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Continuous Estimation of the Key Components Content in the Isomerization Process Products

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Soft sensors for estimating a fraction of key components in the products of a Low-temperature isomerization process equipped with a deisohexanizer distillation column are developed. Real plant data from the refinery distributed control system (DCS) are used. A considerable attention is paid to data selection, selection of key input variables, data processing and analysis.
Dynamic soft sensor models for estimating the fraction of 2,2-Dimethylbutane, 2,3-Dimethylbutane, 2-Methylpentane and 3-Methylpentane in the products of the process are developed based on linear and nonlinear regression techniques. The development of a linear dynamic Finite Impulse Response (FIR), Autoregressive with Exogenous Inputs (ARX), Output Error (OE), as well as Nonlinear Dynamic Autoregressive with Exogenous Inputs (NARX) and Hammerstein-Wiener (HW) models are presented. Developed models were evaluated by validation techniques including Root Mean Square Error (RMSE), Absolute Error (AE), Final Prediction Error (FPE) and FIT coefficients.
The results show that the developed soft sensors can reliably estimate the content of key components and thus replace process analysers in the case of failure. This will contribute to the operation stability of the column, the rise in product quality, the reduction in energy consumption as well as the improvement of whole isomerization process. Also, the developed soft sensors can be applied in the Advanced Process Control scheme of the deisohexanizer column.

1. Introduction

Legislation requirements for the limitation on pollutants emission into the environment demand strict following to prescribed concentration of pollutants emission from plants, vehicles and other devices. There are also requirements for continuous improvement in product quality and minimizing energy consumption. Continuous measurement of the key process variables is necessary for both requirements. However, process analysers are usually very expensive; they can suffer from a large analysis time and they are subject to failures.
As an alternative for continuous process analysis soft sensors were proposed. Many methods have been developed for estimation and prediction of key process variables by using other easily measured process variables (Kadlec et al., 2009). They are applied for process monitoring and can be a part of advanced process control strategy where they are used for estimating the key variable behaviour.
Various model structures can be developed for real process modelling. In complex industrial processes, the development of first principles models can be very demanding, time-consuming and with a large number of uncertain parameters. Data-driven models with parametric polynomial structures like linear autoregressive models with external inputs and their nonlinear versions are more convenient, but model order and time delays have to be predefined (Ujević Andrijić et al., 2017).
Typical soft sensor design procedure includes the following steps: selection of historical data from plant database, outlier detection and data filtering, model structure and regressor selection, model estimation and validation (Fortuna et al., 2007). Choosing the optimal model structure is often crucial for soft sensor performance (Kadlec et al., 2009).
Many papers in recent years were covered various design techniques and application of soft sensors in the process industry. However, there is a lack of research on the application of soft sensors in the isomerization

process. Xianghua et al. (2009) proposed an inferential model for online estimation of the para-xylene concentration at the reactor outlet stream in the industrial isomerization unit. Very often soft sensor design is based on neural networks, support vector machine and principal component analysis (PCA). Mei et al. (2017) used Gaussian process regression and PCA to overcome process non-linearity, shifting operating modes, dynamics and uncertainty in the development of a multi-model strategy based soft sensor in fermentation processes. Cao and Luo (2014) proposed a soft sensor model derived from Wiener model structure to effectively describe dynamic and static characteristics of a system. The study presented by Mollaiy-Berneti (2014) describes the development of a committee machine based soft sensor. The proposed inferential sensor combines the results of linear and nonlinear auto-regression exogenous input, neural network and adaptive neuro-fuzzy inference system (ANFIS) for overall oil flow rate prediction. The work presented by Shakil et al. (2009) demonstrates the application of dynamic neural networks for developing soft sensors used for the NO_x and O_2 emission prediction due to combustion operation in industrial boilers. Chen et al. (2009) used FIR model to develop a dynamic soft-sensor based on OE method for prediction of the immeasurable outputs of product quality variables in dual-rate sampling systems.

In this work, several types of dynamic linear and nonlinear parametric polynomial models are developed, including FIR, ARX, OE, NARX and HW models which predict the key components content of the sidecut and overhead products at the deisohexanizer distillation column.

