

Can artificial neural networks help the experimentation in catalysis?

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Abstract

This work is focused on the practical application of artificial intelligent techniques in chemical engineering. Specifically, it describes an application of artificial neural networks for modelling the kinetics of a chemical reaction using methods not based in a kinetic model. Thus, neural networks have been used to model the behaviour of one catalyst under different reaction conditions for a specific reaction, i.e. *n*-octane isomerisation. Secondly, trained neural networks were used to model successfully another reaction with a similar reaction network.

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1. Introduction

Two issues of paramount importance in combinatorial catalysis are high-throughput experimental tools and data management. The new development of high throughput experimentation techniques in the frame of heterogeneous catalysis is enabling the screening of large number of new materials and, therefore, is increasing exponentially the number of catalytic data, derived from the parallel synthesis, characterisation and catalytic testing. However, the rapid progress of those experimental tools [1–3] requires the development of more powerful data management techniques adapted to this specific research methodology. Data management is referred here to software techniques for (i) the efficient administration and schedule of large

amounts of experimental data, (ii) the comprehension and modelling of the organised data and (iii) the global search strategy to optimise the catalytic performance.

Traditionally, the processing and understanding of the experimental *outputs* (characterisation and catalytic performances) was accomplished by the researchers, who applied previous experiences or fundamental knowledge in order to carry out the experimental design and to establish relationships between the different experimental results. In the case of combinatorial catalysis, the large number of variables in play and the application of complex optimisation algorithms for the experimental design makes difficult the direct human interpretation of data derived from high throughput experimentation. Recently, data mining techniques have been applied [4–7] in order to find relationships and patterns between the input and output data derived from accelerated experimentation. Hence, artificial intelligence (AI) techniques

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have an important potential for modelling and prediction of complex high-dimensional data. Among these techniques, artificial neural networks (NN) could be useful in the chemical field.

Artificial neural networks have been mainly used in classification problems [8,9], in character recognition [10,11], in negotiation problems, in information processing [12], in control and automation, in prediction problems [13,14]. Artificial neural networks have successfully been applied to conventional catalytic modelling and design of solid catalysts. Those applications [15] include: design of ammoxidation of propylene catalyst [16], design of methane oxidative decoupling catalyst [17], analysis and prediction of results of the composition of NO over zeolites [18]. Also, NN has been used combined with genetic algorithms for the design of propane ammoxidation catalyst [19]. A recent work reports the viability of NN in the analysis and prediction of catalytic results within a population of catalysts produced by combinatorial techniques [20].

The purpose of this paper is the modelling of kinetic results in a chemical reaction using methods not based in a kinetic model. In contrast to the referred applications [15–20], where NN were applied to predict the catalyst performance based on catalyst composition, in the present work NN were trained to predict reaction results based on reactor conditions (Fig. 1). Therefore, NN were applied to model the behaviour of one catalyst under different reaction conditions (partial pressures, contact time and temperature) for a specific reaction. Hydroisomerisation of linear alkanes was used for the study of the NN structure and settings.

A secondary aim of this work is to study the possibility of using the already trained neural networks for modelling different reaction processes (changing the reactant or the catalyst) with a similar reactive

scheme. In this way, neural networks were retrained with a small number of experimental data from a new reaction.

With this methodology, it would be possible to obtain rapidly a *black box* model of a kinetic process, which can be useful for further modelling or scaling up of the catalyst, minimising the number of experimental results required.

2. Experimental

2.1. Artificial neural network fundamentals

Artificial neural networks consist of a number of simple interconnected processing units, also called neurons, which are analogous to the biological neurons.

Two important features of neural networks (NN) are the ability of supplying fast answers to a problem and the capability of generalising their answers, providing acceptable results for unknown samples. In this way, they need to learn about the problem under study and this learning is commonly named *training process*. This process usually starts with random values for the weights of the NN. Then, NN are supplied with a set of samples belonging to the problem domain and they establish mathematical correlation between the samples [21], modifying the values of their weights. In a *retraining process*, initial weights are not random but are obtained by means of a previous training process. In this way, NN retraining with data from similar problems would require a much lesser amount of data in order to achieve a good prediction performance.

