Neural Network Modelling of the Equilibrium Anionic Polymerization of Cyclic Siloxanes

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The kinetics of the equilibrium anionic polymerization of some cyclic siloxanes is modelled by using neural networks. Feedforward neural networks with one or two hidden layers have been used to appreciate the rates of disappearance of octamethylcyclotetrasiloxane and aminopropyl disiloxane at different catalyst concentrations (direct modelling). Alternatively, another neural model has been developed to estimate the amount of catalyst, which leads to an imposed final concentration of siloxane (inverse modelling). Experimental data for the polymerization of octamethylcyclotetrasiloxane in the presence of KOH as a catalyst and 1,3-bis(aminopropyl)tetramethyldisiloxane as a functional endblocker were used as training data sets for neural models. Satisfactory agreement between experimental data and network predictions obtained in validation phases proved that the projected models have good generalization capacities and, consequently, they describe well the process.

Keywords: neural networks, direct and inverse neural modelling, polysiloxane, cyclic siloxanes, anionic ring opening polymerization

The recent years proved that neural networks have become a powerful tool in chemical processes area, especially for modelling and prediction of nonlinear systems [1].

Usually, experimental and industrial practices use two types of models: mechanistic models (classical/ phenomenological models) based on the physical and chemical features and data-based empirical models. Each of these categories presents advantages and disadvantages, and, in this order, a comparison of them is necessary. The mechanistic models present the advantage to be valid upon a large area of operating conditions and reflect the process phenomenology. For this reason, whenever it is possible, the main recommendation should be to use the physic and chemical knowledge for the process. The disadvantages of these models, could be the difficulties concerning the specificity of the process and the problems in designing a system mathematical model. The difficulties regarding the chemical process refer to many aspects as follows: the absence of on-line testing (measurements), the considerable delays at testing, the possibility of many answers determined by the different operating conditions. Concerning the design of the mathematical model, several aspects can be mentioned: the complexity of reactions' mechanisms or the fact that the phenomenology of the processes are insufficiently known, the great number of chemical species into the system, the great number of model equations and the special methods in giving the solutions.

An overlooking from the studies on neural network for modelling or control allows the observation of some advantages: parallel organization permits solutions to problems where multiple constraints must be satisfied simultaneously; graceful degradation and the rules are implicit than explicit [2].

On the other hand, the disadvantages seem to be upon the necessity to obtain a perfect neural network with the experimental or operational history data. Also neural network needs large amount of good quality data for its training, which is normally difficult to obtain in practice. Data sparsity, 'overfitting' and poor generalization are other problems faced by researchers when using the basic neural network alone [3]. A special attention should be to paid to an uniform distribution of data throughout the design space [4]. In the idea of identification data which cover the whole range of the process variable, any applications prove that if properly trained and validated, these neural network models can be used to accurately predict the process behaviour, hence, leading to process optimization and control performance improvement [5].

Roy et al [6] have shown that multilayer perceptron with at most two hidden layers can solve any non-linear problem provided there are sufficient numbers of hidden nodes.

An important and widely studied class of semi-organic polymers is constituted by polyorganosiloxanes.

Polyorganosiloxanes possess a variety of interesting and desirable properties such as low glass transition temperatures, high lubricity, UV stability, good thermal stability, low toxicity and unique surface properties.

Two general methods are well known and widely used for linear polysiloxane synthesis: polycondensation of bifunctional siloxanes and ring-opening polymerization (ROP) of cyclic oligosiloxanes [7]. ROP is the most traditionally and significant route to obtain high molar mass linear polysiloxanes, cyclic tetramer and trimer being usually the starting monomers. This polymerization may be carried out either anionically or cationically [7, 8]. In principle, any compound that can split the siloxane bond by ionic (either electrophilic or nucleophilic) mechanism can initiate polymerization of cyclosiloxanes with involvement of the positive or negative reaction centers of the growing chains. There are a wide variety of compounds that can initiate the ROP polymerization of cyclosiloxanes including strong organic and inorganic acids or bases and metal oxides [9, 10].

It is well known that, in the presence of the strong acids or bases, the Si-O bonds in both unstrained cyclosiloxanes and linear macromolecules (which have comparable

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energy) can be split, and a mixture of cyclic and linear polysiloxanes will be obtained. The siloxane bonds are continuously broken and reformed until the reaction reaches a thermodynamic equilibrium. In the presence of a functionalized disiloxane, oligomers having such ending functional groups resulted, the molecular mass being controlled by the ratio between cyclosiloxane and disiloxane.

The anionic polymerization of cyclosiloxanes and other cyclic compounds that contain the siloxane bond is accomplished in most cases either in bulk or in solution, and rarely in emulsion, in suspension, in the solid phase, and under zone melting conditions.

The most active catalysts for the polymerization of cyclosiloxanes are hydroxides, alcoholates, phenolates, silanolates, siloxanolates of the alkali metals, quaternaty ammonium and phosphonium bases and their siloxanolates, organolithium, sodium and potassium compounds. Besides these, other catalysts used for the anionic polymerization of cyclosiloxanes are the alkali metal or lead salts of carboxylic acids or the metal derivatives of carboxylic acid esters.

