

Determination of Data Driven Soft Sensors in Dimethyl Ether Production by Reactive Distillation Column

Budi Husodo Bisowarno^{1a*}, Putri Ramadhany^{2,b}
and Tjioe Gerry Sebastian Wibowo^{3,c}

¹⁻³Department of Chemical Engineering, Faculty of Industrial Technology, Parahyangan Catholic University, West Java, Indonesia

^abudih@unpar.ac.id, ^bpramadhany@unpar.ac.id, ^csebastiangerry2@gmail.com

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Abstract. DME production by methanol dehydration using reactive distillation has a lot of potentials. However, the DME purity and methanol conversion is hard to be controlled and need inferential variable to be controlled. Data driven soft sensors can be utilised to select inferential variables, which can be used to control DME production by using reactive distillation. The data was collected from process simulation using ASPEN and analyzed by using PCA (Principal Component Analysis) and PLSR (Partial Least Squares Regression). The results show that based on the data driven soft sensors method, the DME purity can be controlled by using T4 as an inferential variable and ratio reflux as the manipulated variable. However, the methanol conversion is hard to be controlled because the potential inferential temperature was not significantly affected by reflux ratio and reboiler duty as the candidate manipulated variables.

Introduction

Fuel is one of the most important aspects of our life, in 2020 Indonesia needed almost 8,02 million ton LPG (Liquefied Petroleum Gas) in which 80% of it was still fulfilled by imports. One of the alternative of LPG is DME (Dimetil Eter) which is dubbed to be more efficient than LPG and environmentally friendly [1]. Beside its use as LPG alternative, DME can also be used as Diesel fuel alternative. DME can be produced by direct or indirect reaction. The direct reaction is a reaction in which the syngas formation process can be produced through the coal/biomass gasification process or the partial oxidation of natural gas, which is then converted into DME. Indirect reaction is a reaction in which the process begins with the manufacture of MeOH or methanol, followed by dehydration of MeOH in a separate reactor for producing DME [2].

In this research, it will be focused on the indirect reaction by using reactive distillation. The methanol dehydration can be shown in Eq. 1. Reactive distillation has advantages as reducing operational cost as the reaction and separation process will be done in single equipment [3]. In addition, reactive distillation also can increase the reactan conversion and selectivity [4]. However, the reactive distillation should be tightly controlled in term of the product purity and reactan conversion. These disadvantages can be solved by using data driven soft sensor.



Data driven soft sensors or black box model is a model based on measuring data on industrial processes. In the modeling procedure the relationship between inputs and outputs data of the factory can be emphasized while advanced process knowledge can be ignored. The use of soft sensors with the help of data is useful for extracting important information behind the data, so as to build better soft sensors performance. A wide variety of artificial intelligence and machine learning techniques provide a powerful modeling toolbox for black box models. Besides, the statistical method can also used to provide black box models [5]. This research utilized statistical method to make data driven soft sensors by using PCA (Principal Component Analysis) and PLSR (Partial Least Squares Regression).

Experimental Procedure

The research was conducted by analyzing the data generated from simulation using ASPEN Plus® and ASPEN Plus Dynamic®. The steady state simulation model was based on the simulation that has been conducted by Bildea and the scheme can be shown in Fig. 1. The dynamic simulation data was collected by changing the value of input variables, which were reflux ratio and reboiler duty $\pm 5\%$ from the initial values. The selection of these two input variables as manipulated variables for controlling the DME purity and methanol conversion with inferential temperatures T5 and T47 was based on the research by Wahid and Putra [6].

