

Production optimisation in
the petrochemical
industry by hierarchical
multivariate modelling.

Phase 2: On-line implementation

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B1862

July 2009

This report approved
2009-07-09


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Organization IVL Swedish Environmental Research Institute Ltd.	Report Summary
Address P.O. Box 5302 SE-400 14 Göteborg	Project title Production optimisation in the petrochemical industry by hierarchical multivariate modelling in real-time. Project sponsor Swedish National Energy Administration The foundation IVL (SIVL) Emerson Process Management Nynas AB
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Title and subtitle of the report Production optimisation in the petrochemical industry by hierarchical multivariate modelling. Phase 2: On-line implementation	
Summary <p>IVL, together with Emerson Process Management, has developed a decision support system (DSS) based on multivariate statistical process models. The system was implemented at Nynas AB's refinery in order to provide real-time TBP curves and to enable the operator to optimise the process with regards to product quality and energy consumption.</p> <p>The project resulted in the following proven benefits at the industrial reference site, Nynas Refinery in Gothenburg:</p> <ul style="list-style-type: none"> • Increased yield with up to 14 % (relative terms) for the most valuable product • Decreased energy consumption of 8 % <p>Validation of model predictions compared to the laboratory analysis showed that the prediction error lay within 1°C throughout the whole test period.</p> <p>(For a more extended Summary, see page 2. For a summary in Swedish, see page 4.)</p>	
Keyword Petrochemistry, petrochemical industry, crude oil distillation, process optimisation, energy efficiency, multivariate modelling, MVA, soft sensor, TBP	
Bibliographic data IVL Report B1862	
The report can be ordered via Homepage: www.ivl.se , e-mail: publicationservice@ivl.se , fax+46 (0)8-598 563 90, or via IVL, P.O. Box 21060, SE-100 31 Stockholm Sweden	

Foreword

This project was accomplished within the Process Integration program of the Swedish National Energy Administration with additional funding from IVL Swedish Environmental Research Institute, Emerson Process Management and Nynas AB. The tight collaboration with process operators at the demonstration site during the course of the project has been vital for the success of this project.

We want to give a special thanks to Michael Thengberg, Boris Gelin and Lars Hidfors at Nynas AB, for their great enthusiasm and eager engagement in the project.

Summary

In oil refining, properties such as flash point, density and viscosity of the fractions used to blend the speciality oils are important to the quality of the final products. The True Boiling Point (TBP) curve provides good characterization for the multiple-component products typical of oil refining.

At Nynas AB's refinery in Gothenburg, TBP curves were usually measured by off-line gas chromatography. The measurement frequency was three per day and the analysis took several hours. More frequent TBP data would provide better opportunities for efficient process control and effective performance monitoring. Nynas AB sought a reliable, cost-effective method to provide operators with a more frequent, real-time measure of TBP.

IVL, together with Emerson Process Management, has developed a decision support system (DSS) based on multivariate statistical process models. The system was implemented at Nynas AB's refinery in order to provide real-time TBP curves and to enable the operator to optimise the process with regards to product quality and energy consumption. It was shown that the use of existing measurements in the process i.e. pressure, flow and temperature, to mention a few, enabled development of mathematical models that predict, monitor and give alarms for different process behaviours.

Multivariate statistical models were used to identify which of the large number of data parameters from the different process steps were most significant for process performance and which could be correlated to the manual TBP analyses. After implementation of the resulting models, the system provided on-line predicted TBP curves and was a valuable tool when changing products or optimising the process. Results, trends and model diagnostics could be seen directly in the control system so the operator quickly could see whether the process were working as it should or whether adjustments was needed to achieve the desired product quality. The refinery's existing three-time daily manual analysis was thus complemented by real-time predictions for the product properties without the need to invest in extra analyses.

Another important goal was to enable experienced operators to share their knowledge of the refinery process with new staff. Changes made in the process parameters are rapidly propagated into the prediction system and these changes can be tracked in the information presented in the user interface. This is an extremely effective way to learn about the process.

The system can also be used to monitor the process and identify deviations from expected operations. The models were calibrated against normal process conditions and an alarm based on model statistics was set to trigger whenever there was excessive deviation from these conditions. The system not only check that all the parameters lay within their approved range, but also that the relationships between all parameters is correct. When the alarm is activated, the drill-down-investigation functionality of the user interface makes it easy for the operator to investigate which parameters cause the alarm. This is useful support for deciding on appropriate actions.

Prediction models were calibrated, validated and implemented for the three most common modes (production recipes) of the refinery. For each mode the TBP curves of a number of fractions, ranging between three and four, were modelled. The criteria for model accuracy set in advance, in terms of prediction error, were met for 94% of the results from validation.

The project resulted in the following proven benefits at the industrial reference site, Nynas AB's refinery in Gothenburg:

- Increased yield with up to 14 % (relative terms) for the most valuable product
- Decreased energy consumption of 8 %

The result is from a two weeks evaluation period. If the decreased energy consumption can be maintained during the whole production year then it leads to a reduction of CO₂ emissions with 1 500 ton per year. The potential energy saving is equivalent to the yearly fuel oil consumption required by 220 family houses.

Validation of model predictions compared to the laboratory analysis showed that the prediction error lay within 1.5 °C throughout the whole test period.

Due to the positive results the project was given large publicity. It is always encouraging with good publicity but the main goal is to extend our approach to other industries and processes. Our experience is that through proper optimization, large economic and environmental benefits are possible to achieve in many processes.

Sammanfattning

Inom oljeraffinering är flampunkt, densitet och viskositet viktiga egenskaper hos de fraktioner som tas ut och blandas till specialoljor. Med rätt egenskaper nås rätt kvalitet på den slutliga produkten. Fraktionernas kokpunktskurvor (True Boiling Point, TBP) är direkt relaterade till dessa parametrar och andra viktiga produkttegenskaper.

Vid Nynas AB's raffinaderi i Göteborg analyseras uttagna prover på laboratoriet. Två till tre prover per fraktion och dag samlas normalt in och TBP-kurvan erhålls efter en tidskrävande analys med gaskromatograf. Högre frekvens på TBP-resultatet och snabbare återkoppling till processoperatörerna skulle avsevärt förbättra processövervakningen och bana väg för effektivare processstyrning. Nynas AB letade efter en kostnadseffektiv lösning för att förse processoperatörerna med TBP-kurvor i realtid.

I samarbete med Emerson Process Management har IVL utvecklat ett operatörsstödsystem baserat på processmodeller från multivariat statistik. Systemet implementerades på Nynas AB's raffinaderi för att ge operatörerna tillgång till TBP-kurvor i realtid vilket möjliggör optimering av produktkvalité och energiförbrukning. Projektet visade att matematiska prediktions-, övervaknings- och larmhanteringsmodeller kunde baseras på befintliga mätdata från processen, t.ex. tryck, flöden och temperaturer.

Multivariat statistik användes för att identifiera det urval av flera hundra mätdata från olika processteg som var mest signifikant för processens beteende och som därmed kunde användas för korrelation med de manuellt analyserade TBP-kurvorna. När sedan modellerna implementerats i systemet gav de on-line prediktioner av TBP vilket blev ett värdefullt verktyg vid produktbyte och processoptimering. Resultat, tidstrender och modelldiagnostik gjordes tillgängligt i kontrollsystemet så att operatörerna kunde använda dessa för att se om processen fungerade som den skulle eller om det behövdes justeringar för att nå önskad produktkvalitet. Raffinaderiets manuella analys av TBP kompletterades därmed med realtidsprediktioner av produkttegenskaperna. Man fick TBP-svar med högre frekvens utan att investera i extra analyser.

En annan viktig del i projektet var att underlätta för erfarna processoperatörer att dela med sig av sin kunskap om raffinaderiets beteende till nyanställda och/eller mindre erfarna operatörer. När en processparameter ändras propageras resultatet av förändringen snabbt genom operatörsstödsystemet och kan studeras av användaren, vilket är ett mycket bra sätt att lära känna processen.

Systemet kan även användas för processövervakning och identifiering av avvikelser från förväntat beteende. Modellerna kalibrerades för normala processförhållanden. Larm baserade på modelldiagnostik användes för att varna operatören vid avvikelser från normala förhållanden. Hänsyn tas inte bara till att varje parameter i sig ligger innanför sitt godkända intervall utan även till att den inbördes relationen mellan parametrar stämmer. Gränssnittet innehåller funktionalitet för klicka sig vidare från en graf till en annan och på så sätt snabbt och enkelt få information om vilka parametrar som bidragit till ett larm samt tidsserie för dessa, vilket ger ett bra stöd för operatörernas beslut om åtgärder vid larm.

