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# Prediction of Variance in the Product Quantity and Quality of HDPE through PLS Modeling - An Introductory Study

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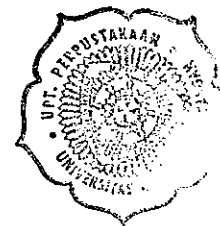
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# Summary

In this thesis, a study was undertaken to model the product quantity and quality in a HDPE production process, Partial Least Squares and Recursive Least Squares were investigated. The modeling steps are data collection, data conditioning, performing a Principal Component Analysis for variable selection, performing the PLS/RLS modeling and the model validation.

Data was collected for five different production types, although modelling was primarily done for one production type with model validation for the other production types.

There are 75 variables including two output variables (production level and melt index) that were collected from the plant. There are 19 variables that have to be removed from the input matrix because they show a zero and a constant values. Some of data the variables also need to be changed because these data can be marked as potentially bad data. Some correlated variables were found after performing a Principal Component Analysis. As the result of this analysis, the new input matrix with 44 variables was ready to be used for modelling purposes.

For the production quantity, a good model to explain the relationship between the conversion (1-R) and the input variables was obtained. This model can be used to predict the conversion for another condition. The model can predict actual values very well by capturing 85% of the variance and producing not more than 5% of the error. It was found that only seven variables of the data set of 44 variables were needed for a good prediction of the conversion.

For prediction of the melt index, a relatively good model with 15 variables was obtained. This model can capture 76% of the variance of the actual value. However, the model can not be used to predict the melt index of another production type. Application of the PLS model show very poor prediction, the predicted value deviates far from the real value.

An adaptive model based on the recursive least squares method was developed and resulted in a very good prediction. However, a recursive least squares method can not be used to predict far away in the future since the model always adapting all the time. Further investigation is therefore required to identify how the melt index can best be modeled, such as the use of hierarchical models.



# Table of Contents

Summary	1
Table of Contents	2
Acknowledgements	4
1. Introduction	5
1.1 General	5
1.2 Research Goals	5
1.3 Outline of the Report	5
2. Polyethylene	7
2.1 General	7
2.2 HDPE Process Technology	10
2.2.1 HDPE Process based on the Phillips Process with a Slurry Loop Reactors	10
3. Process or System Identification	13
3.1 General	13
3.2 Identification Steps	14
4. Data Collection	15
5. Data Conditioning	17
5.1 General	17
5.2 Project Evaluation	18
5.2.1 Examining the Data	18
6. Principal Component Analysis	24
6.1 General Theory	24
6.2 PCA Decomposition	25
6.3 Project Evaluation	27
6.3.1 Load Evaluation in section 1	30
7. Partial Least Squares	39
7.1 General Theory	39
7.2 Dealing with non-linearities	42
7.3 Dynamic extensions of PLS	42
8. Product Quantity Modeling	44
8.1 Variables Selection	44
8.2 Model Development	47
8.3 Model Comparison	54
8.4 Model Validation	56
9. Product Quality Modeling	64
9.1 Model Development	67
9.2 Model Comparison	70
9.3 Model with time delay	71
9.4 Model Validation	72
9.4.1 A new PLS model development using the same 15 variables as the original model	74
9.4.2 A PLS model with a new set of variables	79
9.5 A recursive least squares model	81
9.5.1 Result of recursive least squares method	82
10. Conclusions and Suggestions	86
References	87
Appendix A HDPE process flowsheet	88

Appendix B Detailed information about the collected variables	89
Appendix C List of matlab files	
C.1 Data conditioning	92
C.2 Variables selection	93
C.3 Model validation	102
C.4 Model with time delay	104
C.5 A recursive least squares	108
Appendix D Result of variables selection	
D.1 Variables selection for product quantity	111
D.2 Variables selection for product quality	117
Appendix E A recursive least squares method	132

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# Chapter 1

## Introduction

### 1.4 General

In polyethylene production, a reaction in a long tubular reactor at high pressure or in slurry reactor, which work at a medium pressure can be conducted.

The product quantity is controlled by controlling the ethylene mass flow going into the reactor. However, from field experiences, the ratio between these two measurements (the product quantity and the ethylene mass flow) seems to be influenced by others process measurements.

The product quality is determined by several measurements such as the melt index, the flow index and the density. The product quality is not constant, it can fluctuate considerably between different campaign. A model that can be used to predict the product quality, in this case the melt index is desirable.

Through PLS (Partial Least Squares) modeling a model can be developed to predict the output variable, by relating the output variable with all available measurements. In this project, two models are being developed, first is the product quantity model, the other is the product quality model. All important measurements have been collected for modeling purposes. Prior to modeling, the process data needs to be conditioned and it has to be determined which process variables do affect the product quantity and quality.

After a suitable model has been developed, it should be concluded whether a sufficient part of the variance in the product quantity and the quality can be explained from the process measurements. If so, the process can be controlled, if not, additional measurements may be required.

All data required for the research project are taken from the HDPE (High Density Polyethylene) production plant at SABIC Euro Petrochemicals.

### 1.5 Research Goals

The research goals are development of model, which can predict the output variable and to determine which part of the variance in the output variable can be explained from measured process data and which part of variance remains unknown.

### 1.6 Outline of the Report

The report is divided into ten chapters as describe in the following paragraph :

Chapter 2 represents a general explanation about the polyethylene processes including the High Density Polyethylene (HDPE) process technology.

Chapter 3 shows a general information about process identification. The identification steps used in the research project is described in this chapter.

Chapter 4 until chapter 7 are the main part of this report. Chapter 4 shows the information about the data collection from the plant.

Chapter 5 represents the general information about data conditioning. In this chapter, several important things in data conditioning such as detecting and removing bad data are included. The data conditioning results are described in chapter 5.2.

Chapter 6 introduces the Principal Component Analysis as the method for reducing the dimensionality and eliminating the correlated variables. The result of the PCA is described in chapter 6.3.

Chapter 7 deals with the description and mathematical background of the Partial Least Squares modeling. The evaluation of the model is explained in chapter 8 and chapter 9.

Chapter 10 shows the conclusions and suggestions of this research project.