One of the most well-known structures of neuronal networks for supervised learning is the multi-layer perceptron, which is generally used for classification

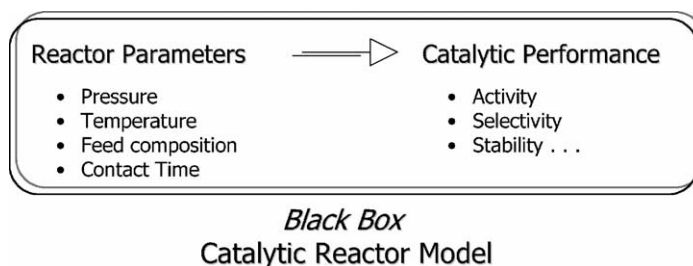


Fig. 1. Scheme of the application of the neural network to catalysis, as a black box model.

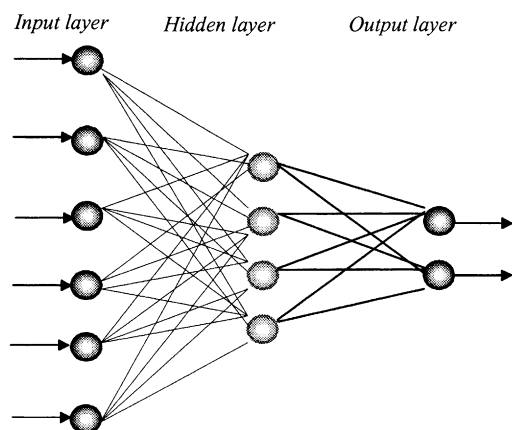


Fig. 2. Scheme of a multi-layer perceptron.

and prediction problems. In the multi-layer perceptron, neurons are grouped into layers. An example of a layered network is shown in Fig. 2. In this network there are d inputs, m hidden units and c output units. The output of the j th hidden unit is obtained by first forming a weighted linear combination of the d input values, giving:

$$a_j = \sum_{i=0}^d w_{ji} x_i \quad (1)$$

Here, w_{ji} denotes a weight going from input i to hidden unit j and x_i denotes the input i of the neuron. Then, using an activation function g , final output of neurons are obtained:

$$z_j = g(a_j) \quad (2)$$

Sigmoidal activation functions are widely applied. In this work, logistic and tangential sigmoidal functions have been employed for the hidden units.

$$g(a_j) = \frac{1}{1 + e^{-a_j}} \quad (\text{logistic sigmoidal function}) \quad (3)$$

$$g(a_j) = \frac{e^{a_j} - e^{-a_j}}{e^{a_j} + e^{-a_j}} \quad (\text{tangential sigmoidal function}) \quad (4)$$

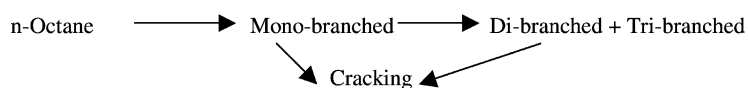
Additional neural network functions used in multi-layer perceptron can be found elsewhere [22].

2.2. Neural networks applied to n -paraffin isomerisation modelling

One of the possible methods for increasing the octane number (ON) in gasoline is the isomerisation of linear paraffin to yield its branched isomers. For example, the isomerisation of n -hexane to its mono-branched isomers produces an increase of 50 points in ON, and 70 for the di-branched isomers. A reaction scheme (Fig. 3) involves the sequential isomerisation of the paraffin into the mono-, di- and tri-branched isomers. Undesired cracking side reactions can occur, producing the break of the carbon chain, decreasing the benefits of the isomerisation process. Isomerisation reaction is catalysed over bi-functional catalysts (acid + hydrogenating metal), like Pt-chlorinated alumina for low temperature and Pt-mordenite [23]. A proposed mechanism (Fig. 4) would involve the dehydrogenation of the sorbed n -paraffin over the metal, rearrangement of the n -olefin over the acid site and final re-hydrogenation of the *iso*-olefin to produce the final *iso*-paraffin. Therefore, a good isomerisation catalyst requires strong acid sites and an adequate balance between metal and acid function [24,25].

It was analysed the application of NN for the prediction of three different catalytic performances: n -paraffin conversion, mono-branched and di-branched yields. Input variables for the prediction were reaction conditions: n -octane partial pressure (P_O), hydrogen partial pressure (P_H), reactor temperature and contact time.

Training data for n -octane isomerisation was obtained from theoretical simulations of a fixed bed reactor model. The necessary kinetic parameters for the

Fig. 3. Reaction scheme for the isomerization of n -alkanes.