Prediktionsmodeller för TBP kalibrerades, validerades samt implementerades för raffinaderiets tre vanligaste körmoder (produktionsrecept). Tre till fyra fraktioner per körmod modellerades. Valideringen visade att de på förhand uppsatta målen för modellnoggrannhet, uttryckt som prediktionsfel, klarades i 94 % av fallen.

Projektet kunde visa på följande vinster för den industriella referensanläggningen, Nynas AB's raffinaderi i Göteborg:

- Upp till 14 % ökat utbyte av den mest värdefulla produkten (relativ ökning).
- 8 % minskad energiförbrukning.

Det var resultatet efter en två veckor lång utvärderingsperiod. Om samma minskning av energiförbrukningen kan realiseras under hela produktionsåret så leder det till en minskning av CO₂-utsläpp med 1 500 ton per år. Den potentiella energibesparingen motsvarar årsbehovet för 220 oljeuppvärmda villor.

Valideringen visade att prediktionsfelet vid jämförelse mellan modellprediktioner och laboratorianalys låg inom 1,5°C under hela denna utvärderingsperiod.

Projektet har fått en hel del publicitet, mycket tack vare intensiv marknadsföring av de lyckade resultaten. Det är alltid roligt med bra publicitet men nu blir målet att kunna testa samma lösning på andra anläggningar för att utöka de miljömässiga vinsterna som kan uppnås efter optimering. Det behöver inte nödvändigtvis röra sig om raffinaderier eftersom de metoder som använts kan appliceras på de flesta typer av industrier.

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1 Introduction

The petrochemical industry stands for 7 % of the total energy consumption in the Swedish industry, 11 300 GWh [1], which has a large impact on both the global and the local environment. The industry is overall well optimised with regards to energy efficiency and emissions but new possibilities for improvements with model based optimisation integrated in the process control have arisen.

This project builds on the results from a previous project “Production optimisation in the petrochemical industry by hierarchical multivariate modelling” [2], [3]. Software and process prediction models needed to be developed further to take them to an on-line installation. The previous project showed that operators could gain knowledge from and hence control the process better if they had the information in real time. The reference site is Nynas AB's crude oil refinery in Gothenburg, the same refinery that participated in the previous project.

Refining crude oil is very complex with a huge amount of variables affecting the product throughout the process. Desired information would be to have the True Boiling Point (TBP) curve presented in the control room updated with real time predictions to make sure that product quality is within boundaries and to improve active control by the operators. Before this project, the TBP curves were only available to the operators after laboratory analysis of samples taken from the production line three times a day. Analysis times of a couple of hours made the information to the operators reflect a past process behaviour, rather than showing the current status of the process. A real time prediction of the TBP curve gives the possibility to alter process variables without gambling since there is a quick response to changes in the process giving that yield and energy consumption could be optimised. A very experienced operator can from the TBP curve understand how the process steps with fractionation, mixing and raw material properties are correlated but for most operators this is very difficult. By presenting variables with most impact on the TBP curve they can increase their understanding of how the different variables correlate and thus improve their process control.

Another reflection from the first project is to implement models that give an overview of the whole process and suggest how to steer the process into the most desirable state. The model also gives early warning signals of process variation that are outside normal conditions.

This project is a natural continuation of the previous project and is aimed to integrate the off line models to achieve the same or better results when used in real time to optimise the process. To succeed, there was a need for development of both models and decision support system (DSS) to be able to gather data, predict parameters and to show the operator results in an easy and user friendly environment. The development work of the DSS was performed in close collaboration with Emerson that has the process control software used at the refinery reference site Nynas AB.

2 Objectives

The objective of this project is to contribute with means that could be exploited for the purpose of forming an even stronger and more diversified Swedish petroleum industry, to be a part to count on internationally when it comes to energy and cost reduction in processing but most importantly reduce environmental impact and have a safer system. The vision is to exploit the concept to other energy intense industries.

The project aims to show the potential of multivariate modelling, especially when it comes to use in real time, and to contribute with a reference case to ease further dissemination and exploitation. It should prove the benefits of using real time model based process integration to increase the process knowledge and be used as a powerful tool to optimize the process with regards to energy, quality and raw material usage.

Goals in figures for the reference site:

- Energy efficiency increased by 7 %
- Product yield increased by 10 %
- Process variation decreased by 35 %

Project milestones

- Models for on-line monitoring calibrated and validated
- On-line monitoring software developed and implemented at the reference site
- Start-up of the model based process integration system
- Educate operators in using the system
- Dissemination of results through workshops, seminars, fairs and press.

3 Research and Technical Development

3.1 Methods

Process data in a factory is a resource of information not always used to its full potential. In this project process data was captured from existing sensors, instrument, valves, machines and other sources of equipment generating information that might be of interest to use for modelling. The process data captured from the process control system (PCS) was stored in a historical database to be easily available. To build statistical predictive models there is a need for reference data for the parameters of interest. The parameter of most interest in this case was the True Boiling Point (TBP) curve which was analysed manually by a GC analyser. For statistical modelling it is important that reference data and process data are well determined to have as accurate results as possible. Only data from periods where the process and GC analysis were sure to be stable and correlated were used for calibrating the models. This means that data close to product changes where the relation between process and GC analysis could differ was not used for modelling.

The statistical modelling method used in this work is standard Partial Least Squares (PLS), [4][5]. Process modelling by multivariate statistical modelling methods, such as PLS, 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.

PLS models can be used for predicting product properties from process data, which is sometimes referred to as a soft sensor, but also for process monitoring, fault detection, fault identification and process optimisation. In this project the inherent model statistics Squared Prediction Error (SPE) and Hotellings T^2 (T^2) were implemented together with the real time predictions of TBP and used both as indicators of model validity and for fault detection.

Different forms of the Root Mean Square Error (RMSE) statistic were used as a measure of model accuracy. In the model calibration work, cross-validation of the models was made from excluding in turn one sequence of data to calculate the RMSECV (CV for Cross-Validation). In the validation, model predictions were compared to measured data that had not been part of the calibration data for the models, thus resulting in the RMSEP statistic (P for Prediction).

A study similar to this one has been performed, developing soft sensors to predict quality parameters in refineries [6]. Conclusions drawn are that PLS modelling are a powerful tool for reducing vast amounts of data without losing understanding of what the models actually do. In the study the feature of insight in the models is important for faultfinding and safety since compared to more black box methods such as neural network you can easily find variables responsible for abnormal process conditions.

Another study [7] was looking into on-line monitoring, with dynamic PLS, of the de-aromatization process. The results showed that it was possible to achieve early detection of process deviations which, if handled correctly, improves safety, improves the product quality and gives less maintenance.

3.2 Process description

The reference site in the present study is Nynas AB's refinery in Gothenburg, Sweden. The process is outlined in Figure 1. At the refinery crude oil is fractionated 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 largest by volume product of this refinery but lighter products are also of importance.

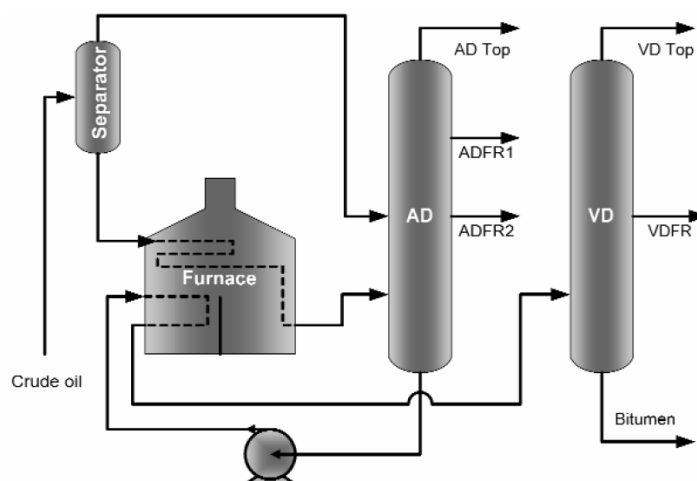


Figure 1. Schematic outline of the distillation process at Nynas AB's refinery in Gothenburg. The initial products are the fractions ADTOP, ADFR1, ADFR2, VDTOP, VDFR and bitumen. Mixing of some of these products to form new products also occur.

