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# Production optimisation in the petrochemical industry by hierarchical multivariate modelling

Concise report

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Production optimisation in the petrochemical industry by hierarchical multivariate modelling - Concise report


**Sammanfattning/Summary**

This project demonstrates the advantages of applying hierarchical multivariate modelling in the petrochemical industry in order to increase knowledge of the total process. The models indicate possible ways to optimise the process regarding the use of energy and raw material, which is directly linked to the environmental impact of the process. The refinery of Nynäs Refining AB (Gothenburg, Sweden) has acted as a demonstration site in this project. The models developed for the demonstration site resulted in:

- Detection of an unknown process disturbance and suggestions of possible causes.
- Indications on how to increase the yield in combination with energy savings.
- The possibility to predict product quality from on-line process measurements, making the results available at a higher frequency than customary laboratory analysis.
- Quantification of the gradually lowered efficiency of heat transfer in the furnace and increased fuel consumption as an effect of soot build-up on the furnace coils.
- Increased knowledge of the relation between production rate and the efficiency of the heat exchangers.

The project is also reported, with a higher level of detail, in the IVL report B1586-B.



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# Summary

This project demonstrates the advantages of applying hierarchical multivariate modelling in the petrochemical industry in order to increase knowledge of the total process. The models indicate possible ways to optimise the process regarding the use of energy and raw material, which is directly linked to the environmental impact of the process. The refinery of Nynäs Refining AB (Gothenburg, Sweden) has acted as a demonstration site in this project. The investigation was performed with data from the existing process. Since the basic distillation process is similar at most refineries, the general results of this project can be incorporated at other sites.

Three general objectives have been considered during the project.

- Reach a more effective production and thereby lower the energy demand and the environmental impact of the process.
- Obtain improved process economics through an increase in productivity and a decrease in energy and raw material consumption.
- Capture the present process knowledge of the individual operators in statistical and mathematical models, and thereby turning this knowledge into company knowledge.

The project has shown that:

- There are large oscillations present in the upper half of the AD tower. This leads to more inefficient process operation and higher consumption than necessary of resources and energy. Suggestions of possible causes are given.
- A hierarchical model of the entire process has shown large potential for increased yield of the most valuable product in combination with energy savings by process optimisation.
- It is possible to predict product quality in the form of True Boiling Point (TBP) curves for at least four of the six distillation fractions. For most of the products the accuracy of the model predictions are similar to the accuracy of the laboratory analysis method used today, which is run every 8 hours and gives results with approximately 4 hours delay. Model predictions can be executed continuously and the models can act as soft sensors of the product quality. This leads to entirely new control possibilities. Key personnel at Nynäs estimates that the yield of the most valuable product could be increased by 0.5% absolute (approximately 5% relative) if the TBP soft sensors were implemented on-line, which can be translated into energy savings by the same amount per kg product. The economical benefits are also substantial; approximately 4 MSEK/year in increased income is a rough estimate by Nynäs. Nynäs view is that it would be very valuable to put the TBP prediction models on-line.
- The models show and quantify the gradually lowered efficiency of heat transfer in the furnace and increased fuel consumption as an effect of soot build-up on the furnace coils.
- The efficiency of the heat exchangers is significantly lower at higher production rate, which should be taken into account when optimising the process with respect to energy consumption.

# Sammanfattning

Detta projekt demonstrerar de fördelar som kan uppnås genom att använda hierarkisk multivariat modellering för öka kunskapen om processer i petrokemisk industri. Modellerna visar på möjligheter att optimera processen med avseende på energi- och materialförbrukning, vilket direkt påverkar processens miljöpåverkan. Nynäs Refining AB raffinaderi på Hisingen i Göteborg har varit demonstrationsanläggning i projektet. Undersökningen utfördes baserat på historiska data från processen. Eftersom destillationsprocessen är mycket vanlig i petrokemisk industri kan projektresultaten utnyttjas på andra anläggningar.

Övergripande mål för projektet är att:

- Minska miljöbelastningen från anläggningen genom en resurseffektivare produktion
- Erhålla bättre processekonomi genom ökning av produktiviteten och minskning av energi- och materialförbrukning
- Fånga den kunskap som idag finns hos erfarna operatörer om hur processen fungerar och ska köras i modeller och därmed omvandla denna från personkunskap till företagskunskap.

Resultaten visar att:

- Det finns stora svängningar i den övre halvan av AD-tornet, vilket leder till lägre effektivitet och högre resursförbrukning än nödvändigt. Förslag på möjliga orsaker ges i rapporten.
- En hierarkisk model av hela den studerade processen visar på en stor potential att genom optimering öka utbytet av den värdefullaste produkten i kombination med energibesparing.
- Det är möjligt att utifrån processdata som mäts on-line prediktera kokpunktskurvorna för fyra av de sex destillationsfraktionerna. För de flesta fraktioner har modellen ungefär samma noggrannhet som den laboratorieanalys som idag används för att mäta kokpunktskurvorna. Denna analys utförs var åttonde timma och svaret erhålls med ca fyra timmars fördröjning. Modellprediktioner kan beräknas kontinuerligt och modellerna kan användas som virtuella sensorer för produktkvalitet. Detta ger helt nya möjligheter att styra och reglera processen jämfört med dagens läge. Nynäs anser att man skull kunna nå mycket stora fördelar genom att implementera de virtuella sensorerna on-line i realtid. Man uppskattar att utbytet av den värdefullaste produkten kan ökas med 0,5%, vilket motsvarar ca 5% relativ ökning, om de virtuella sensorerna implementeras on-line. Detta kan räknas om till en lika stor energibesparing per kg produkt och de ekonomiska vinsterna är också avsevärda; en intäktsökning med ca 4 MSEK/år är en grov uppskattning.
- Modellerna kvantifierar hur en gradvis försämring av värmeöverföringen i ugnen leder till ökad bränsleförbrukning på grund av uppbyggnad av sot på rören i ugnen.
- Värmeväxlareffektiviteten är signifikant lägre vid hög produktionshastighet. Hänsyn till detta bör tas på processen optimeras med avseende på energiförbrukning.