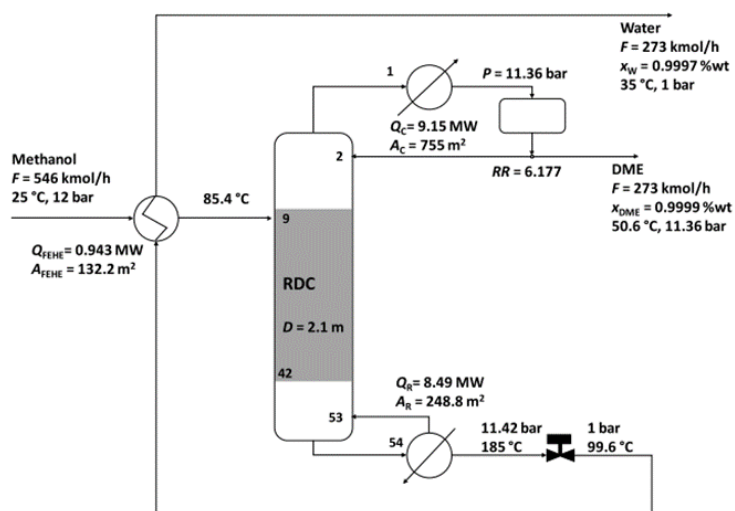


Fig. 1 Simulation scheme of DME production using reactive distillation [7]

The collected data was then analyzed by using PCA and PLSR method in The Unscrambler X™ software. The first statistical analysis was used to analyze the influence of temperatures stages to DME purity and methanol conversion. The second statistical analysis was used to analyze the influence of input variables (reflux ratio and reboiler duty) to temperature stages especially temperatures that have significant influence to DME purity and methanol conversion.

Results and Discussion

Process Simulation. Based on the steady state simulation process, the results obtained are in accordance with the literature where for the existing flow rate specifications are shown in Table 1. Based on the dynamic simulation, if the the reflux ratio increased, the purity of DME increased while distillate flow rate and temperature profile decreased. If the reboiler duty increased, the purity of DME decreased while distillate flow rate, methanol conversion, and temperature profile decreased. The opposite happened if the two variables were decreased.

Table 1 . Steady state process simulation results

Parameter / [Unit]	Feed	Distillate	Bottom Product
Total flow rate / [kmol/h]	546	273	273
Methanol flow rate / [kmol/h]	543,27	2,73	$4,41 \times 10^{-6}$
Water flow rate / [kmol/h]	2,73	$1,33 \times 10^{-5}$	273
DME flow rate / [kmol/h]	0	270,27	$5,46 \times 10^{-12}$

PCA Method on DME Purity and Methanol Conversion Values. Based on the descriptive statistics results that can be shown in Fig. 2, for simulation range $\pm 5\%$ methanol conversion has wider range than DME purity with the minimum value of DME purity is 97.94% and minimum value of methanol conversion is 95.39%. The total data analyzed were 25,896 data.

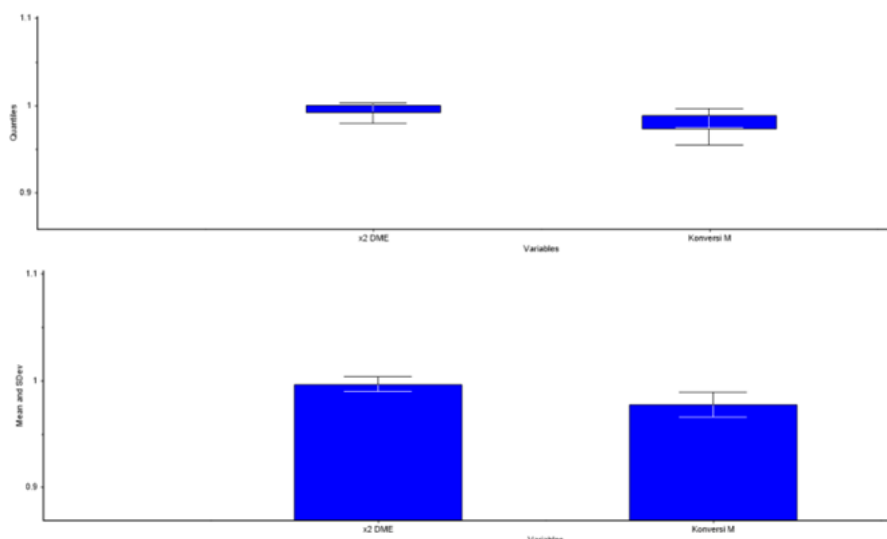


Fig. 2. Descriptive statistics result of DME purity and methanol conversion

Based on the correlations loadings as shown in Fig. 3, the DME purity has negative correlation with methanol conversion.

