

An online application of dynamic PLS to a dearomatization process

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Abstract

Early detection of process disturbances and prediction of malfunctions in process equipment improve the safety of the process, minimize the time and resources needed for maintenance, and increase the uniform quality of the products. The objective of online-monitoring is to trace the state of the process and the condition of process equipment in real-time, and to detect faults as early as possible.

In this article the different properties of the online-monitoring methods applied in the process industries are first reviewed. A description of the systematic development of the online-monitoring system for an industrial dearomatization process, specifically for flash point and distillation curve analysers, is then presented. Finally, the results of offline and online tests of the monitoring system using real industrial data from the Fortum Naantali Refinery in Finland, are described and discussed. The developed online-monitoring application was successful in real-time process monitoring and it fulfilled the industrial requirements. PACS: 07.05.Mh; 07.05.Tp; 83.85.Ns

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1. Introduction

According to several studies, inadequate managing of abnormal situations causes annual losses of US\$ 20 billion for the petrochemical industry in the USA. This, together with many other similar estimates, has led to extension of the field of diagnostic methods during the last decade. Since then, hundreds of successful applications of different monitoring methods have been reported (Lennox & Sandoz, 2002).

According to Venkatasubramanian, Rengaswamy, Yin, and Kavuri (2003), diagnostic methods can be divided into three categories: quantitative model-based, qualitative model-based and process history-based methods, as shown in Fig. 1.

A fundamental understanding of the functionality of the studied process is necessary for model development in model-

based methods. The quantitative models use mathematical functional relationships, whereas qualitative models apply qualitative functions that focus on different units in a process in order to capture the relationships between input and output of the system (Venkatasubramanian, Rengaswamy, Yin, et al., 2003).

The process history-based approach, which is especially suitable for process monitoring purposes, requires a large amount of data in order to capture and model the features of the process. The history-based models can be subdivided into qualitative and quantitative models. The basis of qualitative models consists of rule-based and trend modelling methodologies, whereas the quantitative methods are divided into statistical and non-statistical, neural networks-based pattern recognition models (Venkatasubramanian, Rengaswamy, Kavuri, & Yin, 2003).

Common features of the statistical methods used are their ability to reduce correlations between variables, compress data, and reduce the dimensionality of the data. These characteristics enable efficient extraction of the relevant information

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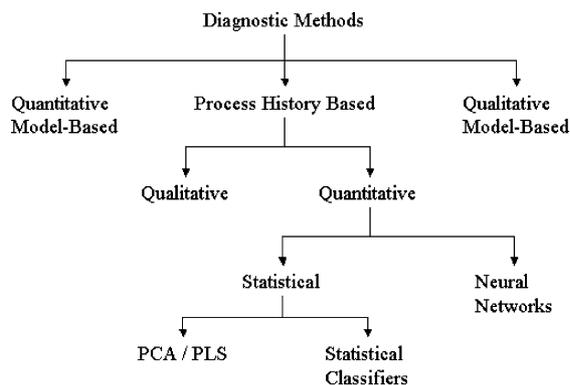


Fig. 1. Categories of the diagnostic methods.

and analysis of the data. The most important statistical monitoring methods are based on principal component analysis (Jackson, 1980) and partial least squares regression (Gerlach, Kowalski, & Wold, 1979).

The idea of principal component analysis (PCA) is to make a compact, orthogonal representation of the multivariable data with linear combinations of the original variables. The downside of the method is its inability to model non-linearities but, because the method is effective in its simplicity, the variations of this method are widely used for monitoring and diagnostic purposes.

The partial least squares (PLS) method, or projection to latent structures, is an extension of PCA. PLS regression forms a linear relationship between the input data matrix X and the output data matrix Y . The relationship is found, for example, between process variables and product quality variables. The method has the ability to analyse data with many, noisy, collinear and incomplete variables in both X and Y (Wold, Sjöström, & Eriksson, 2001).

Dynamic methods of PCA and PLS consider the dynamic nature of the monitored process and analyse both cross-correlation and autocorrelation. The dynamic characteristic is achieved by introducing time-lagged variables into the data matrices in a similar manner as in time series analysis. The dynamic methods are especially suitable for continuous processes with long time delays and varying throughputs on process variables (Ku, Storer, & Georgakis, 1995; Wold, Sjöström, & Eriksson, 2001).

