Application of partial least squares regression method for mathematical modeling of rocket aerodynamic data

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Abstract
Partial Least Squares regression (PLS) is utilized for mathematical modeling of the aerodynamic data of the rocket with control surfaces. Based on the available trigonometric mathematical model of the rocket and the cross-validation method, the PLS model with good generalization capability is constructed and verified with two examples. The results show that PLS is feasible and effective and the modeling results are comparative with the results of Orthogonal Least Squares regression (OLS) method. Moreover, the PLS is robust and has a good generalization capability, and it may be utilized for more diverse applications in engineering practice.

1. Introduction

Partial Least Squares regression (PLS) is a new multivariate data analysis method taking advantage of the Least Squares regression, Principal Component Analysis (PCA), and Canonical Correlation Analysis (CCA). It was originated in chemical field and was used to solve the problems of multiple correlations of independent variables and problems whose sample size is less than variables. This method integrates application of multivariate linear regression, PCA and CCA, and realizes a synthetic application of multiple multivariate statistical analysis methods. The advantage of this method lies in three aspects. First, PLS could deal with the situation that there exist correlations among the input variables. Second, it could handle the modeling problems whose sample size is less than the variables. Last, through integrating the PCA and regression modeling, the mechanism of complex system can be analyzed more effectively by the PLS[1][2].
The PLS method has now been widely used in chemical metrology, industrial design, social sciences, and other research fields, but there are few works about the application of PLS method in aeronautical and astronautical researches. So, in this paper, the PLS method is extended to treat the problem of aerodynamic characteristic modeling of rocket. Especially, mathematical modeling of the axial force and normal force of a rocket is discussed.

2. Partial least squares regression method

Assume that a single dependent variable y, independent variables$\{x_1, x_2,\dots, x_p\}$ and n sample points constitute a data table, $\boldsymbol{X}=(x_{ij})_{n\times p}$ and $\vec{y}=(y_i)_{n\times 1}$, the basic principle of PLS is to select the components of $\vec{t}_1$, $\vec{t}_2,\dots,\vec{t}_h$ （$h\le p$） sequentially to making both the variance of $\mathrm{Var}(\boldsymbol{t}_i)$ and the covariance of $\mathrm{Cov}(\boldsymbol{t}_i, \boldsymbol{y})$ as great as possible. And by establishing the regression equation between $\vec{y}$ and $\vec{t}_1$, $\vec{t}_2,\dots,\vec{t}_h$, the regression equation between $\vec{y}$ and $x_1, x_2,\dots, x_p$ can be founded. The detailed steps are as follows[1].
(1) Standardize independent variables matrix $\boldsymbol{X}$ and dependent variable $\vec{y}$, then can get standardized variables matrix $\boldsymbol{E_0}$ and standardized column vector $\vec{f}_0$, i.e.,

$$\boldsymbol{E}_0=\left(x_{ij}^*\right)_{n\times p};\ \vec{f}_0=\left(y_i^*\right)_{n\times 1};\ x_{ij}^*=x_{ij}-\bar{x}_j,\ \bar{x}_j=\frac{1}{n}\sum_{i=1}^{n}x_{ij};\ y_i^*=y_i-\bar{y},\ \bar{y}=\frac{1}{n}\sum_{i=1}^{n}y_i \tag{1}$$

(2) Extract the first component from $\boldsymbol{E}_0$,

$$\vec{t}_1 = \boldsymbol{E}_0 \vec{w}_1 \,; \quad \vec{w}_1 = \boldsymbol{E}_0^T \cdot \vec{f}_0 \tag{2}$$

And carry out the regression of $\boldsymbol{E_0}$ and $\vec{f}_0$ on $\vec{t}_1$,

$$\boldsymbol{E}_0 = \vec{t}_1 \vec{p}_1^T + \boldsymbol{E}_1 \,; \; \vec{f}_0 = \vec{t}_1 r_1 + \vec{f}_1 \,; \; \vec{p}_1 = \frac{\boldsymbol{E}_0^T \cdot \vec{t}_1}{\left\| \vec{t}_1 \right\|^2} \,; \; r_1 = \frac{\vec{f}_0^T \cdot \vec{t}_1}{\left\| \vec{t}_1 \right\|^2} \tag{3}$$

Where $\boldsymbol{E_1}$ and $\vec{f}_1$ are regression residual error matrix and residual error vector respectively.