2. Soft sensor model structures

In the book by Ljung (1999) system identification methods are briefly explained. The simplest dynamical process model is the FIR, which represents the linear regression over the past measuring input samples. The model predictor is presented by the following equation:

$$\hat{y}(t) = \mathbf{B}(q)u(t - nk) \tag{1}$$

where $\mathbf{B}(q) = \mathbf{B}_1 + \mathbf{B}_2 q^{-1} + ... + \mathbf{B}_{nb} q^{-nb+1}$ is polynomial matrix by q^{-1} of dimensions $n(y)\times n(u)$. nb is the number of past process input samples and nk is input time delay expressed by the number of samples.

One of the frequently used linear dynamic process model which takes into account a noise occurrence is the ARX. The model predictor is:

$$\hat{y}(t) = [1 - \mathbf{A}(q)]y(t) + \mathbf{B}(q)u(t - nk) \tag{2}$$

where $\mathbf{A}(q) = 1 + \mathbf{A}_1 q^{-1} + \mathbf{A}_2 q^{-2} + ... + \mathbf{A}_{na} q^{-na}$ is polynomial matrix by q^{-1} of dimensions $n(y)\times n(y)$. na is the number of past process output samples.

One of the commonly used linear models for the online estimation is the OE model:

$$\hat{y}(t) = [1 - \mathbf{F}(q)]\hat{y}(t) + \mathbf{B}(q)u(t - nk) \tag{3}$$

where $\mathbf{F}(q) = 1 + \mathbf{F}_1 q^{-1} + \mathbf{F}_2 q^{-2} + ... + \mathbf{F}_{nf} q^{-nf}$ is polynomial matrix by q^{-1} of dimensions $n(\hat{y}) \times n(\hat{y})$. nf is the number of past model predicted output samples.

A linear dynamic model can be sufficient for the applications in many cases, but most of industrial processes show nonlinear dynamic behaviour. The structure of linear models is fully defined by the selected regressors, while the nonlinear model structure additionally depends on attributes of a nonlinear function. Such a nonlinear function can be presented by various types of networks such as wavelet, sigmoid, piecewise-linear and other.

NARX is a nonlinear version of ARX model. The predictor has a linear regression form with the addition of a nonlinear part:

$$\hat{y}(t) = f_n(y(t-1),...,y(t-na),u(t-nk),...,u(t-nk)-nb+1) \tag{4}$$

where f_n is a nonlinear function containing a number of nonlinear units. When the system dynamics can be well described by a linear model but if there is a presence of a static nonlinearity at inputs and outputs the HW model can be applied. HW model has a block structure described by 3 functions:

- $w(t) = f(u(t))$ is a nonlinear function transforming input data u(t)
- $x(t) = (\mathbf{B}/\mathbf{F})w(t)$ is a linear transfer function where **B** and **F** are polynomials of the OE model
- $\hat{y}(t) = h(x(t))$ is a nonlinear function mapping output data x(t) from the linear block to the model output

The nonlinear functions of the HW model are described in the same as at a NARX model.

3. Process description

Refinery process of catalytic isomerization of pentane, hexane and their mixtures improves the octane of light straight-run naphtha. The reactions take place in the presence of hydrogen over a fixed bed of catalyst and at operating conditions that promote isomerization and minimize hydrocracking (Meyers, 2003).
The dominant reaction of the isomerization process is the conversion of n-paraffins to i-paraffins, i.e., to high-octane structure (Cerić, 2012). The reaction is controlled by thermodynamic equilibrium that is more favorable at a low temperature. The isomerized product is stabilized in the stabilizer distillation column where it is separated as a liquid product at the bottom and fuel gas at the top of the column. The basic isomerization process is improved by adding a deisohexanizer column where the stabilizer bottoms are separated into normal and isoparaffin components. In the deisohexanizer column sidecut stream, the non-converted n-paraffins and the new-formed low-octane methylpentanes are concentrated and returned to the reactor section as shown in Figure 1 (Meyers, 2003).