## Preface

This project was accomplished within the Process Integration program of the Swedish National Energy Administration with additional sponsoring from Nynäs Refining AB. The tight collaboration with process operators at the demonstration site during the course of the project has been vital for the many interesting results achieved. The project is also reported, with a higher level of detail, in the IVL report B1586-B.

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# 1 Introduction

The petrochemical industry is not commonly associated with terms like renewable energy and sustainability. Nevertheless it is fair to assume that the products of this industry will stay a commodity of our society for quite a long time. So even though the vision is that the use of non-renewable resources in time will be restricted, there is much reason to address issues like process optimisation, energy savings and reduced environmental impact of the petrochemical industry.

There is great potential for environmental improvement within the Swedish petrochemical industry. Along with the pulp, paper, metal, iron and steel industries the chemical industry is one of the largest industrial resource consumers of Sweden. 36 000 TJ of combustion energy per year is used by the Swedish petrochemical industry alone [1]. Although Swedish refineries today are well adapted regarding energy efficiency and emissions to the environment, they still have a considerable environmental impact, locally as well as globally. Thanks to enhanced computer capacity, there has been huge improvements in model based monitoring and optimisation techniques, which means that there can exist new optimisation opportunities even for such processes that are considered well optimised today.

Refining of crude oil comprises a number of process steps, e.g. fractionated distillation and mixing of fractions to obtain products with desirable qualities. This makes the overall process extremely complex, since all process steps affect each other through material and energy flows. It is desirable to understand the effect that variations in crude oil quality, process disturbances and control parameters have on the final result, and to be able to optimise the process on account of material and energy consumption. This requires deep knowledge about the specific process steps as well as interactions between steps. Statistical modelling is an established method to give increased knowledge of processes. The fact that petrochemical industries generally are well documented by on-line instrumentation and highly automated makes it possible to extract a lot of data suitable for process modelling.

The refinery of Nynäs Refining AB (Gothenburg, Sweden) has acted as a demonstration site in this project. Frequent meetings have been held between the modellers at IVL and the process operators at Nynäs Refining to discuss the process and to assure that results are relevant. Since the basic process is similar at most refineries, the general results of this project can easily be incorporated at other petrochemical sites. Naturally, more specific results such as the actual models will be site specific.

# 2 Objective

The intention of this project is to demonstrate the advantages of applying hierarchical multivariate modelling in order to increase knowledge of the total process in the demonstration site. The models should also indicate possible ways to optimise the process regarding the use of energy and raw material as well as the environmental impact of the process.

Three general objectives have been considered during the project.

- Reach a more effective production and thereby lower the energy demand and the environmental impact of the process.
- Obtain improved process economics through an increase in productivity and a decrease in energy and raw material consumption.
- Capture the present process knowledge of the individual operators in statistical and mathematical models, turning this knowledge into company knowledge.

It is also expected that unwanted variation in the product quality will be reduced as a result of the increased understanding of the process and the enhanced monitoring possibilities given by the models.

# 3 Scope and data

The scope of the study is to investigate data from the existing process, capturing current process variation in models and interpreting the effect it has on the product quality. Hence, retro fitting of the process is not considered.

The study is based on real process data from the demonstration site. Historical data from the on-line process documentation of one particular operational mode, from the period of June 2002 to June 2003, was used. This corresponds to 110 days of data, in coherent periods of 2.5 days up to 11.5 days.

Data from laboratory analyses of the true boiling point (TBP) curve of four fractions from the distillation towers (see section 5 below) have also been included in the study, since the curve gives a very good characterisation of many important properties of the products. Analysis is normally carried out 3 times a day.

# 4 Methods

The statistical modelling methods used in this work are standard as well as multi-block Principal Component Analysis (PCA) and Partial Least Squares (PLS). Process modelling by multivariate statistical modelling methods, such PCA [2,3] and PLS [3, 4] and modifications thereof, are increasingly used and accepted in industry. This can be explained by their ability to handle the large amounts of process data generated in well-instrumented modern process industries and to extract relevant information from the data.

Standard modelling methods are efficient in handling large amounts of data. However, when applied to very large multi-step processes there is a risk that the increasing model size and complexity can decrease the usefulness of the model by hampering interpretation and making model maintenance difficult. If the data is organised in meaningful blocks, usually according to the sections of the process, so called multi-block models [5] can be applied, which can increase the utility and interpretation abilities of the models significantly.

Multi-block modelling methods use a two level model structure: a sub-level that contains model structures for the individual blocks and a super-level that connects the blocks. A scheme of a process and a multi-block model structure is given in Figure 1. The common variations and interactions between process sections are modelled on the super level, while details about the contributions and effects in each section are obtained on block level. Multi-block PCA models can be used for process monitoring, fault detection, fault identification and process optimisation. The structure makes fault detection easier by providing easier interpretation of which process section is having problems on super level and details about the problems on block level. Multi-block PLS models can be used for predicting e.g. product properties from process data, similar to ordinary PLS, but with increased model interpretability.

Multi-block modelling have been used successfully in a smaller application in a cracking unit by Wold *et al* [6]. Westerhuis and Coenegracht [7] describes an application from the pharmaceutical industry that demonstrates the advantages of multi-block modelling, although only two blocks are used. The advantages can be expected to be greater when studying a more complex process like in the project described in this report.

Previous applications of multivariate modelling in the refinery industry include the use of ordinary PCA and PLS on e.g. a fluid catalytic cracking unit and a crude distillation unit [8-11]. Several authors have recognised the lack of good on-line sensors in distillation processes and the unsatisfactorily long response times for laboratory determinations of properties for products from the processes, which hampers quality control and efficient process control.