(3) Extract the second component from $\boldsymbol{E_1}$ and $\vec{f}_1$, and make regression on $\vec{t}_2$, i.e.,

$$\vec{t}_2 = E_1 \vec{w}_2 \,; \; \vec{w}_2 = E_1^T \cdot \vec{f}_1 \,; \; \boldsymbol{E}_1 = \vec{t}_2 \vec{p}_2^T + \boldsymbol{E}_2 \,; \; \vec{f}_1 = \vec{t}_2 r_2 + \vec{f}_2 \,; \; \vec{p}_2 = \frac{\boldsymbol{E}_1^T \cdot \vec{t}_2}{\left\| \vec{t}_2 \right\|^2} \,; \; r_2 = \frac{\vec{f}_1^T \cdot \vec{t}_2}{\left\| \vec{t}_2 \right\|^2} \tag{4}$$

(4) Continue to extract component from $\boldsymbol{E_2}$ and $\vec{f}_2$, and repeat the process for m steps, then, m components ($\vec{t}_1$, $\vec{t}_2$, …, $\vec{t}_m$) can be got. Carry out the regression of $\vec{f}_0$ on $\vec{t}_1$, $\vec{t}_2$, …, $\vec{t}_m$, i.e.,

$$\hat{\vec{f}}_0 = r_1 \vec{t}_1 + r_2 \vec{t}_2 + r_3 \vec{t}_3 + \ldots + r_m \vec{t}_m$$

and it can be rewritten as the form of:

$$y = x_1 \alpha_1 + x_2 \alpha_2 + \ldots + x_p \alpha_p \,; \alpha_i = \sum_{k=1}^{m} r_k \vec{w}_{k,i}^* \,, \; \vec{w}_k^* = \left[\prod_{j=1}^{k-1} \left(I - \vec{w}_j \vec{p}_j^T \right) \right] \vec{w}_k \tag{5}$$

In the aforementioned process of the modeling, there exists a key problem that how to decide the number of component m, which is treated with the following cross validation method. Successively one by one deleting the i_th (i=1, n) sample from the n sample points, new sample groups can be marked as $\boldsymbol{X}_{(-i)}$ and $\vec{y}_{(-i)}$. Building a PLS model with h components from $\boldsymbol{X}_{(-i)}$ and $\vec{y}_{(-i)}$ and using this model to predict value of the previously-deleted i_th sample $\hat{y}_{h(-i)}$. So for different h, the sum of the square error of this prediction could be defined as,

$$PRESS_h = \sum_{i=1}^{n} \left[y_i - \hat{y}_{h(-i)} \right]^2$$

This value is now used as a measure of the model's prediction ability, i.e., when $PRESS_h$ reach a minimum value, the model has the best prediction ability. Then the number of component m can be selected as the value of h^* to minimize $PRESS_h$,

$$PRESS(h^*) = \min_{1 \le h \le r} PRESS_h \quad ; \quad r = rank(\boldsymbol{X}^T \boldsymbol{X}) \tag{6}$$

3. Aerodynamic coefficient modeling of rocket with control surfaces

In principle, aerodynamic data of rocket with control surfaces is a six-dimensional function of Mach number, attack angle, body rolling angle and three control surface deflection angles. Since the range of the flight Mach number, attack angle and control surface deflection angles might be wide in the flight envelop, it's hard to get all the aerodynamic data by CFD or wind tunnel experiments. In the past practices, a mathematic model was established on the linearization of aerodynamics coefficients and the aerodynamic derivatives to get aerodynamic characters in different Mach number, different attack angle and different control surface deflection angles. But at present, with the improvement of the attack angle and the maneuverability of modern rocket, the nonlinear aerodynamic characteristics comes out and the linear method of aerodynamic modeling can not satisfy the engineering requirement, so it's necessary to develop some new method to build nonlinear aerodynamic model from a certain number of experiment or CFD data.

