PRODUCT DESIGN VIA PLS MODELING: STEPPING OUT OF HISTORICAL DATA INTO UNKNOWN OPERATING SPACE

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Abstract: A product design and analysis method is given in this paper to step out of the historical data space to search for operating conditions meeting new quality specifications. Iterative piecewise PLS modelling is adopted as the implementation framework for this purpose. The historical linear PLS model is extended systemically and iteratively to track the likely nonlinear property in the newly discovered operating space. Application to an injection molding process shows the good feasibility of the proposed method.

Keywords: Product design, Multivariate quality control, Modelling, Piecewise analysis, Iterative method.

1. INTRODUCTION

Modern industrial processes can be operated over a range of operating conditions to produce a wide variety of products to meet the rapidly changing market. To respond to such frequent product changeover, it is necessary to develop methods that can quickly and economically find new operating conditions to achieve the desired product qualities. Existing solutions to this subject can be grouped into three categories: theoretical model based, design of experiment (DoE) based, and experience based. Although theoretical model can cover complete operating space, such a model is rarely available due to complicated process physical and chemical behaviours. Factorial design of experiment can provide balanced and representative data covering the design space. The number of experiment can be still large for a process with large number of variables. Experience based methods are highly dependent on the knowledge of the experts, and they are applicable only to specific processes.

For a modern industrial process, there exists many historical data that can be explored to reveal the relationship between the existing product and its corresponding operating condition. For a new quality specification, it may be useful to start with the analysis of the historical data using multivariate statistical methods to extract information guiding experiments for searching for operating conditions to meet the new product requirement. This procedure is referred as product design via multivariate analysis. The first work was reported by Moteki & Arai (1986), where Principal Component Analysis (PCA) is combined with a theoretical method for operation planning and quality design. More recently, Jaeckle & MacGregor (1998) developed a methodology based on latent variable techniques using historical data to determine a window of process operating conditions for new quality specifications. This method has been successfully applied to a semi-batch emulsion polymerization process and a batch solution polymerization process (Jaeckle and MacGregor, 2000). Industrial case study has been reported by Chen & Wang (2000) and Sebzalli & Wang (2001), using PCA and clustering method to identify operating spaces and operating strategies for desired products. A product design method combining PCA with genetic programming has also been reported by

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Lakshminarayanan et al. (2000) to determine new operating conditions.

The above methods are all data-based with a common implicit assumption that new product quality specifications and operating conditions are within the range and structure of historical data. This assumption, stated in the work of Jaeckle & MacGregor (1998), will limit the applications to a certain degree. For many industrial processes, it may be common that the process has been only operated in the past under certain specific operating conditions, which span only a narrow subspace of the entire feasible operating space. The operating condition for a new quality specification may be highly likely to be outside, rather than within, the range of historical data. It is thus necessary to develop methods to search for operating conditions outside the historical envelope. This paper attempts to do so. Section 2 analyzes possible conditions when stepping out of the historical data into new operating space. An iterative piecewise PLS modelling method is proposed in section 3 as a possible solution to the problem. The results are illustrated on an injection molding process in section 4. Finally, conclusions are drawn in section 5.

2. PROBLEM ANALYSIS

Let's first have a brief review on the key ideas of the existing methods. Based on the available historical data, the existing methods attempt to build an empirical model (M_{method}) between operating conditions (X) and product quality (Y). Under the assumption that the relationship between new product quality $\mathbf{y}_{des}$ and new operating condition $\mathbf{x}_{new}$ still obey the model (M_{method}), the new operating condition is obtained by $\mathbf{x}_{new}^T = \mathbf{y}_{des}^T \cdot M_{method}^T$ (Jaeckle & MacGregor, 1998).

For industrial processes, if the historical database indeed covers the entire operating space, the existing methods can be directly and successfully applied. This, however, is a quite ideal case. It is more likely that the historical data is only a small sub-set of the full scope of products. For this case, we should consider the following two scenarios: Scenario A, where the historical model (M_{method}) can be applicable to new operating space, and Scenario B, where the historical model can no longer be accurately applied in the new operating space. As the behaviour over the entire product range is typically nonlinear for many industrial processes, Scenario B can widely exist, which is the focus of this paper.