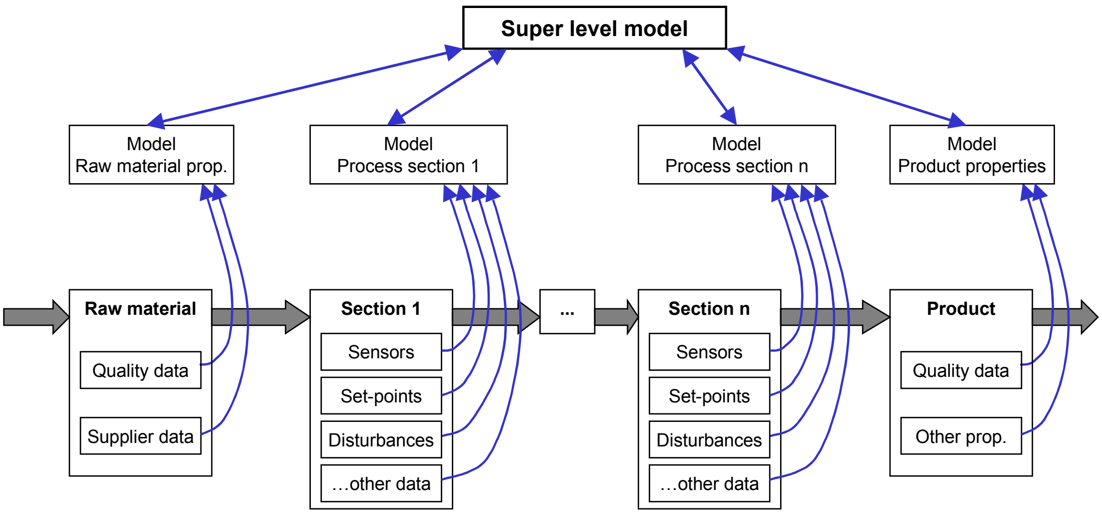



Figure 1. Schematic picture of a multi-block model applied to a multi-step process.

# 5 Process description

The demonstration site in the present study is Nynäs Refining AB's refinery in Gothenburg, Sweden. The process is outlined in Figure 2. At the refinery crude oil is fractioned into more desirable products through the process of distillation. The refinery has two distillation towers, one with atmospheric distillation (AD) and the other with vacuum distillation (VD). Bitumen, which is used in the making of asphalt, is the main product of this refinery but lighter products are also of importance.

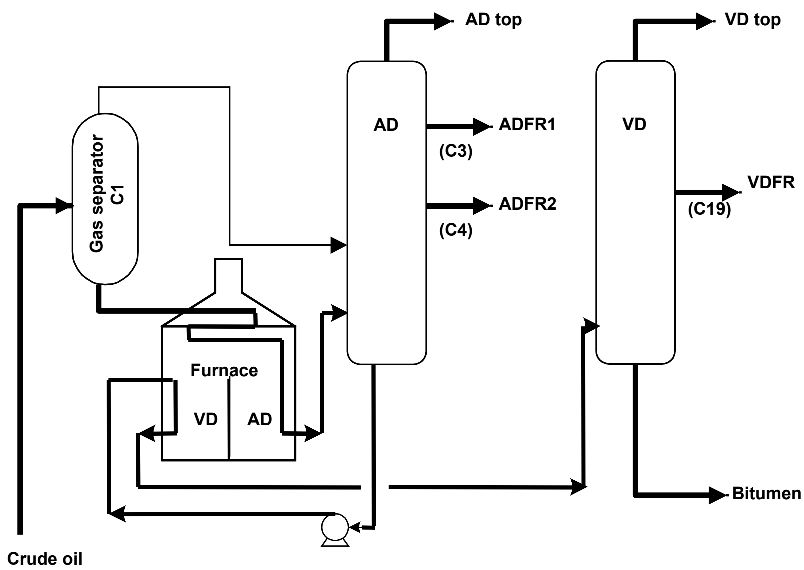



Figure 2 Simplified outline of the distillation process at Nynäs Refining AB. The initial products are the fractions ADTOP, ADFR1, ADFR2, VDTOP, VDFR and bitumen. Mixing of some of these products to form new products also occur.

For modelling purposes, the process was divided into several logical blocks and measured parameters within each block were grouped together. The blocks are listed below in the order of appearance in the process, but it should be noted that there is heat exchange between the warmer products and the cooler feed of crud oil, which of course has an effect on previous blocks.

- **Raw material.** The crude oil is heated in a series of heat exchangers, recovering the excess energy in the products. Typical process parameters in this block are feed rate and temperatures.

- **AD furnace.** In the AD furnace the crude oil is heated to the right temperature before it enters the AD tower. The fuel consumption in the furnace is of course of high interest in the modelling work. It should be noted that the AD and the VD parts of the furnace are not completely isolated from each other.

- **AD tower.** Distillation at atmospheric pressure. This block also includes so-called side strippers of the fractions ADFR1 and ADFR2, denoted C3 and C4 respectively. Process parameters of particular interest in this block are the temperature profile through the tower, steam supply (to the bottom of the tower and to the side strippers) and fraction yields.

- **VD furnace.** What is left of the crude oil after extraction of the three fractions in the AD tower is further heated in the VD part of the furnace. Similarly to the AD furnace, the fuel consumption is of interest in the modelling work.

- **VD tower.** Distillation at very low pressure. This block also includes the side stripper of the fraction VDFR, denoted C19. As for the AD tower, process parameters of particular interest in this block are the temperature profile through the tower, steam supply (to the bottom of the tower and to the side stripper) and fraction yields.

- **Product properties.** The block for the product properties refers to the laboratory analyses of true boiling point (TBP) curves of the four fractions ADFR1, ADFR2, VDTOP and VDFR. The analyses are performed three times a day and the curves can be linked to important qualities of the fractions, e.g. their viscosity, density and flash point.