In recent years, many nonlinear modeling methods have been put forward which can be classified to be two categories. One is the base function superposing method such as the polynomial function model, the spline function model and the differential/integral equation method, the other is the artificial intelligence modeling method such as the neutral network model, the fuzzy logic model. By comparison, the base function superposing method is more physically meaningful and the artificial intelligence modeling method often fits the sample data better[3-5]. For rocket, the aerodynamic model often can be expressed as a trigonometric series function of the roll angle and the control surface deflection angles because there exits some geometric symmetry nature in the data. And for certain Mach number and attack angle, the aerodynamic coefficient could be expressed as the sum of two parts, one is the aerodynamic coefficient with control surfaces at the neutral position, the other is the influence of control surface deflection[6][7]. Taken the longitudinal aerodynamic coefficient as an example, it could be written as,

$$F = a_0 + \sum_{i=1}^{m_1} a_i \cos(n_i\phi) + \sum_{j=1}^{m_2} a_{m_1+j}[f_j(\delta_x,\delta_y,\delta_z)\cos(n_j\phi)] + \sum_{k=1}^{m_3} a_{m_1+m_2+k}[g_k(\delta_x,\delta_y,\delta_z)\sin(n_k\phi)] \tag{7}$$

where ϕ is roll angle; a_i is coefficients of series; n_i、n_j、n_k are positive integers; m_1 is the number of trigonometric function terms without control surface influence; m_2 and m_3 are the number of cosine and sine base function terms taking control surface deflection influence into accounts; f_j, g_k are the polynomial function of control surface deflections; more details can be found in Ref.[7].

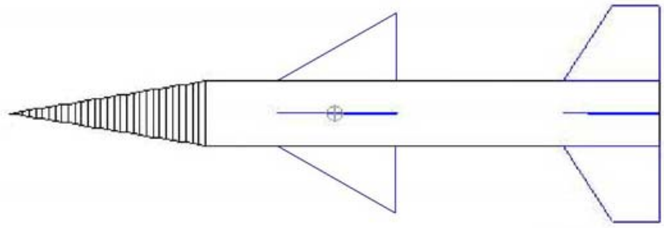

Figure 1: A typical rocket geometry

4. Application cases

4.1 Case 1

A typical rocket shown in Fig.1 is investigated in the test cases. In the first case, the control surfaces deflect with same direction and same angle, then the equivalent rolling control surface deflection angle δ_x equals the single control surface deflection angle and the normal force coefficient can be written as,

$$\begin{aligned} C_N &= a_0 + a_1\cos(\phi) + a_2\cos(2\phi) + a_3\cos(3\phi) + a_4\cos(4\phi) + a_5\cos(5\phi) + a_6\cos(6\phi) \\ &+ a_7\delta_x\cos(4\phi) + a_8\delta_x^2\cos(4\phi) + a_9\delta_x^3\cos(4\phi) + a_{10}\delta_x\cos(8\phi) + a_{11}\delta_x^2\cos(8\phi) \\ &+ a_{12}\delta_x^3\cos(8\phi) + a_{13}\delta_x\sin(4\phi) + a_{14}\delta_x^2\sin(4\phi) + a_{15}\delta_x^3\sin(4\phi) + a_{16}\delta_x\sin(8\phi) \\ &+ a_{17}\delta_x^2\sin(8\phi) + a_{18}\delta_x^3\sin(8\phi) \end{aligned} \tag{8}$$