One-dimensional examples are given in Fig. 1 to illustrate the two scenarios, where Fig.1(a) is for Scenario A and Fig.1(b) is for Scenario B. The rectangle represents the historical operating region; solid line is the true model (f_*) over the entire operating space; the dashed line is the model (f_0) derived from the limited historical data. Generally, the true model, i.e., the global model, is nonlinear; while the historical model, i.e., the local model, may be linear for most industrial processes over a narrow operating space, as shown in Fig. 1(b).

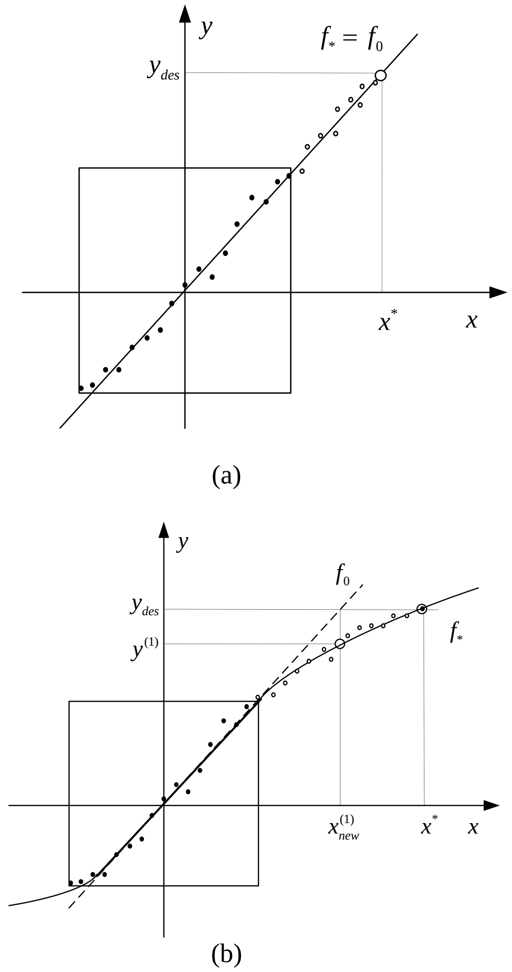


Fig. 1. Illustration of two scenarios in discovering new operating space
(a) Scenario A; (b) Scenario B.

For Scenario A, the local model can be directly applied to new operating space. But for Scenario B, the operating condition ($x_{new}^{(1)}$) obtained from the historical model (f_0) result in the actual quality ($y^{(1)}$), rather than the desired quality (y_{des}). To find the desired operating condition (x^*), relationship between product qualities and operating conditions in the new operating space is necessary. Product design in this case can be viewed as a coupled procedure of model updating. The challenge in such model updating lies in that, there is no data available in the unknown operating space. New experiments need to be designed in searching for the desired operating condition quickly and economically. New model in the desired local operating space can be typically represented by a linear model; a procedure needs to be developed for obtaining such a model to track the globally nonlinear process behaviour.

Based on the above analysis, a strategy is proposed in the next section to migrate the historical model to new operating space in the frame of PLS modelling for the aforementioned product design issue.

3. METHODOLOGY

In the following, we assume that, (1) a set of historical data is available, consisting of existing product quality (Y) and the corresponding settings on all manipulated process variables (X); (2) X and Y have been mean-centred and scaled; (3) a PLS model, introduced in section 3.1, has been built on X and Y, which can represent the relationship between X and Y in the historical data space; (4) new quality specification is feasible for the process, satisfying all physical constraints; (5) In the entire operating space of the process, the relationship between operating conditions and qualities changes mildly and continuously.

3.1 PLS

Partial Least Squares (PLS) is a popular regression method that can project high dimensional correlated process data down to a few number of latent variables and then model the latent variables by one-dimensional linear regression. It had many successful applications in process monitoring, fault detection and diagnosis, quality prediction, product design, etc. Mathematically, PLS is formulated by an outer relationship in X and Y (Eq.1) and an inner relationship between X and Y (Eq.2),

$$\begin{aligned} X &= T \cdot P^T + E = \sum_a \mathbf{t}_a \mathbf{p}_a^T + E \\ Y &= U \cdot Q^T + F = \sum_a \mathbf{u}_a \mathbf{q}_a^T + F \end{aligned} \quad (1)$$

$$\begin{aligned} \mathbf{u}_a &= \mathbf{t}_a \cdot b_a + r \\ b_a &= \mathbf{u}_a^T \mathbf{t}_a / \mathbf{t}_a^T \mathbf{t}_a \\ (a &= 1, \cdots, A) \end{aligned} \quad (2)$$

where $\{\mathbf{t}_a, \mathbf{u}_a\}$ is a pair of latent variables in X and Y spaces; $\{\mathbf{p}_a, \mathbf{q}_a\}$ are the corresponding loading matrices; T, U, P and Q are in the matrix form; E, F and r are model residuals; *a* is the index of latent variable; and *A* is the number of latent variables retained. The detailed PLS algorithm can be found in literature (Geladi and Kowalski, 1986; Höskuldsson, 1988).