Chen, McAvoy, and Pivoso (1998) proposed a multivariate statistical controller based on dynamic PCA. The method was tested successfully with a binary distillation column. The DPCA model constructed from tray temperature measurements represented the process. Komulainen (2003) developed an online-monitoring system for a dearomatization process in Fortum's Naantali Refinery, Finland. The monitoring system was based on dynamic PLS methods, extended with computed variables.

Recursive methods for PLS have been proposed by Dayal and MacGregor (1997) and Helland, Bernsten, Borgen, and Martens (1992). The recursive methods are especially suitable for time-dependent processes with slow changes like

catalyst deactivation, aging and contamination of equipment and drifting of the process and measurements. The methods include updating of mean and or variance, computation and determination of the optimal amount of principal components or latent variables, and updating of the Hotelling T^2 and SPE indices. The methods can be applied blockwise or after every new measurement. The use of a time window or forgetting factor is recommended.

Li, Yue, Valle-Cervantes, and Qin (2000) reported an application of recursive PCA to the rapid thermal annealing of semiconductors. Contamination and cleaning of sensors cause drifting in the measurements, which has resulted in the static monitoring methods giving false alarms. Monitoring is important in this batch process, because failures at the beginning of the batch lead to off-specification product quality. The RPCA application alarmed only when real failures occurred, and the number of false alarms was reduced significantly compared to the application of statistic PCA.

Dayal and MacGregor (1997) applied recursive PLS with a constant and variable forgetting factor to a mineral flotation process. The aim was to predict the future process output variables. Compared to the recursive least squares method, the best results were obtained with an RPLS with a changing forgetting factor.

Multi-scale principal component analysis (MSPCA) is a combination of PCA and wavelet analysis. The idea of MSPCA is to remove autocorrelations of every variable with wavelet analysis, and to eliminate cross-correlations between variables with PCA (Misra, Yue, Qin, & Ling, 2002). The method is suitable for processes with autocorrelated measurements and time-varying characteristics. Misra et al. (2002) reported on the application of MSPCA to a tubular gas phase reactor system. A moving time window approach was applied. The slow drifting of the process was visible from the approximation matrix. The monitoring system gave early warnings of the process faults and identified the causes of malfunctions.

Non-linear principal component analysis (NLPCA) is a combination of neural network and PCA. The idea is that the network fits a non-linear model to the data, and PCA removes the cross-correlations. The first NLPCA, proposed by Kramer (1991), consisted of a five-layer auto-associative neural network. The second and fourth layers consisted of non-linear nodes and the third layer of the bottle-neck nodes representing the principal components. The first and last layers were composed of linear input and output nodes. Determining the number of nodes in each layer is the drawback of this method. Dong and McAvoy (1996) proposed an NLPCA method, which integrates principal curve algorithm and neural networks. The idea of this method is to fit curves instead of lines to the data with the help of a three-layer feedforward network. The network consists of one linear input layer, one sigmoidal non-linear layer, and one linear output layer. The principal curves are first extracted. The network is then taught to map the original data to the principal curves, and another

neural network is then taught to map the principal curves back to the original set of variables.

Shao, Jia, Martin, and Morris (1999) applied NLPCA to monitor a spray dryer. The noise was removed with wavelet analysis and the NLPCA method was used for the wavelet coefficients. The combination of wavelet analysis and NLPCA-IT-net structure of 10-18-3-12-10 gave considerably better results in fault detection and identification than the linear PCA.

Non-linear PLS utilizing neural networks (NNPLS) has been proposed by Qin and McAvoy (1992). Berglund and Wold (1997) have reported non-linear PLS called implicit non-linear latent variable regression (INLR).

Neural network architectures can be divided into three categories, feedforward, feedback and self-organizing networks. According to Kohonen (2001), neural networks are the most applicable to classification and regression problems, which do not need perfect precision. The availability of large amounts of data is especially important.

