the highest order model possible) the rank of matrix X is analyzed. If it is found that the number of model terms requested is greater than the rank of X, the *rsmodel* function performs an exhaustive search for the "best" combination of allowed number of model terms (defined by the condition number of $X'X$) before performing the least squares regression.

After performing the regression the *modelvalidate* fuction is called to obtain some information regarding the usefullness/validity of the model. The *rsmodel* function gives as output a response surface model object that can later be used to make predictions and displays in the command window a table with the values (or mean values) of the calculated coefficients b_j and an ANOVA Table.

modelvalidate

This function takes as inputs the *rsmodel* object and the vector of parametrized data objects used to obtain the model. The outputs of this function are: the predicted values for the same parameter values as the original data, the error of the prediction (data value minus predicted value), the estimated of the standard deviation (also known as the standard error) of each parameter, the coefficient of determination (R^2), the total number of observations (n), the number of terms in the fitted model (p), the sum of squares of the residuals (SSE), and the total sum of squares (SST).

modeloutput

This function predicts the value/form of the point/wafer map for a given set of parameter values. The inputs needed for this function are the model obtained using *rsmodel* and the values and names of the parameters of interest.

getbcoeff

The *getbcoeff* function takes as input the model obtained from *rsmodel* and present as output the calculated parameters b_j's. If the data used to calculate the model was a single point in the wafer, *getbcoeff* gives the value for b_0, a vector b containing the linear terms b_j, and a triangular matrix B containing the cross-product terms b_{ij}.

If the data used to calculate the model was a full wafer, *getbcoeff* gives as output scalarfields with the information of b_0, b, and B.

plotb

When a complete wafer map is modeled, an easier way to view the estimated parameters, as oposed to using the *getbcoeff* function, is to present the resulting scalarfields graphically. The *plotb* function takes as input the model obtained from *rsmodel* and gives as output plots of the scalarfields of the estimated parameters.

bttest

The *bttest* function performs a t-test to each individual parameter obtained using *rsmodel*. The null hypothesis H_0 for the testing is that the "true" parameter β_j is zero, while the alternative hypothesis is that $\beta_j \neq 0$. If the level of significance (α) is not specified a default value of 0.05 is used, giving a 95% confidence in the test. If the null hypothesis for a given parameter cannot be rejected that parameter assumes the value of zero. In other words, that parameter is removed from the model.

If the calculations are for a full wafer, a parameter β_j is assumed to be zero, thus removed from the model, if the null hypothesis cannot be rejected in at least a *pp* percentage of the points of the quadrature grid. If the *pp* value is not specified a value of 75 is used (i.e. β_j has to be zero in at least 75% of the points in the quadrature grid for it to be removed form the model).

The *bttest* function gives as output an array of the terms that are considered relevant with a 100(1-α)% confidence. This array is then used in the *rsmodel* function to obtain an updated model for the data.

comptest

The *comptest* function is used to compare two models in order to determine which one is a more appropriate fit to the data. This function takes as inputs a vector of parametrized data objects, two cell arrays with the terms of the models to be compared, and the level of significance α for the comparison. If α is not specified a default value of 0.05 is assumed.

If the calculations are for a full wafer, the *comptest* function accepts the model with the larger number of terms as the "best" fit if it is considered so in at least a *pp* percentage of the points of the quadrature grid. If the *pp* value is not specified a value of 75 is used.

This function gives as outputs the number of parameters used in each model, the actual ratio of the sum of residuals of the models (if the comparison is for one point), the percentage of points where the model with a larger number of terms is considered better (if the comparison involves full wafers), the critical value for the ratio, and the conclusion that follows the comparison of both ratios.

Additional Tools

There are other functions that do not belong exclusively to the *rsmodel toolbox*, but that are helpful in manipulating the data.

waferpoint

The *waferpoint* function returns the value of a point in a wafer. This function takes as inputs the wafer profile and the polar coordinates (r,θ) of the point.

plotsequence

As its name implies, the *plotsequence* function plots a sequence of wafer maps. The input for this function is a vector of scalarfield objects containing the information of the wafers.

xmlwrite

The *xmlwrite* function is used to write a data file marked up in XML from a MATLAB struct object. By applying this function the information stored in MATLAB objects may be easily shared and can even be posted online.

urlxmlread

The *urlxmlread* function takes as input the url address where the data is stored in a XML format and returns an array structure from which the data is retrieved.

Example

Consider the two-variable second order polynomial system presented in the previous chapter (Table 2.1). The same analysis is now performed in MATLAB using the computational toolbox.

First, the data is transformed to a parametrized data object that containes the response value (y_{data}), the name of the independent variables (x_1 and x_2), and the values for these variables. Then, the object is sent as input to the *rsmodel* function.

```
>> M2=rsmodel(E)

rsmodel object "M2"

Parameters: mean value
----------
x1 : 0.5
x2 : 2.5
Those used in model:
    'x1'    'x2'

  Term : value       (std error)
--------------------------------
    b0 : 4.70799e+000 (2.54756e-001)
    b1 : -7.55316e+000 (4.16014e-001)
    b2 : 1.32913e-001 (2.08007e-001)
  b1,1 : -4.22771e+000 (3.39674e-001)
  b1,2 : 1.45324e+000 (8.77035e-002)
  b2,2 : 9.86204e-001 (4.00310e-002)

R^2 : 0.99982


                                          ANOVA Table
-------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)               (MS)
-------------------------------------------------------------------------------
Regression           5              655.660            131.1319    6819.22    3.574e-011
Residual             6                0.115              0.0192
Total               11              655.775
```

E is the parametrized data object that contains the example data and $M2$ is the second order response model obtained. The values obtained for the coefficients, standard deviations (i.e. standard errors), and ANOVA Table are the same as the ones obtained in the previous chapter.

Next, a *bttest* is performed to determine which coefficients are relevant and the resulting cell array is used to update the model.

```
>> mterm=bttest(M2);
>> M2u=rsmodel(E,mterm)

rsmodel object "M2u"

Parameters: mean value
----------
x1 : 0.5
x2 : 2.5
Those used in model:
    'x1'    'x2'

  Term : value       (std error)
--------------------------------
    b0 : 4.85567e+000 (1.02536e-001)
    b1 : -7.58269e+000 (3.95579e-001)
  b1,1 : -4.22771e+000 (3.25001e-001)
  b1,2 : 1.46505e+000 (8.20290e-002)
  b2,2 : 1.01082e+000 (1.04244e-002)

R^2 : 0.99981


                                          ANOVA Table
-------------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)              (MS)
-------------------------------------------------------------------------------------
Regression           4              655.652           163.9130    9310.96    4.092e-013
Residual             7                0.123             0.0176
Total               11              655.775
```

In the updated model the value of b_2 if forced to be zero and the model is recalculated. Again, the values obtained are the same as the ones obtained in the previous chapter.

The full second order model is compared to the updated model using *comptest*.

```
>> c=comptest(E,2,mterm)

c =

           p1: 6
           p2: 5
        ratio: 1.0681
    criticalr: 1.9979
       pvalue: 0.5464
   conclusion: 'model 1 IS NOT significantly better than model 2'
```

Model 1 refers to the full second order model and Model 2 refers to the updated second order model. The conclusion from this comparison is the same as the one reached in the previous chapter, the updated model is prefered over the original full

second order model.

If a first order model is fitted to the data the resulting b values are:

```
>> M1=rsmodel(E,1)

rsmodel object "M1"

Parameters: mean value
----------
x1 : 0.5
x2 : 2.5
Those used in model:
    'x1'    'x2'

  Term : value       (std error)
--------------------------------
    b0 : -1.68727e+000 (1.17984e+000)
    b1 : -8.14777e+000 (1.05528e+000)
    b2 : 5.79055e+000 (3.85335e-001)

R^2 : 0.96943


                                          ANOVA Table
-------------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)               (MS)
-------------------------------------------------------------------------------------
Regression          2               635.730            317.8649    142.72    1.526e-007
Residual            9                20.045              2.2272
Total              11               655.775
```

The result of comparing this model to the updated second order model is

```
>> c=comptest(E,1,mterm)

c =

           p1: 3
           p2: 5
        ratio: 162.6650
     criticalr: 2.3535
       pvalue: 1.8217e-008
    conclusion: 'model 2 IS significantly better than model 1'
```

Model 1 refers to the first order model, Model 2 refers to the updated second order model, and the conclusion is that Model 2 is better than Model 1.

Chapter 4

Artificially Generated Wafers Study

Three diferent sets of artificial wafers were generated in order to test the *Response Surface Model computational toolbox*. All sets were obtained using a full factorial design of experiment for values of the independent variables (i.e. "fake" operational conditions) p and q equal to -2, 0, and 2. The first set represents a full second order response and behaves as $W = Wo + WA\ (p+6)\ (p-0.3) + WB\ (q+5)\ (q-0.1) + WA\,WB\ (p-0.3)\ (q-0.1)$. The second set correspons to a second order response that has one parameter equal zero (i.e. is missing a term) and behaves as $W = Wo + WA\ (p-0.3) + WB\ (q+5)\ (q-0.1) + WA\,WB\ (p-0.3)\ (q-0.1)$. Lastly, the third set follows a third order response and behaves as $W = Wo + WA\ (p-3)\ (p+6)\ (p-0.3) + WB\ (q+5)\ (q-0.1) + WA\ WB\ (p-0.3)\ (q-0.1)$. For all three cases Wo is a flat wafer of thickness 1 plus the data noise, and WA and WB are shown in Figure 4.1.

Single Point Analysis

The single point analysis of the artificially generated wafers takes as data points the mean thickness of each wafer. Once these values are calculated they are stored in parametrized data objects that also contain the values for the independent variables p and q, and their names. The *rsmodel* function is then applied to these

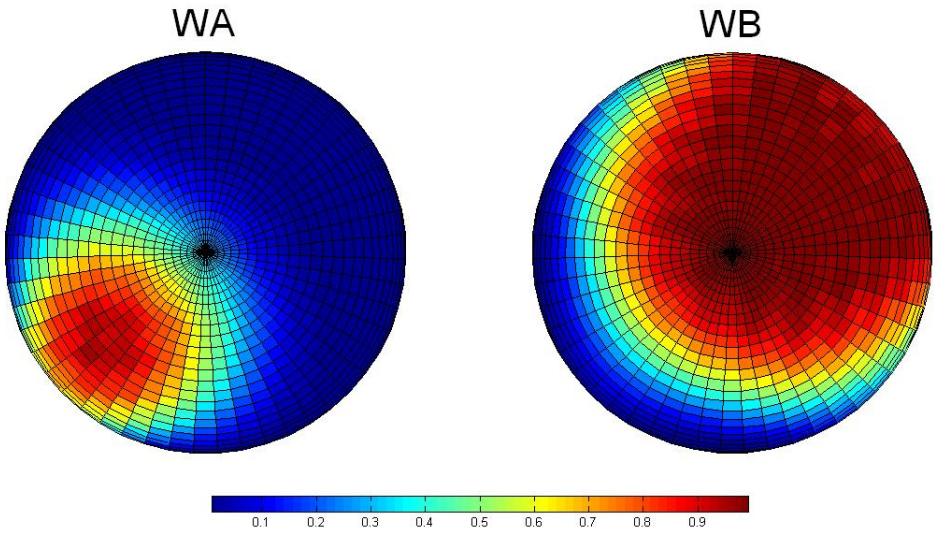

Figure 4.1: *WA and WB used to generate the artificial wafers*

objects.

Full second order behavior

The independent variables and mean thickness when the artificial wafers follow the equation $W = Wo + WA\ (p+6)\ (p-0.3) + WB\ (q+5)\ (q-0.1) + WA\ WB\ (p-0.3)\ (q-0.1)$ are tabulated in Table 4.1. These data are fitted to a second order model using the *rsmodel* function, the relevance of each individual parameter is tested using *bttest*, and an updated model is calculated.