3.2 Piecewise regression

Piecewise regression is a popular nonlinear regression method, where linear regression models over different regions are lumped together to approximate a globally nonlinear model. The simplest piecewise-regression model that joins two straight lines sharply at the changepoint is formulated as,

$$y = \begin{cases} f_1(x, \theta_1) & x \le \alpha \\ f_2(x, \theta_2) & x > \alpha \end{cases} \quad (3)$$

where the model parameters θ and the changepoint α are typically unknown and must be estimated. For details on piecewise regression, one can refer to the literature (Seber and Wild, 1989).

3.3 Iterative piecewise PLS method

For easy understanding, we shall first illustrate the iterative piecewise regression method using the one-dimensional example of Fig. 1(b). The first thing is to check the validity of the old model in a new operating space, where new experiment is unavoidably needed. With the assumptions, the operating condition of the first new experimental trial can be calculated by the historical model (f_0), e.g., $x_{new}^{(1)} = f_0^{-1}(y_{des})$, as illustrated in Fig. 2, where the desired quality data and all new experimental data in future are mean-centred and scaled by the same normalization parameters obtained from historical data. The actual quality value will be $y^{(1)} = f_*(x_{new}^{(1)})$, rather than y_{des}. If the difference $\left\| y^{(1)} - y_{des} \right\|$ is beyond the tolerance limit, that is, the old model is no longer valid for new data $(x_{new}^{(1)}, y^{(1)})$, piecewise regression can be performed here for modelling the relationship between operating conditions and qualities in the expanded operating space.

To do so, the changepoint and parameters of the new linear model have to be determined. With the assumption that the historical local model has reasonable performance for the historical data, and the newly obtained data that does not obey the historical model, the "boundary" point $(x_{b+} = f_0^{-1}(y_{b+}), y_{b+})$ can be chosen as the changepoint between the historical model $f_0(x)$ and a new linear model $f_1(x)$, where y_{b+} stands for the closest quality data in the historical envelope to the desired quality. The piecewise model that joins the above two models is formulated as,

$$y = \begin{cases} f_0(x) & x \in R^0 \\ f_1(x) & x \in R^1 \end{cases} \quad (4)$$

where R^0 is the historical data space; and R^1 is the new data space, e.g. $R^0 = [x_{b-}, x_{b+}]$ and $R^1 = [x_{b+}, \infty]$ for the example of Fig. 2. The linear model $f_1(x)$ can be roughly determined by the changepoint (x_{b+}, y_{b+}) and new experimental data $(x_{new}^{(1)}, y^{(1)})$. Although it is impossible to ensure the confidence of the new model derived only from the two data points from the statistical point of view, it can still be used to provide the right direction in searching for the desired operating condition from the application point of view, supposed that the new experimental data is clean and informative.

After the first experimental trial, there are two possible results in terms of the newly obtained quality data $y^{(1)}$. For case I, as illustrated in Fig. 2, $y^{(1)}$ is still smaller than the desired value, indicating that the optimal operating condition is still outside the newly explored space. Further experimental trial $(x_{new}^{(2)}, y_{new}^{(2)})$ is needed in the unknown space based on the local model f_1, and a three-piece regression model will be derived with the new changepoint $(x_{new}^{(1)}, y^{(1)})$ as,

$$y = \begin{cases} f_0(x) & x \in R^0 \\ f_1(x) & x \in R^1 \\ f_2(x) & x \in R^2 \end{cases}, \tag{5}$$

where $R^0 = [x_{b-}, x_{b+}]$, $R^1 = [x_{b+}, x_{new}^{(1)}]$ and $R^2 = [x_{new}^{(1)}, \infty]$ for the example of Fig. 2.