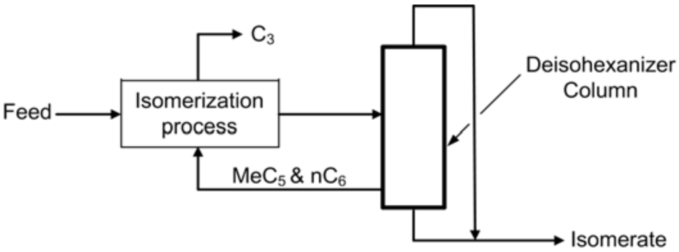

Figure 1: Isomerization process and deisohexanizer column (Meyers, 2003)

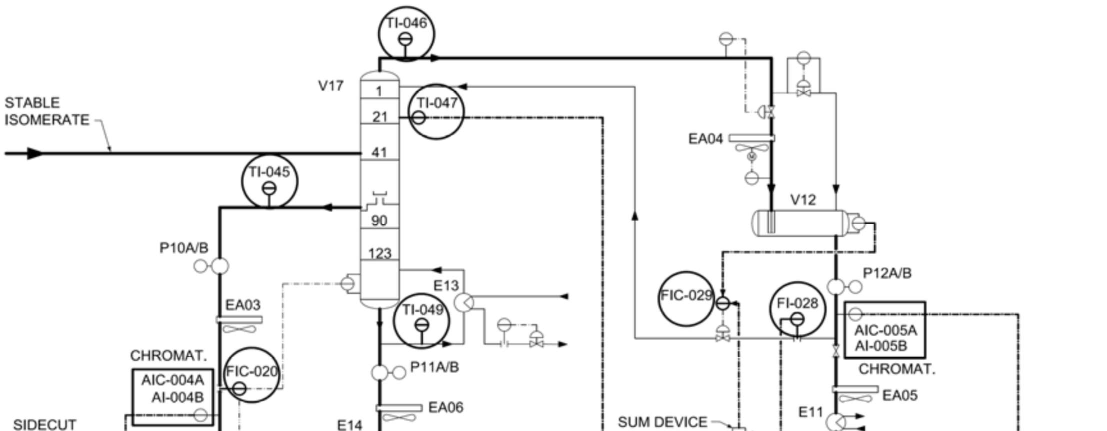

Figure 2: Deisohexanizer column and influential variables

The key components of the isomerization process products are the high-octane 2,2-DMB, 2,3-DMB and the low-octane 2-MP, 3-MP. Their content is measured by on-line chromatographic analyzers where high-octane sample is taken from the deisohexanizer side-cut stream and low-octane sample is taken from the deisohexanizer overhead stream as shown in Figure 2. The fraction of the components is also determined by laboratory analyses. The goal is to maintain high-octane 2,2-DMB and 2,3-DMB in the overhead stream and to maintain low-octane 2-MP and 3-MP in the sidecut stream by controlling the fraction of these key components. Usually, the challenge is long process analyzing time that contributes to overall process control dead time and unstable column operation. Analyzers are also frequently under maintenance. For that reason, soft sensors are developed for continuous estimating the fraction of the key components to enable inferential control.

Based on process expert experience the following variables are chosen as the influential variables on the key components content: TI-046, V17 column overhead stream temperature; TIC-047, V17 column 21st tray temperature; TI-045, V17 column sidecut stream temperature; TI-049, V17 column bottom stream temperature; FI-028, V17 column reflux flow; FIC-029, V17 column reflux flow and isomerate outlet flow sum; FIC-020, V17 column sidecut stream flow and FIC-026, V17 column bottom stream flow, see Figure 2.

4. Model development

Data from the refinery DCS were collected over period of 2–3 weeks and checked with laboratory assays. According to the process dynamics, the sampling interval was chosen to be 3 minutes. Data preprocessing included detection of outliers and missing data and detrending. The coefficients of the ARX and FIR models were optimized by least-squares method, for the OE models that was numerical search method, and for the NARX and HW models a combination of Gauss-Newton, Levenberg-Marquardt and Trust-region methods were used. The models were developed using the MATLAB System Identification Toolbox. The models were evaluated by statistical criteria based on root mean square error (RMSE), absolute error (AE), final prediction error (FPE) and FIT coefficients (MathWorks, 2014), Eq(5)–(6):

$$\mathrm{FPE} = V\left(1 + 2d / n\right) \tag{5}$$

$$\mathrm{FIT} = 1 - \left(\sqrt{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2} \Big/ \sqrt{\sum_{i=1}^{n} (y_i - \bar{y})^2} \right) \cdot 100 \tag{6}$$

where y is the measured output, $\hat{y}$ is the model output, $\bar{y}$ is the mean of y, V is the loss function, d is the number of estimated parameters and n is the number of values in the estimation data set.