Taking the flight condition as Mach number M=2.36, and attack angle α=4°, the normal force coefficients of 63 states with 7 rolling deflection angle(δ_x=-10°, -5°, -2°, 0°, 2°, 5°, 10°) and 9 body rolling angle(ϕ= (i-1)*90°/8) are calculated with DATACOM software[8] and the calculated results are added with 2% measurement noise to simulate the experimental data. 21 out of the 63 states are taken as the training sample of modeling. the 21 states includes, rolling control surface deflection is 0°, with body rolling angle is 0°, 11.25°, 22.5°, 33.75°, 45°, 56.25°, 67.5°, 78.75°, 90°; rolling control surface deflection is 5°, with body rolling angle is 0°, 11.25°, 22.5°, 33.75°, 45°, 90°; rolling control surface deflection is 10°, with body rolling angle is 0°, 11.25°, 22.5°, 33.75°, 45°, 90°. Based on these 21 samples, the Orthogonal Least Squares regression method (OLS) presented in [7] can be used to get the following aerodynamics model,

$$C_N = a_0 + a_2\cos(2\phi) + a_4\cos(4\phi) + a_7\delta_x\cos(4\phi) + a_8\delta_x^2\cos(4\phi) + a_{11}\delta_x^2\cos(8\phi)$$
$$+ a_{13}\delta_x\sin(4\phi) + a_{15}\delta_x^3\sin(4\phi) + a_{17}\delta_x^2\sin(8\phi)$$

From the expression, it can be seen that the OLS method ignores some trigonometric series' terms of formula (8), and build mathematic model based on nine terms. Obviously, although this method could overcome the singularity of matrix in regression, some useful information in the deleted terms has also been discarded. So, the PLS method now is tried to build the model. In the PLS model, all the 17 trigonometric terms in Eq.(8) are treated as base functions. With cross validation of the 21 samples, the prediction error of $PRESS_h$ can be calculated as,

$PRESS_1$=1.9599134; $PRESS_2$=0.7383252; $PRESS_3$=0.4406658; $PRESS_4$=0.2161127;
$PRESS_5$=0.03616128; $PRESS_6$=0.01781333; $PRESS_7$=0.01657417; $PRESS_8$=0.01987823;
$PRESS_9$=0.02364244; $PRESS_{10}$=0.02597883; $PRESS_{11}$=0.03118961.

So, the number of component of h is selected to be 7, and the corresponding $a_i(i$=0,18) in formula (8) can be computed through Eqs.(1)-(5). In Fig.2, the comparison of two modeling results for training states of δ_x=0° and 5° was given in which "OLS" is the result of OLS modeling, "PLS(h=7)" is the result of PLS modeling, and "Exp." is the training data. The two models also are used to predict the rest 42 samples. The predicted states of δ_x=-10° and 2° are shown in Fig.3. It can be seen that modeling results of PLS is generally better than OLS.