From the previous study [2] it was concluded that for modelling the total process the gain by dividing

the process into logical blocks were marginal and not worth the extra complexity. The same results could be obtained by using the parameters directly into the models without time lagging, provided that the models are used during stable process conditions. The blocks are however a good way for visualisation of the process and group parameters used in the model. Blocks are listed below in the order of appearance in the process.

- **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. 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. 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, VDT and VDFR. In addition to these four products, there is also a special product which consists of a mixture of the two fractions ADFR2 and VTOP. In this report that product is referred to as MIX. The TBP curve shows the distillation temperature of the extracted fraction by weight percent, see Figure 2. The analyses are performed once every working shift (2-3 analysis a day) and the TBP curves can be linked to important qualities of the fractions, e.g. their viscosity, density and flash point. Parameters used in the modelling are the temperatures at 0.5, 1, 2, ..., 99, 99.5 weight percent of each fraction. Consequently there are 101 variables per fraction.

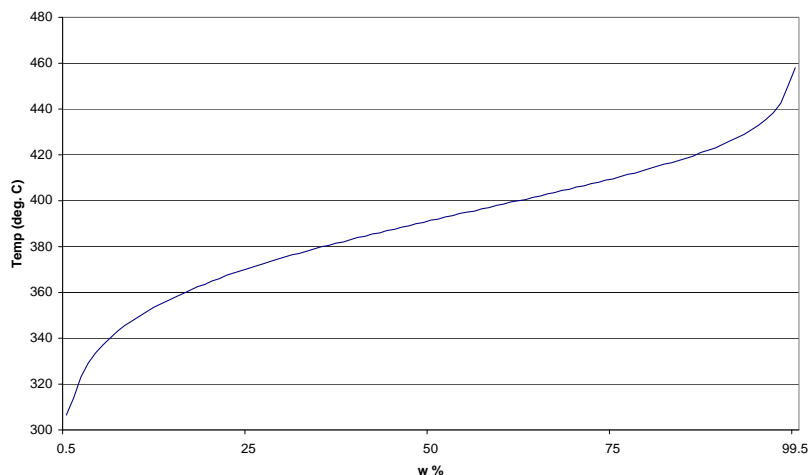


Figure 2. Example of a TBP curve where 50 weight percent of the molecules in the fraction have a boiling point above 390 °C.

3.3 Scope of the work

The scope of this study is to model the TBP curves of selected fractions by the use of measurements readily available in the process control system. The models should be integrated in the DSS developed by Emerson.

The production at the reference site is run according to different modes (recipes) that are alternated over time depending on the current properties of the crude oil and the desired product properties. This project includes modelling of the three main production modes, called M300, M601 and M604.

The MIX fraction is only produced for some of the production modes of the refinery and can thus only be modelled for those particular modes. Furthermore, it became apparent in the previous project that the lightest fraction, ADFR1, was not suitable for modelling from the process measurements. So ADFR1 was excluded from the work in this project. The modes and fractions included in the modelling work in this project are presented in Table 1.

Table 1. Production modes and fractions included in the model calibration.

Mode	Fraction
M300	ADFR2 MIX VDT VDFR
M601	ADFR2 VDT VDFR
M604	ADFR2 MIX VDT VDFR

Criteria for acceptable model accuracy was set up based on the results from the previous project, see Table 2. Since TBP curves of the MIX fraction were not included in the predecessor project it was not possible to set up any specific criteria for them. It should be expected that it is possible to achieve model accuracy for MIX in the same order as the model accuracy of the other fractions.

Table 2. Criteria for model accuracy, in RMSE, °C

TBP	ADFR2	VDT	VDFR
5%	2.5	3.0	5.0
50%	2.5	2.8	3.3
95%	4.0	3.0	5.0

3.4 Development phases

The model development and implementation was conducted according to the schedule presented below.

1. Data acquisition - Process data and GC analysis data from the Nynas refinery
2. Model calibration
3. Data acquisition - New data (process and GC) for use in validation of models from step 2.
4. Model validation
5. Start models for on-line use at Nynas - End of august 2007.
6. First model evaluation period - September to November 2007.
7. Model re-calibration - Updating the models with the data from step 3.
8. Second model evaluation period - May to June 2008

Development of the DSS was performed in parallel with 1-4, in order for it to be functioning at the time of 5.

3.5 Results and discussion

The system was evaluated during two evaluation periods. In the first evaluation the focus was on model accuracy, up-time and analysis frequency. The second evaluation was to optimise by working with the system to keep close track of the process while adjusting the variables to find the best settings.

3.5.1 Model calibration

As far as possible, the models were calibrated using data from all production modes in the same model, but with different scale factors for the different production modes. This was possible for the fractions ADFR2, MIX and VDFR. For the VDT fraction the model statistics (RMSECV) showed that a better result was reached by calibrating one separate model for each of the production modes. The model accuracy, presented as RMSECV for the model calibration and re-calibration, is listed in Table 3.

For some of the models the model accuracy is slightly better (lower RMSECV) before re-calibration, but since more calibration data means that the model covers more information on possible process variation all of the re-calibrated models were implemented in the DSS before the start of the second evaluation period.

Table 3. Results from the model calibration and model re-calibration.
Model accuracy (RMSECV, ° C)

Fraction		Calibration Model accuracy (RMSECV)	Re-calibration Model accuracy (RMSECV)
ADFR2	5%	1.9	2.2
	50%	2.0	2.1
	95%	2.8	3.4
VDT	5%	1.7 - 1.6 - 2.8	1.9 - 2.1 - 1.4
	50%	2.2 - 1.7 - 2.3	2.1 - 1.7 - 1.4
	95%	2.4 - 1.9 - 3.0	2.2 - 1.3 - 1.7
VDFR	5%	6.2	6.4
	50%	2.0	1.9
	95%	1.2	1.8
MIX	5%	1.7	1.5
	50%	1.7	1.4
	95%	2.2	2.2

3.5.2 Model validation

Before the models were started at Nynas for on-line use they were validated using new data that was not included in the calibration work. Validation was done by comparing results from the models predicting the True Boiling Point (TBP) curve with results from the laboratory analysis performed with the GC instrument. Samples with an apparent error in the GC analysis (e.g. the curve takes a "step" in the middle) were excluded from the calculation of prediction error. The validation results, calculated as Root Mean Square Error of Prediction, were excellent, see Table 4. The light end of VDFR is the only part that does not fulfil the criteria in Table 2. The reason might be the large variation in the light end of VDFR from the GC analysis. It had increased compared to the analysis results in the predecessor project. Other than this it looks very good. Model validation is based on a different number of samples from the respective fractions corresponding to the availability of GC analysis data, see Table 5.

Table 4. Result from the model validation period. Model accuracy (RMSEP, °C).

Fraction		Model accuracy (RMSEP)	
M300, M601 and M604			
ADFR2	5%	2.2	
	50%	1.5	
	95%	2.0	
M300 - M601 - M604			
VDT	5%	2.8	3.0 - 0.9
	50%	2.1	2.8 - 0.8
	95%	2.0	1.7 - 1.4
M300, M601 and M604			
VDFR	5%	8.0	
	50%	2.1	
	95%	1.8	
M300 and M604			
MIX	5%	1.0	
	50%	1.4	
	95%	3.0	

Table 5. Number of test samples (validation data)

Fraction	Validation data
ADFR2	196 GC analyses from May to Aug 2007
VDT M300	94 GC analyses from May to Aug 2007
VDT M601	13 GC analyses from May to Aug 2007
VDT M604	43 GC analyses from May to Aug 2007
VDFR	127 GC analyses from May to Aug 2007
MIX	71 GC analyses from June to Aug 2007

3.5.3 First model evaluation period

The evaluation period comprises September, October and November 2007. During this period the modes 300 and 601 were used. The models were evaluated with regards to 1. Time-frame, 2. Up-time and 3. Model accuracy.

1. Models were set to execute every 5th minutes, an interval chosen by the operators which was enough for calculation of new TBP curves.
2. The models were running the entire evaluation period, apart from the short periods of time (less than 10 s) that it takes for the system to automatically close old models and load new models after a change of modes. When changing a mode, the process changes from one state to another. Naturally, this does not happen in a few minutes. A detailed follow-up of 2 mode changes showed that the time it takes from starting a mode change to the process having settled in its new state was 60 and 80 minutes respectively. The models domains were restricted

to within the respective modes (i.e. transitions between modes are not covered by the models). Thus, models predictions were not reliable during the time it takes to change the process into a new mode. This was also indicated by the T^2 - and SPE statistics, See Figure 3, which can be used as a tool for the operator to verify when the process has settled in the new mode. For the evaluation period, unreliable model predictions due to mode changes corresponded to <1% of the time.