5. Results and discussion

All models were additionally evaluated on the validation data set. In the tables 1 and 2 the results of the linear (FIR, ARX, OE) and nonlinear (NARX, HW) models for estimating the content of 2,3-DMB in the deisohexanizer column sidecut stream and 2-MP content in the deisohexanizer overhead stream are shown, respectively.

Table 1: 2,3-DMB model evaluation

	FIR	ARX	OE	NARX	HW
FIT	65.84	73.15	72.62	72.99	73.76
FPE	0.0524	1.17×10^{-7}	0.0345	1.44×10^{-7}	0.1017
RMSE (% mole)	0.266	0.209	0.213	0.206	0.200
AE (% mole)	0.213	0.163	0.156	0.163	0.149

Table 2: 2-MP model evaluation

	FIR	ARX	OE	NARX	HW
FIT	62.0	82.89	88.02	83.5	88.91
FPE	1.181	5.9×10^{-8}	0.0856	6.39×10^{-8}	0.1822
RMSE (% mole)	0.856	0.386	0.270	0.386	0.260
AE (% mole)	0.681	0.320	0.201	0.326	0.196

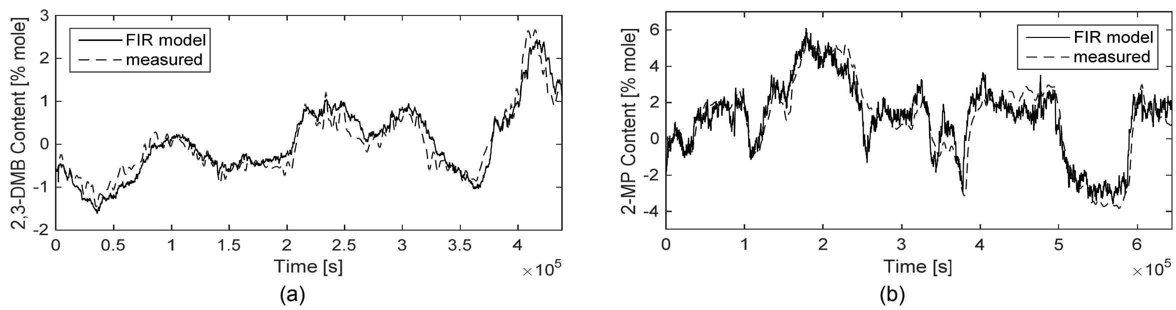

Figure 3: Comparison between measured data and FIR model. (a) 2,3-DMB content. (b) 2-MP content

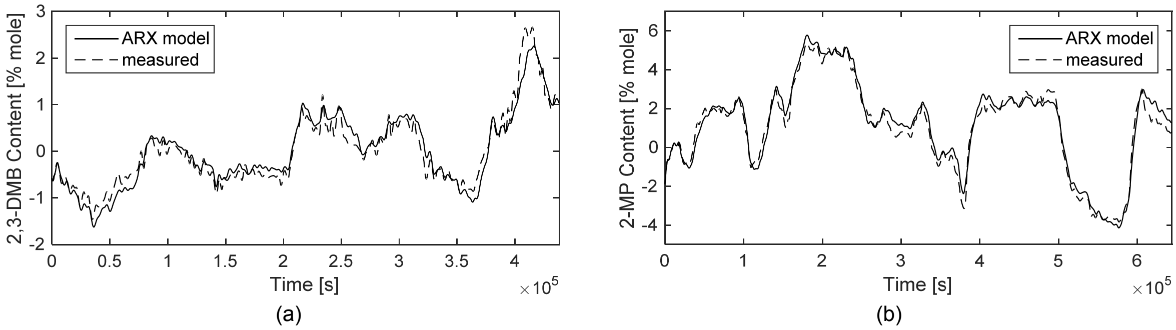

Figure 4: Comparison between measured data and ARX model. (a) 2,3-DMB content. (b) 2-MP content