The self-organizing map, introduced by Kohonen, is an unsupervised neural network that classifies data on the basis of the similarities of the weight vectors of the neurons. The neural network consists of a grid of neurons, in which the neighbouring neurons are competing for weight coefficients. The accuracy of the map is influenced by the size and shape of the map, and the size of the neighbourhood of the neurons. These parameters have to be determined before teaching the map (Alhoniemi, Hollmén, Simula, & Vesanto, 1999; Kohonen, 2001). The states of the neighbouring neurons are usually similar. To increase the accuracy of the classification, the use of a linear vector quantization (LVQ) algorithm is recommended (Kohonen, 2001). SOM has been compared to non-linear PCA, because it adapts to the structure of the data, and the weight of the neurons tend to set the densest regions of the data and form an approximation of a curve fitted to the data.

An application of SOM for monitoring the Outokumpu Harjavalta flash smelter was described by Jämsä-Jounela, Vermasvuori, Endén, and Haavisto (2003). The system detected equipment malfunctions and monitored process states using SOM in conjunction with heuristic rules. Kämpjärvi, Sourander, and Jämsä-Jounela (2004) developed an online-monitoring system which used a combination of PCA, SOM and RBFN to detect and identify faults. The system was successfully tested online at the Borealis ethylene plant in Porvoo, Finland.

A neural net based on adaptive resonance theory differs fundamentally from a self-organizing map in the fact that the size and shape of the map are not determined beforehand, but they are formed in the teaching phase. The only parameters needed are the vigilance parameter, which determines whether a new input vector is close enough to an existing neuron, and the step size, which determines the degree of change of the weights of the winning neuron. One problem is the possible incoherence of the map. The ART map has many modifications, including combinations of ART maps, like ART3 and

ARTnet, and hybrids of ART maps and fuzzy logic in FuzzyARTMAP (Wienke et al., 1996). Rallo, Ferre-Giné, Arenas, and Giralt (2002) reported the application of FuzzyARTMAP to a polymerisation process. FuzzyARTMAP was applied to develop a virtual sensor system, which predicted the properties of low density polyethylene on the basis of process variables.

2. Description of the dearomatization process

Dearomatization processes are widely used in the petroleum oil refining industry. The purpose of the dearomatization process is to remove aromatic compounds from the feedstock by hydrogenating them in a continuous process. The process consists of two trickle-bed reactors with packed beds of catalyst, a distillation column, several heat exchangers and separation drums and other unit operations. The process is presented in Fig. 2.

The seven different types of feedstock used in the process are petroleum oil cuts with clearly differing properties. A change of feed type is made, on the average, once every 4 days. The cold, liquid feedstock fed to the unit is heated in heat exchangers EA1 and EA2, and then fed to reactor DC1 together with hydrogen and recycle liquid. Exothermic saturation reactions in the first reactor remove most of the aromatic compounds. After dearomatization in reactor DC1, the reaction product is cooled in heat exchanger EA1 and then fed to gas separation drum FA1. Gaseous and liquid reaction products are separated in the drum. Part of the liquid is circulated back to reactor DC1. The rest of the liquid, together with separated gas and fresh hydrogen, are fed to the second reactor DC2, where the aromatics level of the product drops to near zero. After the second reactor, the reaction product is cooled in heat exchangers EA2 and EA3 and fed to the second gas separation drum FA2. Gas separated from the liquid mainly consists of unreacted hydrogen, which is recycled back to the first reactor, and the rest of the gas is removed. The separated liquid is heated in heat exchangers EA3 and EA4 and then fed to distillation column DA1.

The overhead of the column is cooled in a cooler and then fed to separation drum FA3, where the gaseous part is re-

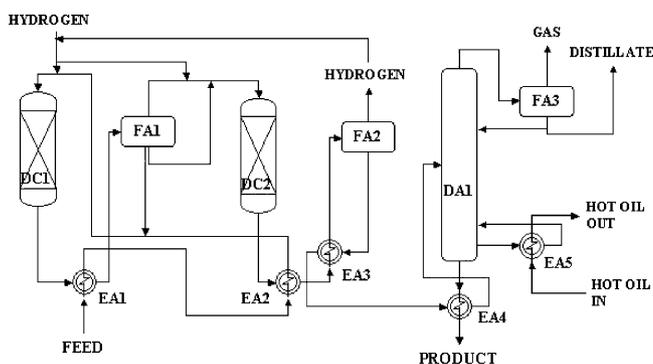


Fig. 2. The dearomatization process.

moved and the liquid is divided into reflux and distillate. The distillate consists of the lightest compounds of the reaction product.