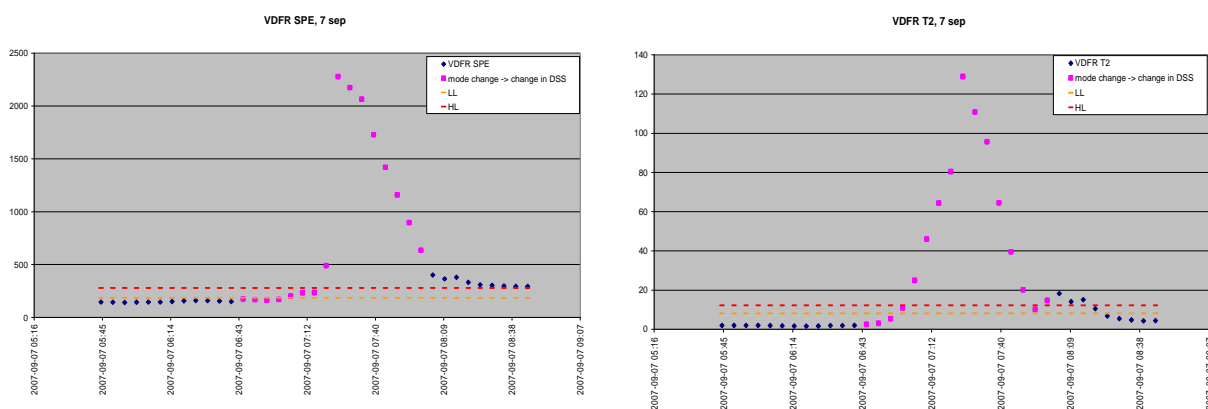


Figure 3. Model statistics of VDFR during a change of modes, M300 to M601, 2007-09-07. The operator started the mode change 6:45. The process has stabilized in the new mode at 8:05 and the decision support system automatically changes to the settings used for M601. (LL=Low limit alarm, HL=High limit alarm for T^2 and SPE respectively)

- During the entire evaluation period, the refinery had production problems resulting in bad distillates from the VD tower. On account of this the process was operated in a different way compared to operation at normal process conditions. These problems resulted in that the models were used in their respective domain, which was also verified by the T^2 and SPE statistics. The criterion on model accuracy was only evaluated for periods when neither of the T^2 and SPE statistics exceeded their low limit alarm. Table 6 shows how much of the models' active time during the evaluation period that they were used within their domain.

Table 6. The models active time during the first evaluation period that they were used within their domain (T^2 and SPE statistics was below low limit alarm).

	M300	M601
ADFR2	35%	35%
VDT	85%	0.1%
VDFR	95%	16%

No GC analyses were made on VDT or VDFR during the evaluation period because of the bad distillates from the VD tower. Therefore there were no samples to use for evaluation of the criteria for these fractions. For ADFR2 there were a few (18) samples that were analyzed on the same GC instrument that was used for calibration of the models. Out of these 18, only 3 were sampled when the ADFR2 model was operated within its domain. All 3 were from M300. Table 7 shows the prediction error between ADFR2 from the GC instrument and the model predictions for those 3 samples.

Table 7. Result from the evaluation period. Model accuracy (RMSEP, °C).

	Fraction	Model accuracy (RMSEP)
ADFR2	5%	0.4
	50%	1.8
	95%	1.6

3.5.4 Second model evaluation period - Process optimisation

The second evaluation period took place in the period 26/5 – 13/6 2008. By then the problems with bad distillates from the first evaluation periods had been solved by Nynas during the yearly winter maintenance brake. The second period was limited in time and focused on showing the benefits from refinery optimisation using on-line process monitoring. During the evaluation period, the most experienced operator of Nynas was put to the task of actively using the information from the DSS with the goal to enhance production results with respect to the yield of the MIX fraction whilst keeping the product quality within its specification.

The results from the evaluation period were compared to the situation prior to the active use of the DSS and the relative increase in the yield of MIX was calculated, see Table 8. It could be concluded that during the optimisation period there was an:

- Increased yield with up to 14 % (relative terms) for the most valuable product
- Decreased energy consumption of 8 %

Table 8. Relative increase in yield of MIX during evaluation period, compared to the production in spring 2008 up to 25/5.

Mode	Relative increase in yield of MIX
M300	9.6 %
M604	14 %

The result also showed a decrease in the amount of fuel oil required for the furnace per ton of produced MIX fraction with 10 kg/ton. This corresponds to an 8% decrease in energy use per ton of produced MIX.

Burning of fuel oil generates 75 g CO₂ emissions / MJ [8]. Assuming that it is possible to maintain the same results over the whole production year, the reduction in fuel oil leads to 1 500 ton less CO₂ emissions per year.

The following example is given for comparison. An average family house requires 20 MWh for heating and the energy efficiency of a modern household boiler using fuel oil is approximately 80% [9]. With a heating value of fuel oil (Eo1) at 35.9 GJ/m³ [8] the yearly energy savings made possible at the Nynas refinery are equivalent to the yearly fuel oil consumption required by 220 family houses.

3.5.4.1 Validation for process optimisation period

For the second evaluation period where the aim was to optimise the yield of the MIX you could suspect that the process was sometimes stressed and out of bounds since the operators were trying out different settings to increase the performance. The model validity parameters in Figure 5 and Figure 5 shows that SPE exceeded the low alarm limit during mode 300 and the high alarm limit during mode 604, while the T^2 parameter never exceeded its limits.

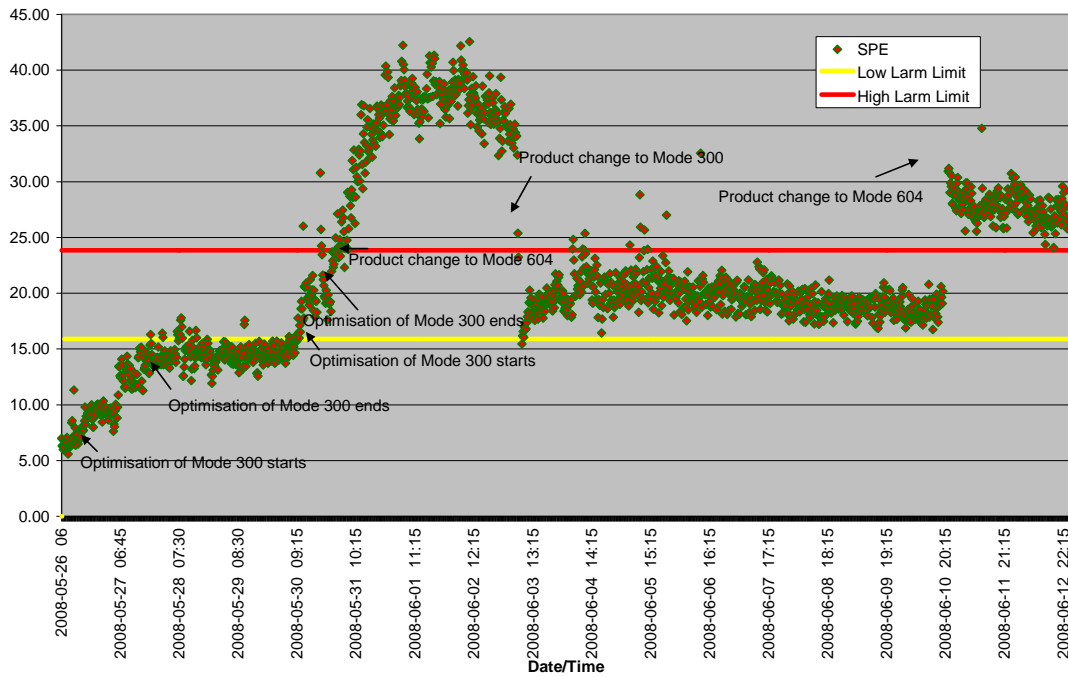


Figure 4. Model validity parameter SPE for MIX model during the optimisation period.

