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Variable Influence Analysis of an In-Situ Catalytic Adsorption (ICA) Steam Gasification using Multivariate PLS

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ABSTRACT

In this paper, multivariate data analysis based on Partial least squares projection to Latent Structure (PLS) is utilized as an alternative approach to study the process variables-output responses relationship on a published data from an In-situ catalytic adsorption steam gasification pilot plant for H2 production. Performance comparison between the multivariate PLS analysis is compared with the reported data in literature obtained using RSM, ANOVA analysis and three dimensional surface plots. Results show promising capability of the multivariate PLS approach in allowing the variables-responses relationship to be studied simultaneously**.**

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INTRODUCTION

Gasification technologies offer the opportunities to convert lignocellulose biomass into clean fuels i.e. hydrogen or synthesis gases which is mixture of CO and H_2 (Chaubey, Sahu, James, & Maity, 2013); (Yusup, Khan, Ahmad, & Rashidi, 2014). Biomass gasification is usually added up by steam and catalyst to improve the product gas composition towards hydrogen rich gas production. More recently, the addition of in-situ CO_2 adsorbent in gasification process makes biomass as a negative CO_2 emitter. Palm oil waste is considered to be a source of renewable hydrogen especially in Malaysia which produced huge amount of oil palm wastes.Gasification using palm kernel shell (PKS) can be done either by using air or steam gasification using either fixed or fluidized bed reactor (Esfahani, Wan Ab Karim Ghani, Mohd Salleh, & Ali, 2011); (Mohammed, Salmiaton, Wan Azlina, Mohammad Amran, & Fakhru'l-Razi, 2011).

PKS gasification typically involves a number of process variables, and various studies have been done to investigate the effect and interaction of these process variables (Yusup *et al*., 2014); (Fermoso *et al*., 2010). In (Yusup *et al*., 2014) particularly, the interactions among temperature, steam to biomass mass ratio, adsorbent to biomass mass ratio, superficial velocity and biomass particle size for in-situ catalytic adsorption (ICA) steam gasification process of palm kernel shell for H_2 production were studied. In their paper, the influence of the five process variables on two output responses (H_2 composition and yield) were analyzed using Response Surface Methodology (RSM) based on Centered Composite Rotatable Design (CCRD) approach. ANOVA analysis and three dimensional surface plots were utilized to study and visualize the interaction of any two process variables at a time on a specific output response variables.

In this paper, an alternative approach in studying the process variables interactions and influences on the same data presented in (Yusup *et al*., 2014) is investigated using the multivariate data analysis (MVDA) methods. Based on statistical projection method, MVDA is a cutting edge technology that provides graphical plots and projections by extracting information from multivariate and complex series of data (i.e. multiple variables measured on multiple samples or at multiple time points) simultaneously. In comparison to classical statistical methods such as Multiple Linear Regression, MVDA offers certain advantages in handling dimensionality problem, handling short and fat and long and lean data tables, dealing with missing data and affording helpful as well as investigative graphical tools (Eriksson, Johansson, Kettaneh-Wold, & Wold, 2001; Tauhid-Ur-Rahman, 2005). In this paper, Partial Least Squares projections to latent structures or PLS will be employed.

Methods:

Assume X is an N x K matrix of predictor or input variables, and Y is an N x M matrix of response

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or output variables, where N is the number of observations corresponds to, for example, the chemical samples, and K and M are the number of input and output variables, respectively. In MVDA, principal component analysis (PCA) forms the basis for most multivariate data analysis (Eriksson *et al*., 2001);(Lindgren, Geladi, & Wold, 1993; Saikat & Jun, 2008; Wold, 1987). However, one drawback of PCA technique is that it captures only the characteristics of the *X*-matrix or the input variables (Saikat & Jun, 2008). Any sort of relation that may exist between each input variable and the response or output variable is not captured. In multivariate regression analysis however, significant benefits can be achieved if as much information in the *X*-matrix can be captured as well as in the relation between the input variables *X*-matrix and the output variable *Y*-matrix. PLS provides an alternate approach that allows us to achieve this balance (Saikat & Jun, 2008).

Partial least squares projection to Latent Structures:

The PLS technique works by successively extracting principal components from both X and Y such that covariance between extracted principal components is maximized. PLS method tries to find a linear decomposition of X and Y such that $X = TP^T + E$ and $Y = UC^T + F$ where the information related to the observations are stored in the score matrices T (N x A) and U (N x A); the information related to the variables are stored in the X-loading matrix P^T (K x A) and the Y-weight matrix C^T (M x A). The variation in the data that was left out of the modelling form the E (N x K) and F (N x M) residual matrices (Eriksson *et al*., 2001; Saikat & Jun, 2008).