Table 4.1: Full second order wafers' mean thickness

p	q	mean Thickness
-2	-2	-4.8388
-2	0	-1.3438
-2	2	7.5288
0	-2	-3.6906
0	0	0.2000
0	2	9.6543
2	-2	-0.6735
2	0	3.7737
2	2	13.5661

```
>> M=rsmodel(Wm)

rsmodel object "M"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : value       (std error)
--------------------------------
    b0 : 2.44938e-001 (3.10391e-002)
    b1 : 1.27667e+000 (8.50042e-003)
    b2 : 3.32935e+000 (8.50042e-003)
  b1,1 : 2.36878e-001 (7.36158e-003)
  b1,2 : 1.17003e-001 (5.20542e-003)
  b2,2 : 6.78611e-001 (7.36158e-003)

R^2 : 0.99998
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	5	322.554	64.5109	37199.86	2.199e-007
Residual	3	0.005	0.0017		
Total	8	322.559			

Table 4.2: Predicted mean thickness and residuals

data	pred. value	residual
-4.8388	-4.8371	-0.0016
-1.3438	-1.3609	0.0171
7.5288	7.5442	-0.0154
-3.6906	-3.6993	0.0087
0.2000	0.2449	-0.0449
9.6543	9.6181	0.0363
-0.6735	-0.6665	-0.0070
3.7737	3.7458	0.0279
13.5661	13.5869	-0.0208

```
>> mterm=bttest(M);
>> Mud=rsmodel(Wm,mterm)

rsmodel object "Mud"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : value       (std error)
--------------------------------
    b0 : 2.44938e-001 (3.10391e-002)
    b1 : 1.27667e+000 (8.50042e-003)
    b2 : 3.32935e+000 (8.50042e-003)
  b1,1 : 2.36878e-001 (7.36158e-003)
  b1,2 : 1.17003e-001 (5.20542e-003)
  b2,2 : 6.78611e-001 (7.36158e-003)

R^2 : 0.99998
```

The updated model is exactly the same as the original second order model. Thus, it is clear that, according to the *bttest*, all terms are considered relevant.

The predicted thickness using the calculated model and the residuals are displayed in Table 4.2.

Table 4.3: Second order wafers' mean thickness

p	q	mean Thickness
-2	-2	-3.2706
-2	0	0.2244
-2	2	9.0970
0	-2	-3.3497
0	0	0.5409
0	2	9.9952
2	-2	-3.3781
2	0	1.0691
2	2	10.8615

Second order behavior

The second set of artificial wafers has the form $W = Wo + WA\ (p - 0.3) + WB\ (q + 5)\ (q - 0.1) + WA\ WB\ (p - 0.3)\ (q - 0.1)$. The mean thickness and independent variable values for this set of data appears in Table 4.3.

The model obtained for these data when *rsmodel* is used is:

```
rsmodel object "M"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : value       (std error)
--------------------------------
    b0 : 5.85851e-001 (3.10391e-002)
    b1 : 2.08477e-001 (8.50042e-003)
    b2 : 3.32935e+000 (8.50042e-003)
  b1,1 : 9.60337e-003 (7.36158e-003)
  b1,2 : 1.17003e-001 (5.20542e-003)
  b2,2 : 6.78611e-001 (7.36158e-003)

R^2 : 0.99998
```

```
                                        ANOVA Table
-------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)              (MS)
-------------------------------------------------------------------------------
Regression          5             282.688             56.5375    32602.07    2.681e-007
Residual            3               0.005              0.0017
Total               8             282.693
```

When this model is tested with *bttest* and an updated model is calculated the result is:

```
>> mterm=bttest(M);
>> Mud=rsmodel(Wm,mterm)

rsmodel object "Mud"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : value       (std error)
--------------------------------
    b0 : 6.11460e-001 (2.60667e-002)
    b1 : 2.08477e-001 (9.21598e-003)
    b2 : 3.32935e+000 (9.21598e-003)
  b1,2 : 1.17003e-001 (5.64361e-003)
  b2,2 : 6.78611e-001 (7.98128e-003)

R^2 : 0.99997


                                        ANOVA Table
-------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)              (MS)
-------------------------------------------------------------------------------
Regression          4             282.685             70.6712    34669.49    2.496e-009
Residual            4               0.008              0.0020
Total               8             282.693
```

Note that the b_{11} term disappears in the updated model because, according to the results of *bttest*, it is not considered important. To verify that the updated model is in fact a "better" fit that the full second order model, a model comparison is performed.

Table 4.4: Predicted mean thickness and residuals

data	pred. value	residual
-3.2706	-3.2817	0.0112
0.2244	0.1945	0.0299
9.0970	9.0996	-0.0026
-3.3497	-3.3328	-0.0169
0.5409	0.6115	-0.0705
9.9952	9.9846	0.0107
-3.3781	-3.3838	0.0058
1.0691	1.0284	0.0407
10.8615	10.8696	-0.0080

```
>> c=comptest(Wm,2,mterm)

c =

            p1: 6
            p2: 5
         ratio: 1.5673
     criticalr: 4.3760
        pvalue: 0.2831
    conclusion: 'model 1 IS NOT significantly better than model 2'
```

The comparison shows one more time that the b_{11} term is not significant since its addition in the full second order model does not represent an improvement. The predicted thickness and the residuals are presented in Table 4.4.

Third order behavior

The last set of artificial data generated follows the equation $W = Wo + WA\ (p-3)\ (p+6)\ (p-0.3) + WB\ (q+5)\ (q-0.1) + WA\ WB\ (p-0.3)\ (q-0.1)$. The mean thickness for each wafer and the "operating conditions" (i.e. independent variable values) are found on Table 4.5.

When *rsmodel* is used on these data the following b coefficientes and ANOVA

Table 4.5: Third order wafers' mean thickness

p	q	mean Thickness
-2	-2	7.7068
-2	0	11.2018
-2	2	20.0744
0	-2	-2.0543
0	0	1.8364
0	2	11.2907
2	-2	-6.8554
2	0	-2.4082
2	2	7.3842

table are obtained:

```
rsmodel object "M"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : value       (std error)
--------------------------------
    b0 : 1.88132e+000 (3.10391e-002)
    b1 : -3.40519e+000 (8.50042e-003)
    b2 : 3.32935e+000 (8.50042e-003)
  b1,1 : 6.23246e-001 (7.36158e-003)
  b1,2 : 1.17003e-001 (5.20542e-003)
  b2,2 : 6.78611e-001 (7.36158e-003)

R^2 : 0.99999


                                          ANOVA Table
-------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)             (SS)              (MS)
-------------------------------------------------------------------------------
Regression          5             572.360            114.4720    66009.68    9.304e-008
Residual            3               0.005              0.0017
Total               8             572.365
```

Notice that, as explained in the previous chapter, the *rsmodel* function fits the data up to a full second order model. Regardless, acording to the coefficient of determination ($R^2 = 0.99999$) and the sum of square of residuals ($SSE = 0.005$)

the second order model appears to be a good fit.

The relevance of each of the terms of the second order model is tested using *bttest* and an updated model is calculated.

```
>> mterm=bttest(M);
>> Mud=rsmodel(Wm,mterm)

rsmodel object "Mud"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : value       (std error)
--------------------------------
    b0 : 1.88132e+000 (3.10391e-002)
    b1 : -3.40519e+000 (8.50042e-003)
    b2 : 3.32935e+000 (8.50042e-003)
  b1,1 : 6.23246e-001 (7.36158e-003)
  b1,2 : 1.17003e-001 (5.20542e-003)
  b2,2 : 6.78611e-001 (7.36158e-003)

R^2 : 0.99999
```

The updated model is the same as the full second order model demonstrating that all second order terms are considered relevant.

Table 4.6 has the predicted values and the residuals. The small values of the residuals confirm that, even though the "true" response is a third order, a second order model is a good approximation for the response.

Full Wafer Maps

For the full wafer analysis of the artificially generated wafers the parametrized data objects have the full wafer information, the values for the independent variables p and q, and their names. The *rsmodel* function is then applied to these objects.

Table 4.6: Predicted mean thickness and residuals

data	pred. value	residual
7.7068	7.7085	-0.0016
11.2018	11.1847	0.0171
20.0744	20.0898	-0.0154
-2.0543	-2.0629	0.0087
1.8364	1.8813	-0.0449
11.2907	11.2545	0.0363
-6.8554	-6.8483	-0.0070
-2.4082	-2.4361	0.0279
7.3842	7.4051	-0.0208

Full second order behavior

The artificial wafers with the full second order behavior follow the equation $W = Wo + WA\,(p+6)\,(p-0.3) + WB\,(q+5)\,(q-0.1) + WA\,WB\,(p-0.3)\,(q-0.1)$. The plot for the generated wafers is obtained using the *plotsequence* function. The resulting graph is found in Figure 4.2. These wafers are fitted to a second order model using the *rsmodel* function.

```
>> WM=rsmodel(W)

rsmodel object "WM"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : mean value (mean std error)
-------------------------------------
    b0 : 2.50712e-001 (1.03443e-001)
    b1 : 1.28254e+000 (2.83289e-002)
    b2 : 3.32412e+000 (2.83289e-002)
  b1,1 : 2.28715e-001 (2.45335e-002)
  b1,2 : 1.18623e-001 (1.73478e-002)
  b2,2 : 6.84453e-001 (2.45335e-002)

mean(R^2) : 0.99868
```

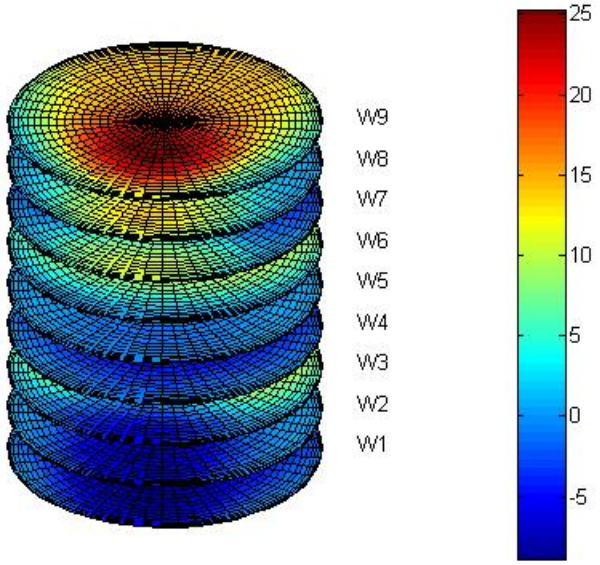

Figure 4.2: *Full second order artificial wafers*

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	5	460.797	92.1593	4088.30	6.034e-006
Residual	3	0.068	0.0225		
Total	8	460.864			

The obtained coefficients are plotted using *plotb* (Figure 4.3).

The relevance of each individual parameter is tested using *bttest*, and an updated model is calculated.

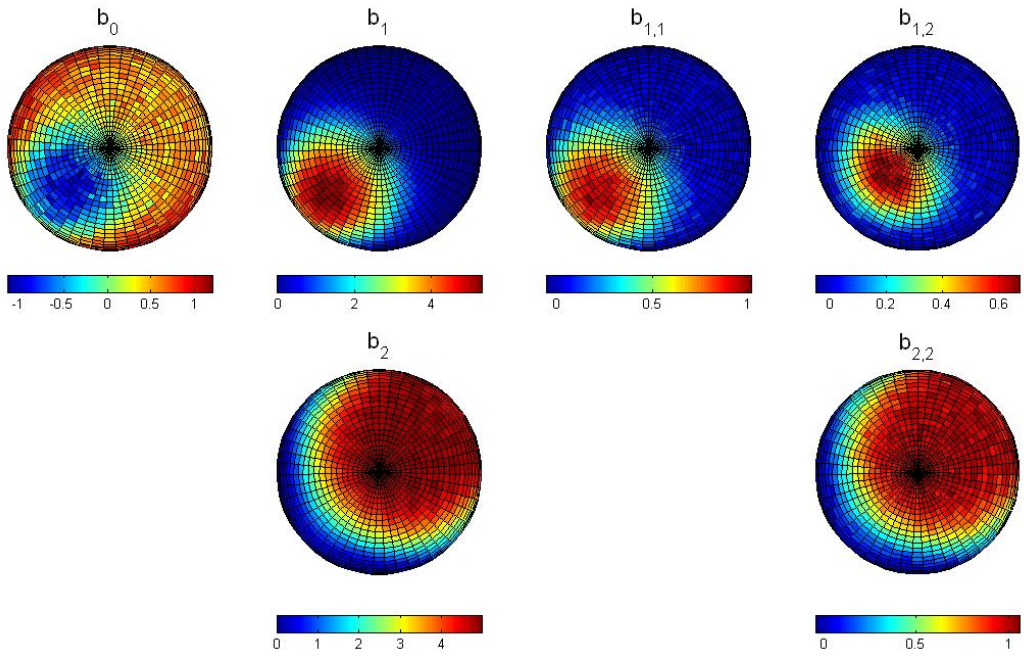

Figure 4.3: *Full second order b_j coefficients*