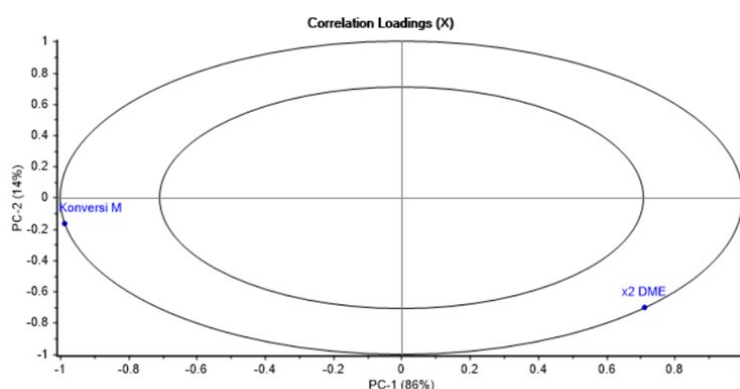


Fig. 3 Correlation loadings between DME purity and methanol conversion

The potentially outliers data was analysed by using score plot and influence plot that can be seen in Fig. 4. Based on the the score plot, the potential outliers are marked by black color. However in the influence plot those data only have high residual value and low leverage value, because of it the data can be assumed not outliers.

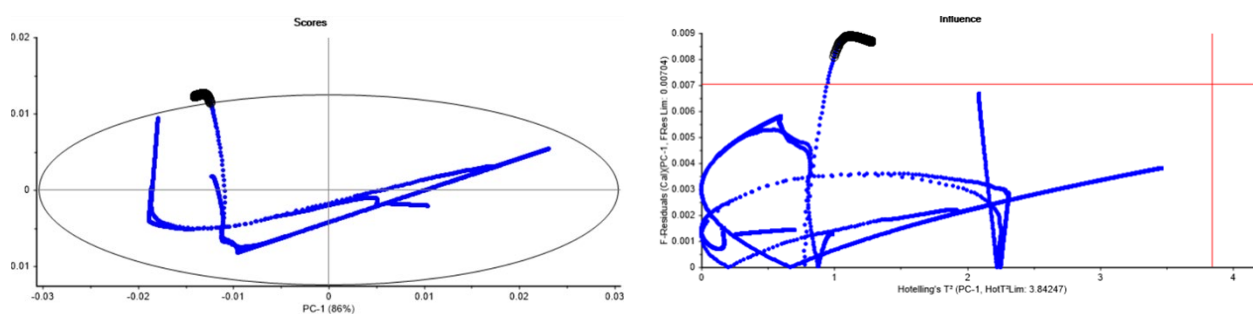


Fig. 4 Score plot and influence plot of DME purity and methanol conversion

Influence of Temperatures Stage to DME Purity and Methanol Conversion. The correlation loadings of stage temperatures as input data and DME purity and methanol conversion as output data that can be shown in Fig. 5. Based on the correlation loadings, the DME purity has negative correlation with the stage temperatures in general while the methanol conversion has positive correlation with the stage temperatures in general.

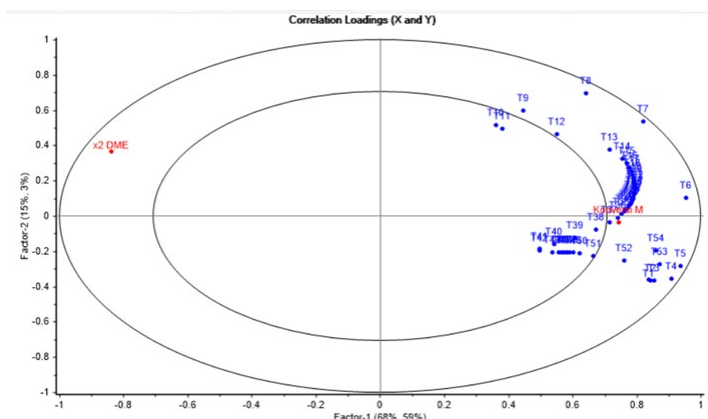


Fig. 5 Correlation loadings of stage temperature with DME purity and methanol conversion