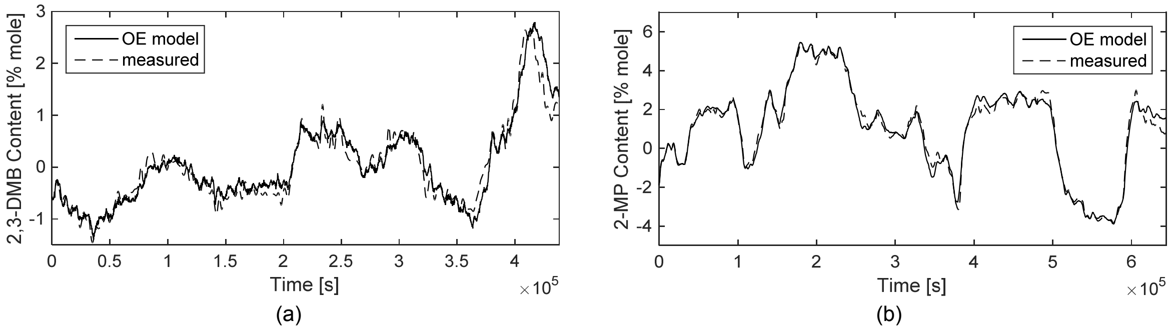

Figure 5: Comparison between measured data and OE model. (a) 2,3-DMB content. (b) 2-MP content

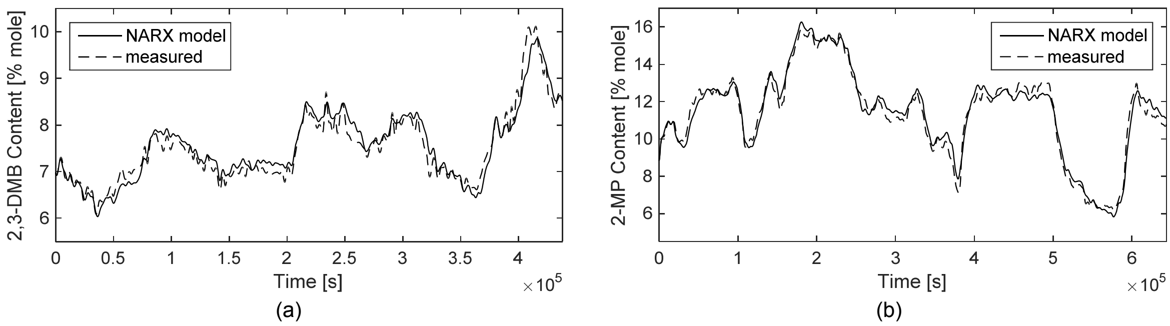

Figure 6: Comparison between measured data and NARX model. (a) 2,3-DMB content. (b) 2-MP content

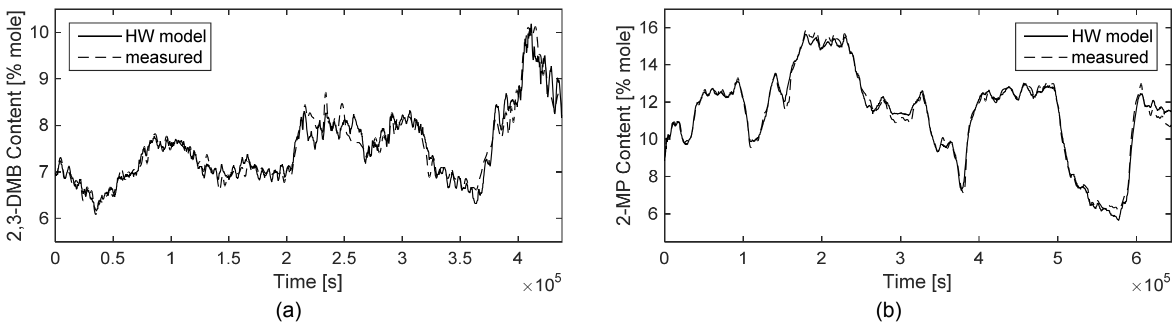

Figure 7: Comparison between measured data and HW model. (a) 2,3-DMB content. (b) 2-MP content

Figures 3, 4, 5, 6 and 7 show the comparison between measured data and model output for the estimation of the content of 2,3-DMB and 2-MP, respectively. The comparison is shown for validation data set.