# 6 Results and discussion

This section presents some selected results of the modelling efforts carried out in the project. For deeper technical presentation of the results, please see IVL report B1586-B. Models and results most relevant to improving process performance have been selected and are discussed below. The models discussed are of both PCA and PLS type as well as both single block and multi-block.

## 6.1 Effect of production rate

A PCA model based on data from the AD tower and TBP data from ADFR1 and ADFR2 clearly shows effects of production rate on the product properties. The two products get lower flash points when the production rate is high. The interpretation of the model is rather straightforward. It shows that lower flash points are obtained when higher production rates are not compensated with higher steam flows to the side strippers for each product respectively. Note that the production rate and side stripper steam flows are not the only factors contributing to varying flash points of the two products.

### 6.1.1 Conclusions and recommendations

It is suggested to add relative steam flows to operator process screens and to use this in process operation. Examples are kg steam to AD bottom per ton crude oil that enters the AD tower and kg steam to each side stripper per ton fraction extracted of the product going to that side stripper. This simple measure would facilitate correct steam flows and thus, better control of the TBP curves of the products.

## 6.2 AD tower oscillations

The analysis showed that an oscillation with a period of approximately 85 minutes is present in a number of variables related to the top half of the AD tower. The oscillation corresponds to a significant part, 8%, of the total process variability in this tower. A detailed analysis, using dynamic PCA [12], was undertaken based on data with high time resolution: 30 seconds.

The model shows that only a few variables related to the upper half of the AD tower have a major contribution to the oscillation. The ADTOP yield oscillates between 0 and 0.5%. The density of the ADTOP flow to cistern is oscillating between approximately 0.70 and 0.71 $kg/dm^3$, which, since it cannot be attributed to temperature changes, indicates oscillating ADTOP product properties. The same is true for ADFR1 product properties, since ADFR1 density is oscillating but not the temperature of the ADFR1 flow to cistern. The temperature amplitude in the ADFR1 extraction point, which is related to product properties, is approximately 5°C, which is a major change[1]. Thus, the

[1] The standard deviation of the 50% point in the TBP curve for this fraction is 3°C

oscillations seem to have a marked effect on the AD tower and product streams. The oscillating changes in product properties are not possible to detect from the TBP curves, since sampling and analysis is done only once every 8 hours

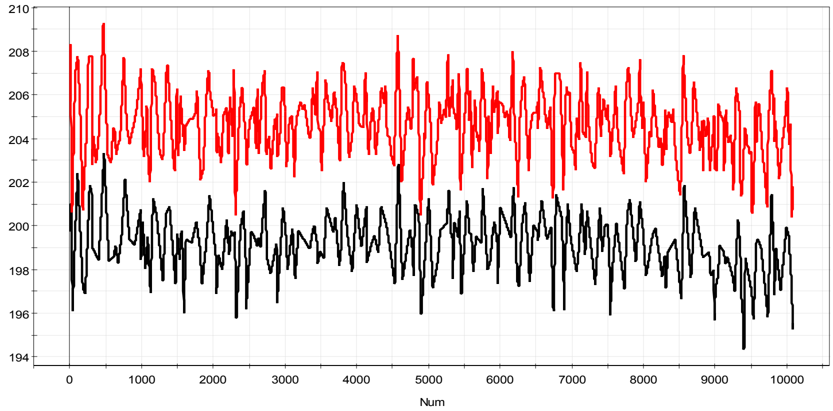



Figure 3. Data from the period 14-17 June 2002: temperatures in the extraction point of ADFR1 (red) and side stripper of ADFR1 (black).

Notably the temperature of the ADTOP reflux and the pressure in the top of the AD tower are not oscillating while the temperatures of the ADFR1 extraction and the corresponding side stripper, C3, are. Also the flow of gas from the gas separator on the ADTOP stream is oscillating. Furthermore, it was found that there seems to be small phase shifts between the oscillating variables. The variable "leading" the oscillation is the temperature in the ADFR1 side stripper, about 5 minutes ahead of the ADTOP flow oscillation.

Three possible explanations to the oscillations were identified. The possible origins are:

- **The water separator of the ADTOP flow** In discussions with the process operators, it was put forward that the extraction of the ADTOP fraction from the water separator to tank is irregular, which can give rise to the oscillations in ADTOP flow and yield. It has not been considered a problem since it was not known to influence the AD tower itself. The present analysis, however, strongly indicates such an influence. A possible mechanism may be that the irregular flow from the water separator causes pressure changes in the connected gas separator and the ADTOP, which would then influence the rest of the tower.

- **The gas separator for the crude oil**. Oscillations in the gas flow from the gas separator of the crude oil, C1, caused by poor pressure control in that separator is another possible cause. If the pressure in C1 builds up during some time and is suddenly released by opening the valve for the gas flow to the AD tower, the amount of low-boiling components (including water) and possibly also the pressure in the AD tower can oscillate. Unfortunately the gas flow from C1 to the AD tower that would be the primary indicator is not logged.

- **The side stripper of ADFR1**. The third potential explanation to the oscillations is that the cause is related to the side stripper of ADFR1, C3. This is supported by the fact that the temperature in C3 is "leading" the oscillations, about 5 minutes before the ADTOP flow. The oscillations in C3 would then influence the AD tower by either the flow from the tower to the side stripper or the gas flow in the opposite direction.

No signs of a similar oscillation are found in the individual analysis of other process sections, which indicates that the phenomenon observed is local and does not influence other process sections significantly. This is also confirmed in the multi-block models.

### 6.2.1 Conclusions and recommendations

From the above results, it can be concluded that PCA and dynamic PCA are extremely powerful tools for identification of process disturbances such as oscillations. This is true both for variables where the oscillation is the dominating variation and variables where the oscillation is only a minor contribution or where the effect is partially hidden by database compression.