```
>> mterm=bttest(WM,0.01);
>> WMud=rsmodel(W,mterm)

rsmodel object "WMud"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : mean value (mean std error)
-------------------------------------
    b0 : 2.50712e-001 (1.03443e-001)
    b1 : 1.28254e+000 (2.83289e-002)
    b2 : 3.32412e+000 (2.83289e-002)
  b1,1 : 2.28715e-001 (2.45335e-002)
  b1,2 : 1.18623e-001 (1.73478e-002)
  b2,2 : 6.84453e-001 (2.45335e-002)

mean(R^2) : 0.99868
```

The updated model is the same as the original model. Thus, all terms are considered relevant and the response follows a full second order behavior.

The *modeloutput* function is used to predict the wafer map when $p = 0.3$ and

$q = 0.1$ and the result is found in Figure 4.4. According to the equation used to generate the artificial wafers, these values should give a uniform wafer with mean thickness of 1nm.

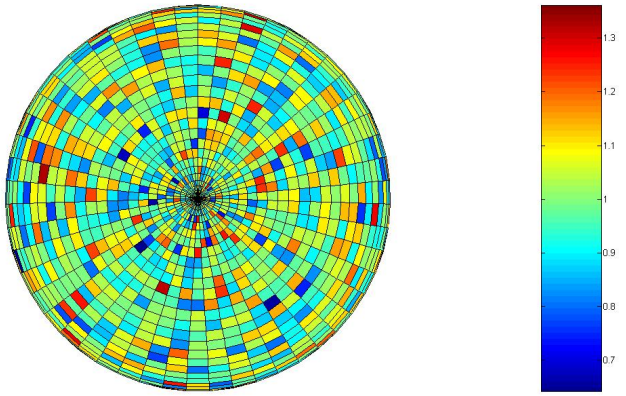

Figure 4.4: *Predicted wafer p=0.3, q=0.1*

Second order behavior

The second set of artificial wafers follow a second order behavior where one coefficient is zero. Figure 4.5 shows the nine wafers generated according to the equation $W = Wo + WA\,(p-0.3) + WB\,(q+5)\,(q-0.1) + WA\,WB\,(p-0.3)\,(q-0.1)$.

A model for these wafers is obtained using *rsmodel*. Then a *bttest* is performed to determine the importance of each term and an updated model is calculated.

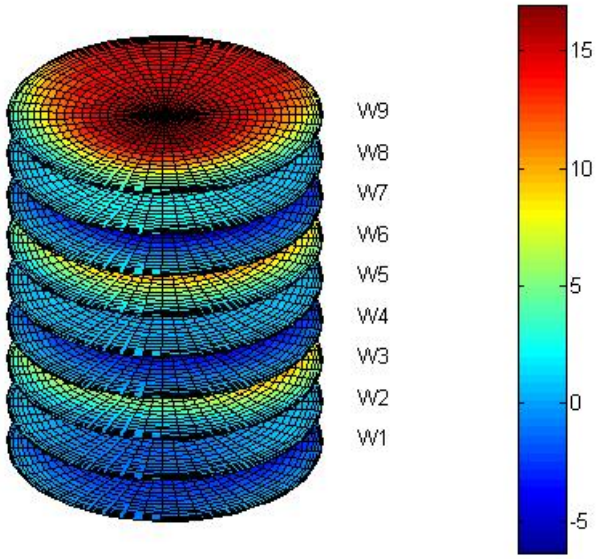

Figure 4.5: *Second order artificial wafers*

```
>> WM=rsmodel(W)

rsmodel object "WM"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : mean value (mean std error)
-------------------------------------
    b0 : 5.91624e-001 (1.03443e-001)
    b1 : 2.14348e-001 (2.83289e-002)
    b2 : 3.32412e+000 (2.83289e-002)
  b1,1 : 1.44051e-003 (2.45335e-002)
  b1,2 : 1.18623e-001 (1.73478e-002)
  b2,2 : 6.84453e-001 (2.45335e-002)

mean(R^2) : 0.9945
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	5	354.483	70.8966	3145.06	8.943e-006
Residual	3	0.068	0.0225		
Total	8	354.551			

```
>> mterm=bttest(WM,0.01);
>> WMud=rsmodel(W,mterm)

rsmodel object "WMud"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : mean value (mean std error)
-------------------------------------
    b0 : 5.95466e-001 (8.18213e-002)
    b1 : 2.14348e-001 (2.89282e-002)
    b2 : 3.32412e+000 (2.89282e-002)
  b1,2 : 1.18623e-001 (1.77148e-002)
  b2,2 : 6.84453e-001 (2.50525e-002)

mean(R^2) : 0.99215
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	4	354.460	88.6151	3914.65	1.956e-007
Residual	4	0.091	0.0226		
Total	8	354.551			

The b_{11} term is not consider relevant and it dissapears from the updated model. The obtained b coefficients are plotted in Figure 4.6. Note that the plot for the b_{11} coefficient is a constant field with zero value.

The obtained updated model is compared to the original full second order model using *comptest*.

```
>> c=comptest(W,2,mterm)

c =

                p1: 6
                p2: 5
    pointpercentage: 0.6839
         meanpvalue: 0.3876
          criticalr: 4.3760
         conclusion: 'model 1 IS NOT significantly better than model 2'
```

The comparison shows that the full second order model is consider a "better" model only in 0.7% of the points. Thus, the updated second order model is chosen as the "optimal" fit for the data.

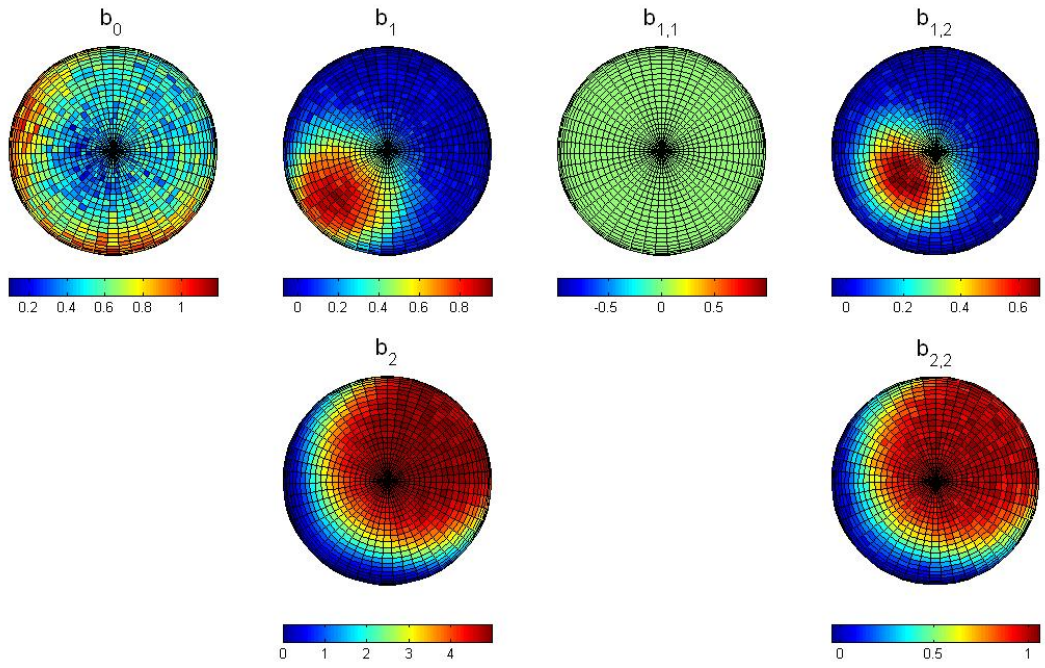

Figure 4.6: *Second order b_j coefficients*

Figure 4.7 shows the prediction wafer when $p = 0.3$ and $q = 0.1$. The resulting wafer is approximately uniform with a mean thickness of 1nm, which in concordance with the equation used to generate the artificial wafers.

Third order behavior

The third set of artificial wafers follows the form $W = Wo + WA\ (p-3)\ (p+6)\ (p-0.3) + WB\ (q+5)\ (q-0.1) + WA\ WB\ (p-0.3)\ (q-0.1)$. The generated wafers are plotted in Figure 4.8.

The resulting model when *rsmodel* is applied to these wafers is:

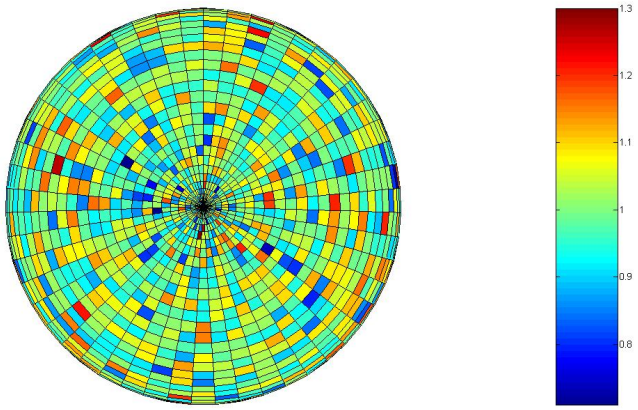

Figure 4.7: *Predicted wafer p=0.3, q=0.1*

```
>> WM=rsmodel(W)

rsmodel object "WM"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : mean value (mean std error)
-------------------------------------
    b0 : 1.88709e+000 (1.03443e-001)
    b1 : -3.39932e+000 (2.83289e-002)
    b2 : 3.32412e+000 (2.83289e-002)
  b1,1 : 6.15083e-001 (2.45335e-002)
  b1,2 : 1.18623e-001 (1.73478e-002)
  b2,2 : 6.84453e-001 (2.45335e-002)

mean(R^2) : 0.99951
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	5	1117.468	223.4936	9914.44	1.598e-006
Residual	3	0.068	0.0225		
Total	8	1117.536			

Then, the relevance of the individual coefficients is tested and an updated model is calculated.

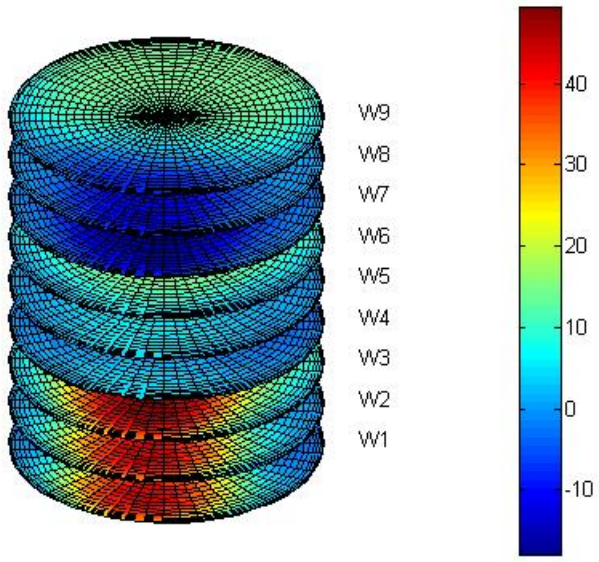

Figure 4.8: *Third order artificial wafers*

```
>> mterm=bttest(WM,0.01);
>> WMud=rsmodel(W,mterm)

rsmodel object "WMud"

Parameters: mean value
----------
p : 0
q : 0
Those used in model:
    'p'    'q'

  Term : mean value (mean std error)
-----------------------------------
    b0 : 1.88709e+000 (1.03443e-001)
    b1 : -3.39932e+000 (2.83289e-002)
    b2 : 3.32412e+000 (2.83289e-002)
  b1,1 : 6.15083e-001 (2.45335e-002)
  b1,2 : 1.18623e-001 (1.73478e-002)
  b2,2 : 6.84453e-001 (2.45335e-002)

mean(R^2) : 0.99951
```

Since the updated model is the same as the original model it can be concluded that all terms are important. Figure 4.9 shows the calculated b coefficients.

The predicted wafer obtained for values of $p = 0.3$ and $q = 0.1$ is presented

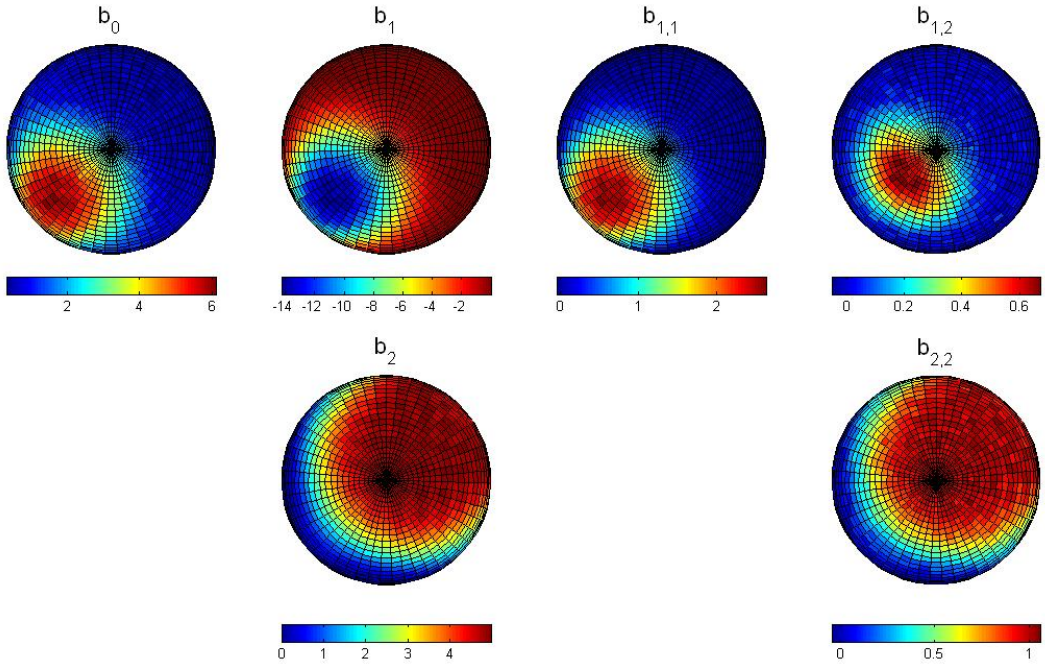

Figure 4.9: *Third order b_j coefficients*

in Figure 4.10. The resulting wafer is close to uniform with except of the lower left corner. The deviation from uniformity in the predicted wafer is due to difference in the order of the model and of the form used to generate the wafers ($W = Wo + WA\ (p-3)\ (p+6)\ (p-0.3) + WB\ (q+5)\ (q-0.1) + WA\ WB\ (p-0.3)\ (q-0.1)$).