For case II, as illustrated in Fig. 3, $y^{(1)}$ is larger than the desired value. In this case, we should search for the desired operating condition within the newly explored operating space. Similarly, a new experimental data $(x_{new}^{(2)}, y_{new}^{(2)})$ is obtained based on the model f_1. Then, the local model $f_1(x)$ will be replaced by two sub local models as,

$$y = \begin{cases} f_0(x) & x \in R^0 \\ f_{02}(x) & x \in R^{02} \\ f_{21}(x) & x \in R^{21} \end{cases}, \tag{6}$$

where $R^0 = [x_{b-}, x_{b+}]$, $R^{02} = [x_{b+}, x_{new}^{(2)}]$ and $R^{21} = [x_{new}^{(2)}, x_{new}^{(1)}]$ for the example of Fig. 3. The new linear models f_{02} and f_{21} are determined by the data { (x_{b+}, y_{b+}) , $(x_{new}^{(2)}, y_{new}^{(2)})$ } and { $(x_{new}^{(1)}, y_{new}^{(1)})$, $(x_{new}^{(2)}, y_{new}^{(2)})$ }, respectively.

The above piecewise regression modelling can be repeated further until the updated process model can approach the true relationship around the desired operating condition (x^*).

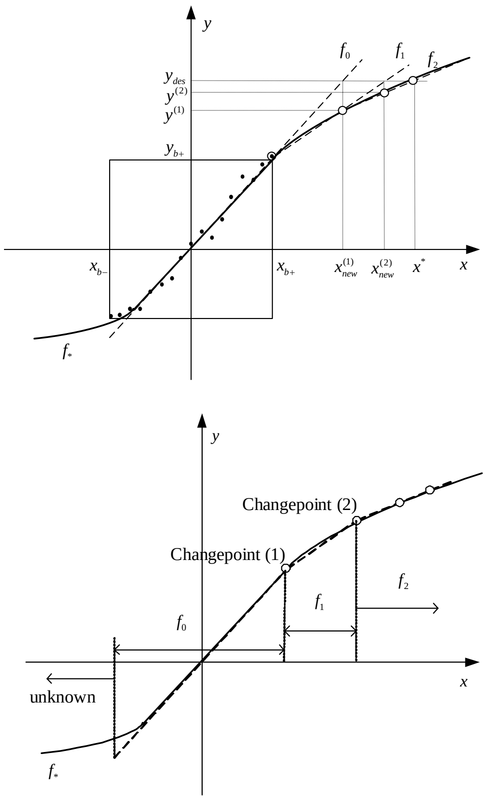


Fig. 2. Illustration of iterative piecewise regression modelling (Case I).

The above iterative piecewise modelling is simple and easy to be implemented in the one-dimensional case. For high dimensional and highly correlated industrial data, the above procedures can also be implemented with the aid of PLS modelling. In the implementation, the outer relationships of the historical PLS model will be kept unchanged, only the inner relationship is updated to track the nonlinearity in the expanded operating space, where piecewise regression is performed in each pair of latent variables $\{\mathbf{t}_a, \mathbf{u}_a\}$ $(a = 1, \cdots, A)$. This is feasible as discussed by Qin & McAvoy (1992) in their nonlinear PLS method, where neural network is used to approximate the nonlinear inner relationship and the outer relationships are kept in linear structure to attain the robust generalization property.

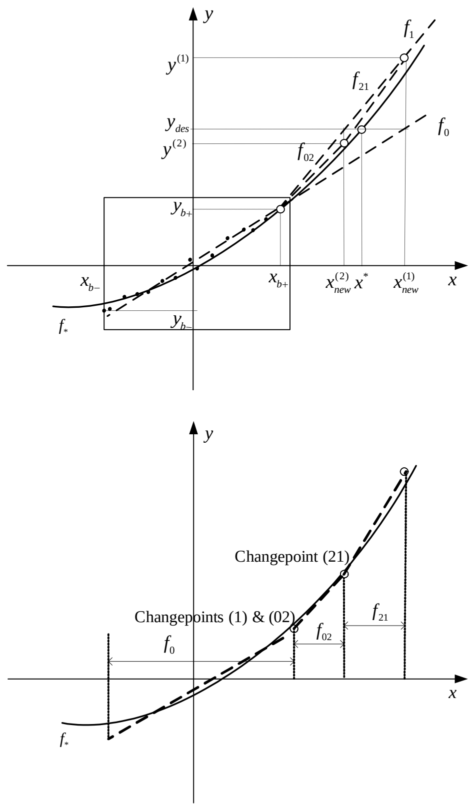


Fig.3. Illustration of iterative piecewise regression modelling (Case II).