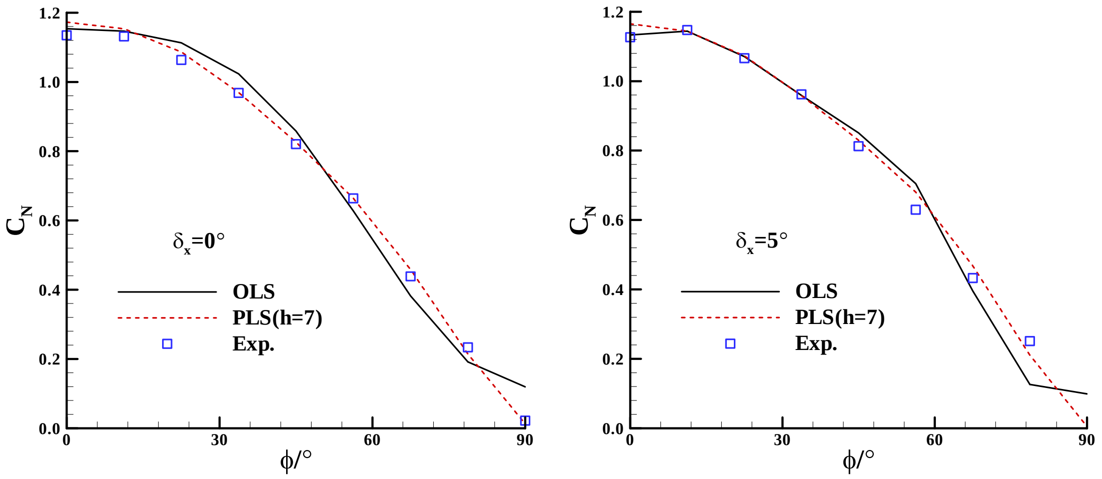

Figure 2: Comparison of modeling results for training states

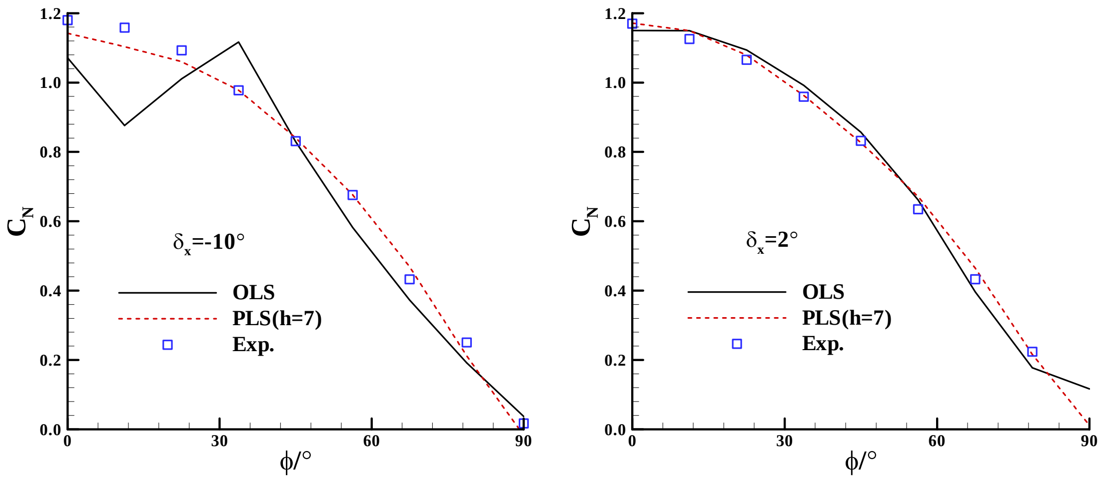

Figure 3: Comparison of modeling results for predicted states

4.2 Case 2

In the second case, the Mach number is 1.5 and the attack angle is 6°. Four control surfaces deflect schematically to generate the 216 combination of three equivalent rolling, yawing, and pitching control surface deflections of δ_x= 0°, 5°, 10°; δ_y= -15°, -10°, -5°, 0° , 5°, 10°, 15°, 20°; and δ_z= -15°, -10°, -5°, 0° , 5°, 10°, 15°, 20°. And every combination corresponds to 8 body roll angles, so, there are totally 216×8=1728 states. DATACOM software is also used to calculate the axial force coefficient of these states and the calculated results are added with measurement noise of standard deviation being 0.1 to simulate the experimental data.

65 out of the 1728 states are picked out to build the aerodynamic model, and the 65 samples are "δ_x= 0°, δ_y= 0°, δ_z= 0°, ϕ= 0°, 22.5°, 45°, 67.5°, 90°"; "δ_x= 0°, δ_y=δ_z=5°, 10°, 15°, ϕ= -135°, -45°, 45°"; "δ_x=5°, δ_y=5°, δ_z=10°, ϕ=0°"; "δ_x=10°, δ_y=-15°, δ_z=10°, ϕ=45°". A model containing 24 trigonometric base function terms[7] is now chosen as the standpoint of the modeling. When OLS is used to model the 65 samples and the significance level below which the model term's contribution can be ignored is set to be 5×10^{-5}, a model with 14 terms can be got. Using this model to predict all the 1728 states, the prediction error is,

$$E_{OLS} = \sum_{i=1}^{1728}\left[C_{AOLS}(\delta_{xi},\delta_{yi},\delta_{zi},\phi_i) - C_{A\exp}(\delta_{xi},\delta_{yi},\delta_{zi},\phi_i)\right]^2 \tag{9}$$