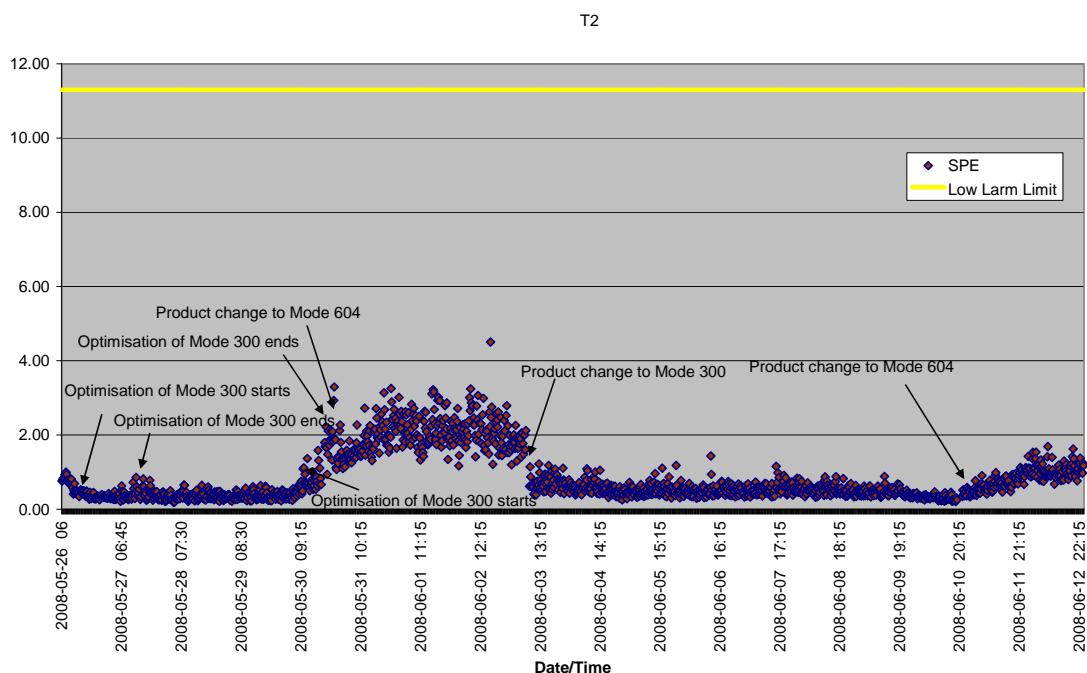


Figure 5. Model validity parameter T2 for MIX model during the optimisation period.

Validation was done by comparing results from the predicted TBP curve with results from the laboratory analysis performed with the GC instrument. The actual error for the boiling point predictions at 5%, 50% and 95% has an average standard deviation of 1.0 degrees for the whole test period, see Table 9. The model accuracy was calculated as RMSEP based on 36 samples of M300 and 8 samples of M604. The actual predicted and measured values are shown in Figure 6 and Figure 7.

Table 9. Model accuracy for the three set point values used in the operator interface. The Root Mean Square Error of Prediction (RMSEP, °C) was as low as 0.8 degrees compared to reference analysis for 50%.

Fraction	Model accuracy (RMSEP)	
MIX	5%	1.0
	50%	0.8
	95%	1.3
	Mean	1.0

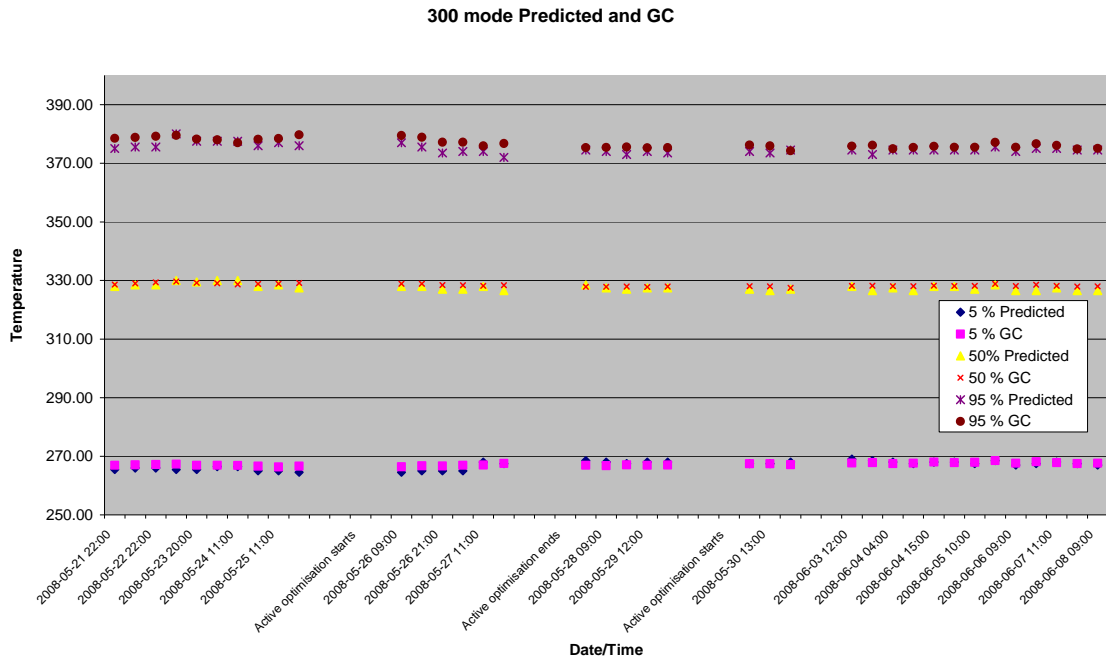


Figure 6. Predicted and measured (analysed by GC) values of the 5%, 50% and 95% points of the TBP curve for mode 300 during the second evaluation period.

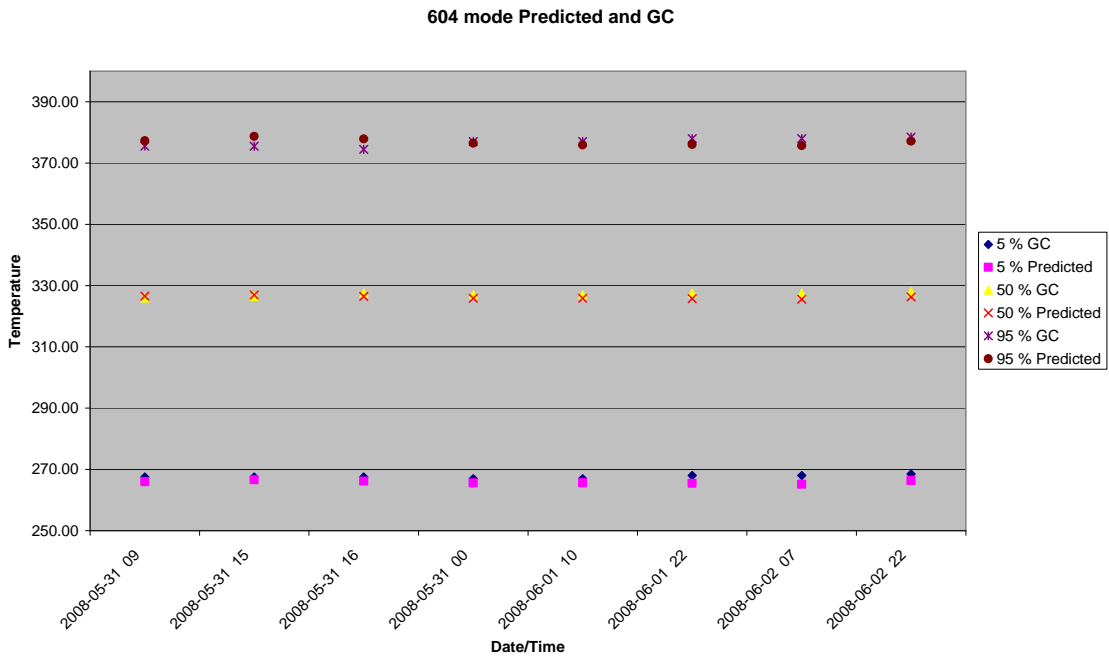


Figure 7. Predicted and measured (analysed by GC) values of the 5%, 50% and 95% points of the TBP curve for mode 604 during the second evaluation period.

3.5.5 Operator user interface

The goal was to develop an easy-to-use interface for advanced process information. The basic view, see Figure 8, gives the operators information on the entire TBP curve of each fraction (charts on the left) as well as time series of important points on the TBP curve (charts on the right). Supervisory control limits, based on information from the entire process, lets you know if the process is "on track". The colour of the model indicator shows either *green* for OK, *orange* for low limit alarm (warning) or *red* for high limit alarm.