Comparing the evaluation results for 2,3-DMB and 2-MP content in linear and nonlinear models, it can be seen that the later give better results for the ARX, OE, NARX and HW models, while the FIR models give roughly the same performance examining the FIT values.
For both 2,3-DMB and 2-MP content, FIR models give the weakest performance comparing to other models. The reason is their simple parametric structure that takes into account only past measured input values for model output calculations. For the 2-MP content, the OE shows better matching in the comparison with ARX. Comparing with nonlinear models, based on overall FIT, FPE, RMSE and AE, the best results are obtained with the HW model. 2,3-DMB content ARX, OE, NARX and HW model gives roughly the same performance although it was expected that nonlinear modeling will result with certain improvements. Figures 3–7 show a good matching between measured data and model output for both 2,3-DMB and 2-MP content. Also, the overall absolute errors of around 0,2 % mole is satisfying for planned online implementation.
The results for 2,2-DMB and 3-MP content model have been omitted due to limited space, but similar conclusions can be drawn as well as for above-analysed cases.

6. Conclusions

Linear and nonlinear dynamic models for estimating the content of 2,2-DMB, 2,3-DMB, 2-MP and 3-MP as key components in the products of a low-temperature isomerization process equipped with a deisohexanizer distillation column were developed. The results show that the process dynamics can be reliably described. The results obtained by both 2,3-DMB and 2-MP content models are acceptable for the soft sensor application in the plant. Due to the tendency that optimal model for implementation in the real plant is the simplest model with a good FIT and a small prediction error the OE models is best selection for on-line analyser temporary replacement, while the ARX models can be applied in the advanced process control scheme.

References

Cao P., Luo X., 2014, Soft Sensor Model Derived from Wiener Model Structure: Modeling and Identification, Chinese Journal of Chemical Engineering, 22, 538–548.

Cerić E.,2012, Nafta, procesi i proizvodi, IBC d.o.o., Sarajevo, BA.

Chen C., Mo S., Chen X., 2009, Dynamic soft-sensor based on finite impulse response model for dual-rate system, 2009 Chinese Control and Decision Conference, Guilin, CN, 2173–2178.

Fortuna L., Graziani S., Rizzo A., Xibilia M.G., 2007, Soft Sensors for Monitoring and Control of Industrial Processes (Advances in Industrial Control), Springer, London, UK.

Kadlec P., Gabrys B., Strandt S., 2009, Data-driven soft sensors in the process industry, Computers & Chemical Engineering, 33, 795–814.

Ljung L., 1999, System Identification: Theory for the User, 2nd edition, Prentice Hall, New Jersey, US.

Mei C., Chen Y., Zhang H., Chen X., Liu G., 2017, Development of a multi-model strategy based soft sensor using gaussian process regression and principal component analysis in fermentation processes, Chemical Engineering Transactions, 61, 385–390.

Meyers R.A. (Ed), 2003, Handbook of Petroleum Refining Processes, Third Edition, Chapter In: N A Cusher (Ed.), UOP Penex Process, McGraw-Hill, New York, US, 9.15–9.27.

Mollaiy-Berneti S., 2014, A committee machine based soft sensor as an alternative to multiphase flow meter for oil flow rate prediction of the wells, Journal of Intelligent & Fuzzy Systems, 26, 2719–2729.

Shakil M., Elshafei M., Habib M.A., Maleki F.A., 2009, Soft sensor for NO_x and O_2 using dynamic neural networks, Computers & Electrical Engineering, 35, 578–586.

System Identification Toolbox: User's Guide, Release 2014a, 2014, The MathWorks, Inc., Natick, US.

Ujević Andrijić Ž., Mohler I., Bolf N., Dorić H., 2017, Development of Inferential Models for Fractionation Reformate Unit, 2017 21st International Conference on Process Control (PC), Strbske Pleso, SK, 143–148.

Xianghua C., Ouguan X., Hongbo Z., 2009, Recursive PLS soft sensor with moving window for online PX concentration estimation in an industrial isomerization unit, 2009 Chinese Control and Decision Conference, Guilin, CN, 5853–5857.