The column reboil is generated in heat exchanger EA5. The non-aromatic product is drawn off as the bottom product and cooled in heat exchanger EA4. The quality of the cooled product is measured online by flash point and distillation curve analysers. Laboratory measurements of the product are performed twice a day.

The dearomatization process has no noticeable effect on the heaviest part of the distillation curve of the feedstock, but the properties of the lightest cuts are strongly affected by the distillation.

3. Objective of the online process monitoring

The objective of this study was to develop an online-monitoring system for an industrial dearomatization process.

First, the monitoring target was specified. The process historian, where the process faults and disturbances in the process were documented, provided a precise insight into the problem. The process historian of one year was examined in order to select the most frequently occurring disturbances.

One of the most common disturbances in the dearomatization process historian was a fault in the analysers. The occurrence of faults and the possibility of identifying related phenomena with process analysis methods, made the monitoring of process analyser faults the most important task of the study.

The aim of the monitoring was to detect whether the analysers were working correctly and to provide a reliable prediction of the analyser measurements also at the time when faults occurred. Prediction was needed in order to compensate for the temporary unavailability of measurements from the flash point analyser, which was used for half of the time for another process.

The monitoring methods used were the process history-based, quantitative methods falling within the categories of statistical or neural network methods.

4. Systematic approach for development of the online-monitoring system

Due to the complex nature and non-linearity of the process and product properties, a nine-stage systematic approach was introduced for the development of the online-monitoring system. First, the direct process variables that affected the flash point and distillation curve of the product were determined, and the selected variables were then time-lagged. Next, computed variables capable of capturing the characteristics of the dearomatization process were created on the basis of the time-lagged, direct process variables. The combination of direct process variables and computed variables with the strongest influence on the flash point and distillation curve, was then

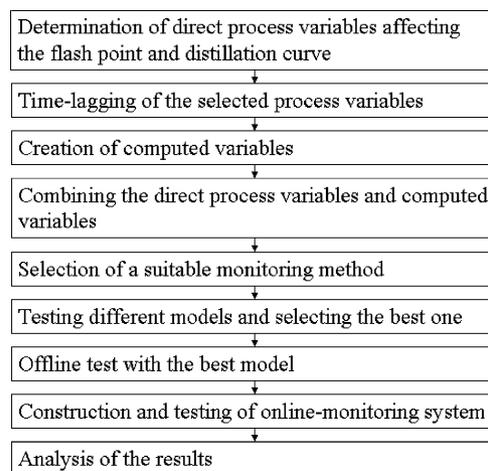


Fig. 3. The development stages of the online-monitoring system.

selected. After the combination of variables had been created, the most suitable method for monitoring proved to be dynamic PLS. Different models for monitoring were developed and tested. The offline test was performed with the most suitable models. When the results of the offline tests were satisfactory, an online-monitoring system was developed and tested. Finally, the results of the online test were analysed. The sequential development stages, shown in Fig. 3, are described and discussed in more detail in the following.

4.1. Determination of direct process variables affecting the flash point and distillation curve

Plant data from the dearomatization unit of the Naantali Refinery consisted of about 100 different measurements of temperature, pressure, flows, levels, and set points of the control valves. The measurements were collated in a real-time process historian. The most important measurements were used with a sampling interval of 1 min in this study.

The bottom product of the distillation column is measured online with the flash point and distillation curve analysers. The distillation curve analyser gives values for the initial, 5%, 10%, 50%, 90%, 95% and end point of the distillation curve every 40 min. The flash point analyser makes a measurement every second minute. As the dearomatization process has a noticeable effect only on the flash point and the initial, 5% and 10% points of the distillation curve, the other four points of the distillation curve were excluded from the study. The amount of distillate strongly affects the flash point and the front end points of the distillation curve, because these values reflect the amount of light compounds remaining in the bottom product.

The process variables affecting the analyser variables were selected on the basis of correlation analysis and process knowledge.

The selected variables were the following:

- 10 temperature measurements from reactors DC1 and DC2.

- 10 temperature measurements from overhead (2), reflux, bottom product (2), feed of distillation column (2), upper, middle and lower part of the distillation column.
- 10 flow measurements including the flow of the feedstock, hydrogen, circulated reaction product and hydrogen to the first reactor, hydrogen and reaction product to the second reactor, reaction product and reflux to the distillation column, distillate and bottom product from the distillation column.
- Pressure at the top of the column and its set point.
- Three level measurements from the bottom of the distillation column (measurement and set point) and separation drum FA3.
- Two computed variables, temperature difference and enthalpy from the reboiler of the column.