As for PLS, through cross validation method, it can be seen that the optimal number of components number of h is 11, and this value is used to calculate a_i and get the model. Also use this model to predict all the 1728 states, the prediction error is,

$$E_{PLS} = \sum_{i=1}^{1728}\left[C_{APLS}(\delta_{xi},\delta_{yi},\delta_{zi},\phi_i) - C_{A\exp}(\delta_{xi},\delta_{yi},\delta_{zi},\phi_i)\right]^2 \tag{10}$$

These results show that the modeling result of PLS is wholly better than OLS. Further calculations reveal that for 216 sets of control surface deflection combinations, the PLS results of 121 sets are better than OLS and the OLS results of other 95 sets are better than PLS. The comparison of modeling results for two sets of control surfaces deflection ("δ_x=10°, δ_y=10°, δ_z=-20°" and "δ_x=10°, δ_y=15°, δ_z=20°") with PLS results better than OLS is given in Fig.4. and another comparison of two sets ("δ_x=10°, δ_y=-5°, δ_z=20°" and "δ_x=5°, δ_y=-10°, δ_z=-15°") with OLS results better than PLS is given in Fig.5. From Fig.4, it can be seen that there is no obvious non-physical oscillation in the model results of PLS and they are comparative or slightly better than the result of OLS.

In order to validate the effectiveness of the estimation algorithm, the calculated temperature history on measurement locations is firstly used as measurement data to estimate the heat flux. The estimated result is shown as the dashed line("Qestimated(σ=0K)") in Fig.4, agreeing with the specified heat flux well except for the final time. The difference may be due to the damping nature of the heat conduction and the influence of surface heat flux at the final time can not be manifested from the simultaneous temperature history at the measurement point which is a bit far from the heating surface.

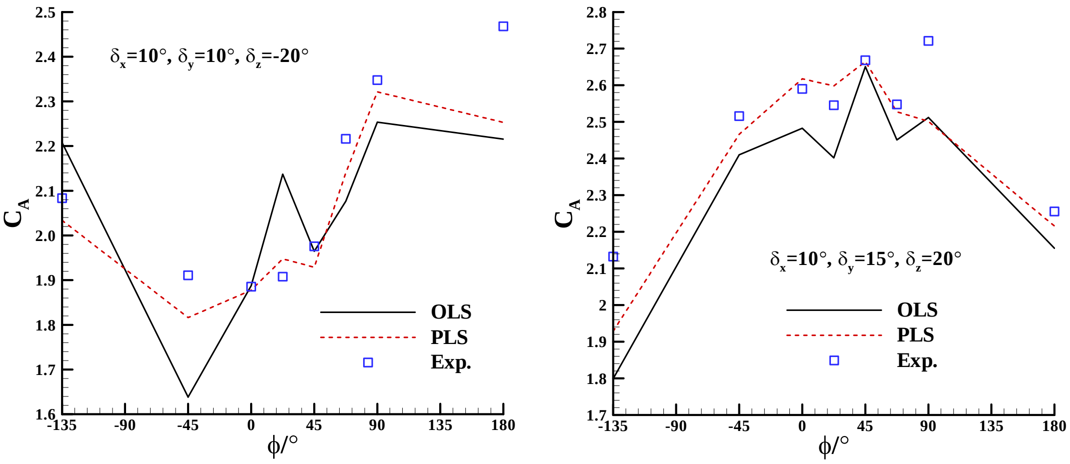

Figure 4: Comparison of modeling results for two sets of control surfaces deflection