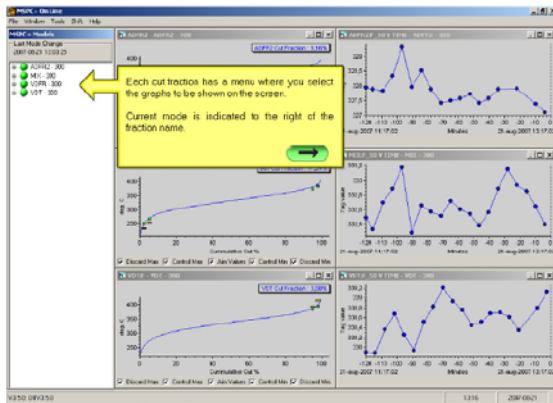


Figure 8. Screen shot from the basic view of the DSS in use at the Nynas Gothenburg refinery. The qualities of three products are presented as model results of the TPB curves. Supervisory control limits are applied to the aggregated information from more than 150 process variables per product.

Alarm and fault detection uses the supervisory control that takes into account all of the process variables presented in a time series in Figure 9. If the limit is exceeded an alarm sets off. The faulting sensor(s) is easily identified in a chart that sorts all variables according to their contribution to the alarm, see Figure 10. Thus, not only the faulting sensor is identified but information is also gained on which other variables are connected to the fault. The operator gets further details on the fault by looking into the trend curves of involved variables, see Figure 11. The functionality of the interface allows the user point-and-click access from the supervisory control curve (Figure 9) to the contribution plot (Figure 10) and from the contribution plot to the time series of the selected variable (Figure 11)

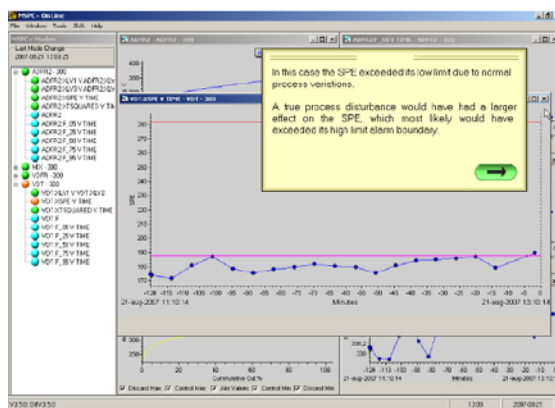


Figure 9. Time series for Standard Prediction Error (SPE), which is used for supervisory control. The T^2 statistic is also used for supervisory control in the same way as SPE.

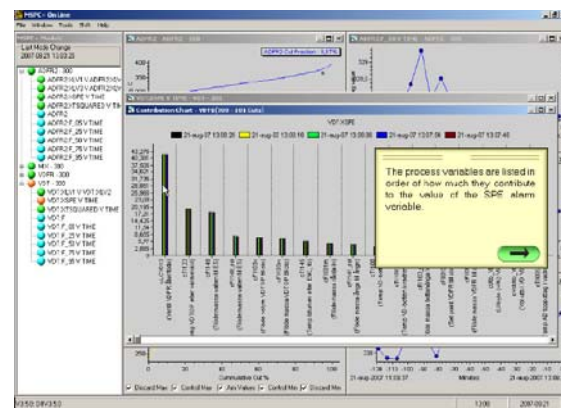


Figure 10. Contribution plot from each variable sorted by highest impact on model deviation.

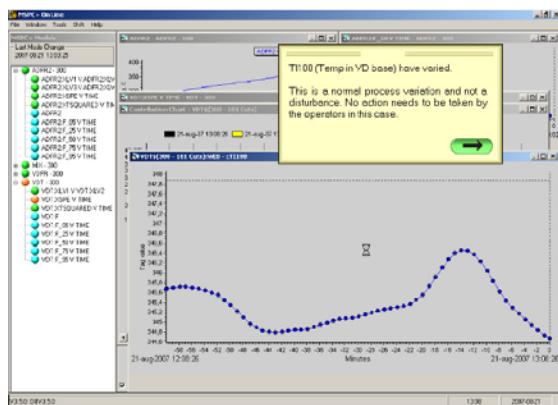


Figure 11. Time series for a selected process variable.

All of the screen shots presented above were extracted from the interactive training material developed in this project, cf. the section on Training of process operators. The yellow boxes of information are only for training purposes. They are not visible in the operators' interface that is used in the day to day process control.

4 Dissemination activities

When summarizing the dissemination activities it was obvious that prioritizing this activity early in the project benefited how well the results were spread. The project has had a great deal of positive publication in the press and results have been presented in several fairs and seminars. Below there is an overview for some of the major activities and publications.

4.1 Press

A press release went out to all major news papers which resulted in that the main economical news paper in Sweden, Dagens Industri [10], published one whole page with interviews from both IVL and the industrial partner Nynas AB explaining the project. The project has also been published in Nordisk Industri [11] and Kemivärlden [12]. These three articles (all in Swedish) are included in the Appendix.

4.2 Fairs and seminars

Emerson Global Annual User Meeting in September 2008. This meeting is one of the major technical conferences for the refinery sector. There are about 3000 people working in refineries from around the world that participates. The response from the presentation of the results during the conference was very positive from both industry and Emerson. Most of the people in the refinery sector now know that it is possible to use multivariate modelling in real-time for optimising their process with regards to energy efficiency and yield increase.

The 7th – 9th October the project was the major exhibitor at Processteknikmässan held in Gothenburg (www.processteknik.info). Swedish Fair invited IVL to present the solution developed

in this project showing on the possibilities of future operation support systems. The support system tied all aspect of the fair together covering everything from sensors, engines and control. On the dedicated space of 150 m² there was a stage for invited speakers, a control room with screens and demo software, a barista and 7 people involved with the project to handle all questions and to hand out information. On the three daily speak sessions scientist from other areas with similar experience presented their results and thoughts about the future. One of the sessions was re-occurring and that was the control room presentation made by the operators at Nynas AB presenting the solution live on big screens. An independent evaluation of our participation showed on very positive feedback from fair participants [13].



Figure 12. Boris Gelin, Nynas AB, contributed to the successful presentation of the DSS at the Process Technology Fair, Swedish Fair in Gothenburg 2008.

Following an invitation from the Center of Visualization Göteborg, IVL presented results from the project at the Visual Forum conference, 12th of March 2009, Swedish Fair in Gothenburg. The topic of the conference was *Visualization - A Tool For Decision* and the presentation, entitled *Applied visualization - Examples from industry and society*, was part of the session *Visualization with environmental aspects*.

The project was presented for the IVL theme committee for sustainable production 11th Mars 2009. This committee is a mix between industrial partners and research founders. Participants at this meeting were representatives from Volvo, Vattenfall, Naturvårdsverket, Teknikföretagen, Södra and Formas. The response from the committee was positive and created some new possibilities to look into applications at both Södra and Volvo.

4.3 Training of process operators

The system interface was introduced to the process operators in August 2007. By then the software functionalities, developed by Emerson, were ready and IVL had implemented and launched the first set of models. Thus, from then on the operators had access to the on-line TPB predictions and the process diagnostics provided by the models. In order to establish a good understanding among the operators of how to use the new system, IVL arranged special training sessions at Nynas for each of the operator teams during August and September 2007.

In addition to the training on site, an interactive (point-and-click) training material was created. This material was installed on the same computer as the DSS in the control room at Nynas and can

easily be accessed by the operators at any time when they have questions about using the DSS. The interactive training is divided into four sections, for easy access to answers on specific topics.

1. Introduction to user interface

The user is familiarised with the GUI: Charts of TBP curve, time series for selected boiling points, time series for the supervisory control variables.

2. Shift menu

The user is shown how to easily change settings of the time series to display the last 8 or 12 hours and how to get back to the default view of 2 hours.

3. Alarm

The user is taught about the DSS alarm handling: What does an alarm look like? How to investigate the process variable contribution to alarms. Acknowledgement of alarms.

4. After mode changes

This section teaches the user what happens in the DSS after a change of modes (recipes). The DSS automatically closes down the models of the past mode and starts up the models of the new mode. The user is shown how to select and order the charts to view in the interface.

The starting page of the interactive training material is illustrated in Figure 13

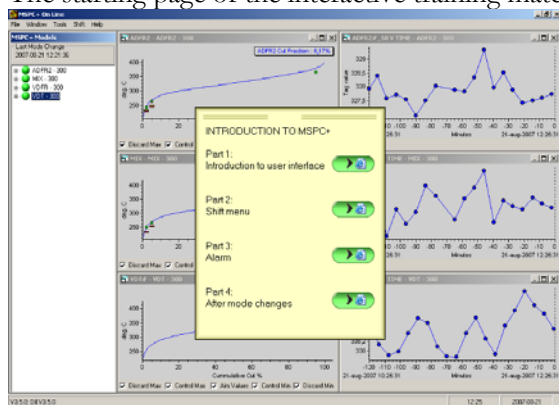


Figure 13. The starting page of the interactive training material gives the user access to four sections of training; Introduction to user interface, Shift menu, Alarm and After mode changes.