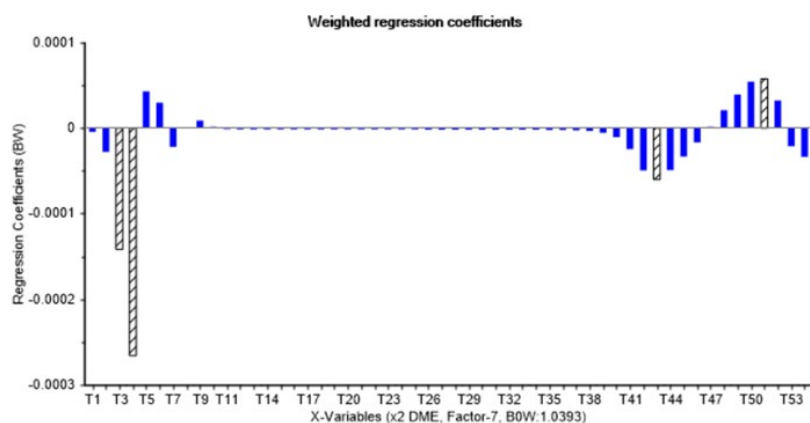


Fig. 6 Weighted regression coefficients distribution of influence of stage temperatures to DME purity

The weighted regression coefficients distribution for influence of stage temperatures to DME purity can be shown in Fig. 6 while influence of stage temperatures to methanol conversion can be shown in Fig. 7. Based on the Fig. 6, the stage temperatures that have significant influence on DME purity sequentially are T4, T3, T45 (positive correlation) and T51 (negative correlation). While based on Fig. 7, the stage temperatures that have significant influence on methanol conversion sequentially are T54, T53, T52 (negative correlation).

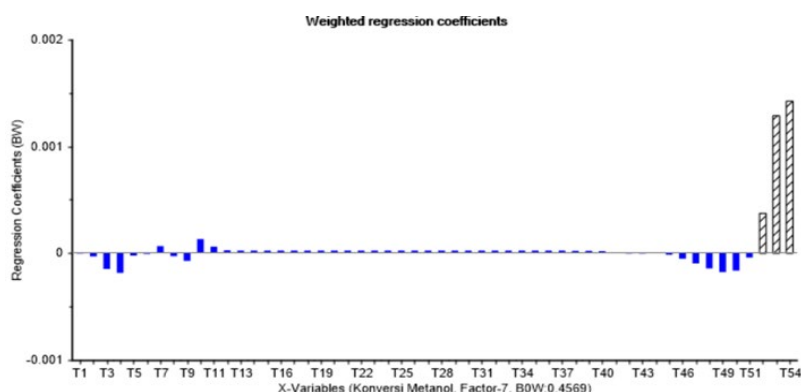


Fig. 7 Weighted regression coefficients distribution of influence of stage temperatures to methanol conversion

PCA Method on Stage Temperatures. Based on the descriptive statistics results that can be shown in Fig. 8. For simulation range $\pm 5\%$ the stage temperatures that has wide range are temperatures from rectifying section. The stage temperatures from stripping section have slightly change but the stage temperatures from reaction section didn't change and can be assumed stable.