In fact, from Eq.(1) to Eq.(5), it can be seen that in PLS, all the candidate series' terms in the model are retained but some latent insignificant modes corresponding to the small eigenvalue of the matrix $E^T \bar{y}\bar{y}^T E$ are ignored by the modulating the coefficients' value of the model terms. While in OLS, some terms in the trigonometric series of the

aerodynamic force model with insignificant contribution are directly truncated to preserve the stability of the model. So, there are some similarities between these two algorithms and the modelling results are comparative. Since the PLS model often contains more candidate trigonometric series' terms than the OLS, it may preserve more useful information and has better modeling accuracy than OLS. Besides, PLS has a good generalization capability and it may be applied for more diverse situations with a same model structure and different coefficient values.
Moreover, after comparing the modeling algorithms of PLS and OLS, it also can be found that the PLS can deal with the situation that some correlation exists among the modeling variables and has a good generalization capability by deciding the number of component of *h* with cross validation method. In contrast, when there is some correlation among the modeling variables, the OLS often fails and its generalization capability is greatly influenced by the selection of model terms, and how to determine the number of model terms of OLS rationally still needs further investigation.

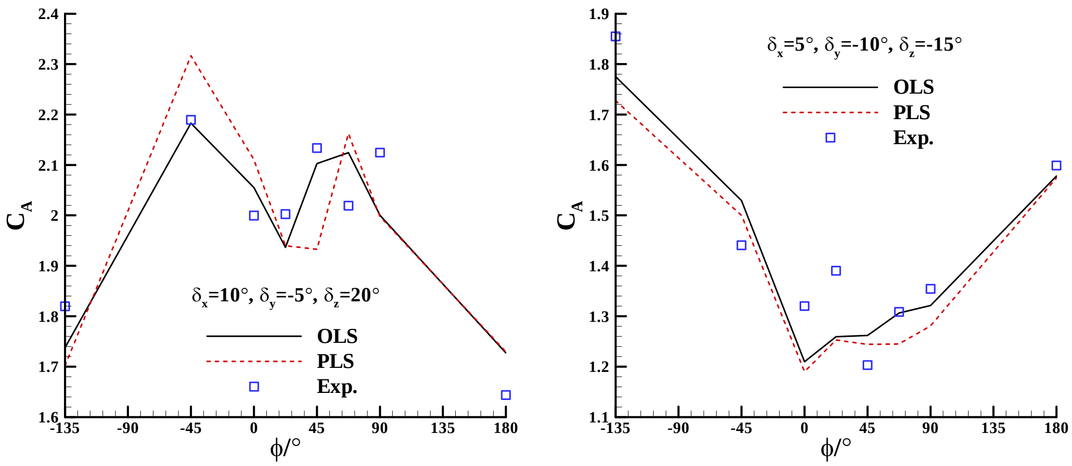

Figure 5: Comparison of modeling results for two sets of control surfaces deflection

6. Conclusion

In this paper, the Partial Least Squares regression modeling method is utilized to describe the aerodynamic characteristic of rocket with control surfaces. Firstly, at a given incidence and Mach number, the aerodynamic forces of the rocket is written as a trigonometric series function of the body roll angle and the control surface deflection angles, so the terms in the series is treated as independent variables and the regression of aerodynamic forces on these terms is carried out by PLS method. Especially, in the PLS, the cross-validation technique is utilized to determine the number of the components and the resultant model exhibits a good generalization capability. Secondly, two examples of the normal force modeling of a rocket with four control surfaces deflecting identically, and the axial force modeling of a rocket with four control surfaces deflecting respectively are studied with PLS and OLS method. The results show that the PLS and OLS try to keep the significant modes of matrix $E^T \vec{y} \vec{y}^T E$ and the terms with greater contributions from the candidate model terms respectively, and exhibit comparative modelling result. The PLS retains all the candidate base function terms in the model, saving more useful information, so its modeling accuracy may be better than OLS. Moreover, the PLS has a good generalization capability and is robust in practical situation, being another effective method for aerodynamic modeling of rockets and other flight vehicles.

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