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DATA-DRIVEN ESTIMATION OF CRITICAL QUALITY ATTRIBUTES ON INDUSTRIAL PROCESSES

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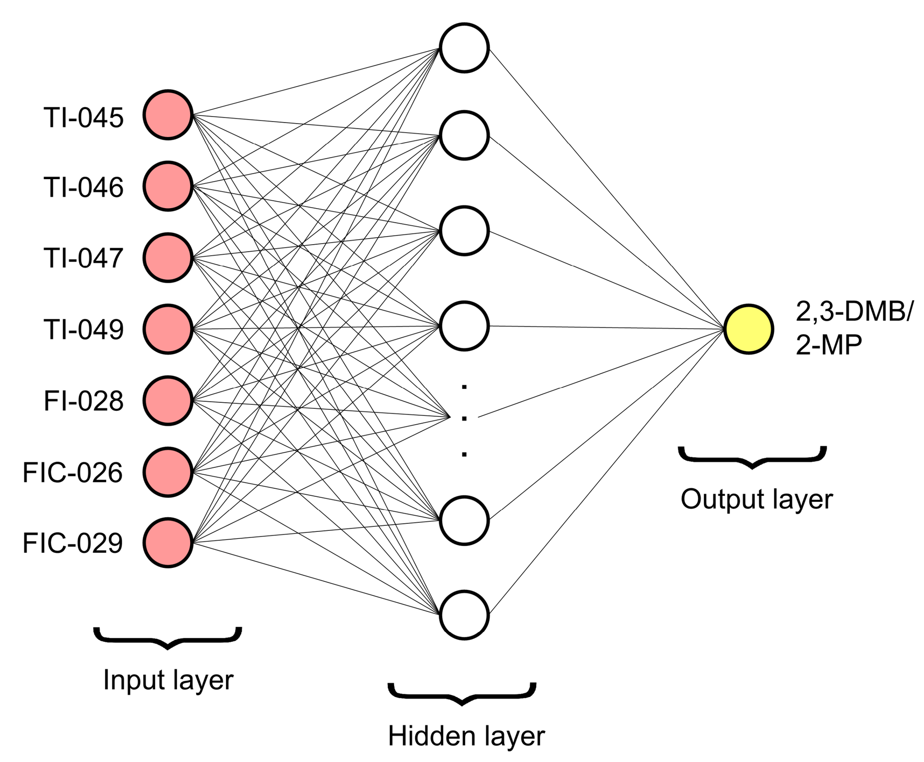
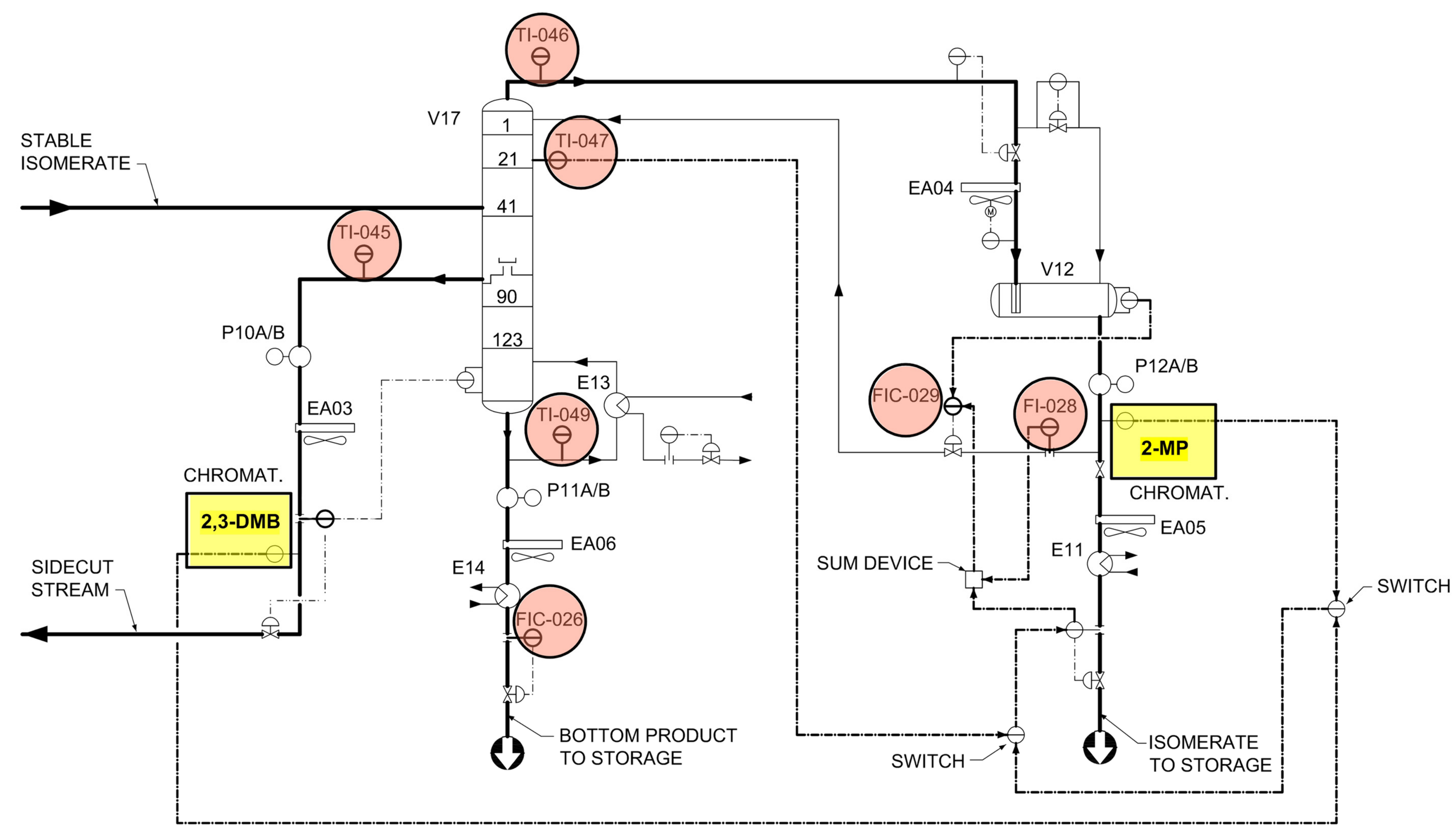
Abstract