Note that the principal components for X and Y are extracted successively and the number of principal components extracted, A, depends on the rank of X and Y. Decomposition is finalized so as to maximize covariance between T and U. There are multiple algorithms available to solve the PLS problem. However, all algorithms follow an iterative process to extract the principal components of X and Y.

Materials and data:

The In-situ Catalytic Adsorption (ICA) Steam Gasification System pilot plant used in this analysis is as described in (Yusup *et al*., 2014). The feedstock used was palm kernel shell. The present study considers five process variables; temperature, steam to biomass ratio, adsorbent to biomass ratio, fluidization velocity and biomass particle size. The data generated using CCRD design in (Yusup *et al*., 2014) with 26 experimental runs are used for the PLS analysis in the next sections. The *X*-block consists of the five process variables, and the *Y*-block consists of the two output response variables, namely H_2 yield and H_2 composition (see (Yusup *et al*., 2014)).

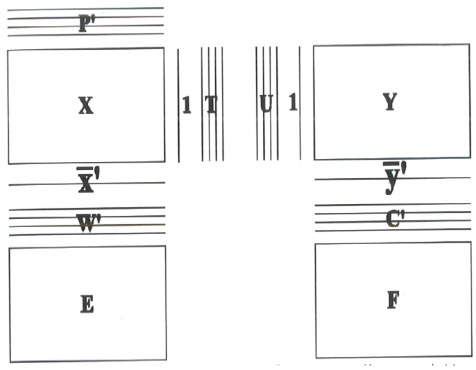

Fig. 1: PLS decomposition parameters.

RESULTS AND DISCUSSIONS

In this paper, the MVDA using PLS is applied using SIMCA-P software by Umetrics AB (Eriksson *et al*., 2001). Applying the PLS analysis on the data set, cross-validation technique inherent in SIMCA-P software generated a PLS model with single significant principal components (*A* = 1) as shown in Figure 2. The amount of variation in Y explained in terms of sum of squares, R2Y is 43%, and it measures how well the model fits the data. On the other hand, the percent of variation of the training set predicted by the model according to cross validation, Q2 is 38% and it indicates how well the models predicts new data. Manually increasing the number of principal components results in greater deterioration in the predictive capability of the PLS model as indicated by the Q2 value shown in Figure 3. Hence, for the subsequent analysis in this paper, only the first principal component is analyzed.

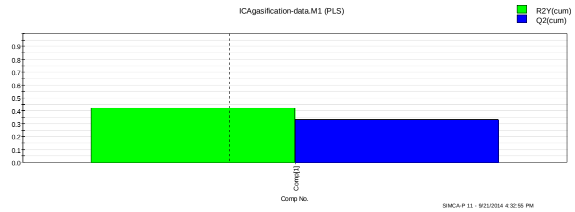

Fig. 2: Significant principal component given by SIMCA-P.

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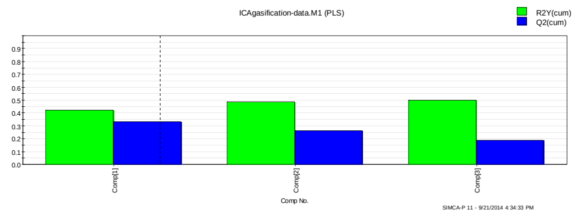

Fig. 3: The effect of increasing number of principal components to three.

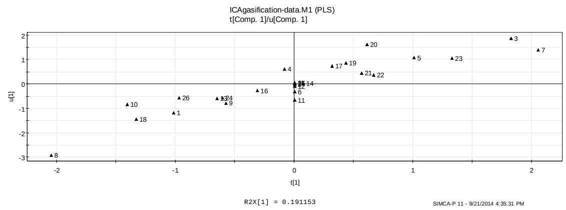

Fig. 4: PLS *t1/u1* scores plot.