The polymerization of cyclosiloxanes under the influence of the alkali metal hydroxides has been studied in greatest detail.

There are many kinetic studies on the polymerization of octamethylcyclotetra- or octamethylcyclotri- siloxane (D_4 and D_3, respectively) in the presence of strong acid or base catalysts carried out in order to evaluate the effect of different parameters (monomer concentration, temperature, catalyst concentration, presence or absence of a endblocker) on the equilibrium position.

Such experimental data were used in this paper for modelling of anionic polymerization of cyclosiloxane. The literature data on the polymerization of D_4 in the presence of KOH as a catalyst and 1,3-bis(aminopropyl)tetramethyl-disiloxane as a functional endblocker [11] were chosen.

The present paper refers to the use of neural networks as efficient and simple tools for process modelling, recommended especially when the reaction mechanism is incompletely known. This type of modelling methodology is applied for the first time in the siloxane polymer field.

Experimental part

The general outline for the preparation of functional oligomers is shown in scheme 1.

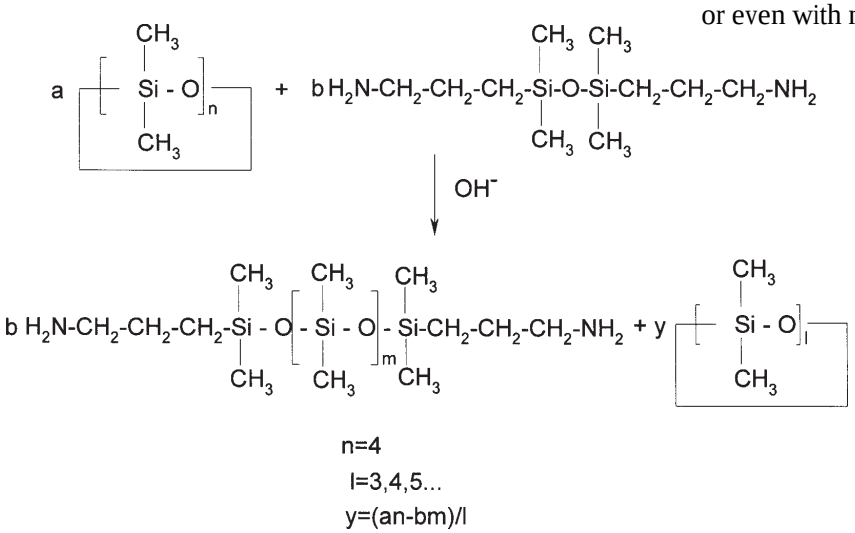
This paper refers the synthesis of equilibration reaction kinetics of D_4 in the presence of functional end-blockers [11]. The considered experimental data are presented in Table 1. Conditions in which these data were obtained are: bulk polymerization of octamethylcyclotetrasiloxane (D_4) (without a solvent), in presence of potassium silanolate (hydroxide) as a catalyst, and 1,3-bis(aminopropyl)tetra-methyldisiloxane (DSX) as an end-blocker, by stirring under argon, at pre-established temperature. In presence of the cyclosiloxane, KOH forms potassium siloxanolate, which is the proper catalyst. Samples were removed (withdrawn) at various times and analyzed by high-performance liquid chromatography for the D_4 content and by capillary gas chromatography for the disiloxane concentration. In Table 1, the experimental data show the effect of catalyst concentration on the disappearance of D_4 at 160°C and, also, the decrease of the aminopropyl disiloxane concentration. As can be seen, the rate of disappearance of D_4 increased with increasing KOH concentration. In the reaction containing 0.126 mole % KOH, equilibrium concentration of D_4 is attained faster than at lower catalyst levels. The reaction rate of DSX in the presence of potassium siloxanolate (KOH) is significantly slower as compared with D_4 reaction rate.

Neural network modeling

Generally speaking, a neural network consists of processing neurons and information flow channels between the neurons, usually called „interconnections". Each processing neuron calculates the weighted sum of all interconnected signals from the previous layer plus a bias term and then generates an output through its activation transfer function.

A general problem of a neural network modelling represents the transformation of a set of inputs into a set of outputs. The neural network model is obtained by trying, with input/output pairs, which have to be related by the transformation which is being modeled. The adjustment of the neural network function to experimental data (learning process or training) is based on a non-linear regression procedure. Trying is done by assigning random weights to each neuron, evaluating the output of the network and calculating the error between the output of the network and the known results by means of an error or objective function. If the error becomes too large, the weights are adjusted and the process goes back to evaluate the output of the network. This cycle is repeated till the error become low or the stop criterion is satisfied [12].

The main advantage of a neural network is the capacity in *generalization* from the examples to other inputs that were not seen yet. As a rule, the model is sought from an available set of data that clearly contain a number of very interesting relationships, feature correlations and other information, which cannot be deduced in a straightforward manner from the first principles, by theoretical calculations or even with numerical methods.