5 Conclusion

The project has successfully demonstrated implementation of multivariate prediction models in an on-line environment at the reference site, the Nynas AB refinery in Gothenburg. Despite the unforeseen and unpreventable production problems occurring during the first model evaluation period the project has shown that on-line prediction of the TBP curves is indeed a good solution for enhanced process monitoring and control. The operators get accurate feedback on the current product qualities. When they change settings in the process they can follow the response of the TBP curve promptly, instead of waiting for the laboratory analysis of a product sample.

Prediction models were calibrated, validated and implemented for the three most common modes (production recipes) of the refinery. For each mode the TBP curves of a number of fractions, ranging between three and four, were modelled. The criteria for model accuracy set in advance, in terms of prediction error, were met for 94% of the results from validation (17 out of 18 reference points met the criteria).

All of the milestones set out for the project were accomplished. The goals for the reference site were achieved, exceeded even, with respect to energy efficiency and yield, as proven by the second evaluation period. The third goal, i.e. that the installation would lead to a decrease in process variation by 35%, has not been possible to verify. The intention was to compare normal production, before active use of the DSS, with a longer period when the operators used the system in their daily process control. Neither of the two evaluation periods were suitable for that purpose. The first one due to the process problems with black distillates and the second one due to the fact that the operators pushed the model (and thus the process) to its boundaries in order to test its full potential. However, it is reasonable to believe that the on-line information on TBP curves provided by the DSS will be a helpful tool for the operators, assisting them to keep the production more stable due to the fast feedback on changes in the resulting product. This should also smooth out process variation, but how much remains to be proven.

When the operators used the models for active control of the MIX yield the model's validity parameter SPE was pushed outside its alarm limits. This is not surprising since the data used in calibration of the model was collected from normal process operation. There is a need for model updates in order to reflect the new strategies employed by the operators. This is a natural aspect of model improvement. Models should be maintained and frequently updated to account for recent changes in production, changes which can be either an effect of improved process control or of drifting production equipment (due to e.g. clogging of valves, deteriorated sensors, broken and replaced components). A recommendation is to refresh the models at least once per year to keep them up to date with the current status of production.

Thanks to the successful results and to proactive dissemination strategies of the project participants the project has reached a large audience, both within the petroleum industry and in general. It can be expected that the attention drawn to the project has opened the eyes of several potential users of similar applications and that multivariate statistics in process control will gain trust by the industrial users in the future.

6 Future work

The installation at Nynas AB is planned to be maintained and used in daily manufacturing by operators at the plant. A support package will have to be developed to secure continuous operation without downtime.

Nynas AB has expressed an interest in taking the system one step further and to use it as Advanced Process Control (APC). This is to improve production even further and to minimise process variation by letting a control software take over manual operator control.

To spread the results and to have bigger environmental benefits IVL will also look into the possibilities to implement this solution at other refineries. The methodology is however not restricted to refineries so other industrial sectors will be exploited. Contacts have already been

established within the food processing industry, the pulp and paper industry and construction material industry to investigate the possibility to implement the system in their production.

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- [10] Dagens Industri 30/9-08 p. 28 (MILJÖ, in Swedish)
- [11] Nordisk Industri nr 4 2008 p. 63 (in Swedish)
- [12] Kemivärlden Biotech 2008-10-02 (in Swedish)
- [13] Mässa- och process- och tekniska utställningen 2008_IVL.pdf (in Swedish)

Appendix 1 - Articles from the Swedish press

Kemivärlden Biotech
Kemisk Tidskrift

chemicalnet.se

Kemivärlden Biotech med Kemisk Tidskrift. Skriver om kemi och bioteknik i Sverige och världen.
Medlemstidning för Svenska Kemistsamfundet och SKR.

Lyckad processoptimering

2008-10-02

IVLs nya processoptimeringssystem gav en vinst på 850 000 kronor på 14 dagar när det testades hos Nynas. Nu knoppar IVL av sitt första bolag någonsin.

IVL Svenska miljöinstitutet har utvecklat ett nytt operatörsstödsystem för processindustrin, kallat POP, Process optimizing pack. I systemet används statistiska processmodeller för att simulera kurvor som ger realtidsinformation, vilket gör det möjligt för operatörerna att snabbt anpassa processen till optimal drift.

Systemet testades under våren 2008 för att kontrollera kokpunktskurvan vid Nynas raffinaderi i Göteborg. Idag mäts kokpunktskurvan, som ger indirekt information om densitet, flampunkt och svavelhalt, med hjälp av analyser tre gånger per dygn.

Försöket gav hela 14 procent ökat utbyte på en av deras specialoljor under de 14 dagar som försöket pågick, vilket motsvarar en vinst på 850 000 kronor.



– Det är väldigt bra resultat, prediktionen vi fick av kokpunktskurvorna varierade högst ett par grader mot verkligheten. Kurvorna gör det lättare för operatörerna att anpassa processen för att få ut önskad produkt, berättar Åsa Nilsson, civilingenjör på IVL och tekniskt ansvarig för Nynasprojektet.

Under projektet upptäcktes flera andra förbättringsområden, som fluktuationer i det atmosfäriska destillationstornet, att ångtillförseln inte är anpassad till skillnader i produktionstakt och att värmeväxlarna för råoljan har mycket sämre effektivitet vid hög tillverkningsstakt.

– Vi har testat samma metoder i ståltillverkningen hos SSAB och hos kommunala avloppsreningsverk också, i princip går tekniken att använda överallt där man mäter något, säger Åsa Nilsson.

IVL tänker nu för första gången knoppa av ett bolag med namnet EEQ, Environment, Economy, Quality. Det amerikanska systemutvecklingsföretaget Emerson har varit inblandade i en del tillämpningar av POP, och Emerson är en tänkbar partner för EEQ när systemet ska kommersialiseras. Projektet att dra igång bolaget leds av Magnus Andersson på IVL.

– Han är i USA på Emerson Global Users Exchange conference just nu och presenterar systemet, det är verkligen spännande, säger Åsa Nilsson, som troligen kommer att vara inblandad i teknikdelen i EEQ också.

– Jag hoppas det i alla fall, det här är det roligaste projektet jag har jobbat med under mina åtta år på IVL.

[Hilda Hultén](#)

MILJÖ

Redaktör: Peter Lundgren, peter.lundgren@di.se, 08-573 651 78

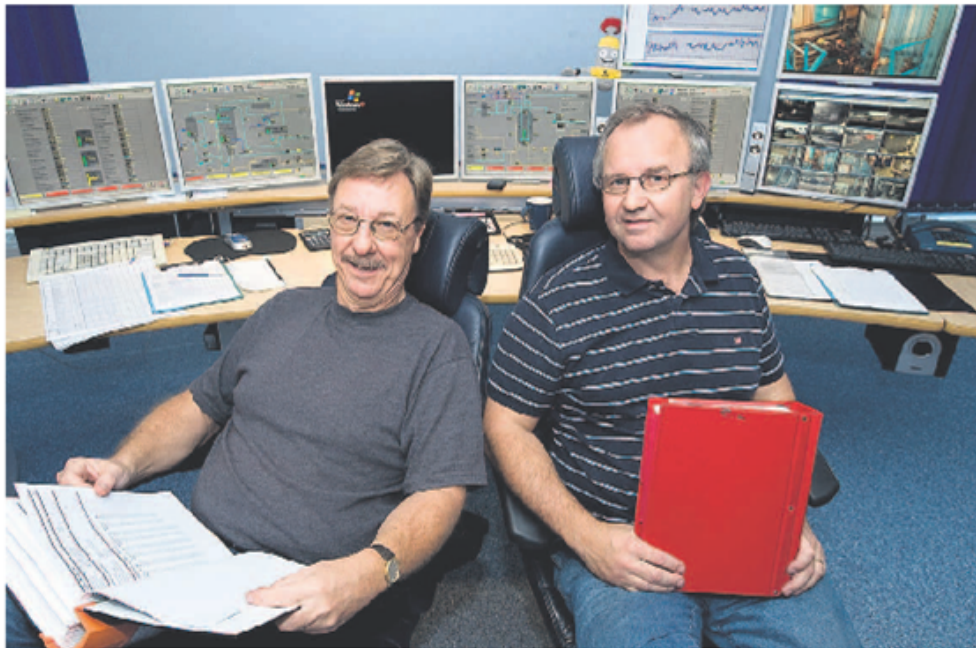
Varje tisdag om företagande inom miljöområdet

Vad vill du läsa om på Miljö?