The effect on product properties can, to some extent, be expected to be averaged out in the storage tank. However, the oscillations clearly contribute to a wider boiling point interval for ADFR1 with a lower flash point as a consequence. Further, process control is to a large extent based on the TBP curves determined by GC for samples taken every 8 hours. With the large oscillations present in the process, the precise timing of sampling has a large influence on the determined TBP curve and thus accurate process control is not possible. Thus, the oscillations can be expected to impair process performance with respect to energy consumption, process economy and product quality but it is very difficult to quantify the effect.

The PCA has pointed out some candidate causes to the oscillations but in order to determine the cause of the problem, it is necessary to have access to higher quality data for some of the variables measured in the process and stored in the history database. It is recommended to increase the quality of data in the history database by decreasing compression for some process. When the necessary changes in the data history collection are done, it should be possible to identify the cause of the oscillation and to take the necessary measures to correct it, which would most likely mean to tune a control loop or repair a faulty valve.

## 6.3 Prediction of product quality

It is reasonable to believe that variation in product quality reflects variation in how the process is operated and changes in the raw material. It is also reasonable to believe that, under some circumstances, changes in raw material composition will be reflected in the process variables that are measured on-line. Therefore it can be possible to model product quality based upon the values of the process variables. In order to investigate this further, PLS models for TBP-curves of four fractions were calibrated. The advantage of these models over e.g. regular multiple regression models and artificial neural network models are that they can be used both for prediction and for interpretation of the underlying phenomena that causes the variation in the predicted parameters. A further advantage is the prediction diagnostics obtained by PLS that can be used to increase the reliability of the model by detecting an outdated model.

Previous work in modelling of petrochemical processes has indicated that linear models are not adequate to describe the non-liner process behaviour. However, in this report it is shown that by using "smart" variable transformations, i.e. by including knowledge about process non-linearity in the data transformation strategy prior to the regression step, it is possible to use linear models to accurately describe the process and to predict the product quality.

### 6.3.1 Variation in TBP data

An initial PCA investigation of the TBP-curves of the fractions ADFR1, ADFR2, VDTOP and VDFR showed that, between the two towers, the quality of the products did not display any distinct co-variation. Variation in the TBP-curves of fractions from the AD and the VD tower were mainly described in separate components of the PCA model. On the other hand, fractions from the same tower were highly correlated and only a few components were needed to explain a majority of the variance in data. Therefore the continued approach was to further investigate the fractions from each tower in separate PCA models, including the process variables related to the tower, and then evaluate individual PLS models. One model is made for the fractions of the AD tower and one for the fractions of the VD tower.

### 6.3.2 Estimation of prediction errors

For the results presented in this study, the model prediction errors are expressed as RMSECV (*root mean square error of cross validation*). RMSECV is a measure of the average prediction error (given in the same unit as the response variable) calculated from data unknown to the model. The cross validation scheme used in the validation of the PLS-models is based on a *leave-one-production-period-out* approach, which means that the production periods (2.5-11.5 days, different number of samples) are used as cross validation segments. Thus, no data from a certain production period is present in the calibration data when the TBP curves for that production period is being predicted. This is believed to give better prediction error estimates than other cross validation schemes since there are major differences between operating conditions, and possibly raw material properties, between the periods but much smaller differences within periods. The larger differences are representative for future production and, hence, RMSECV based on leave-one-production-period-out should be realistic for future use of the model.

When estimating the performance of a model prediction it is also important to have an estimate of the error in the reference method for two reasons. 1) The prediction is compared to the reference value so the error estimate is actually influenced by the uncertainty in the reference value. 2) The purpose of modelling is usually to replace the reference method or to make the values from it available more frequently. It is then of great interest to know the relative performance of the methods. The uncertainty of the reference TBP curves used for modelling was estimated based on the method specifications and discussions with the laboratory personnel. The standard gives estimates of reproducibility and repeatability. The actual error is believed to be between these two, since repeatability considers two samples analysed in sequence on the same instrument, while reproducibility considers different laboratories. Hence, the two error estimates where pooled. The resulting reference errors were in accordance with the experience of the laboratory personnel.

### 6.3.3 Prediction results

The PLS models show that it is possible to predict product quality in the form of TBP curves for ADFR1, ADFR2, VDTOP and VDFR from the on-line process data. The prediction error estimates along with the TBP reference errors and the TBP standard deviations are shown in Table 1.

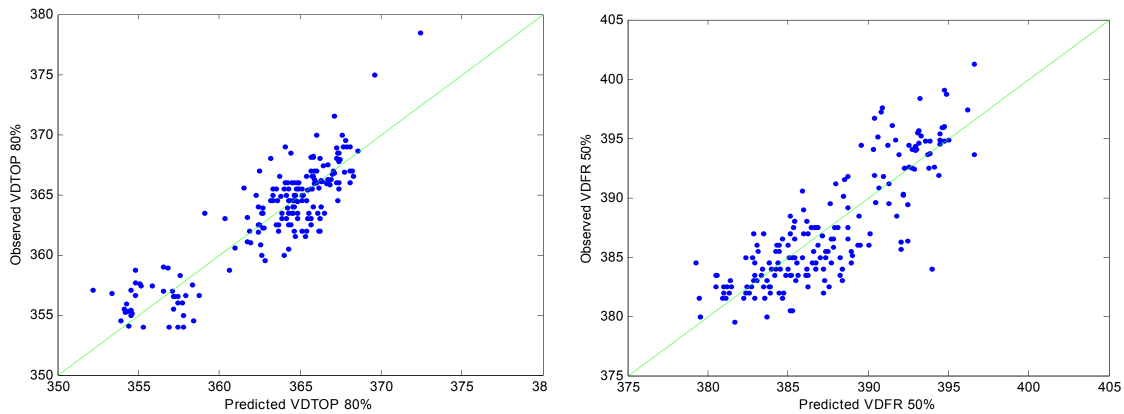



Figure 4 Observed vs. predicted during cross validation, VDTOP 80% (left) and VDFR 50% (right).