The proposed iterative piecewise PLS modelling can be summarized as below.

Step I: Use the historical PLS model to get a new operating condition ($\mathbf{x}_{new}^{(1)}$), the corresponding quality data ($\mathbf{y}^{(1)}$), and the latent variable scores $\mathbf{t}_{new}^{(1)}$ and $\mathbf{u}_{new}^{(1)}$, as shown in Table 1.

Step II: Keep the outer relationship unchanged, piecewise updating the inner relationship to track the nonlinearity in the expanded operating space similar to Eq.(5) or Eq.(6).

Step III: Repeat step I & II using the historical PLS outer model and the updated inner model until achieving the desired operating conditions and quality.

Based on the updated nonlinear PLS model over the expanded operating space, the existing product design methods can be applied to find the feasible operating conditions for new quality specifications, as illustrated in the next section.

Table 1. Procedures in the first step of iterative piecewise PLS modelling method

Historical PLS model parameters:

Outer model: P_0 and W_0 for X;
Q_0 and C_0 for Y

Inner model: B_0 between T and U

Step I of recursive piecewise PLS method:

(1) $\mathbf{u}_{des} = \mathbf{y}_{des} C_0$;

(2) $\mathbf{t}^{(1)} = \mathbf{u}_{des} (B_0)^{-1}$;

(3) $\mathbf{x}_{new}^{(1)} = \mathbf{t}^{(1)} P_0^T$;

(4) Modify $\mathbf{x}_{new}^{(1)}$ to satisfy physical constraints;

(5) Do experiment under $\mathbf{x}_{new}^{(1)}$ to get quality data $\mathbf{y}^{(1)}$;

(6) $\mathbf{t}_{new}^{(1)} = \mathbf{x}_{new}^{(1)} W_0$ and $\mathbf{u}_{new}^{(1)} = \mathbf{y}^{(1)} C_0$, { $\mathbf{t}_{new}^{(1)}$, $\mathbf{u}_{new}^{(1)}$ } for step II.

4. ILLUSTRATION

The proposed iterative piecewise PLS modelling method for product design is applied to an injection molding process to demonstrate its feasibility and effectiveness.

Injection molding process can be operated over a wide range of operating conditions. For the machine in our lab, when processing high-density polyethylene (HDPE), the normal settings of Packing Pressure (P.P.), Barrel Temperature (B.T.) and Mold Temperatures (M.T.) can be within the ranges of 150bar ~ 450bar, 180 ºC ~ 220 ºC, and 15 ºC ~ 55 ºC, respectively. The relationship between these settings and dimensional qualities such as part weight and length can be accurately described by the first pair of PLS latent variables, as detailed in the authors' previous work (Lu & Gao, 2005). It is clearly nonlinear over the entire operating space, as shown in Fig. 4.

To illustrate the proposed method, data from 9 different operating conditions are collected to form the "historical data", as shown in Table 2, where the ranges of product weight and length are 23.36g ~ 27.41g and 116.67cm ~ 117.27cm, respectively. The linear PLS model derived from these historical data have good performance in quality prediction, as shown in Fig. 5. A new product quality specification, weight= $27.86g$ and length= $117.52cm$, is required now, which is beyond the range of historical products, but achievable on the machine. The results of the proposed iterative piecewise PLS method are shown in Fig. 6 and Table 2, where the method of Jaeckle & MacGregor (1998) is adopted to invert the PLS model to find the corresponding operating conditions. From Fig. 6, the final PLS model has three-piece inner relationships (B_0 , B_1 , and B_2), and the desired operating conditions for the new quality setting can be achieved by the third inner model (B_2). Only two trials are conducted by the proposed method in searching for the right operating condition to achieve the desired product qualities. This obviously reduces the effort and time in designing new products.