A total of 35 direct process measurements and two computed variables of the reboiler were selected.

4.2. Time-lagging of the selected process variables

The time lags in the dearomatization process are long, approximately 2 h from the first temperature measurement to the analysers of the bottom product.

Total time lags, i.e. dead time and process lag, between the temperature measurements were estimated using a cross-correlation function. The maximum value of the cross-correlation function was selected for the total time lag for the measurement. The reference measurement was the first temperature measurement of the process unit. The total time lags for flow, pressure and level measurements were estimated on the basis of the nearest temperature measurement. The sampling interval was 1 min, resulting in total time lags of full minutes.

The data were time-lagged according to the estimated total time lags.

4.3. Creation of the computed variables

Computational variables were created in order to capture the basic characteristics of the dearomatization process. The characteristics of the distillation especially were investigated, because distillation has a strong effect on the flash point and the initial point of the distillation curve. The computed variables were constructed from 36 time-lagged process measurements as follows:

- The heat generated in the first and second reactors, and the heat divided by the flow of the fresh feedstock to the first reactor.
- Temperature differences in the reactors were computed between the highest and the lowest measurement. Temperature differences in the distillation column were computed between the temperatures of: the middle of the column and the feed, bottom of the column and feed, bottom product and the bottom of the column, top of the column and reflux, bottom product and the overhead of the column.

- Flow ratios were determined for distillate and bottom product, distillate and reflux, distillate and feed of the column, bottom product and feed of the column, and reflux and feed of the column.
- Variables describing enthalpy were represented by simple products of the flow rate and temperature. Instead of direct enthalpies, the enthalpy ratios, i.e. one enthalpy variable divided by another, were used.
- The enthalpy ratios for the distillation column were computed between: distillate and feed, reflux and feed, bottom product and feed, distillate and bottom product, and reflux and bottom product.
- The process measurement describing the enthalpy of the reboiler, divided by the flow of the feed to the column, was also calculated/created.

A total of 23 computed variables were created.

4.4. Combination of the direct process variables and the computed variables

The combination of direct process measurements and computed variables was formed on the basis of the correlations between the variables and the analyser variables.

All the previously described computed variables were used in the combination. Especially temperature measurements of the distillation column, pressure of the overhead and the computed variables of the second reactor had high correlations with the analyser variables.

The final combination contained 21 direct, time-lagged, process measurements and 23 computed variables, which were constructed from the time-lagged process measurements.

4.5. Selecting the most suitable monitoring method

The following requirements were specified for the methods. The method should be able to handle several dozen variables and the output of the method should give accurate predictions of the analyser values. The method should be able to distinguish between process transitions at feedstock changes, and the process and analyser faults. The method should also be able to distinguish between malfunctions of the analysers and process faults as early as possible, and to give the operator an alarm. Only the methods described in the literature survey were considered. A method that could be applied online and based on process history was preferred.

The need for precise prediction ruled out neural nets. The clear relationship between process and computed variables, and the quality variables of the product, led to the use of PLS-based methods.

Owing to the dynamic nature of the process, dynamic partial least squares regression (DPLS) was selected. DPLS fulfilled all the requirements, and the relationship between the process variables and the analyser variables made the structure of the method very simple.

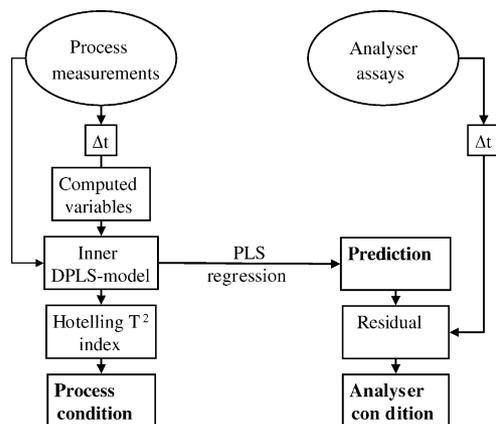


Fig. 4. A schematic picture of the utilization of the DPLS method to detect process disturbances and analyser faults.