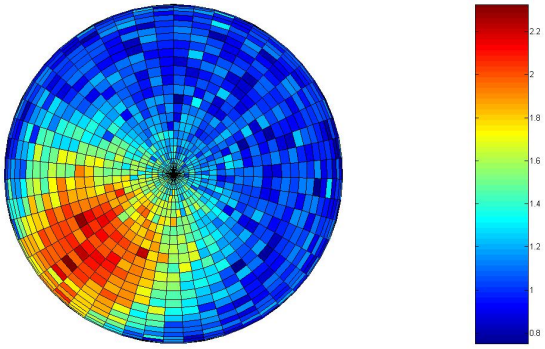

Figure 4.10: *Predicted wafer p=0.3, q=0.1*

Chapter 5

Spatially Programmable CVD Reactor Study

Once the validity of the computational toolbox is demonstrated with the artificial data, it is aplied to "real" wafer data. The Spatially Programmable Chemical Vapor Deposition System (SP-CVD)[3, 4, 10] used for this study has a three-zone showerhead and a "reverse flow exhaust" method of pumping out residual gases from each segment (Figure 5.1. The showerhead allows individual control over the mass flow rate and composition of the precursor gases to each segment making it possible to control the two-dimensional gas concentration patterns over the wafer. The "reverse flow exhaust" minimizes inter-segment convective gas flows in the gap between the showerhead and the wafer. Thus, the transport of gas species in the inter-segment region may be controlled by adjusting the gap size (the inter-segment diffusive flux increases proportionally with the gap size).

The chemical system used consists on tungsten chemical vapor deposition on $4''$ wafers. The percursor gases are WF_6 and H_2, and argon is used as an inert compensatory gas to maintain a constant flowrate. The overall reaction for the tungsten deposition that takes place at the wafer's surface is:

$$WF_{6(g)} + 3H_{2(g)} \rightarrow W_{(s)} + 6HF_{(g)}$$

The reaction rate under the operating conditions can be expressed as

$$r = k(P_{WF_6})^0(P_{H_2})^{1/2}$$

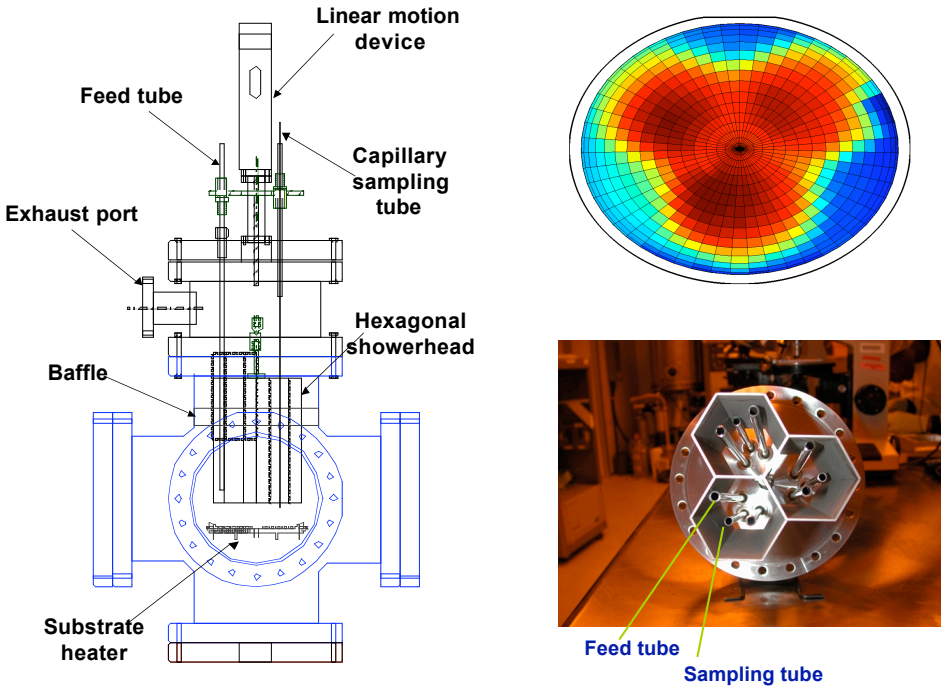

Figure 5.1: SP-CVD reactor system illustrating the reactor chamber design (left), the segmented showerhead design (bottom right), and a representative W film thickness map (top right)

Where k is the temperature dependent kinetic constant, P_{WF_6} is the partial pressure of WF_6 and P_{H_2} is the partial pressure of H_2.

The experiments were carried at a constant total mass flow of 60 standard cubic centimeters (1sccm=7.4x10^{-7} mol/s), a heater temperature of 400 ^{o}C (giving an approximate wafer temperature of 380 ^{o}C), and a reactor pressure of 1 torr. The deposition time for all the wafers was set to 900 seconds. After each deposition the thickness was measured with a four-point probe ex-situ metrology station resulting in a rectangular grid of 900 measurement points.[11] Wafer maps were then generated

by interpolating the thickness data to a numerical quadrature grid defined on a computational domain that has the same physical dimensions as the wafer.

Once the wafer maps are obtained, a single point analysis of the data is perfomed followed by a full wafer analysis.

The hydrogen flowrates used in each run are found in Table 5.1.

Segments' Center Point

The objective of the single point analysis of the SP-CVD reactor data is to find an optimal model for the thickness of the center point of each wafer segment (Figure 5.2) using the rsmodel computational toolbox. The values of thickness at the center points are obtained using the *waferpoint* function.

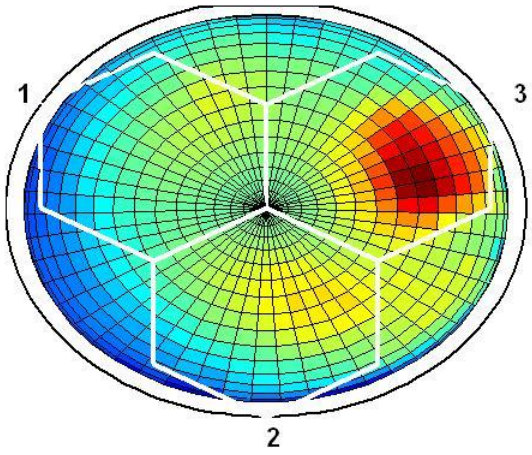

Figure 5.2: *Wafer segments*

According to the kinetics of the chemical system, the rate of the reaction depends on the square root of the hydrogen concentration. Thus, the factors used to fit the model are the square root of the H_2 flowrates to each segment and the

Table 5.1: Operational conditions for each wafer

wafer ID	H2s1 (sccm)	H2s2 (sccm)	H2s3 (sccm)	gap (mm)
w081506_01	16	32	48	3
w081506_02	32	48	16	3
w081506_03	48	16	32	3
w081506_04	32	32	32	3
w081506_05	32	0	0	3
w081506_06	0	32	0	3
w081506_07	0	0	32	3
w081606_01	0	0	32	1
w081606_02	0	32	0	1
w081606_03	32	0	0	1
w081606_04	32	32	32	1
w081606_05	48	16	32	1
w081606_06	32	48	16	1
w081606_07	16	32	48	1
w081606_08	16	32	48	5
w081606_09	32	48	16	5
w081606_10	48	16	32	5
w081606_11	32	32	32	5
w081606_12	32	0	0	5
w081606_13	0	32	0	5
w081606_14	0	0	32	5
w081706_01	0	0	32	3
w081706_02	0	32	0	3
w081706_03	32	0	0	3
w081706_04	32	32	32	3
w081706_05	48	16	32	3
w081706_06	32	48	16	3
w081706_07	16	32	48	3
w081806_01	0	0	32	2
w081806_02	0	32	0	2
w081806_03	32	0	0	2
w081806_04	32	32	32	2
w081806_05	48	16	32	2
w081806_06	32	48	16	2
w081806_07	16	32	48	2
w082406_01	0	0	32	4
w082406_02	0	32	0	4
w082406_03	32	0	0	4
w082406_04	32	32	32	4
w082406_05	48	16	32	4
w082406_06	32	48	16	4
w082406_07	16	32	48	4
w082406_08	32	32	0	4
w082406_09	0	32	32	4
w082406_10	32	0	32	4

distance between the showerhead and the wafer (gap).

The results for segment 1 are presented in this chapter. The results for segment 2 and segment 3 may be found on Appendix A.

Full second order model

The values of the calculated b coefficients obtained when a full second order model is fitted to the data are presented bellow. The subscripts 1, 2, and 3 correspond to the square roots of the hydrogen flowrate to segment 1 ($sqh2s1$), segment 2 ($sqh2s2$), and segement 3 ($sqh2s3$) respectively. The subscritp 4 corresponds to the dimension of the gap.

The coefficients and ANOVA Table obtained for segments 1 (P1) are:

```
rsmodel object "P1"

Parameters: mean value
----------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

  Term : value       (std error)
--------------------------------
    b0 : 1.28464e+001 (8.68478e+002)
    b1 : 2.15982e+002 (5.15459e+002)
    b2 : -1.58555e+002 (5.15459e+002)
    b3 : 1.78296e+002 (5.15459e+002)
    b4 : 3.44785e+002 (2.53537e+002)
  b1,1 : -1.29014e+001 (8.47732e+001)
  b1,2 : -5.36840e+000 (2.01761e+001)
  b1,3 : 1.78973e+001 (2.01761e+001)
  b1,4 : -1.20266e+001 (1.93581e+001)
  b2,2 : 2.45365e+001 (8.47732e+001)
  b2,3 : 5.41842e+000 (2.01761e+001)
  b2,4 : 2.52856e+001 (1.93581e+001)
  b3,3 : -3.36424e+001 (8.47732e+001)
  b3,4 : 1.84806e+001 (1.93581e+001)
  b4,4 : -5.33030e+001 (3.73601e+001)

R^2 : 0.8067
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	14	2.12025e+007	1.51447e+006	8.94	3.224e-007
Residual	30	5.08063e+006	1.69354e+005		
Total	44	2.62832e+007			

The standard deviation of the individal parameters (i.e. standard errors) are large in comparison with the parameters' values making the hypothesis testing of the individual coefficients (*bttest*) impractical. Hence, to determine the "optimal" model different model forms are tried and compared.

Other models fitted

The models fitted (in addition to the full second order model) are presented in Table 5.2. T represents the thickness in nanometers(nm), $sqh2s1$ the square root of the hydrogen flow (sccm) into segment 1, $sqh2s2$ the square root of the hydrogen flow (sccm) into segment 2, $sqh2s3$ the square root of the hydrogen flow (sccm) into segment 3, and gap is the distance between the showerhead and the wafer in mm.

Model 1

This model is a full first order of the form $T = b_0 + b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_4(gap)$. The results for segment 1 ($m1s1$) are:

Table 5.2: Models fitted

Model 1	$T = b_0 + b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_4(gap)$
Model 2	$T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3)$
Model 3	$T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_4(gap) + b_{12}(sqh2s1)(sqh2s2) + \ldots$ $b_{13}(sqh2s1)(sqh2s3) + b_{14}(sqh2s1)(gap) + b_{23}(sqh2s2)(sqh2s3) + \ldots$ $b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$
Model 4	$T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_4(gap) + \ldots$ $b_{14}(sqh2s1)(gap) + b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$
Model 5	$T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + \ldots$ $b_{14}(sqh2s1)(gap) + b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$

```
rsmodel object "m1s1"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b0 : -2.48147e+002 (2.13624e+002)
    b1 : 1.54984e+002 (2.39113e+001)
    b2 : 1.10413e+002 (2.39113e+001)
    b3 : 8.65440e+001 (2.39113e+001)
    b4 : 1.49412e+002 (4.85250e+001)

R^2 : 0.73913
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	4	1.94266e+007	4.85665e+006	28.33	3.363e-011
Residual	40	6.85656e+006	1.71414e+005		
Total	44	2.62832e+007			

Model 2

The second model forces the independent term and the gap term to be zero because if there is no hydrogen flow to any of the segments the deposition thickness should be zero regardless of the distance between the showerhead and the wafer. Thus, $T = b_1(sqh2s1)+b_2(sqh2s2)+b_3(sqh2s3)$. The parameter values and ANOVA tables resulting for segment 1 ($m2s1$) are:

```
rsmodel object "m2s1"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 1.69691e+002 (2.36619e+001)
    b2 : 1.25119e+002 (2.36619e+001)
    b3 : 1.01250e+002 (2.36619e+001)

R^2 : 0.66461
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	2	1.74681e+007	8.73405e+006	41.61	1.088e-010
Residual	42	8.81507e+006	2.09883e+005		
Total	44	2.62832e+007			

Model 3

Model 3 takes into account all the independent variables ($sqh2s2$, $sqh2s2$, $sqh2s3$, and gap) and their interactions. The form of the model is $T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_4(gap) + b_{12}(sqh2s1)(sqh2s2) + b_{13}(sqh2s1)(sqh2s3) + b_{14}(sqh2s1)(gap) + b_{23}(sqh2s2)(sqh2s3) + b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$.

The calculated b coefficients and ANOVA table for segment 1 are:

```
rsmodel object "m3s1"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 2.09081e+002 (7.04206e+001)
    b2 : 6.47923e+001 (7.04206e+001)
    b3 : 3.27484e+001 (7.04206e+001)
    b4 : 3.96112e+001 (1.14599e+002)
  b1,2 : 3.98821e+000 (1.14378e+001)
  b1,3 : -3.57487e+000 (1.14378e+001)
  b1,4 : -1.42772e+001 (1.92233e+001)
  b2,3 : -4.88963e+000 (1.14378e+001)
  b2,4 : 1.79405e+001 (1.92233e+001)
  b3,4 : 2.45039e+001 (1.92233e+001)

R^2 : 0.76257
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	9	2.00428e+007	2.22698e+006	12.49	1.421e-008
Residual	35	6.24034e+006	1.78295e+005		
Total	44	2.62832e+007			

Model 4

In the third model, the parameters of the flow interactions ($(sqh2s1)(sqh2s2)$, $(sqh2s1)(sqh2s3)$, and $(sqh2s2)(sqh2s3)$) are relatively small. Therefore, the fourth model does not take into account those interactions and is of the form $T = b_1(sqh2s1)+ b_2(sqh2s2)+b_3(sqh2s3)+b_4(gap)+b_{14}(sqh2s1)(gap)+b_{24}(sqh2s2)(gap)+b_{34}(sqh2s3)(gap)$.