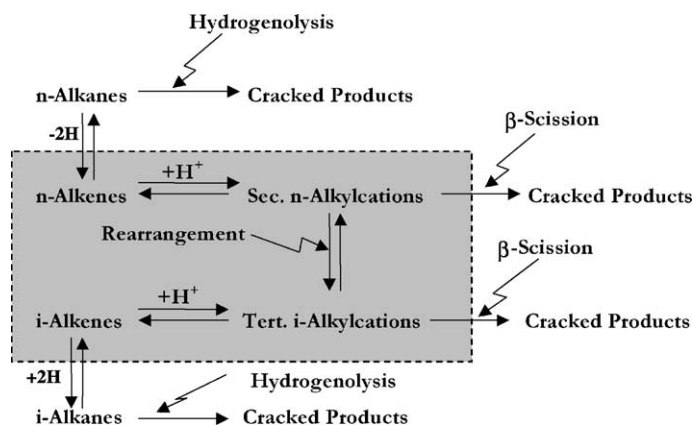


Fig. 4. Mechanism for *n*-alkane hydroisomerisation.

Langmuir–Hinshelwood model were previously obtained [26] by experimentation with a fixed bed microreactor, using a Pt- β -based catalyst and different C_8 isomers as feedstream. For the training process, a set of 34,000 simulated samples was available, with input value ranges as follows: P_O between 0.5 and 2 bar; P_H between 6 and 18 bar; temperature between 503 and 543 K; and contact time between 0.16 and 8 h.

(Fig. 5). Retraining data for *n*-hexane was obtained as well by simulation using the same kinetic model determined for *n*-hexane isomerisation.

2.3. Training process

In order to obtain a good NN prediction performance for a determined problem, the following points

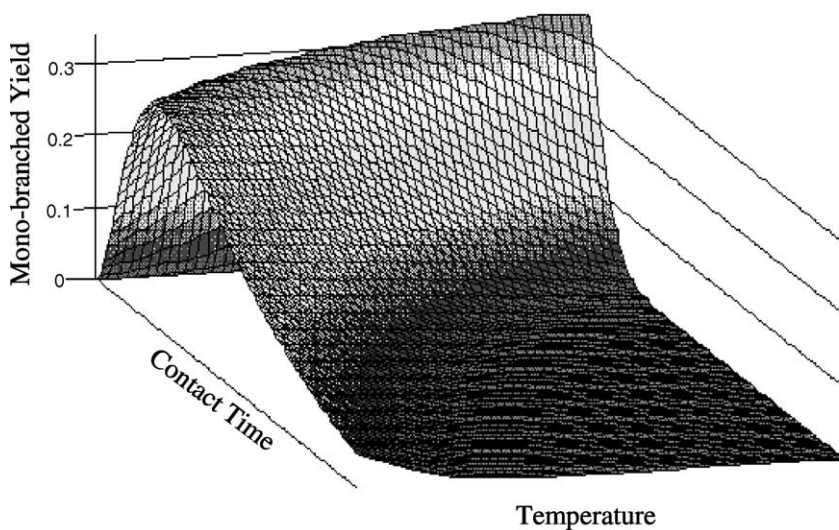


Fig. 5. Simulated data available. Variation of mono-branched isomers yield vs. contact time and temperature, for fixed values of $P_O = 0.5$ and $P_H = 18.18$ bar.

Table 1
Neural network topologies and training sets of samples employed for the optimisation of the neural network model

Input layer	1st layer	2nd layer	Output layer	Activation functions	Training set
4	6	0	3	Logistic	10
	8	3		Tangential	20
	10	5			30
	20	6			50
	40	10			80
	100				100
					170
					850
					1700
					4250
					17000

have to be optimised: (i) network topology including number of hidden layers and number of neurones in each layer, (ii) training algorithm (usually, Backpropagation, Backpropagation with Momentum) and training parameters, and (iii) number of training data. Table 1 summarises the NN topologies and the different training sets employed for the NN optimisation.

A first study of both the topology and the number of training data was carried out employing the Backpropagation algorithm with learning parameter 0.5. Therefore, using supervised learning, an incremental method was applied for the test of different neural network topologies based on the multi-layer perceptron. The topology was modified increasing the number of neurons and the number of hidden layers, starting with one hidden layer with few neurons. Moreover, logistic (3) and tangential (4) sigmoidal activation functions were independently used in neurons of hidden layers. Each NN was trained each time with a different number of samples, from 10 to 17,000. In particular, the whole set of 34,000 samples was divided into 11 training sets of 10, 20, 30, 50, 85, 100, 170, 850, 1700, 4250 and 17,000 samples, respectively. Another set of 300 samples was used for testing the predictions of the neural networks. A fixed number of cycles (1000 cycles) was established as a stopping method. In Table 1, neural network topology and number of samples used for each training process is displayed.