A flowchart of the DPLS method used is illustrated in Fig. 4. First, the direct process measurements were time-lagged and the computed variables were created. The direct process variables and the computed variables formed the input block and time-lagged analyser assays the output block of the PLS regression. The predictions of the analyser variables were made using the input block. The residuals between the predicted and the real analyser values indicated whether the analysers were functioning correctly. A possible process fault was detected with the Hotelling T^2 statistics, calculated as the sum of normalized squared scores of the input block.

4.6. Testing different models

The first task in the model development phase was to select the proper training data. The models were first constructed using the training data of one feed type. As expected, the models did not describe the other feed types. Next, the training data were constructed using the data for several feed types. The more feed types the training data contained, the better were the results. Equal amounts of data from all the feed types were used, totalling 57 h. The data included only normal processing situations with some changes in the feed rate.

An appropriate number of latent variables of the DPLS model was selected for the offline test with the help of the cumulative variance percent table and the root mean square of the calibration (RMSEC) curve. The lower the value of RMSEC, the better the model fits the training data. The RMSEC value was approximately the same for latent variable number 5 and larger ones, as shown in Fig. 5.

The satisfactory values of the cumulative variance percent (above 80%), shown in Table 1, also support this conclusion. With five latent variables the variance percent for the input block was 90.2% and for the output block 99.6%, reflecting the expected level of random noise and mismatch in the process data.

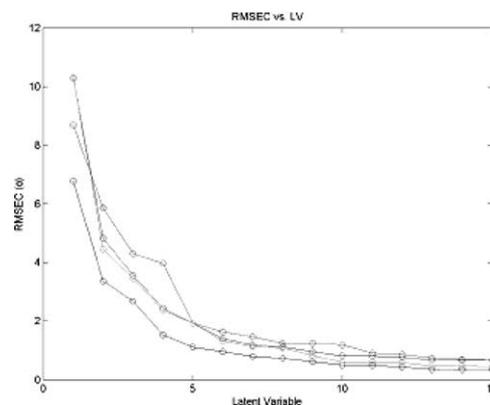


Fig. 5. The RMSEC values for flash point, initial 5% and 10% points of the distillation curve with different numbers of latent variables.

4.7. Offline test

The data set for the offline test contained process data for about 455 h with a resolution of 1 min. The data included several changes in the feed type and faults in the analysers. Most of the data were collected from normal situations.

The values of the process and computed variables were monitored with the Hotelling T^2 index. If the Hotelling T^2 value of the current measurements was over the Hotelling T^2 limit, the process state was classified incorrectly and the predictions of the analysers were not reliable.

If the process state was normal, i.e. the Hotelling T^2 value was below the Hotelling T^2 limit, the predictions of the analyser measurements were computed and the residuals between the real and predicted value were also computed. The monitoring limits for the analyser residuals were defined as half the mean variance of the training data set. If the absolute value of the residual was below the limit, then the analyser was in the normal state. If the limit was crossed, an alarm was given and the analyser measurement was classified as faulty.

The process faults and analyser faults were marked on the basis of the process historian, and the results of the monitoring method and the real faults were compared.

The results of the offline test are presented in Table 1. Monitoring the flash point gave the best results; 97% of the faults were detected correctly and 99% of the normal states were classified properly. Monitoring the initial point of the distillation curve was slightly more complicated because the analyser was occasionally lagging changes in the feedstock.

Table 1
Cumulative variance percentages captured by the PLS model

| Latent variables | CVP input block (%) | CVP output block (%) |
|------------------|---------------------|----------------------|
| 1 | 36.81 | 87.71 |
| 2 | 66.76 | 96.72 |
| 3 | 75.81 | 98.12 |
| 4 | 84.42 | 98.94 |
| 5 | 90.15 | 99.56 |
| 6 | 95.99 | 99.73 |
| 7 | 97.03 | 99.80 |

Table 2
Results of the offline test

| | Flash point | Initial point | 5% point | 10% point |
|--------------------------|-------------|---------------|----------|-----------|
| Faults | 5666 | 937 | 694 | 723 |
| Detected correctly (%) | 97 | 67 | 71 | 66 |
| Detected incorrectly (%) | 3 | 33 | 29 | 34 |
| Normal states | 21625 | 26354 | 26597 | 26568 |
| Detected correctly (%) | 99 | 98 | 96 | 96 |
| Detected incorrectly (%) | 1 | 2 | 4 | 4 |