This work presents an industrial case study of data-driven models based on multilayer perceptron (MLP) neural networks (NN) for refinery light naphtha isomerisation process. The models for the estimation of critical quality attributes of the product were developed. Significant attention was paid to the selection and analysis of data sets for different periods with the aim of capturing enhanced process dynamics. Optimal models were obtained by changing the types of learning function and transfer function, as well as the number of neurons in the hidden layer. Models based on MLP neural networks have shown better generalization abilities in comparison with earlier developed polynomial linear and non-linear models for isomerisation process. This makes the developed MLP neural network models desirable for application to such a process, especially in the field of advanced process control.

Process & model



Multilayer perceptron (MLP) NN model



Deisohexanizer section of isomerisation process

Pearson correlation coefficient

$$R = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}}$$

Determination coefficient

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}$$

Root mean squared error

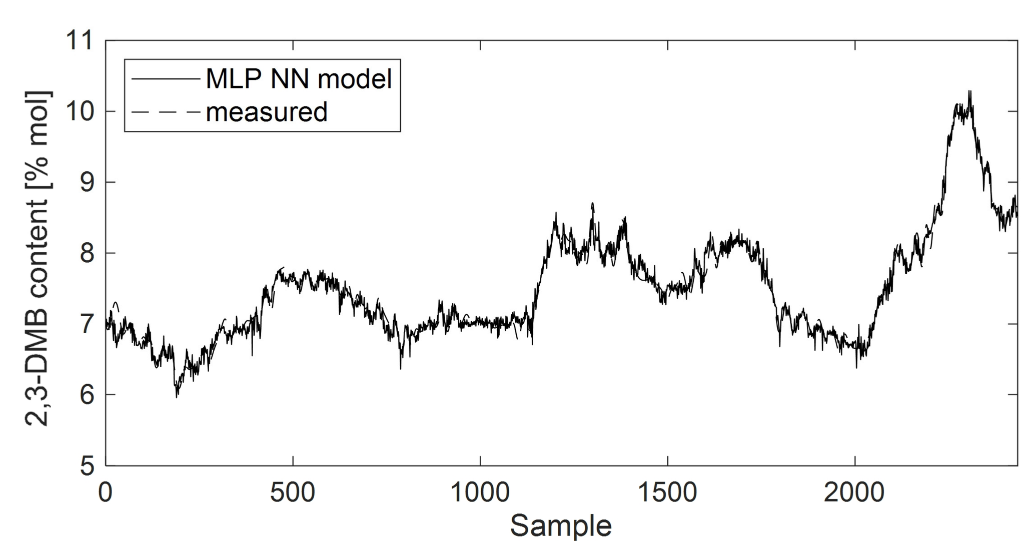
$$RMSE = \sqrt{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2 / n}$$