The model accuracy is low for ADFR1 but higher for the more interesting fractions ADFR2 and VDTOP. The prediction errors (RMSECV) differ among the four products with highest accuracy for VDTOP, 2.0-2.2 °C, and lowest for the light end of VDFR, 4.3 °C at TBP 5%. Two examples of observations vs. predictions on cross validation data are shown in Figure 4. For most of the products the accuracy of the model predictions are similar to or better than the accuracy of the GC method used today.

Table 1. PLS model prediction error estimates for the TBP curves.

| Fraction | TBP % | RMSEC | RMSECV | TBP reference error | TBP reference std deviation |
|---|---|---|---|---|---|
| **ADFR1** | 5 | 2.5 | 2.8 | 2.0 | 2.8 |
| | 20 | 2.2 | 2.7 | 2.4 | 2.9 |
| | 50 | 1.9 | 2.7 | 2.2 | 3.0 |
| | 80 | 1.7 | 2.7 | 2.2 | 3.0 |
| | 95 | 1.6 | 2.8 | 2.6 | 3.1 |
| **ADFR2** | 5 | 1.4 | 2.1 | 2.8 | 2.0 |
| | 20 | 1.5 | 2.5 | 3.0 | 2.6 |
| | 50 | 1.7 | 2.5 | 2.2 | 3.3 |
| | 80 | 2.3 | 2.7 | 2.2 | 5.0 |
| | 95 | 3.1 | 3.2 | 2.6 | 7.5 |
| **VDTOP** | 5 | 1.1 | 2.2 | 2.8 | 2.3 |
| | 20 | 1,4 | 2.2 | 3.1 | 2.4 |
| | 50 | 1.7 | 2.2 | 2.2 | 3.2 |
| | 80 | 1.8 | 2.1 | 2.2 | 4.2 |
| | 95 | 1.6 | 2.0 | 2.6 | 5.3 |
| **VDFR** | 5 | 2.2 | 4.3 | 3.4 | 6.7 |
| | 20 | 1.8 | 2.9 | 3.5 | 5.1 |
| | 50 | 1.7 | 2.7 | 2.2 | 5.0 |
| | 80 | 1.7 | 2.6 | 2.2 | 4.9 |
| | 95 | 1.4 | 2.5 | 2.6 | 4.5 |

### 6.3.4 Conclusions and recommendations

It is possible to predict product quality in the form of TBP curves for ADFR1, ADFR2, VDTOP and VDFR from process data in real-time. The model accuracy is low for ADFR1 but higher for the more interesting fractions ADFR2 and VDTOP. The prediction errors (RMSECV) differ among the four products with highest accuracy for VDTOP, 2.0-2.2 °C, and lowest for the light end of VDFR, 4.3 °C at TBP 5%. For most of the products the accuracy of the model prediction are similar to or better than the accuracy of the GC method used today. In addition, TBP curves from GC analyses are obtained once every 8 hours with a delay of up to 5 hours from sampling, which makes process control using these curves difficult.

Model predictions can be made available on-line in real-time which would give entirely new possibilities for process control. This gives the process operators valuable information on process performance much earlier compared to if they have to wait for the result of time-consuming analyses in the laboratory. This facilitates more efficient process operation, which should lead to decreased production cost and environmental impact.

One of the objectives in this study was to transfer the knowledge of the individual process operators into common company knowledge. The goal is achieved if the models are able to describe the relationship between the process data and the product quality. The interpretation of the PLS prediction models gave some new insights but mainly confirms the knowledge kept by experienced process operators. This lends credibility to the models ability and stability and means that the goal of capturing operator knowledge in models and transfer it to company knowledge is reached. The model interpretation is not discussed further in this short report. It is presented in detail in the full technical report from this project, IVL report B1586-B.

## 6.4 Interpretation of models of the full process

This section discusses some interpretations of a hierarchical model developed in this project. There are several other different interesting interpretations but they are not discussed here to limit the length of this report. All interpretations of the hierarchical model reflect the interactions of different process sections, since this is the main advantage of this type of model. The models are based on 9 blocks including both TBP data and process data, see below. Thus they reflect both process state and its influence on product properties.

- TBP curve for ADFR1
- TBP curve for ADFR2
- TBP curve for VDTOP
- TBP curve for VDFR
- Incoming crude oil (heat exchangers)
- AD tower
- VD tower
- AD furnace
- VD furnace

### 6.4.1 Increases of yields and effects

Several components of the hierarchical model contain a large contribution from production rate, since this has a large influence on the process as has been shown in the individual models of process sections. When optimising a process on-line, the production rate is often not possible to adjust since it is given by the current market demand for the product or the supply of crude oil.

To facilitate optimisation at constant production rate, in particular with regard to the yield of the highly desired product D10 (a mix of ADFR2 and VDTOP), the model was modified to eliminate effects of changing production rate. The product yields during one year of operation of the process mode investigated here show clear potential for optimisation of D10 yield, see Figure 5 (left).

The model was used to investigate the possibility to increase the yield of D10 with acceptable product properties and the potential energy savings. One way to visualise the model is to "map" the process parameters according to their mutual relation, see Figure 5 (right). It is also possible to track the process collective status at a given time by weighing together the values of the process parameters and plotting the resulting value in the map. From the model, and hence also in the map, it is possible to find the process settings that give the desired product qualities, if these are achievable. The model shows that (see Figure 5 (right)):

- Movement along the top-left to bottom-right diagonal influences D10 yield by the yields of VDTOP and ADFR1, which is the way yield optimisation is normally done by the process operators.

- Movement along the bottom-left to top-right diagonal does not influence the yield of D10 and changes in this direction can thus be used to optimise the process with respect to energy consumption and product quality at constant D10 yield.