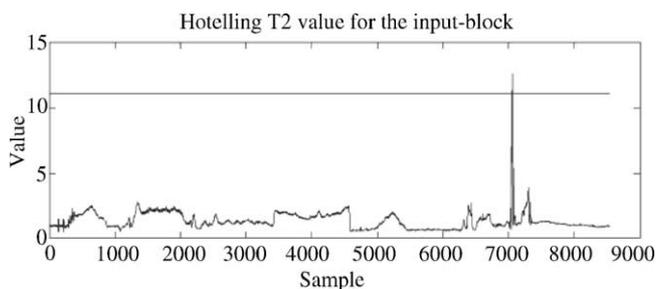


Fig. 6. Hotelling T^2 values for the input block. The limit is marked with a straight line.

The high sensitivity of the initial point of the distillation curve was detected when the measurement of the initial point of the distillation curve was inconsistent with the other analyser measurements.

Overall, the results of the offline test were encouraging; 96–99% of the normal states of the analysers and 67–97% of the fault states were classified correctly as shown in Table 2.

4.8. Online test

An online-monitoring system was developed on the basis of the DPLS model created in the offline test phase. The system was tested online for a time period of 144 h. During this period the type of feedstock changed twice and a disturbance also hit the process once.

The process disturbance at around 7000 min caused a violation of the Hotelling T^2 limit, as shown in Fig. 6. A correct alarm was given for the process disturbance.

The condition of the analysers was monitored with the residual plots. The residuals, presented in Figs. 7–10, re-

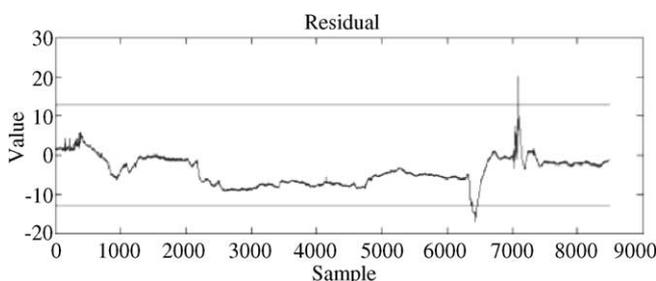


Fig. 7. Residual of the flash point. Limits are marked with straight lines.

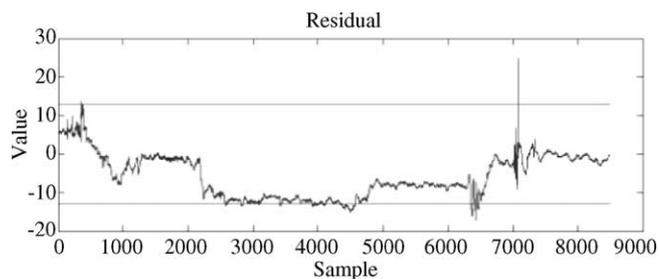


Fig. 8. Residual of the initial point of the distillation curve. Limits are marked with straight lines.

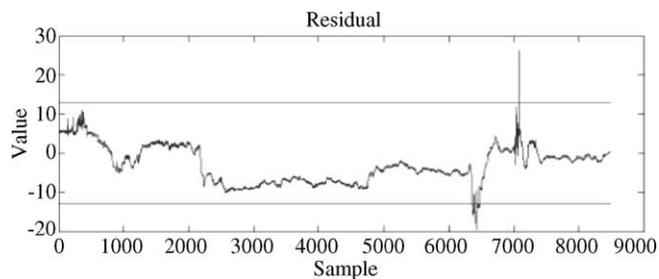


Fig. 9. Residual of the 5% point of the distillation curve. Limits are marked with straight lines.

mained inside the residual limits throughout the experiment, except for two cases. The first alarm occurred around 6500 min and the second around 7000 min. The second case was due to a process disturbance and the alarm was given correspondingly.

The first violation of the residual limits was caused by the lag in the analyser results after the change of feedstock type, and an analyser alarm was given accordingly. The monitoring of the initial point of distillation curve resulted in the residual merely riding the monitoring limits between 2500 and 4500 min. Alarms were not given because the riding was followed and the values remained inside the tolerance limit of one unit.