Figure 4 shows the PLS t1/u1 scores plot of the model for the pilot plant data. It can be observed that a fairly strong correlation between the input variables and the response or output variables. There are no outliers, i.e. off-diagonal points, and this is expected as the data on the 26 experimental runs are based on design of experiments (DOE). The loading line plot (Figure 5) displays the major relation between the process variables (X) and the output responses (Y). Responses opposite to each other are negatively correlated and positively correlated to responses situated near them. Variables situated near responses are positively correlated to them and those situated opposite are negatively correlated to the responses. Hence, from Figure 5, it can be clearly observed that for both H_2 composition (Y_1) and H_2 yield (Y_2), temperature seems to be the most important factor. H_2 composition lies on the opposite quadrant of temperature, i.e. they are negatively correlated to each other. In other words, an increase in temperature will result in a decrease of H_2 composition due to reverse carbonation reaction that dominates (Yusup *et al*., 2014) resulting in higher amount of CO_2 in the product gas, and consequently a reduction in the H_2 composition. Further, H_2 yield is positively correlated with temperature (within the temperature range studied, i.e. 600-750^{o}C) since they are in the same quadrant of the plot, indicating that H_2 yield will benefit at higher temperatures. These findings agree with those reported in (Yusup *et al*., 2014).

For a PLS model, SIMCA-P displays the PLS regression coefficient plots with respect to both H_2 composition and H_2 yield are shown in Figures 6-7. It is important to note that if DOE has been used for the generation of X-data, which is the case for the current data set, these coefficients express a causal relationship. In addition, the coefficients are independent in such a way that Y is expected to change by the amount indicated by the coefficient value. The coefficients basically express how strongly Y is correlated to the systematic part of each of the X-variables. It can be clearly observed from the loadings line plot in Figure 5, and the corresponding coefficients plots in Figures 6-7, that for H_2 composition, the most important variables are temperatures and adsorbent to biomass ratio. Even though H_2 composition increases with increased adsorbent to biomass ratio, as previously mentioned, excess amount of adsorbent at high temperatures would only promote reverse carbonation reaction and hence reduces the overall H2 composition in the product gas. For H_2 yield, the response is positively correlated with the most important variables that are temperatures, steam to biomass ratio and adsorbent to biomass ratio. These findings are in agreement with the results reported in (Yusup *et al*., 2014). Increasing the temperature has favorable effect on the H_2 yield because endothermic reactions such as char gasification, steam methane reforming and tar cracking or reforming contribute to more H2 production in the product gas (Yusup *et al.*, 2014).

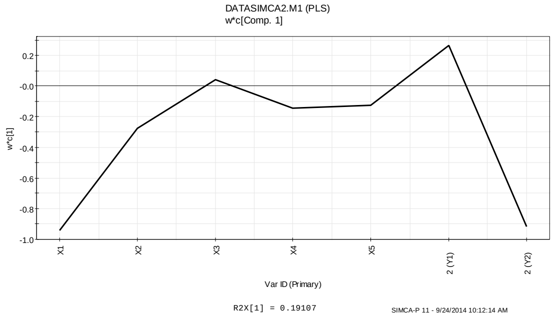

Fig. 5: Loading line plot.

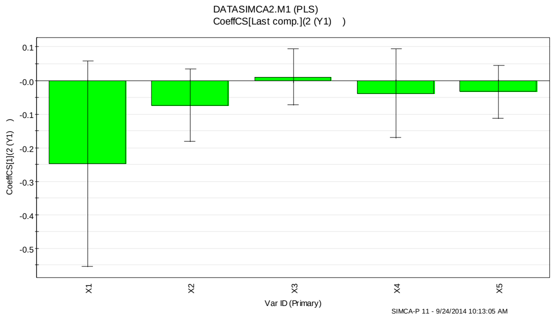

Fig. 6: Coefficient plot for $Y_{1.}$

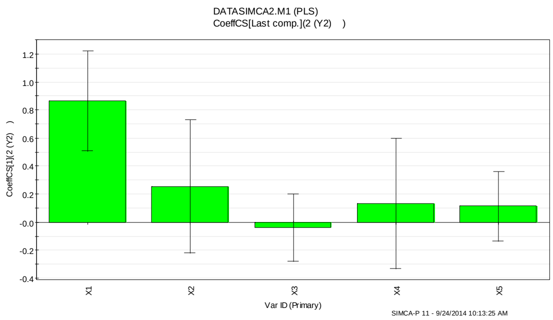

Fig. 7: Coefficient plot for $Y_{2.}$

Conclusions:

An alternative approach in studying the process variables interactions and influences on the same data presented in (Yusup *et al.*, 2014) for H_2 production has been investigated using multivariate PLS method. The results obtained are in good agreement with the reported data in (Yusup *et al.*, 2014) using conventional methods.

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