The values for the parameters obtained when fitting this model to the data for segment 1 ($m4s1$) are:

```
rsmodel object "m4s1"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 2.02664e+002 (5.64551e+001)
    b2 : 5.91090e+001 (5.64551e+001)
    b3 : 2.21239e+001 (5.64551e+001)
    b4 : 5.98703e+001 (4.58022e+001)
  b1,4 : -1.45013e+001 (1.71118e+001)
  b2,4 : 1.72063e+001 (1.71118e+001)
  b3,4 : 2.14077e+001 (1.71118e+001)

R^2 : 0.75942
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	6	1.99601e+007	3.32668e+006	19.99	2.191e-010
Residual	38	6.32310e+006	1.66397e+005		
Total	44	2.62832e+007			

Model 5

Following the same logic as model 2 (i.e. the thickness should be zero when there is no hydrogen flow), the fifth model forces the "gap" term in Model 4 to be zero. Thus, $T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_{14}(sqh2s1)(gap) + b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$. The resulting b coefficients and ANOVA table for segment 1 ($m5s1$) are:

```
rsmodel object "m5s1"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 2.02485e+002 (5.69655e+001)
    b2 : 5.89298e+001 (5.69655e+001)
    b3 : 2.19447e+001 (5.69655e+001)
  b1,4 : -1.02229e+001 (1.69477e+001)
  b2,4 : 2.14847e+001 (1.69477e+001)
  b3,4 : 2.56862e+001 (1.69477e+001)

R^2 : 0.74861
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	5	1.96758e+007	3.93515e+006	23.23	9.566e-011
Residual	39	6.60741e+006	1.69421e+005		
Total	44	2.62832e+007			

Model comparison

At this point it is unclear which one is the best model; however Model 5 ($T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_{14}(sqh2s1)(gap) + b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$) makes physical sense. According to this model, the thickness depends strongly on the flow into that segment and less in the flow into the other two segments. Also, the $(sqh2s1)(gap)$, $(sqh2s2)(gap)$, and $(sqh2s3)(gap)$ take into account the diffusivity of the gases in and out of the segments. Thus, Model 5 is used as basis for the comparisons. In other words, this model will be compared to the other models using a 99% confidence limit ($\alpha = 0.01$) using the *comptest* function.

Full second order vs. Model 5

The comparison results for segment 1 are:

```
Co25S1 =

           p1: 15
           p2: 6
        ratio: 1.3005
    criticalr: 1.9200
       pvalue: 0.4600
   conclusion: 'model 1 IS NOT significantly better than model 2'
```

From these results it is clear that a full second order model does not represent a better fit to the data than a model of the form $T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_{14}(sqh2s1)(gap) + b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$.

Model 1 vs. Model 5

The results when the first order model form is compared to Model 5 for segments 1 ($C15S1$) are:

```
C15S1 =

           p1: 5
           p2: 6
        ratio: 1.0377
    criticalr: 1.1880
       pvalue: 0.2325
   conclusion: 'model 2 IS NOT significantly better than model 1'
```

From these it is infered that , statistically, Model 5 does not represent an improvement over Model 1. However, Model 1 is discarded due to physical reasons (i.e. the thickness has to be zero when the flowrates are zero). Note that, according to this reasoning, b_0 should be zero and in the results from Model 1 b_0 is of order 100.

Model 2 vs. Model 5

When Model 2 is compared to Model 5 the following results are obtained for segment 1:

```
C25S1 =

           p1: 3
           p2: 6
        ratio: 1.3341
    criticalr: 1.3329
       pvalue: 0.0098
   conclusion: 'model 2 IS significantly better than model 1'
```

In this case it is deduced that Model 5 is prefered over Model 2 with a confidence of 99%.

Model 3 vs. Model 5

The comparison of the results of applying Model 3 and Model 5 yield, for the data of segment 1:

```
C35S1 =

           p1: 10
           p2: 6
        ratio: 1.0588
    criticalr: 1.4467
       pvalue: 0.7254
   conclusion: 'model 1 IS NOT significantly better than model 2'
```

It can be concluded that the additional terms obtained when applying Model 3 do not generate a better fit than when Model 5 is applied.

Model 4 vs. Model 5

Finally, Model 4 is compared to Model 5. The results of this comparison for segment 1 ($C45S1$) are:

```
C45S1 =

           p1: 7
           p2: 6
        ratio: 1.0450
    criticalr: 1.1935
       pvalue: 0.1990
   conclusion: 'model 1 IS NOT significantly better than model 2'
```

These results show that the inclusion of the *gap* term is not statistically justified, and it does not make physical sense.

Thus, it can be concluded that Model 5 is the "optimal" form for the wafer thickness of this CVD process. Table 5.3 presents the measured thickness, the thickness predicted when using Model 5, and the residuals for segment 1.

Full Wafer Maps

The 45 wafers obtained using the SP-CVD reactor with the operating conditions shown in Table 5.1 are presented in Figures 5.3, 5.4, and 5.5. As in the case of the segments' center points, the entire wafer maps are fitted to a full second order model and to the model forms in Table 5.2.

Table 5.3: Predicted thickness (Model 5) and residuals for segment 1

T_{data}	T_{pred}	residual
1921.9	2071.1	-149.2
3662.9	2222.8	1440.1
2359.4	2244.0	115.5
2625.1	2230.0	395.2
1390.4	971.9	418.4
1060.1	698.0	362.2
1120.3	560.0	560.3
457.5	269.4	188.0
553.2	454.9	98.3
1117.1	1087.6	29.5
961.0	1811.9	-850.9
2436.0	1923.1	512.9
1873.9	1835.2	38.7
1386.4	1553.9	-167.5
2498.7	2588.4	-89.7
2729.1	2610.3	118.8
1482.8	2564.8	-1081.9
2827.4	2648.0	179.5
1125.0	856.3	268.8
892.6	941.0	-48.4
1086.4	850.7	235.8
525.4	560.0	-34.7
788.8	698.0	90.9
863.8	971.9	-108.1
2671.4	2230.0	441.4
2354.3	2244.0	110.3
2211.9	2222.8	-10.9
2220.1	2071.1	149.0
532.5	414.7	117.7
595.6	576.4	19.2
859.2	1029.8	-170.5
1898.0	2020.9	-122.9
1554.0	2083.5	-529.6
1812.5	2029.0	-216.5
1432.2	1812.5	-380.3
623.7	705.3	-81.7
885.5	819.5	66.0
1145.2	914.1	231.1
2341.9	2439.0	-97.1
2344.4	2404.4	-60.0
2287.7	2416.5	-128.9
1944.3	2329.7	-385.4
1364.5	1733.6	-369.1
1523.1	1524.9	-1.7
1998.9	1619.5	379.4

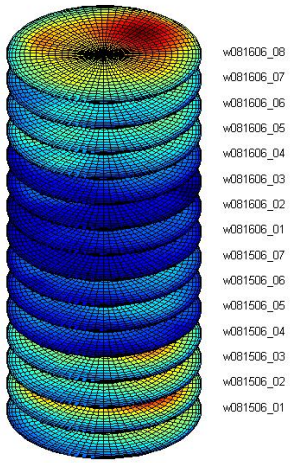

Figure 5.3: *SP-CVD reactor wafer maps 1 to 15*

Full second order model

The results when a full second order is fitted to the data are:

```
rsmodel object "P"

Parameters: mean value
----------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

  Term : mean value (mean std error)
-------------------------------------
    b0 : 2.35851e+002 (6.53083e+002)
    b1 : -5.30688e+000 (3.87618e+002)
    b2 : -2.17055e+002 (3.87618e+002)
    b3 : -7.39654e+000 (3.87618e+002)
    b4 : 2.18828e+002 (1.90656e+002)
  b1,1 : 3.03094e+000 (6.37483e+001)
  b1,2 : -7.00010e-001 (1.51722e+001)
  b1,3 : 1.79590e+001 (1.51722e+001)
  b1,4 : 8.85892e+000 (1.45570e+001)
  b2,2 : 3.61782e+001 (6.37483e+001)
  b2,3 : 5.46879e+000 (1.51722e+001)
  b2,4 : 1.69714e+001 (1.45570e+001)
  b3,3 : 1.40929e+000 (6.37483e+001)
  b3,4 : 1.04919e+001 (1.45570e+001)
  b4,4 : -3.35464e+001 (2.80943e+001)

mean(R^2) : 0.84881
```

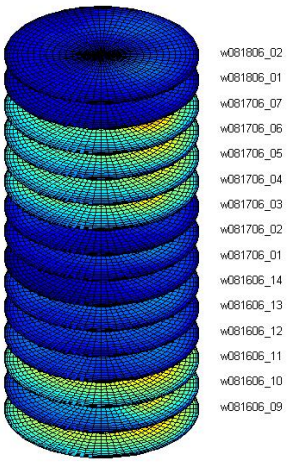

Figure 5.4: *SP-CVD reactor wafer maps 16 to 30*

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	14	1.68464e+007	1.20332e+006	11.57	1.697e-008
Residual	30	3.11957e+006	1.03986e+005		
Total	44	1.99660e+007			

The calculated b coefficients are shown in Figure 5.6. The *bttest* is not performed because of the large standard errors of the individual coefficients.

Other models fitted

Model 1

Model 1 has the form $T = b_0 + b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_4(gap)$. The results when the full wafer data is fitted to this model form is:

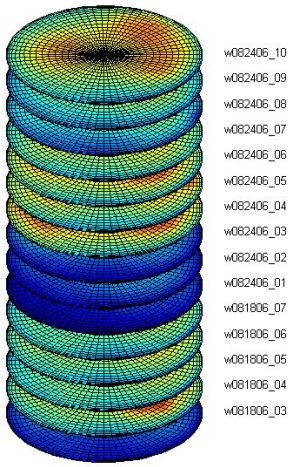

Figure 5.5: *SP-CVD reactor wafer maps 31 to 45*

```
rsmodel object "M1"

Parameters: mean value
----------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

  Term : mean value (mean std error)
-------------------------------------
    b0 : -3.14258e+002 (1.63571e+002)
    b1 : 1.01718e+002 (1.83087e+001)
    b2 : 1.04836e+002 (1.83087e+001)
    b3 : 9.67895e+001 (1.83087e+001)
    b4 : 1.58136e+002 (3.71553e+001)

mean(R^2) : 0.78955
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	4	1.56171e+007	3.90429e+006	35.91	9.615e-013
Residual	40	4.34886e+006	1.08721e+005		
Total	44	1.99660e+007			

Figure 5.7 shows the b coefficients calculated.

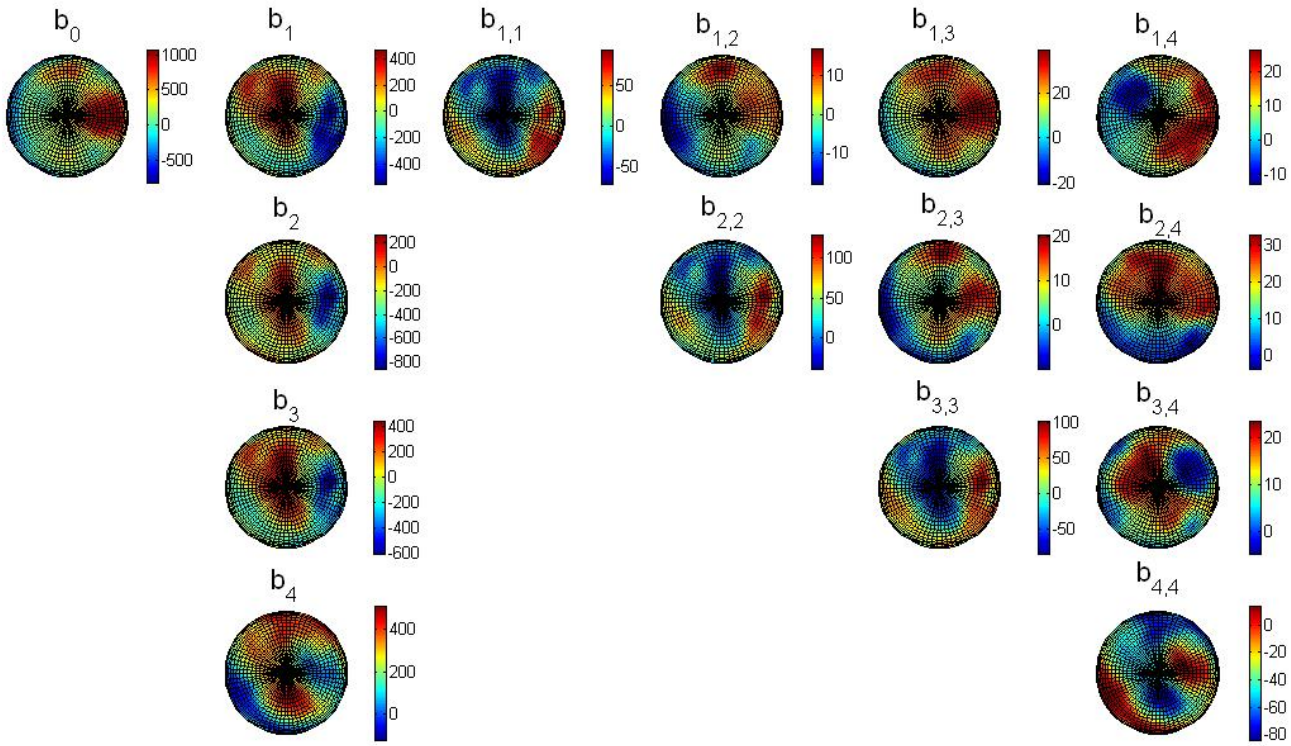

Figure 5.6: *SP-CVD second order b_j coefficients*

Model 2

The independent term and the gap term are forced to be zero in this model form (the thickness of a wafer should be zero if there is no hydrogen flow). Thus, $T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3)$. The model obtained when this form is fitted is:

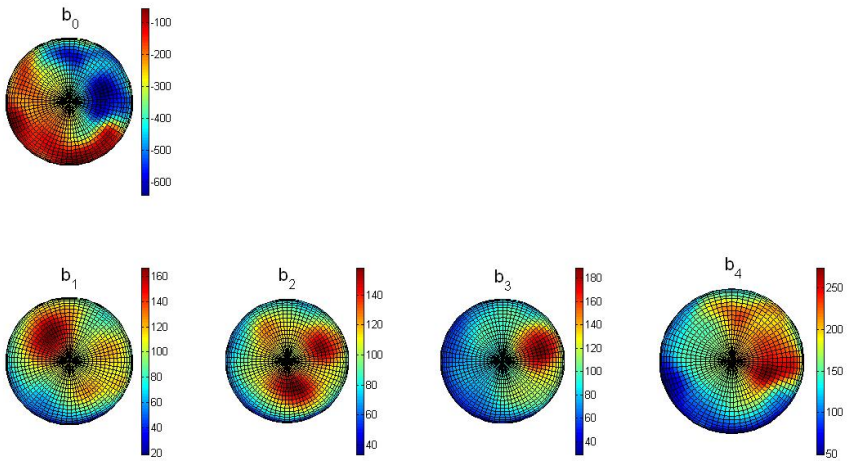

Figure 5.7: *SP-CVD Model 1 b_j coefficients*

```
rsmodel object "M2"

Parameters: mean value
----------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

  Term : mean value (mean std error)
-------------------------------------
    b1 : 1.13660e+002 (1.97492e+001)
    b2 : 1.16778e+002 (1.97492e+001)
    b3 : 1.08732e+002 (1.97492e+001)

mean(R^2) : 0.67838
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	2	1.33478e+007	6.67391e+006	42.35	8.499e-011
Residual	42	6.61817e+006	1.57576e+005		
Total	44	1.99660e+007			

The calculated coefficients are represented in Figure 5.8

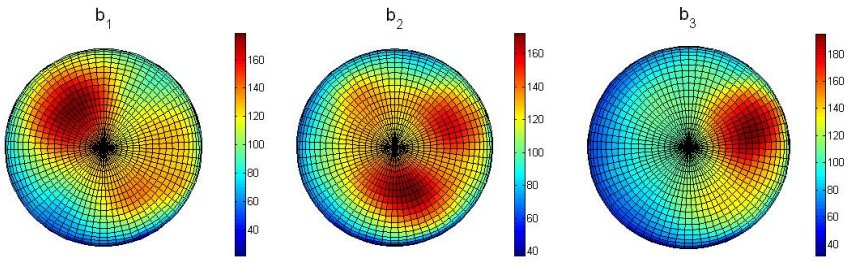

Figure 5.8: *SP-CVD Model 2 b_j coefficients*

Model 3

Model 3 has the form $T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_4(gap) + b_{12}(sqh2s1)(sqh2s2) + b_{13}(sqh2s1)(sqh2s3) + b_{14}(sqh2s1)(gap) + b_{23}(sqh2s2)(sqh2s3) + b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$. In other words, this form includes the independent variables and their interactions.

The results when the data is fitted to this form are:

```
rsmodel object "M3"

Parameters: mean value
----------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

  Term : mean value (mean std error)
-----------------------------------
    b1 : 8.48240e+001 (5.33688e+001)
    b2 : 7.95999e+001 (5.33688e+001)
    b3 : 6.70856e+001 (5.33688e+001)
    b4 : 3.60510e+001 (8.68500e+001)
  b1,2 : 2.07942e-001 (8.66825e+000)
  b1,3 : -1.64142e+000 (8.66825e+000)
  b1,4 : 8.22482e+000 (1.45685e+001)
  b2,3 : -1.00771e+000 (8.66825e+000)
  b2,4 : 1.05165e+001 (1.45685e+001)
  b3,4 : 1.28693e+001 (1.45685e+001)

mean(R^2) : 0.81176
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	9	1.60872e+007	1.78747e+006	16.13	5.078e-010
Residual	35	3.87875e+006	1.10822e+005		
Total	44	1.99660e+007			

Figure 5.9 shows the values of the b coefficients calculated.

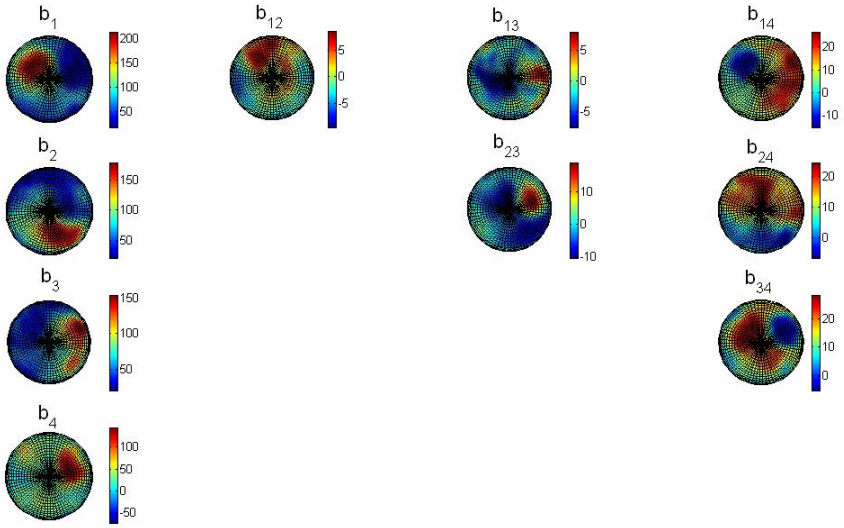

Figure 5.9: *SP-CVD Model 3 b_j coefficients*

Model 4

The fourth model ignores the interactions between the flows to the different segments and has the form $T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_4(gap) + b_{14}(sqh2s1)(gap) + b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$.

The average values of the parameters and the ANOVA Table obtained when fitting this model to the data are:

```
rsmodel object "M4"

Parameters: mean value
----------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

  Term : mean value (mean std error)
-------------------------------------
    b1 : 8.06351e+001 (4.29155e+001)
    b2 : 7.60183e+001 (4.29155e+001)
    b3 : 6.24629e+001 (4.29155e+001)
    b4 : 4.70995e+001 (3.48175e+001)
  b1,4 : 7.55986e+000 (1.30079e+001)
  b2,4 : 1.00374e+001 (1.30079e+001)
  b3,4 : 1.18022e+001 (1.30079e+001)

mean(R^2) : 0.80813
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	6	1.60113e+007	2.66854e+006	25.64	6.039e-012
Residual	38	3.95474e+006	1.04072e+005		
Total	44	1.99660e+007			

The calculated coefficients are represented in Figure 5.10.

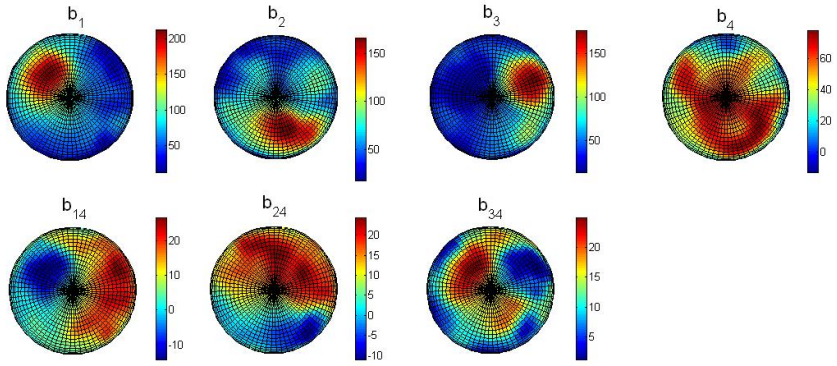

Figure 5.10: *SP-CVD Model 4 b_j coefficients*

Model 5

The last model to be fitted has the form $T = b_1(sqh2s1) + b_2(sqh2s2) + b_3(sqh2s3) + b_{14}(sqh2s1)(gap) + b_{24}(sqh2s2)(gap) + b_{34}(sqh2s3)(gap)$. The resulting b coefficients can be found in Figure 5.11. The mean values of these coefficients and

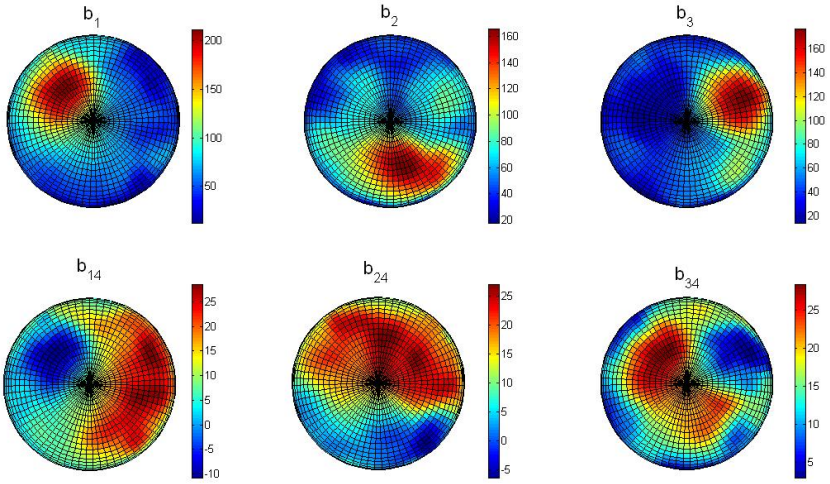

Figure 5.11: *SP-CVD Model 5 b_j coefficients*

the ANOVA table for the model are:

```
rsmodel object "M5"

Parameters: mean value
----------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

  Term : mean value (mean std error)
-------------------------------------
    b1 : 8.04941e+001 (4.35790e+001)
    b2 : 7.58773e+001 (4.35790e+001)
    b3 : 6.23219e+001 (4.35790e+001)
  b1,4 : 1.09257e+001 (1.29651e+001)
  b2,4 : 1.34032e+001 (1.29651e+001)
  b3,4 : 1.51680e+001 (1.29651e+001)

mean(R^2) : 0.79626
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	5	1.58088e+007	3.16176e+006	29.66	2.624e-012
Residual	39	4.15719e+006	1.06595e+005		
Total	44	1.99660e+007			

Model comparison

Model 5 takes into account the dependence of the thickness on the hydrogen flow to the different segments and the interaction between the flows and the gap that represent the diffusivity of the gases in and out of the segments making it a physically feasible model. For this reason, the *comptest* function is used to compare all models against Model 5. The comparisons are made using a significance level of 0.01 (i.e. confidence level of 99%) and considering a point percentage of at least 75%.

The result when the full second order model is compared to Model 5 is:

```
Co25 =

               p1: 15
               p2: 6
    pointpercentage: 42.8913
         meanpvalue: 0.3866
          criticalr: 1.9200
         conclusion: 'model 1 IS NOT significantly better than model 2'
```

This shows that Model 5 is a better fit to the data than the full second order model.

When Model 1 is compared to Model 5 the following result is obtained:

```
C15 =

               p1: 5
               p2: 6
    pointpercentage: 48.6080
         meanpvalue: 0.1877
          criticalr: 1.1880
         conclusion: 'model 2 IS NOT significantly better than model 1'
```

As for the center points case, Model 5 does not represent a significant improvement over Model 1. Nevertheless Model 5 is prefered over Model 1 due to physical reasons.

The comparison between Model 2 and Model 5 yields:

```
C25 =

               p1: 3
               p2: 6
    pointpercentage: 65.6806
         meanpvalue: 3.7153e-004
          criticalr: 1.3329
         conclusion: 'model 2 IS NOT significantly better than model 1'
```

This result shows that Model 5 is not considered better than Model 2 for more than 75% of the points. However, the point percentage indicates that Model 5 is prefered over Model 2 in 65% of the points.

Model 3 is also compared to Model 5 and the result shows that the additional terms of Model 3 do not represent an improvement.