Secondly, an analysis of different training algorithms was carried out with two of the most suitable neural networks obtained from the previous study.

Those neural networks were trained with Backpropagation and Backpropagation with Momentum algorithms, using different learning (μ) and momentum (α) parameters.

All calculations were made on a 500 MHz Pentium processor, using the SNNS neural networks simulator, developed by the Institute for Parallel and Distributed High Performance Systems, at University of Stuttgart [27].

2.4. Retraining process

The prior two studies allowed determining an appropriate neural network for the problem under study. This *n*-octane NN model was lately retrained with a small number of samples of *n*-hexane reaction, which has a similar kinetic scheme. Three NN trained models obtained in the previous studies (using 85, 850 and 17,000 training *n*-octane samples) were retrained with an incremental number of samples of *n*-hexane (10, 20, 30, 50 and 85 samples), employing Backpropagation algorithm. This data has allowed the study of the influence of the number of retraining samples and the influence of the number of training samples of the initial model (*n*-octane model) on the adjustment of the neural weights.

3. Results and discussions

3.1. Results on *n*-octane modelling

Figs. 6 and 7 show the evolution of the absolute error and mean square error² for different neural network topologies (Table 1), trained with an incremental number of samples and Backpropagation algorithm. The most suitable neural network topology turned out to be a multi-layer perceptron (Fig. 8) with four nodes in the input layer (reaction conditions), eight nodes in the first hidden layer (with tangential active functions), six nodes in the second hidden layer (also with tangential active functions) and three nodes in the output layer (reaction results).

A study of the influence of the number of training samples on the error predictions (conversion output)

² Absolute error = $\sum |\text{real-predicted}|/n$; mean square error = $\sum (\text{real-predicted})^2/n$, where *n* is the number of samples.

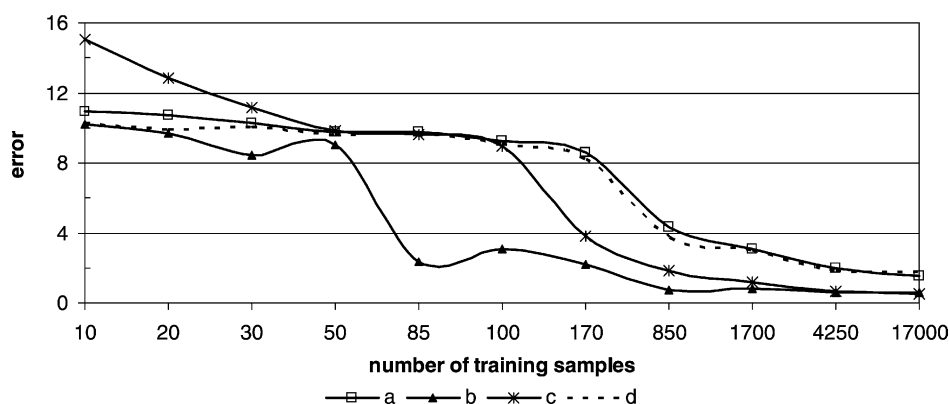


Fig. 6. Mean absolute error (conversion output) for different neural network topologies (test of 300 simulated samples of *n*-octane): (a) four input nodes, ten nodes in 1st hidden layer, three output nodes; (b) four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer, three output nodes (tangential sigmodial function in hidden nodes); (c) four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer, three output nodes (logistic sigmodial function in hidden nodes); (d) four input nodes, eight nodes in 1st hidden layer, three output nodes.

of different topologies can also be observed in Figs. 6 and 7. When increasing the number of samples, the neural network is capable to learn more about the problem under study, decreasing the error predictions. The selected neural network (Fig. 8) can make good quality predictions from 85 training samples. Figs. 9–11 show predicted and real data for the three NN outputs (conversion, mono-branched and di-branched yields) using the selected neural network trained with 850 samples and 300 test samples. The trained NN can pre-

dict properly all the three catalytic performances with small error and thus it can be used as a good kinetic *black box* model.