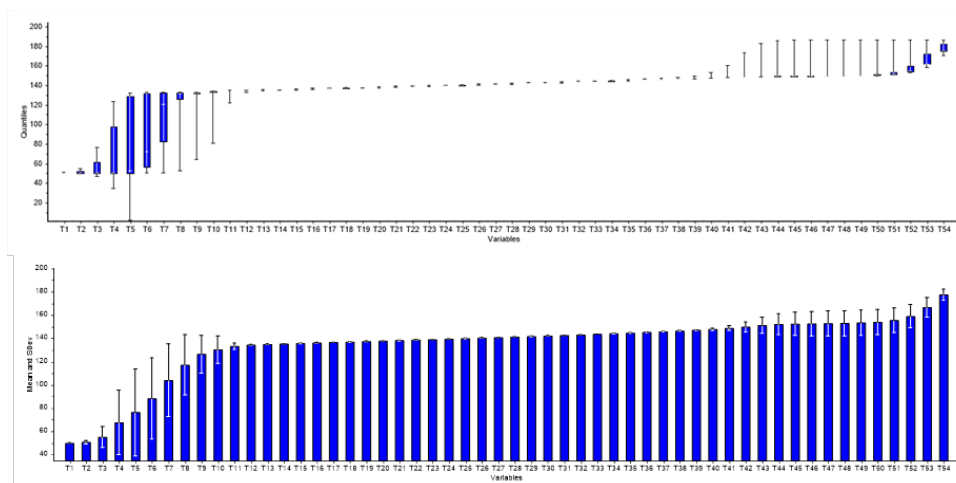


Fig. 8 Descriptive statistics result of stage temperatures

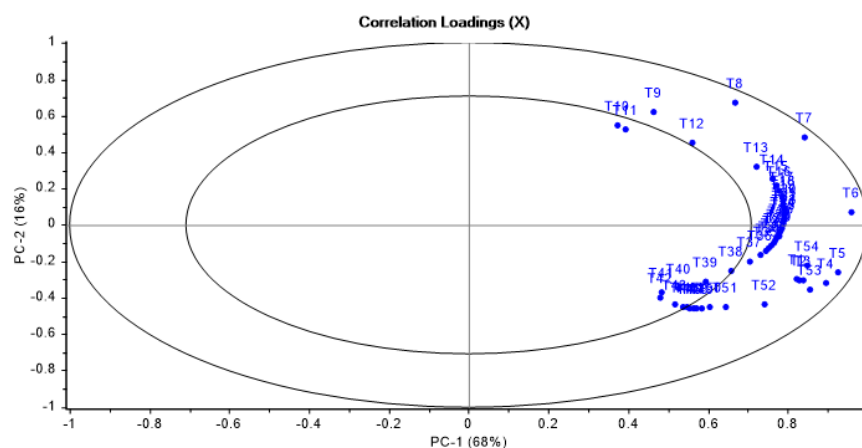


Fig. 9 Correlation loadings of stage temperatures

Based on the correlations loadings that can be shown in Fig. 9, the stage temperatures have positive correlation with each other in general.

The data that are potentially outliers were analyzed using score plot and influence plot as shown in Fig. 10. Based on the the score plot, data that is potentially be an outliers are marked by black color. However in the influence plot those data only have high leverage value and low residual value, because of it the data can be assumed not outliers.

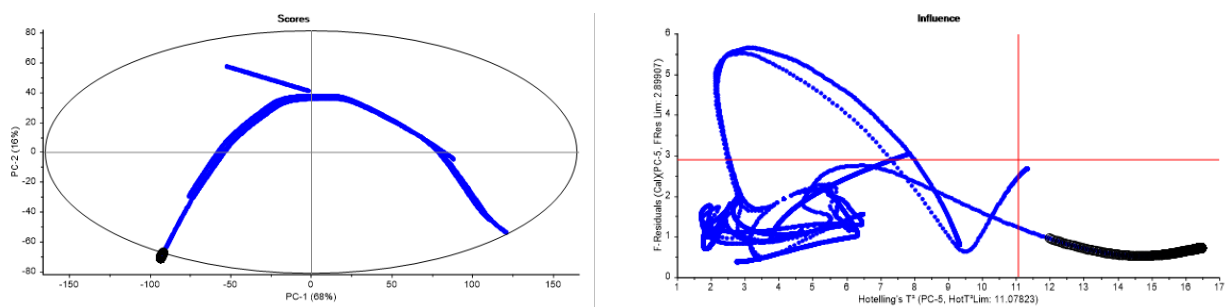


Fig. 10 Score plot and influence plot of stage temperatures

Influence of Reflux Ratio and Reboiler Duty to Stage Temperatures. The correlation loadings of reflux ratio and reboiler duty as input data and stage temperatures as output data can be seen in Fig. 11. Based on the correlation loadings, the reflux ratio has negative correlation with the stage temperatures in general while the reboiler duty has positive correlation with the stage temperatures in general.