```
C35 =

               p1: 10
               p2: 6
    pointpercentage: 36.8968
         meanpvalue: 0.6456
          criticalr: 1.4467
         conclusion: 'model 1 IS NOT significantly better than model 2'
```

Finally, Model 4 and Model 5 are compared demostrating that Model 5 is prefered over Model 4.

```
C45 =

               p1: 7
               p2: 6
    pointpercentage: 52.0230
         meanpvalue: 0.1712
          criticalr: 1.1935
         conclusion: 'model 1 IS NOT significantly better than model 2'
```

Considering the results obtained and the physical knowledge of the system, it can be concluded that Model 5 is the optimal representation for the tungsten deposition in the Spatially Programmable Chemical Vapor Deposition reactor.

A predicted wafer using this model and same operation condition as wafers *w081506_01* and *w081706_07* ($H_2s1 = 16$ sccm, $H_2s2 = 32$ sccm, $H_2s3 = 48$ sccm, and $gap = 3$ mm) is compared to the average of these two wafers in Figure 5.12.

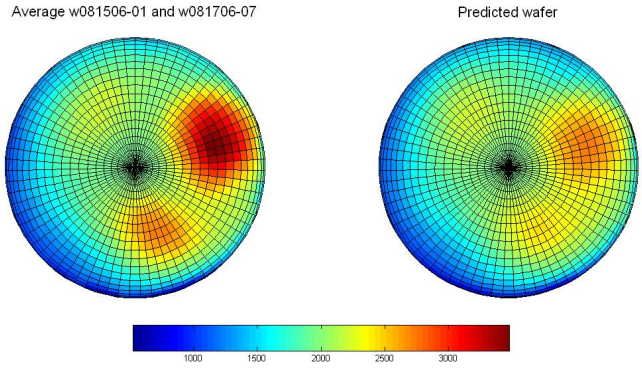

Figure 5.12: *Average wafer and predicted wafer*

Chapter 6

Conclusions and Suggestions for Future Work

The usefulness of the computational toolbox was demonstrated in Chapter 4 using artificially generated data. Afterwards, the toolbox was used to calculate a response surface model for wafers obtained in the Spatially Programmable Chemical Vapor Deposition (SP-CVD) reactor. It is important to note that, even though the calculated model is basically empirical, when any of the physical or chemical principles of the system are known they should be taken into account. Thus, the calculated model for the SP-CVD data, based on the known kinetics of the reaction, uses the square root of the hydrogen flowrates as independent variables.

When the SP-CVD data was analyzed a model of the form $T = b_1(sqh2s1) + b_2(sqh2s2)+b_3(sqh2s3)+b_{14}(sqh2s1)(gap)+b_{24}(sqh2s2)(gap)+b_{34}(sqh2s3)(gap)$ was found to be the most appropriate fit. This conclusion was based in both statistical and physical reasons.

Current work regarding the computational toolbox consists on the development of a graphical user interface (GUI) called *waferview* design for viewing and analyzing wafer objects. This interface compiles the functions discussed in Chapter 3 and more in a user-friendly environment. Another purpose of *waferview* is to automate the toolbox functions as much as possible. Figures 6.1 and 6.2 show two of the windows of this interface.

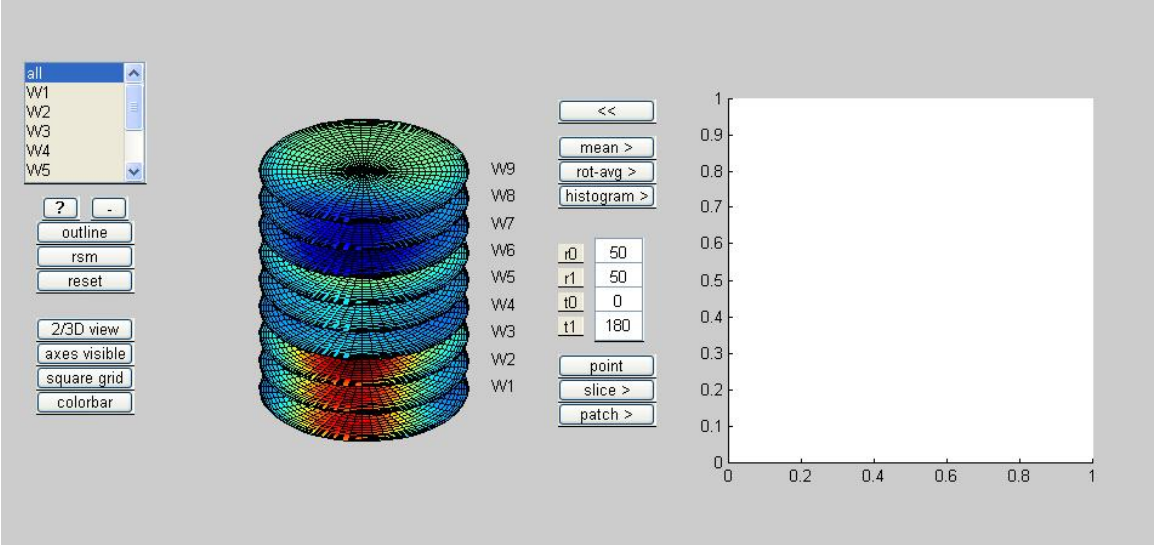

Figure 6.1: *Wafer view*

A future research objective make the necessary modifications to the functions in order to expand the use of the library to other types of substrates. For instance, the computational toolbox could be applied to planetary reactors and rectangular-shaped substrates as the ones used by Hyett and Park in [6].

The large variability of the SP-CVD reactor data bounds the use of the toolbox (i.e. *bttest* cannot be applied), thus more systems should be studied to allow the refinement of the toolbox and make it more useful for combinatorial processes.

Currently, the full wafer analysis of variance is based on a weighted average of the individual grid point's analysis. This is not necessarilly the best approach, thus a more rigorous analysis of the ANOVA for full wafers and distributed parameters should be developed.

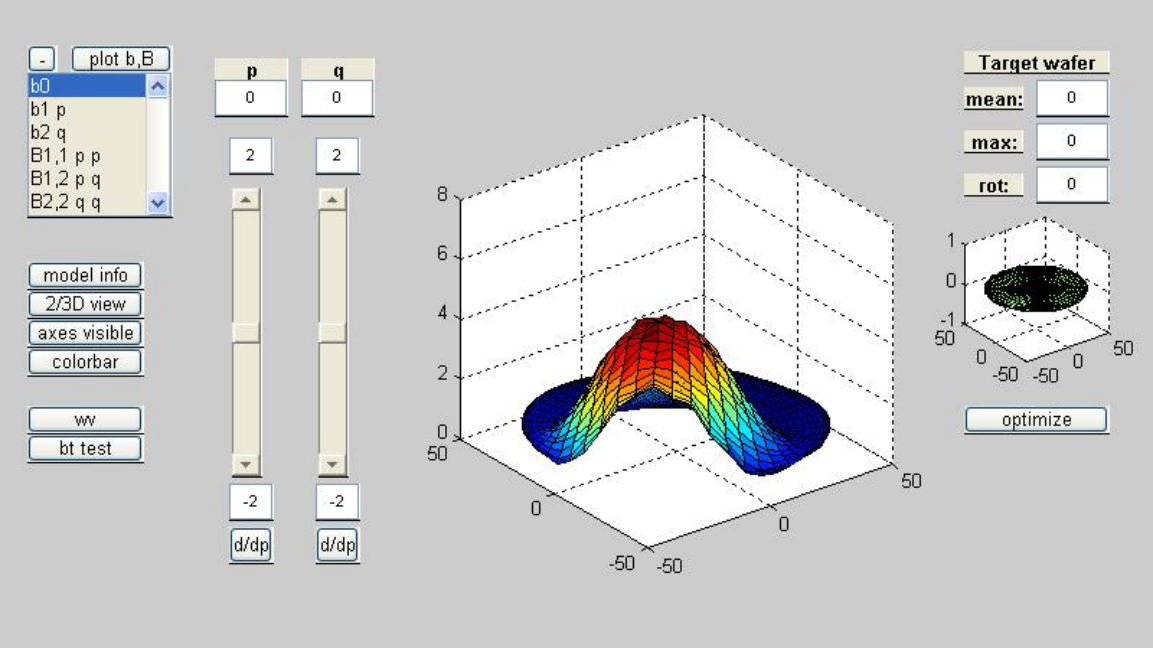

Figure 6.2: *Wafer RSModel view*

Appendix A

Single Point Analysis Results for Segment 2 and Segment 3

Full Second Order Model

The coefficients and ANOVA table obtained when a full second order model is fit to segment 2 (P2) are:

```
rsmodel object "P2"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b0 : 3.42446e+002 (6.57419e+002)
    b1 : 2.76345e+001 (3.90191e+002)
    b2 : -5.90896e+001 (3.90191e+002)
    b3 : 1.17728e+002 (3.90191e+002)
    b4 : 3.71628e+002 (1.91922e+002)
  b1,1 : -1.50451e+001 (6.41715e+001)
  b1,2 : 2.49426e+000 (1.52729e+001)
  b1,3 : 2.38675e+001 (1.52729e+001)
  b1,4 : 1.66108e+001 (1.46537e+001)
  b2,2 : 1.36750e+001 (6.41715e+001)
  b2,3 : 1.17059e+001 (1.52729e+001)
  b2,4 : 6.19871e+000 (1.46537e+001)
  b3,3 : -2.92425e+001 (6.41715e+001)
  b3,4 : 1.47716e+001 (1.46537e+001)
  b4,4 : -6.05300e+001 (2.82808e+001)

R^2 : 0.8677
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	14	1.90941e+007	1.36387e+006	14.05	1.634e-009
Residual	30	2.91128e+006	9.70428e+004		
Total	44	2.20054e+007			

The coeffients and ANOVA table for the second order model fitted to the center point of segment 3 (P3) are:

```
rsmodel object "P3"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b0 : 7.27228e+002 (1.10524e+003)
    b1 : -6.44817e+001 (6.55983e+002)
    b2 : -4.87503e+002 (6.55983e+002)
    b3 : -2.18022e+002 (6.55983e+002)
    b4 : 1.41933e+002 (3.22656e+002)
  b1,1 : -2.80935e+000 (1.07884e+002)
  b1,2 : 9.88785e+000 (2.56765e+001)
  b1,3 : 3.57255e+001 (2.56765e+001)
  b1,4 : 1.37147e+001 (2.46355e+001)
  b2,2 : 6.70991e+001 (1.07884e+002)
  b2,3 : 1.55266e+001 (2.56765e+001)
  b2,4 : 2.69077e+001 (2.46355e+001)
  b3,3 : 3.95721e+001 (1.07884e+002)
  b3,4 : -3.76855e+000 (2.46355e+001)
  b4,4 : -7.56192e+000 (4.75452e+001)

R^2 : 0.80806
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	14	3.46409e+007	2.47435e+006	9.02	2.927e-007
Residual	30	8.22839e+006	2.74280e+005		
Total	44	4.28693e+007			

Other Models Fitted

Model 1

The results when Model 1 is fitted to the center point thickness of segment 2 ($m1s2$) and segment 3 ($m1s3$) are:

```
rsmodel object "m1s2"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b0 : -2.43902e+002 (1.69036e+002)
    b1 : 9.88573e+001 (1.89204e+001)
    b2 : 1.39361e+002 (1.89204e+001)
    b3 : 9.86969e+001 (1.89204e+001)
    b4 : 1.52599e+002 (3.83967e+001)

R^2 : 0.80491
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	4	1.77124e+007	4.42810e+006	41.26	1.090e-013
Residual	40	4.29303e+006	1.07326e+005		
Total	44	2.20054e+007			

```
rsmodel object "m1s3"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b0 : -6.28456e+002 (2.62981e+002)
    b1 : 1.17435e+002 (2.94359e+001)
    b2 : 1.52686e+002 (2.94359e+001)
    b3 : 1.80203e+002 (2.94359e+001)
    b4 : 2.30650e+002 (5.97365e+001)

R^2 : 0.75761
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	4	3.24783e+007	8.11958e+006	31.26	7.914e-012
Residual	40	1.03910e+007	2.59774e+005		
Total	44	4.28693e+007			

Model 2

The estimated parameters and ANOVA tables obtained when Model 2 is fitted to segment 2 ($m2s2$) and to segment 3 ($m2s3$) are:

```
rsmodel object "m2s2"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 1.14546e+002 (2.01099e+001)
    b2 : 1.55050e+002 (2.01099e+001)
    b3 : 1.14386e+002 (2.01099e+001)

R^2 : 0.71065


                                          ANOVA Table
-------------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)               (MS)
-------------------------------------------------------------------------------------
Regression           2          1.56382e+007         7.81912e+006    51.58    4.895e-012
Residual            42          6.36718e+006         1.51599e+005
Total               44          2.20054e+007


rsmodel object "m2s3"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 1.22916e+002 (3.01524e+001)
    b2 : 1.58167e+002 (3.01524e+001)
    b3 : 1.85683e+002 (3.01524e+001)

R^2 : 0.66609


                                          ANOVA Table
-------------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)               (MS)
-------------------------------------------------------------------------------------
Regression           2          2.85550e+007         1.42775e+007    41.89    9.911e-011
Residual            42          1.43143e+007         3.40817e+005
Total               44          4.28693e+007
```

Model 3

The calculated b coefficients and ANOVA table for segment 2 are:

```
rsmodel object "m3s2"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 6.80329e+001 (5.56967e+001)
    b2 : 1.58214e+002 (5.56967e+001)
    b3 : 6.27299e+001 (5.56967e+001)
    b4 : 4.05121e+001 (9.06384e+001)
  b1,2 : 6.75103e-001 (9.04636e+000)
  b1,3 : -9.06858e-001 (9.04636e+000)
  b1,4 : 1.33578e+001 (1.52040e+001)
  b2,3 : -4.17246e+000 (9.04636e+000)
  b2,4 : -1.09659e+000 (1.52040e+001)
  b3,4 : 1.74242e+001 (1.52040e+001)

R^2 : 0.82261
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	9	1.81018e+007	2.01131e+006	18.03	1.108e-010
Residual	35	3.90362e+006	1.11532e+005		
Total	44	2.20054e+007			

The calculated b coefficients and ANOVA table for segment 3 are:

```
rsmodel object "m3s3"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 2.09421e+001 (8.69897e+001)
    b2 : 4.07738e+001 (8.69897e+001)
    b3 : 1.27410e+002 (8.69897e+001)
    b4 : 1.29849e+002 (1.41563e+002)
  b1,2 : 1.07791e+000 (1.41290e+001)
  b1,3 : 2.23049e+000 (1.41290e+001)
  b1,4 : 1.79569e+001 (2.37463e+001)
  b2,3 : 1.85719e+001 (1.41290e+001)
  b2,4 : 1.52900e+001 (2.37463e+001)
  b3,4 : -4.97706e+000 (2.37463e+001)

R^2 : 0.77787
```

```
                                        ANOVA Table
-------------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)              (MS)
-------------------------------------------------------------------------------------
Regression           9          3.33469e+007         3.70521e+006    13.62    4.724e-009
Residual            35          9.52236e+006         2.72067e+005
Total               44          4.28693e+007
```

Model 4

The values for the parameters obtained when fitting this model to the data for segment 2 ($m4s2$) and segment 3 ($m4s3$) are:

```
rsmodel object "m4s2"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 6.18897e+001 (4.45097e+001)
    b2 : 1.50885e+002 (4.45097e+001)
    b3 : 5.38437e+001 (4.45097e+001)
    b4 : 6.04450e+001 (3.61109e+001)
  b1,4 : 1.29012e+001 (1.34911e+001)
  b2,4 : -2.63221e+000 (1.34911e+001)
  b3,4 : 1.54272e+001 (1.34911e+001)

R^2 : 0.82139


                                        ANOVA Table
-------------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)              (MS)
-------------------------------------------------------------------------------------
Regression           6          1.80751e+007         3.01251e+006    29.13    8.850e-013
Residual            38          3.93037e+006         1.03431e+005
Total               44          2.20054e+007
```

```
rsmodel object "m4s3"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 5.20301e+001 (7.09968e+001)
    b2 : 7.89815e+001 (7.09968e+001)
    b3 : 1.69193e+002 (7.09968e+001)
    b4 : 3.08210e+001 (5.76000e+001)
  b1,4 : 2.09516e+001 (2.15194e+001)
  b2,4 : 2.36102e+001 (2.15194e+001)
  b3,4 : 3.52691e+000 (2.15194e+001)

R^2 : 0.76673
```

ANOVA Table

Source of Variation	degrees of freedom (dof)	Sum of Squares (SS)	Mean Square (MS)	fo	P-value
Regression	6	3.28692e+007	5.47821e+006	20.82	1.242e-010
Residual	38	1.00001e+007	2.63159e+005		
Total	44	4.28693e+007			

Model 5

The resulting b coefficients and ANOVA table for segment 2 ($m5s2$), and segment 3 ($m5s3$) are:

```
rsmodel object "m5s2"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 6.17088e+001 (4.55262e+001)
    b2 : 1.50704e+002 (4.55262e+001)
    b3 : 5.36628e+001 (4.55262e+001)
  b1,4 : 1.72207e+001 (1.35444e+001)
  b2,4 : 1.68730e+000 (1.35444e+001)
  b3,4 : 1.97467e+001 (1.35444e+001)

R^2 : 0.80822
```

```
                                        ANOVA Table
-------------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)              (MS)
-------------------------------------------------------------------------------------
Regression           5          1.77853e+007         3.55705e+006    32.87    5.436e-013
Residual            39          4.22017e+006         1.08209e+005
Total               44          2.20054e+007


rsmodel object "m5s3"

Parameters: mean value
----------------------
sqh2s1 : 3.9713
sqh2s2 : 3.9713
sqh2s3 : 3.9713
gap : 3.0667
Those used in model:
    'sqh2s1'    'sqh2s2'    'sqh2s3'    'gap'

 Terms :   Bcoeff     (std error)
---------------------------------
    b1 : 5.19378e+001 (7.03440e+001)
    b2 : 7.88892e+001 (7.03440e+001)
    b3 : 1.69101e+002 (7.03440e+001)
  b1,4 : 2.31541e+001 (2.09279e+001)
  b2,4 : 2.58127e+001 (2.09279e+001)
  b3,4 : 5.72944e+000 (2.09279e+001)

R^2 : 0.76497


                                        ANOVA Table
-------------------------------------------------------------------------------------
Source of   degrees of freedom   Sum of Squares     Mean Square      fo     P-value
Variation         (dof)              (SS)              (MS)
-------------------------------------------------------------------------------------
Regression           5          3.27939e+007         6.55878e+006    25.39    2.653e-011
Residual            39          1.00754e+007         2.58344e+005
Total               44          4.28693e+007
```

Model Comparison

Full second order vs. Model 5

The results for segment 2 ($Co25S2$) and segment 3 ($Co25S3$) for the comparison of the full second order model to Model 5 with a 99% confidence are:

```
Co25S2 =

           p1: 15
           p2: 6
        ratio: 1.4496
     criticalr: 1.9200
       pvalue: 0.1937
   conclusion: 'model 1 IS NOT significantly better than model 2'
```

```
Co25S3 =

           p1: 15
           p2: 6
        ratio: 1.2245
     criticalr: 1.9200
       pvalue: 0.6629
    conclusion: 'model 1 IS NOT significantly better than model 2'
```

Model 1 vs. Model 5

The results when the first order model form is compared to Model 5 for segments 2 ($C15S2$), and 3 ($C15S3$) are:

```
C15S2 =

           p1: 5
           p2: 6
        ratio: 1.0173
     criticalr: 1.1880
       pvalue: 0.4169
    conclusion: 'model 2 IS NOT significantly better than model 1'


C15S3 =

           p1: 5
           p2: 6
        ratio: 1.0313
     criticalr: 1.1880
       pvalue: 0.2758
    conclusion: 'model 2 IS NOT significantly better than model 1'
```

Model 2 vs. Model 5

The results obtained when Model 2 is compared to Model 5 for the data in segment 2 are:

```
C25S2 =

           p1: 3
           p2: 6
        ratio: 1.5087
     criticalr: 1.3329
       pvalue: 0.0010
    conclusion: 'model 2 IS significantly better than model 1'
```

and for segment 3:

```
C25S3 =

           p1: 3
           p2: 6
        ratio: 1.4207
     criticalr: 1.3329
        pvalue: 0.0031
    conclusion: 'model 2 IS significantly better than model 1'
```

Model 3 vs. Model 5

The results when Model 3 is compared to Model 5 for segment 2 ($C35S2$) and segment 3 ($C35S3$) are:

```
C35S2 =

           p1: 10
           p2: 6
        ratio: 1.0811
     criticalr: 1.4467
        pvalue: 0.5909
    conclusion: 'model 1 IS NOT significantly better than model 2'


C35S3 =

           p1: 10
           p2: 6
        ratio: 1.0581
     criticalr: 1.4467
        pvalue: 0.7300
    conclusion: 'model 1 IS NOT significantly better than model 2'
```

Model 4 vs. Model 5

The results when Model 4 is compared to Model 5 are,

for segment 2:

```
C45S2 =

           p1: 7
           p2: 6
        ratio: 1.0737
     criticalr: 1.1935
        pvalue: 0.1024
    conclusion: 'model 1 IS NOT significantly better than model 2'
```

and for segment 3:

```
C45S3 =

            p1: 7
            p2: 6
         ratio: 1.0075
     criticalr: 1.1935
        pvalue: 0.5957
    conclusion: 'model 1 IS NOT significantly better than model 2'
```

Predictions and Residuals

Tables A.1, and A.2 present the measured thickness, the thickness predicted when using Model 5, and the residuals for segment 2 and segment 3, respectively.

Table A.1: Predicted thickness (Model 5) and residuals for segment 2

T_{data}	T_{pred}	residual
2180.6	2116.8	63.8
3013.0	2172.1	840.8
2331.9	2047.2	284.7
2674.4	2161.1	513.3
862.3	641.3	220.9
1419.7	881.1	538.6
1149.3	638.7	510.6
559.4	415.3	144.2
893.9	862.1	31.9
506.5	446.5	60.0
1036.7	1723.8	-687.1
1507.0	1571.7	-64.6
1786.6	1795.9	-9.3
1553.9	1686.4	-132.5
2392.1	2547.3	-155.2
2628.2	2548.3	79.9
2191.5	2522.7	-331.2
2627.7	2598.5	29.2
1020.8	836.2	184.6
986.6	900.2	86.3
1068.1	862.1	206.1
747.9	638.7	109.2
1042.7	881.1	161.5
674.3	641.3	32.9
2448.7	2161.1	287.5
2257.8	2047.2	210.6
2411.4	2172.1	239.3
2558.5	2116.8	441.7
615.9	527.0	88.9
869.2	871.6	-2.4
702.5	543.9	158.6
2157.8	1942.5	215.3
1575.8	1809.4	-233.6
1735.1	1984.0	-248.9
1498.2	1901.6	-403.4
614.8	750.4	-135.6
909.1	890.7	18.4
844.3	738.7	105.6
2111.0	2379.8	-268.8
1736.0	2285.0	-548.9
2146.5	2360.2	-213.7
1726.8	2332.1	-605.3
1234.6	1629.4	-394.8
1543.1	1641.1	-98.0
1739.4	1489.1	250.3

Table A.2: Predicted thickness (Model 5) and residuals for segment 3

T_{data}	T_{pred}	residuals
3318.9	2660.6	658.4
3944.0	2515.0	1429.0
2588.0	2520.2	67.8
2877.2	2624.9	252.4
905.3	686.7	218.6
1046.2	884.3	161.9
1570.5	1053.8	516.6
792.2	989.0	-196.8
436.4	592.3	-155.9
387.0	424.8	-37.8
1303.9	2006.1	-702.2
2304.5	1928.1	376.4
1999.0	1849.5	149.5
2418.1	2103.9	314.2
3738.3	3217.2	521.1
3693.5	3180.4	513.0
2055.5	3112.4	-1056.9
4051.4	3243.7	807.7
1360.4	948.7	411.7
1287.2	1176.4	110.8
1322.2	1118.6	203.5
1016.6	1053.8	-37.2
879.2	884.3	-5.2
704.4	686.7	17.6
2884.5	2624.9	259.6
2550.3	2520.2	30.1
2214.8	2515.0	-300.2
3236.8	2660.6	576.2
754.7	1021.4	-266.7
936.9	738.3	198.6
699.5	555.8	143.7
2128.1	2315.5	-187.4
1637.3	2224.1	-586.8
1621.7	2182.2	-560.5
2597.1	2382.2	214.9
792.3	1086.2	-293.9
924.9	1030.3	-105.5
1046.1	817.7	228.4
2487.1	2934.3	-447.2
2165.3	2816.3	-651.0
2096.9	2847.7	-750.8
2169.2	2938.9	-769.7
1344.3	1848.1	-503.7
1616.8	2116.6	-499.7
2120.6	1903.9	216.6

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