Training algorithm study results are reported in Figs. 12 and 13. The selected neural network topology (Fig. 8) was trained with logistic (Fig. 12) and tangential (Fig. 13) activation functions, using different training algorithms and, subsequently, was tested with 300 samples. Test results expressed as mean square errors (conversion output) did not show

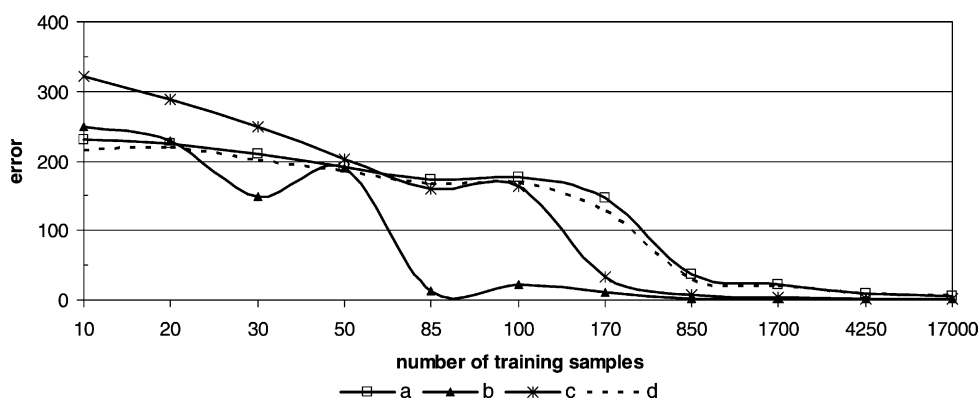


Fig. 7. Mean square error (conversion output) for different neural network topologies (test of 300 simulated samples of *n*-octane): (a) four input nodes, ten nodes in 1st hidden layer, three output nodes; (b) four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer, three output nodes (tangential sigmodial function in hidden nodes); (c) four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer, three output nodes (logistic sigmodial function in hidden nodes); (d) four input nodes, eight nodes in 1st hidden layer, three output nodes.

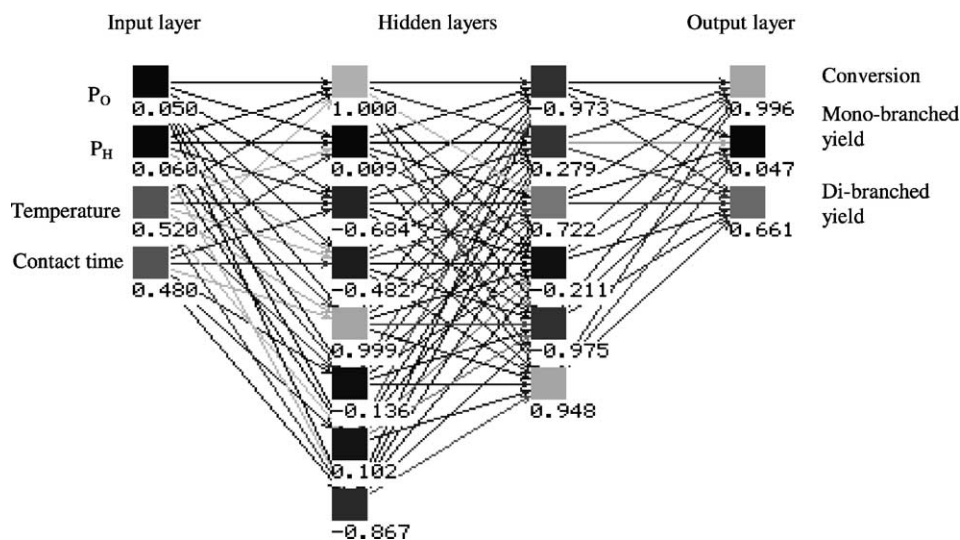


Fig. 8. Neural network selected, with four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer and three output nodes, using activation function in hidden nodes.

any relevant difference between the training algorithms for the problem under study. Furthermore, the number of training samples required for a good prediction degree is reduced by using tangential activation function (Fig. 13) compared with logistic function.

3.2. Results on retraining process

A set of 85 samples for the *n*-hexane was available. It was used to retrain the neural networks modelled

for the *n*-octane, using 10, 20, 30, 50 and 85 samples of this set each time. On the other hand, another set of 300 samples of *n*-hexane was also available for the testing process. Reaction conditions of all samples were inside the same interval as the *n*-octane reaction (see Section 2.2). However, *n*-hexane reaction results present a different distribution from *n*-octane. The distribution of test samples (300 samples) for both reactions is shown in Table 2.