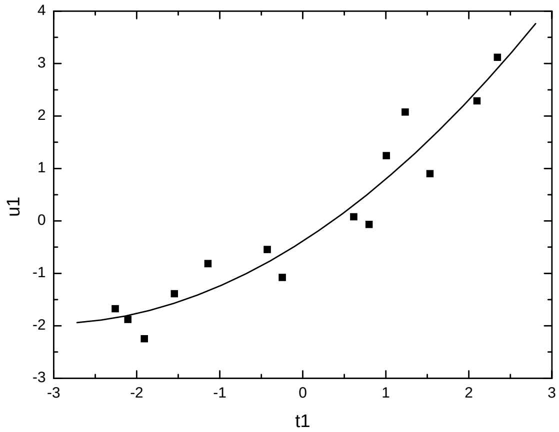
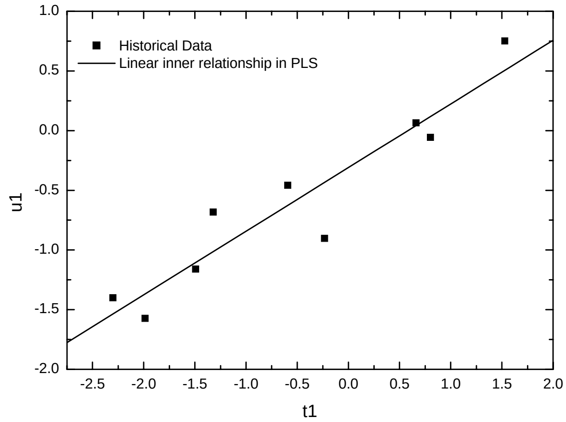
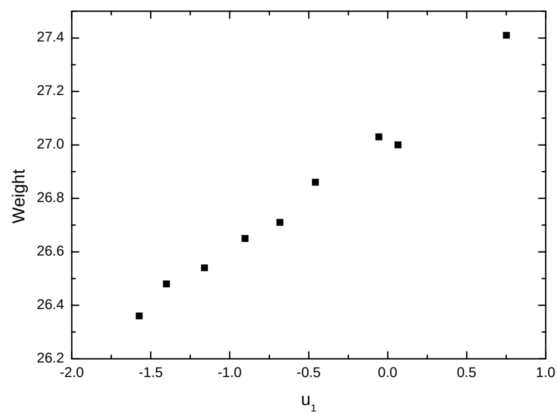


Fig.4. Nonlinear relationship illustration by the first pair of PLS latent variables over the entire operating space.



(a)



(b)

Fig. 5. Illustration of goodness of the historical linear PLS model in the historical operating space. (a) Linear inner relationship; (b) Linear outer relationship in Y.

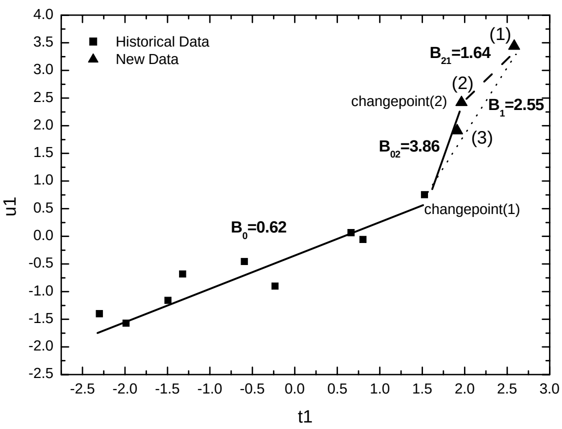


Fig. 6. Iterative piecewise PLS modelling of the inner relationship on the first pair of latent variables.

5. CONCLUSION

Analysis on the product design into unknown operating space has been given in the paper. An iterative piecewise PLS modelling method has been adopted for the above purpose. The application on an injection molding process has demonstrated good feasibility and effectiveness of the proposed method.

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Table 2. Operating conditions, scores of latent variables and quality measurements for historical and new experimental data.

	Operating conditions (P.P., B.T., M.T.)			PLS scores (t1, u1)		quality measurements (Weight, Length)	
	Historical Data						
	150	180	15	-0.59	-0.46	26.86	116.96
	150	180	35	-1.32	-0.68	26.71	116.93
	150	180	55	-2.30	-1.40	26.48	116.69
	300	200	35	0.66	0.06	27.00	117.15
	300	200	55	-0.23	-0.90	26.65	116.85
	120	220	15	-1.49	-1.16	26.54	116.78
	450	220	15	1.53	0.75	27.41	117.27
	150	220	35	-1.99	-1.57	26.36	116.67
	450	220	35	0.80	-0.06	27.03	117.07
	New Experimental Data						
(1)	450	189	15	2.58	3.44	28.17	117.70
(2)	450	193	25	1.96	2.42	27.94	117.56
(3)	440	196	32	1.91	1.91	27.86	117.52