Mean absolute error

$$MAE = \frac{1}{n} \sum_{i=1}^{n} \left| \hat{y}_i - y_i \right|$$

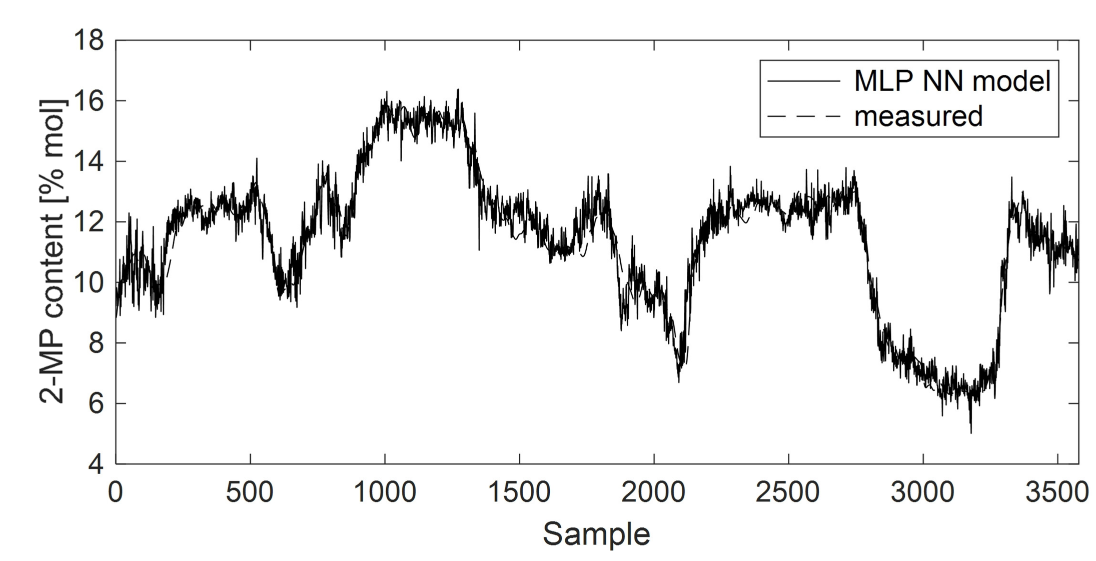
2,3-DMB NN model evaluation results

MLP NN structure	Learning function	Transfer function	Number of neurons	R (test)	R^2 (test)	RMSE [% mol]	MAE [% mol]
7-40-1	Levenberg-Marquardt	Log-sigmoid	40	0.983	0.966	0.147	0.109
7-40-1	Levenberg-Marquardt	Tangent sigmoid	40	0.981	0.963	0.150	0.111
7-15-1	Levenberg-Marquardt	Tangent sigmoid	15	0.972	0.945	0.181	0.138
7-15-1	Levenberg-Marquardt	Log-sigmoid	15	0.970	0.941	0.187	0.141
7-10-1	Levenberg-Marquardt	Tangent sigmoid	10	0.967	0.935	0.194	0.150



2-MP NN model evaluation results

MLP NN structure	Learning function	Transfer function	Number of neurons	R (test)	R^2 (test)	RMSE [% mol]	MAE [% mol]
7-100-1	Levenberg-Marquardt	Log-sigmoid	100	0.981	0.963	0.579	0.415
7-30-1	Levenberg-Marquardt	Log-sigmoid	30	0.972	0.945	0.703	0.518
7-30-1	Levenberg-Marquardt	Tangent sigmoid	30	0.972	0.944	0.697	0.522
7-20-1	Levenberg-Marquardt	Log-sigmoid	20	0.965	0.930	0.781	0.586
7-20-1	Levenberg-Marquardt	Tangent sigmoid	20	0.962	0.925	0.814	0.594



2,3-DMB NN vs. dynamic polynomial models [1]

Model	R (test)	R^2 (test)	RMSE (test) [% mol]	MAE (test) [% mol]
MLP 7-40-1	**0.983**	**0.966**	**0.147**	**0.109**
FIR	0.948	0.878	0.266	0.213
ARX	0.963	0.925	0.209	0.163
OE	0.965	0.928	0.204	0.152
NARX	0.965	0.927	0.206	0.163
HW	0.967	0.934	0.196	0.149

2-MP NN vs. dynamic polynomial models [1]

Model	R (test)	R^2 (test)	RMSE (test) [% mol]	MAE (test) [% mol]
MLP 7-100-1	**0.981**	**0.963**	**0.579**	**0.415**
FIR	0.932	0.866	0.857	0.681
ARX	**0.988**	**0.973**	**0.386**	**0.320**
OE	**0.993**	**0.987**	**0.270**	**0.218**
NARX	**0.987**	**0.973**	**0.386**	**0.326**
HW	**0.993**	**0.986**	**0.277**	**0.204**

[1] S. Herceg, Ž. Ujević Andrijić, N. Bolf, Continuous estimation of the key components content in the isomerization process products, *Chem. Eng. Trans.* 69 (2018) 79.

Conclusion

The MLP neural network models for estimating the content of 2,3-DMB and 2-MP as critical quality components of an isomerization process were developed. The models show good generalization abilities and are able to reliably estimate the content of critical quality attributes. In the case of 2,3-DMB content, MLP NN model show better results in comparison with dynamic polynomial models. However, in the case of 2-MP content, the polynomial models have better results, except of the simple FIR model. In this sense, there is room for further development and testing of dynamic neural networks, and it is possible to assume overall results at the level of dynamic polynomial models or better.