Initially, the neural network selected topology in the previous section (Fig. 8), trained with 85 samples

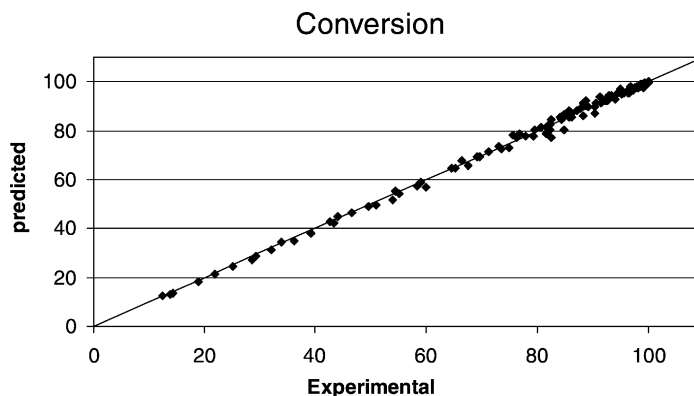


Fig. 9. Conversion predictions obtained with a NN with four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer and three output nodes, using activation function in hidden nodes. Trained with 850 samples of *n*-octane. Test of 300 simulated samples of same reaction.

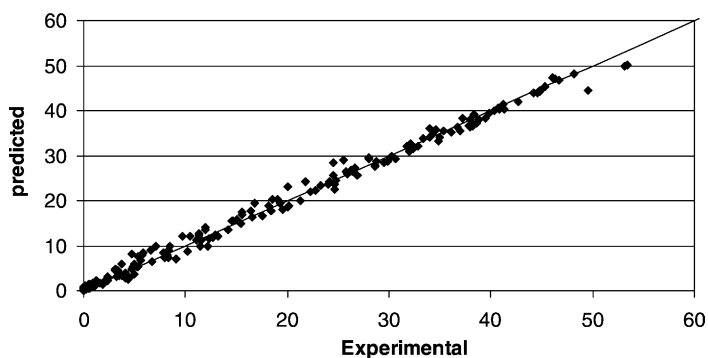


Fig. 10. Mono-branched yield predictions obtained with a NN with four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer and three output nodes, using activation function in hidden nodes. Trained with 850 samples of *n*-octane. Test of 300 simulated samples of same reaction.

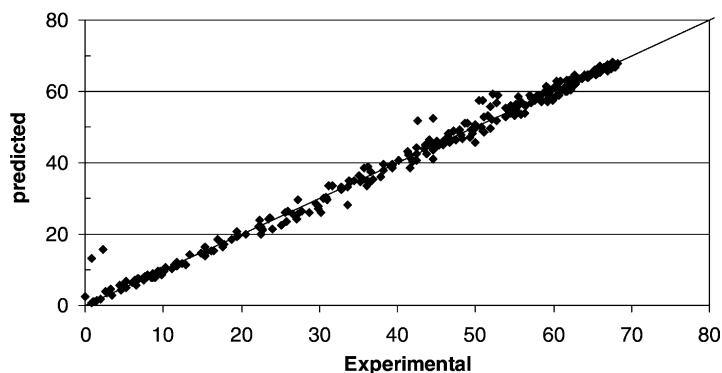


Fig. 11. Di-branched yield predictions obtained with a NN with four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer and three output nodes, using activation function in hidden nodes. Trained with 850 samples of *n*-octane. Test of 300 simulated samples of same reaction.

Table 2

Distribution of test samples (300 samples) for *n*-octane and -hexane reactions

Reaction	Maximum	Minimum	Mean	S.D.
Conversion				
<i>n</i> -Octane	100.00	12.49	91.48	17.91
<i>n</i> -Hexane	100.00	5.41	83.14	23.56
Mono-branched yield				
<i>n</i> -Octane	53.37	0.00	11.42	14.01
<i>n</i> -Hexane	68.37	0.00	20.69	17.94
Di-branched yield				
<i>n</i> -Octane	68.18	0.00	41.77	20.71
<i>n</i> -Hexane	83.86	0.12	53.82	25.96

of *n*-octane, was retrained each time with an incremental number of samples of the *n*-hexane reaction, obtaining new neural network models. Original knowledge about *n*-octane reaction of the trained neural networks is modified with the retraining process, including knowledge about the kinetic process of the *n*-hexane reaction.