The results of the online test are summarized in Table 3. Monitoring the flash point gave the best results, and all the faults were detected correctly. The initial point of the distillation curve classified 93% of the faults and 94% of the normal situations correctly. In total, 94–100% of the normal states of the analysers and 93–100% of the faulty states were detected correctly. The monitoring system classified the

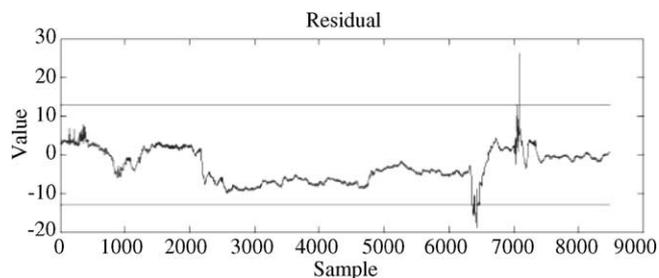


Fig. 10. Residual of the 10% point of the distillation curve. Limits are marked with straight lines.

Table 3
Results of the online test

| | Flash point | Initial point | 5% point | 10% point |
|--------------------------|-------------|---------------|----------|-----------|
| Faults | 72 | 73 | 73 | 74 |
| Detected correctly (%) | 100 | 93.1 | 100 | 100 |
| Detected incorrectly (%) | 0 | 6.9 | 0 | 0 |
| Normal states | 8412 | 8411 | 8411 | 8410 |
| Detected correctly (%) | 100 | 94.3 | 99.7 | 99.9 |
| Detected incorrectly (%) | 0 | 5.7 | 0.3 | 0.1 |

Table 4
Cumulative variance percentages captured by the PLS model

| Latent variables | CVP input block (%) | CVP output block (%) |
|------------------|---------------------|----------------------|
| 1 | 41.09 | 92.78 |
| 2 | 52.94 | 97.17 |
| 3 | 79.88 | 97.85 |
| 4 | 84.41 | 99.59 |
| 5 | 89.78 | 99.74 |
| 6 | 93.99 | 99.77 |
| 7 | 96.34 | 99.80 |

feed type changes correctly as normal states, and gave an alarm for an abnormal process state during the disturbance (Tables 3 and 4).

4.9. Role of the computed variables

To justify the utilization of computed variables in this application, DPLS models with and without computed variables were compared. First, a DPLS model was created using the 37 time-lagged direct process variables. Cumulative variance percents for the DPLS model without computed variables were similar with the cumulative variance percents for the DPLS model with computed variables, as shown in Table 4. The DPLS model without computed variables included five latent variables.

The performance of DPLS with and without computed variables was tested with the online data set. The normal states were detected correctly considerably more often with computed variables than without computed variables as shown in Table 5. DPLS with computed variables classified 94–100% of the normal states correctly where as the DPLS without computed variables classified only 1–88% of the normal states correctly. Therefore utilization of the computed variables was justified in this application.

Table 5
Normal process states detected with and without computed variables

| | Flash point | Initial point | 5% point | 10% point |
|-----------------|-------------|---------------|----------|-----------|
| With CVs | | | | |
| Correctly (%) | 100 | 94.3 | 99.7 | 99.9 |
| Incorrectly (%) | 0 | 5.7 | 0.3 | 0.1 |
| Without CVs | | | | |
| Correctly (%) | 88.1 | 35.3 | 1.1 | 10.8 |
| Incorrectly (%) | 11.9 | 64.7 | 98.9 | 89.2 |

5. Conclusions

The objective of this study was to develop an online-monitoring system for the dearomatization unit of the Naantali Refinery. A systematic nine-stage procedure was used to progress from the problem to the online-monitoring application. The current states of the flash point and distillation curve analysers were monitored and, during malfunctions, their values were predicted using the dynamic partial least squares method.

The results of the offline test were encouraging; 96–99% of the normal states of the analysers and 67–97% of the fault states were classified correctly.

An online-monitoring system was developed and tested for a time period of 144 h. The monitoring system classified the two feed type changes correctly as normal states, and gave an alarm for an abnormal process state during the disturbance.

The developed online-monitoring application fulfilled the industrial requirements and it was successful in real-time process monitoring of the dearomatization process.

In the future the online-monitoring system will be modified to use a non-linear DPLS algorithm to more accurately model the non-linearities of processes. A recursive DPLS algorithm will also be tested.

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