The discussion below quantifies effects on yield, energy consumption and product properties. All quantified effects of changes in the discussion are given as 2 standard deviations of the normal operation variation. This corresponds to a change from the mean operating conditions to the extreme (95% interval end-point) in that direction or vice versa.

It is important to note that no assumption is made that it is actually possible to move outside the domain where the process has been operated during the year studied. The estimates are done based on the actual variation in the historical data. Thus, they are conservative in that it is assumed that domains of operation not visited before are likely to be infeasible. If larger variations in this direction can be made without producing out of specification D10, the savings can be even larger than indicated.

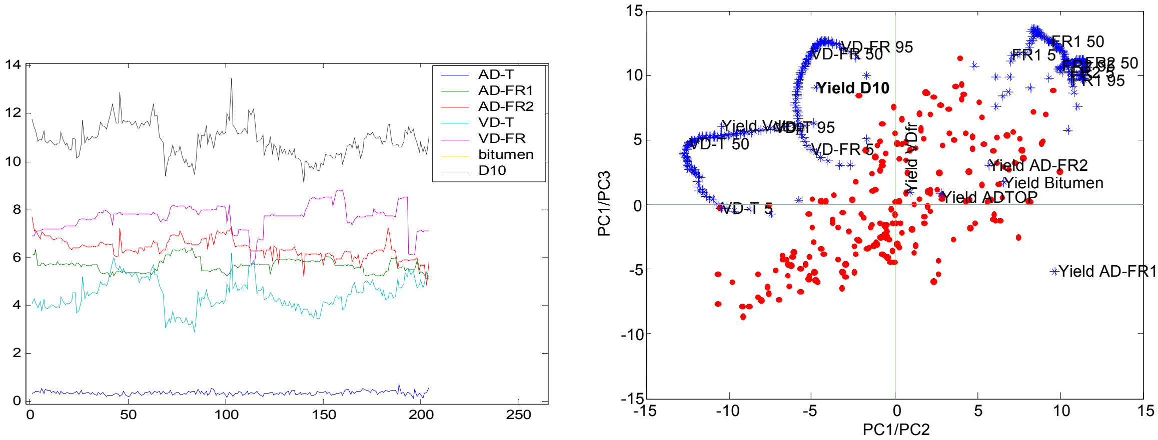
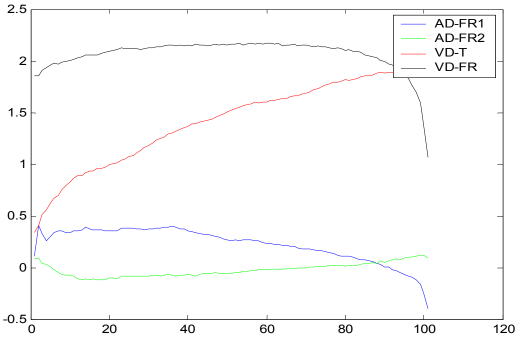



Figure 5. Left: Product yields during June 2002-June 2003. There is a clear potential to optimise the yield of the mixed product D10. (Bitumen yield is about 60-70% and therefore not visible in the chart)
Right: Visualisation of the hierarchical model where production rate has been eliminated. Blue stars represent process variables. Only yields and product property data are shown in this figure, but all variables have their specific position in the map. For graphical visualisation of the complete set of variables, please see IVL Report B1586-B. Red dots represents the status at certain times, showing the operation domain during June 2002-June 2003.

Movement along the first direction influences the D10 yield as well as energy consumption:

- D10 yield is increased by 0.6% by increasing the VDTOP yield at the expense of ADFR1.
- The changes on fuel consumption in the furnaces along this direction are non-significant.
- The main steam flow to be considered is the flow to the AD tower. It is decreased by approximately 10% when the D10 yield is increased. Other steam flows are not influenced significantly.
- The influence on product properties is shown in Figure 6. It can be noted that the AD tower fractions are not influenced significantly, *i.e.* there is no great deviation from zero in Figure 6, while the boiling point of the heavy end of VDTOP is increased by 4°C when the D10 yield is increased 0.6%. This is a natural consequence of the increased yield from the same raw material. The VDFR properties are also changed but this is less important from a process optimisation point-of-view.



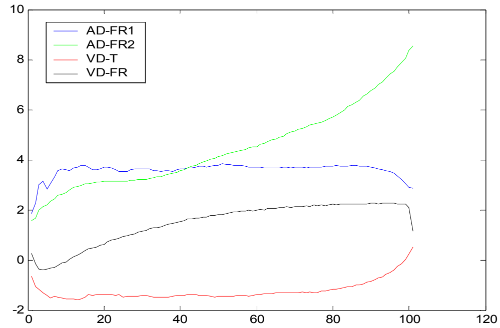




Figure 6. Quantified influence on TBP-curves of fractions from the AD and VD tower as one standard deviation of normal operating conditions (shown by red dots in Figure 5 right).
Left: movement along top-left to bottom-right diagonal in Figure 5 (right).
Right: movement along bottom-left to top-right diagonal in Figure 5 (right).

Movement along the bottom-left to top-right diagonal in Figure 5 (right) does not significantly influence the D10 yield but influences energy consumption and product properties according to:

- The total fuel consumption is decreased by approximately 4% when moving from the centre to the lower left part of Figure 5 (right).
- The steam flows are increased by approximately 5% when moving from the centre to the lower left part of Figure 5 (right).
- The changes in product properties are mainly for ADFR2 as visualised in the right part of Figure 6. Also VDTOP is influenced but in the other direction.