Secondly, the neural network trained with 850 samples of *n*-octane was retrained with the samples of *n*-hexane, improving prediction results. This retraining process was again repeated with the neural network trained with 17,000 samples of *n*-octane. In this case, prediction results were not as good as those obtained with the model of 850 samples of *n*-octane. This behaviour might be due to the fact that the neural network

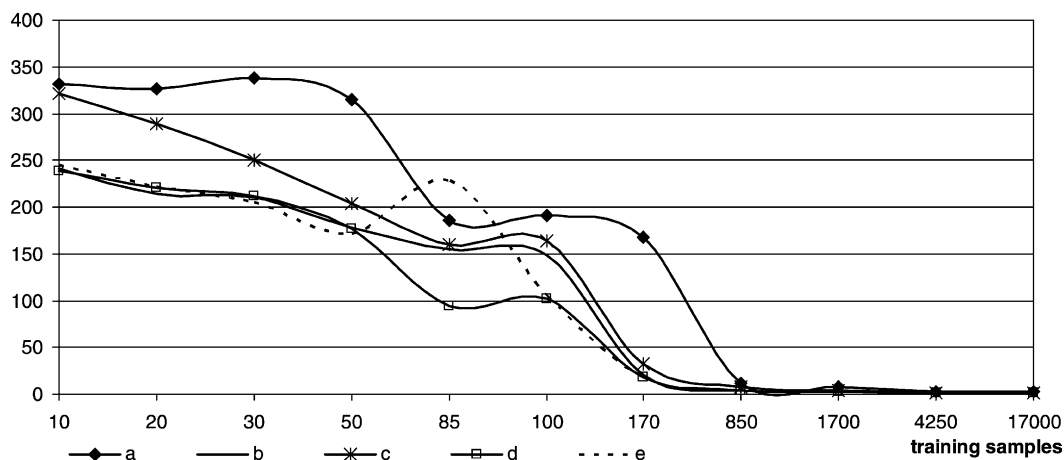


Fig. 12. Mean square error evolution (conversion output). Neural network topology: four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer, three output nodes, logistic sigmoidal active functions in hidden nodes. Training algorithms: (a) Backpropagation ($\mu = 0.2$), (b) Backpropagation ($\mu = 0.8$), (c) Backpropagation ($\mu = 0.5$), (d) Backpropagation with Momentum ($\mu = 0.2$, $\alpha = 0.8$), (e) Backpropagation with Momentum ($\mu = 0.5$, $\alpha = 0.5$).

trained with 17,000 of *n*-octane is over-trained. Hence, it is more difficult to include new knowledge about other reactions by means of the retraining process.

Finally, 85 training samples of the *n*-hexane reaction were used to model neural networks from “scratch” (i.e. training neural networks with no previous knowl-

edge) employing the same neural network topology and training algorithms.

The described retraining study of the NN pre-trained with 850 *n*-octane samples is summarised in Table 3. Retraining results are estimated using the percentage of test samples with prediction absolute error lower than an epsilon value (indicated on the table).