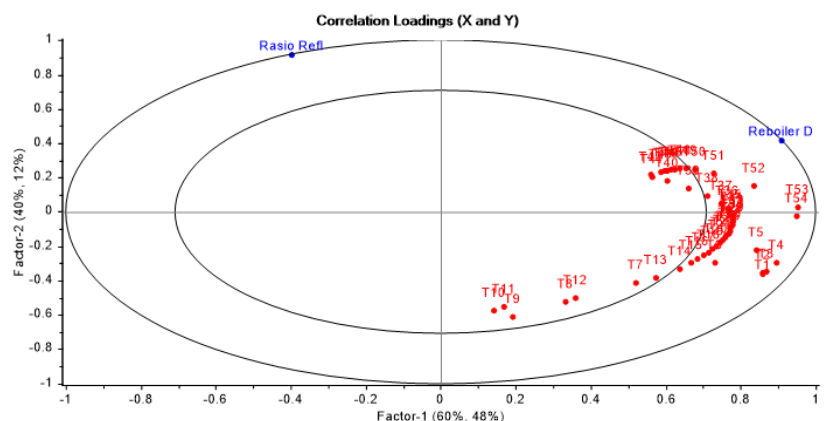


Fig. 11 Correlation loadings of reflux ratio and reboiler duty with stage temperatures

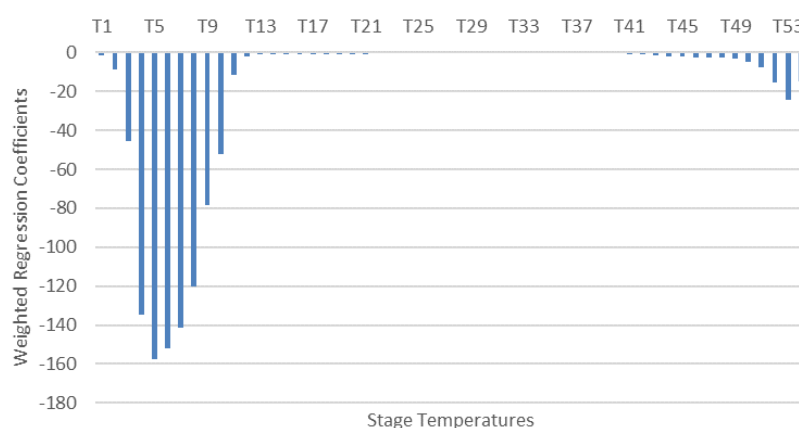


Fig. 12 Weighted regression coefficients distribution of influence of ratio reflux to stage temperatures

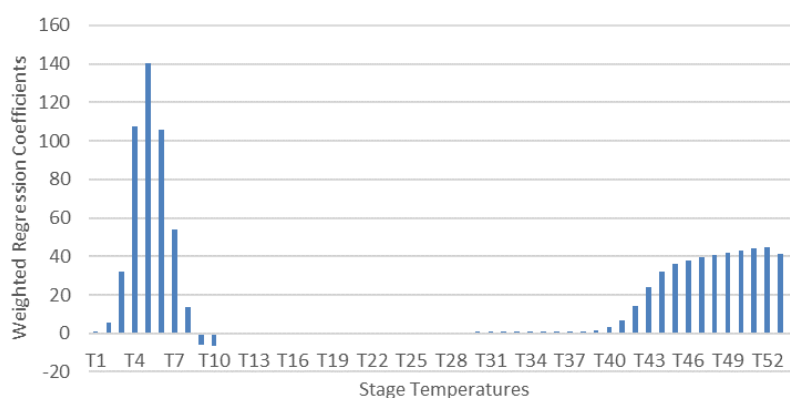


Fig. 13 Weighted regression coefficients distribution of influence of reboiler duty to stage temperatures

The weighted regression coefficients distribution for influence of reflux ratio to stage temperatures can be shown in Fig. 12 while influence of reboiler duty to stage temperatures can be shown in Fig. 13. Based on the Fig. 12, the stage temperatures that significantly influenced by reflux ratio

sequentially are T5, T6, T7, and T4. While based on the Fig. 13, the stage temperatures that significantly influenced by reboiler duty sequentially are T5, T4, T6.

Conclusions

From this research, it could be concluded that based on data driven soft sensors method, the DME purity can be controlled by controlling temperature on stage 4 as the inferential temperature and reflux ratio as the manipulated variable. While based on the data driven soft sensors method, the methanol conversion is difficult to controlled. This is because of the temperature that significantly affect methanol conversion are temperature on stage 52, 53, and 54, which are not significantly affected by either manipulated variables of reflux ratio or reboiler duty.

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