### 6.4.2 Fuel consumption in furnaces

As a result of the hierarchical modelling, attention was drawn to fuel consumption in the furnace. The model reveals the relationship between fuel consumption in the AD and the VD furnace as well as their relation to other process parameters such as crude oil feed flow and the effect of the heat exchangers. It was noted that:

- Build-up of soot on the furnace coils, particularly in the AD furnace, gradually lowers the efficiency of heat transfer and increases the relative fuel consumption. From June to November 2002 there is a gradual increase of the total relative fuel consumption with approximately 1 kg per ton, Figure 7.

- Chemical cleaning of the furnace has a clear effect. The total relative fuel consumption is reduced by at least 1.5 kg per ton after the cleaning in the winter 2002-2003, Figure 7.

- At higher production rate the relative fuel consumption in the AD furnace increases, while the relative fuel consumption in the VD furnace decreases, Figure 8. The effect is about 1 kg fuel per ton crude oil over the entire production rate span.

- The effect of the heat exchangers is lower at higher production rate. Crude oil temperature differences at minimum and maximum feed rate ranges between 5 and 20 °C, with larger differences at the end of the chain of heat exchangers. This is probably one of the reasons why more fuel is needed in the AD furnace during high production rate.

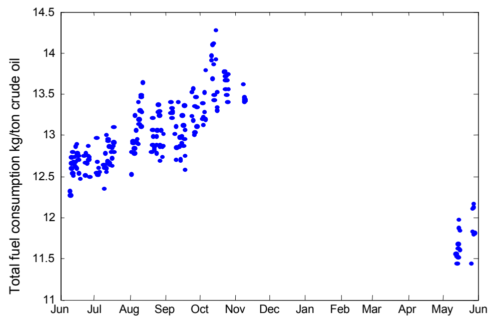



Figure 7 Total relative fuel consumption, variation in time (chemical cleaning during winter stop).

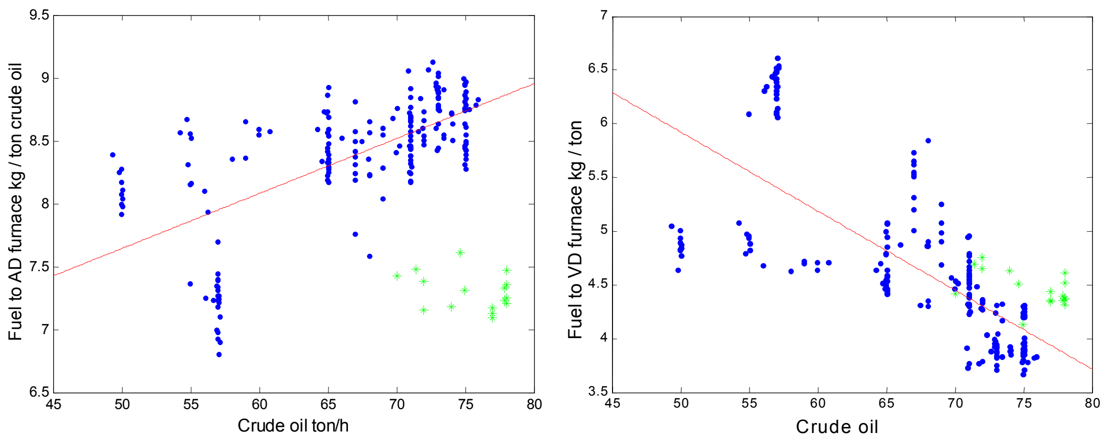



Figure 8 Relation between relative fuel consumption and crude oil feed rate. Left: AD furnace. Right: VD furnace. Before chemical cleaning, blue dots and linear regression, after cleaning, green stars.

### 6.4.3 Conclusions and recommendations

The full process hierarchical model discussed in 6.4.1 has shown large potential for increased yield of D10 and energy savings by optimisation of operating conditions. Due to fluctuations in the process, it can be difficult to achieve the full theoretical benefit in reality for long periods of time. On-line prediction models for TBP curves of ADFR2 and VDTOP as well as process maps from PCA models, as the one shown in Figure 5 (right) above, would be a valuable tool to achieve the potential benefits. Key personnel at Nynäs estimates that the yield of the most important product, D10, could be increased by 0.5% absolute (approximately 5% relative) if the TBP soft sensors were implemented on-line. This can be translated into energy savings by the same amount with respect to kg produced D10 product. The economical benefits are also substantial; approximately 4 MSEK/year in increased income is a rough estimate by Nynäs.

Build-up of soot on the furnace coils gradually lowers the efficiency of heat transfer to the crude oil and increases the relative fuel consumption. These effects can be clearly seen in the models developed. Chemical cleaning of the furnace has a large effect on the total relative fuel consumption, which is reduced to from 13.5-14 kg per ton to approximately 11.5-12 kg per ton after cleaning. This can be used to determine when the cost of chemical cleaning can be motivated by a sufficient decrease in relative fuel consumption.

The effect of the heat exchangers is lower at higher production rate. Crude oil temperature differences at minimum and maximum feed rate ranges between 5 and 20°C, with larger differences at the end of the chain of heat exchangers. This means that less temperature increase is required in the AD furnace at low production rate, which should be taken into account when optimising the process with respect to energy consumption. It should also be kept in mind that, at low production rate, the energy consumption is shifted from the AD part of the furnace to the VD part with roughly the same total energy consumption regarding fuel to the entire furnace.

# 7 Future work

In discussions with process operators and process engineers, possible benefits of putting some of the models developed in this project on-line were investigated. It was agreed that:

- Prediction of the TBP curves would speed up the product quality control significantly.
- PCA models can help monitor current process status and suggest how to steer the process into the most desirable state.

Nynäs current view is that it would be very valuable to put the TBP prediction models on-line and they see potential increases in yield that would correspond to energy savings and improved productivity. In a longer run it would also be interesting to use PCA models for process monitoring on-line.

The promising results obtained in this project show that it would be very interesting to make process models for other operating modes than the one studied in this project. There are at least two more production modes that are frequently used and where the effort would be worthwhile.

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