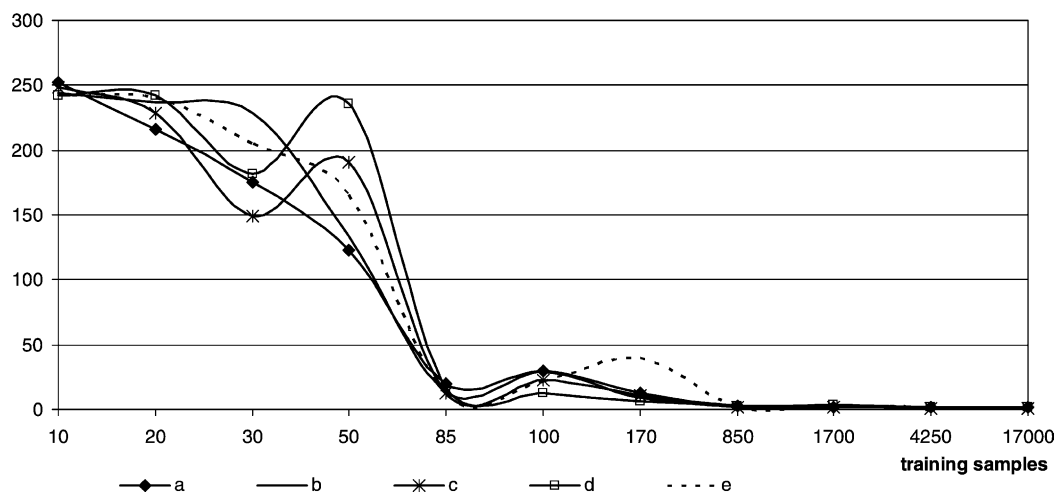


Fig. 13. Mean square error evolution (conversion output). Neural network topology: four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer, three output nodes, tangential sigmoidal active functions in hidden nodes. Training algorithms: (a) Backpropagation ($\mu = 0.2$), (b) Backpropagation ($\mu = 0.8$), (c) Backpropagation ($\mu = 0.5$), (d) Backpropagation with Momentum ($\mu = 0.2$, $\alpha = 0.8$), (e) Backpropagation with Momentum ($\mu = 0.5$, $\alpha = 0.5$).

Table 3

Percentage of test samples with absolute error predictions lower than indicated value, with a neural network of four input nodes, eight nodes in 1st hidden layer, six nodes in 2nd hidden layer and three output nodes, using activation function in hidden nodes

<i>n</i> -Hexane	Conversion (% samples < ε)			Mono-branched yield (% samples < ε)			Di-branched yield (% samples < ε)		
	$\varepsilon = 2$ (%)	$\varepsilon = 3$ (%)	$\varepsilon = 5$ (%)	$\varepsilon = 4$ (%)	$\varepsilon = 5$ (%)	$\varepsilon = 8$ (%)	$\varepsilon = 4$ (%)	$\varepsilon = 5$ (%)	$\varepsilon = 8$ (%)
Without retraining ^a	40	45	50	35	40	55	10	15	25
Retrained with 10 samples ^b	50	60	65	40	50	60	50	55	70
Retrained with 20 samples ^c	60	65	75	60	65	70	60	65	75
Retrained with 30 samples ^d	55	60	70	50	55	70	55	55	65
Retrained with 50 samples ^e	80	90	95	55	60	70	90	95	100
Retrained with 85 samples ^f	85	95	95	75	80	90	90	95	100
Trained with 85 <i>n</i> -hexane samples ^g	20	30	50	30	35	60	25	30	45

^a Trained with 850 *n*-octane samples.

^b Trained with 850 *n*-octane samples and retrained with 10 samples of *n*-hexane reaction.

^c Retrained with 20 *n*-hexane samples.

^d Retrained with 30 *n*-hexane samples.

^e Retrained with 50 *n*-hexane samples.

^f Retrained with 85 *n*-hexane samples.

^g Trained with 85 *n*-hexane samples without prior training with *n*-octane samples.

The selected neural network without retraining process has only knowledge about *n*-octane reaction and would provide poor-quality predictions for a different problem step (other reaction or other catalyst) (see Table 3). However, if this neural network is retrained with a small number of samples of *n*-hexane (30–50 samples), about 80% of test samples are predicted with an absolute error lower than 4 (Table 3). Since for *n*-hexane standard deviation of test samples is about 20 (see Table 2), prediction results can be qualified of good quality. On the other hand, if this neural network topology is initially trained with 85 samples of the *n*-hexane reaction, predictions are worse than those obtained with the retraining process (Table 3).

4. Conclusions

The application of artificial neural networks to modelling and prediction in the field of experimental catalysis is a new powerful tool that could accelerate the development and optimisation of new catalysts. An important characteristic of these models is that they do not require any theoretical knowledge or human experience during their training process.

In this work, the viability of the artificial neural networks for modelling catalytic reactions has been proved. Specifically, the *n*-octane isomerisation process was modelled with different neural networks, obtaining good-quality results. Fundamental knowledge has only been used in the determination of the data structure (parameters, input and output data). However, once those parameters are established, neural networks can be trained and used without further prior knowledge.

Another interesting study of the NN kinetic models is their application to different reactions that present similarities with regard to the reaction used in the training process of the NN. In particular, in this work NN trained with *n*-octane samples were retrained with *n*-hexane samples. In this retraining process a small number of samples is needed to obtain good-quality predictions. Moreover, if those samples are used to train neural networks with no previous knowledge, predictions are much worse than those obtained with the retraining process.

An interesting new methodology for experimentation in catalysis has been shown in this work: the use of a pre-trained NN (so-called *kinetic template*) for the modelling of experimental data from reactions with the same reaction scheme (changing reactant or catalyst).

A future perspective of this method is the possibility of having a library of pre-trained NNs for several reaction schemes and make use of them to build the NN-black box model of new experimental data.

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