Tipsa oss:

E-post: miljo@di.se

Reporter: Maria Ottoson, 08-573 650 59



BÄTTRE STÖD. Lars Hédfors, till vänster, och Boris Gelin på Nynas i Göteborg har fått bättre hjälp i sitt arbete med IVL:s operatörsstödsystem POP. 18.0.000.016.01

Mindre spill med snabbt provsvar

Ojebolaget Nynas har använt IVL:s stödsystem på sitt raffineri i Göteborg. Under en testperiod på två veckor lyckades företaget få ut 14 procent mer ur samma mängd råolja utan att öka energiförbrukningen.

"Det är helt underbart att arbeta med detta system. Det förenklar mitt arbete och det blir jämnare kvalitet", säger Lars Hédfors, processoperatör på Nynas.

Nynasgruppen omsatte förra året 18,7 miljarder kronor och har ett tiotal raffinaderier i världen, varav tre i Sverige.

Boris Gelin är insrumningsingenjör på Nynas bitumenraffinaderi i Göteborg med 40 anställda. För sex år sedan utvaldes han IVL:s Magnus Andersson på en mäsas och de började prata om processoptimering. Samtalet ledde till ett utvecklingsarbete där Nynas har varit med och testat och återkopplat i utvecklingsarbetet av det nya stödsystemet POP.

Bättre än konkurrenterna

"Det här systemet har fler funktioner och är inte så resurskrävande och dyrt som andra system på marknaden. Vi kan producera mer med mindre utsläpp och mindre energiförbrukning", säger Boris Gelin.

Tidigare fanns inget stödsystem utan operatörerna styrde raffineringsprocessen, det vill säga där råoljan heatas upp och separeras till exempelvis bensin, smörjolja och eldningsolja – utifrån mätdata från övervakningssystemet. Arbetet är resurskrävande och sårbart eftersom det kräver stor kunskap och erfarenhet och full koncentration dygnet runt för att få en stabil kvalitet på produkterna.

"I stället för att skicka prov till labbet och få svar efter fyra till tolv timmar på hur produktionen var vid en viss tillfälle kan vi få svar och operatören kan justera direkt. Det betyder att vi får mindre spill", säger Boris Gelin.

Planerar expansion

För Nynas blir miljöfrågorna allt viktigare. Bolaget planerar bland annat att utöka verksamheten i Göteborg.

"Kraven för att få miljöcertifiering idag är mycket högre än tidigare. Vi måste höja oss på många områden och kanske krävs det ett stödsystem som POP för att bättre klara framtida miljökrav", säger Boris Gelin.

MARIA OTTOSON

Smart styrning ger gröna miljonvinster

Att göra nästan samma sak med samma utrustning – fast bättre för miljön och plånboken. Det är grundbulten i det optimerings-system för industrin som IVL Svenska Miljöinstitutet nu ska ta ut i världen.

Oljebolaget Nynas har varit med och utformat systemet som kan ge besparingar på minst 17 miljoner kronor per år.

Efter tio års forskning och utveckling börjar forskningsinstitutet IVL närma sig mållinjen för sitt nya it-system för processindustrin, Process optimisation pack, POP. Arbetet har gått så bra att IVL nu för första gången knoppar av verksamheten och bildar ett eget bolag, EEQ, som ska sälja systemet.

"Det är väldigt intressant och vi hoppas mycket på det här. Det finns många fler idéer inom IVL som vi tror att vi kan göra likadant med framöver", säger Tord Svedberg, vd på IVL.

Kostnaden för systemet

uppgår till närmare 100 miljoner kronor och har fått stöd av EU. POP bygger på att bearbeta de data som redan finns inom industrin och i realtid underlätta operatörernas arbete. Varje delmoment i processen kan därmed göras optimalt utifrån energiförbrukning, råvaru-utnyttjande och kvalitet.

Kan installeras snabbt

"Man uppstår energieffektivisering utan att behöva bygga om vare sig maskiner eller it-system. Det är unikt för POP jämfört med andra liknande system", säger

DI FAKTA

■ **IVL Svenska Miljöinstitutet** är ett fristående, icke vinstdrivande institut som bedriver forskning och uppdragsverksamhet. Det finansieras av staten, näringslivet och anslag.

■ **Nynas hette** från början Nynas och har anor från 1920-talet då Sveriges första raffinaderi byggdes i Nynäshamn.

■ **Idag ägs** Nynas av den finska oje-koncernen Neste Oil och det statliga oljebolaget Petróleos de Venezuela S.A.

Magnus Andersson som har drivit projektet på IVL Svenska Miljöinstitutet.

Självföretaget SSAB testade redan förra året vissa delar av systemet och gjorde besparingar på motsvarande 5 Mkr per år genom mindre kemikalieanvändning samtidigt som slaggproduktions minskade med 1 700 ton per år.

"För många företag är mindre utsläpp en bonus men för oss på IVL är miljöaspekterna det viktigaste", säger Magnus Andersson.

Ska visas upp i USA

IVL har samarbetat med systemutvecklingsföretaget Emerson om en del tillämpningar, och nästa vecka presenteras POP på Emersons årliga kundmäsas i Washington.

Tanken är att Emerson sedan ska börja sälja systemet i hela världen. De potentiella miljonvinsterna av att använda systemet är stora och det

kan användas av alla som arbetar inom processindustrin, enligt Magnus Andersson.

"Det finns 1 100 oljeraffinaderier i världen. Om deras processer optimerades med hjälp av systemet skulle det bidra till oerörliga minskningar i koldioxidutsläpp", säger han.

Räknar med tillväxt

Magnus Andersson är i dag huvudsansvarig för EEQ. Han räknar med att potentialen är stor i hela världen men att tillväxttakten beror på hur samarbetet med Emerson faller ut och hur mycket det nystartade företaget orkar växa.

"I och med att vi jobbar med en stor aktör som Emerson som har 2 500 säljare runt om i världen ger det oss möjlighet att få genomslag ganska fort", säger han.

MARIA OTTOSON
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08-573 650 59

Världsledande Vaisala

Vaisala Oyj ställer ut en hel produktportfölj på mässan, flera är nyheter som lanseras för första gången. Vaisala Group omsatte 224 miljoner EUR förra året och har över 1 000 anställda. Man tillverkar och marknadsför produkter och tjänster för miljö- och industriella mätningar och är världsledande inom sina områden.

Den starkaste tillväxten finns i Vaisala Instruments, som i första hand vänder sig till processindustrin. Bland nyheterna som kommer att presenteras finns bland annat daggpunktsmätare som mäter ett brett område av daggpunkts- och processtemperaturer med snabb svarstid, fuktmätare för mätning av relativ fuktighet i nästan alla miljöförhållanden oberoende av temperatur, tryck och luftfuktighetsnivåer, oljefukthetsmätare för kontinuerlig realtidsmätning av fukthalten/vattenaktiviteten i oljor samt syrehaltsmätare.

IVL visar operatörsstödsystem

Efter tio års utvecklingsarbete är det färdigt och kommer att visas på en speciell aktivitetsyta under hela mässan. Ett operatörsstödsystem som innebär ett helt nytt arbetssätt och kommer att spara miljoner kronor åt användarna. Det är IVL Svenska Miljöinstitutet AB som har utvecklat modellen. Emerson Process Management avser att marknadsföra systemet över hela världen och IVL kommer att knoppa av ett bolag, EEC, som ska driva verksamheten.

Det är det första operatörsstödsystemet i sitt slag i världen där man har aggregerat ett stort antal variabler för att skapa en modell för optimal drift. Övervakningssystemet ger information i realtid, vilket gör det möjligt för operatörerna att snabbt



kunna ställa om processen om kurvan förändras - avviker från optimal produktion.

– Skillnaden mellan vårt och andra övervakningssystem är att man normalt mäter exempelvis temperatur, tryck, viskositet, flödes hastighet etcetera. Alla dessa mätningar sker i realtid och ger en oerhörd mängd information, som ofta är svårtolkad. Vi utnyttjar dessa mätningar - men väger samman alla variablerna i en enda kurva, säger Magnus Andersson, IVL.

Miljö från förra Process
Teknikmässan i Göteborg.