Scheme 1. Preparation of functional siloxane oligomers

Table 1

EXPERIMENTAL DATA FOR THE DISAPPEARANCE OF D_4 AND DSX AT DIFFERENT CONCENTRATIONS OF CATALYST

KOH concentration [Mole %]	Time, [minutes]	$[D_4]/[D_4]_0$	$[DSX]/[DSX]_0$
0.012	0.0	1.00	
0.012	5.0	0.96	
0.012	9.0	0.93	
0.012	15.0	0.91	
0.012	30.0	0.85	
0.012	44.0	0.82	
0.012	61.0	0.79	
0.012	77.0	0.76	
0.012	99.0	0.72	
0.012	120.0	0.68	
0.012	142.0	0.64	
0.012	154.0	0.62	
0.012	165.0	0.60	
0.012	180.0	0.57	
0.062	1.0	0.95	
0.062	5.0	0.72	
0.062	10.0	0.45	
0.062	22.0	0.29	
0.062	31.0	0.28	
0.062	41.0	0.28	
0.062	51.0	0.27	
0.062	61.0	0.26	
0.062	71.0	0.26	
0.062	81.0	0.25	
0.062	91.0	0.25	
0.062	101.0	0.24	
0.062	111.0	0.24	
0.062	121.0	0.23	
0.126	0.0	1.00	1.00
0.126	2.0	0.82	0.94
0.126	4.0	0.59	0.92
0.126	7.0	0.28	0.89
0.126	10.0	0.13	0.87
0.126	15.0	0.10	0.85
0.126	20.0	0.09	0.82
0.126	30.0	0.09	0.78
KOH concentration [Mole %]	**Time, [minutes]**	**$[D_4]/[D_4]_0$**	**$[DSX]/[DSX]_0$**
0.126	40.0	0.09	0.75
0.126	50.0	0.09	0.72
0.126	60.0	0.09	0.71
0.126	70.0	0.09	0.70
0.126	100.0	0.09	0.68
0.126	110.0	0.09	0.67
0.126	120.0	0.08	0.67
0.126	130.0	0.09	0.66
0.126	140.0	0.08	0.65
0.126	155.0	0.08	0.64

The architecture of a neural network has to be determined by the connections between the outputs of neurons with each others. In a standard architecture, the network's neurons are laid in layers. There are possible single and multiple architectures. A multi-layer neural network has input, hidden and output layers consisting of input, hidden and output neurons, respectively. The most common neural network architecture is the multi-layer feed-forward neural network (often called multi-layer perceptron, MLP).

Speaking on the use of neural networks, many papers apply a multilayered, feed-forward, fully connected network of perceptions because the simplicity of its theory, ease of programming and good results obtained. That due to its universal function considering that the network's

topology has allowed to vary freely and it can take the shape of any broken curve [4].

The main steps in neural network modeling are: collecting the experimental data sets, splitting the data in two parts by training and validation process (comparing the network prediction to unseen data), developing the neural network topology (training phase) and checking the generalization capacity of the neural model (validation phase).

Experimental data from table 1 were used to train different neural networks, which model the D_4 concentration as a function of reaction conditions (time and catalyst concentration). 10 % of these data represent validation data set and the remaining data is the training data set.

In this work, the number of hidden layers and units was established by trial and error method over a different range of networks and selecting the one that best balanced generalization performance against network size. The two inputs of neural networks are: concentration of KOH (% mole) and time (minutes) and the network output is represented by the rate for disappearance of D_4, expressed by the ratio of $[D_4]/[D_4]_0$, where $[D_4]$ is the concentration of D_4 at current time and $[D_4]_0$ is the initial concentration of D_4.

The best network topology was determined based upon the mean squared errors (MSE) on the training data. The network was trained using the backpropagation algorithm. The training process is terminated at the point where the network error (MSE) becomes sufficiently low.

The mean squared error was computed using the following formula:

$$MSE = \left(\sum_{j=1}^{P} \sum_{i=1}^{N} (d_{ij} - y_{ij})^2 \right) / (N \cdot P) \qquad (1)$$

where: P is the number of output processing elements (in this case, $P = 1$), N is the number of exemplars in the data set, y_{ij} is the network output for exemplar i at processing element j, and d_{ij} is the desired output for exemplar i at processing element j.

Table 2 presents several neural networks trained with experimental data from table 1. In table 2, **r** represents the correlation between neural network predictions and experimental data and $\mathbf{E_p}$ is the percent error. For instance, MLP(2:3:1) refers to a network with two inputs, one hidden layers with three neurons and one output.

Table 2

DIFFERENT TOPOLOGIES OF NEURAL NETWORKS IN DIRECT MODELING

	Neural network topology	MSE	r	E_p
1	MLP(2:3:1)	0.000763	0.9988	3.7591
2	MLP(2:5:1)	0.000586	0.9991	3.4120
3	MLP(2:7:1)	0.000557	0.9991	3.5796
4	MLP(2:10:1)	0.000475	0.9992	3.0490
5	MLP(2:15:1)	0.000406	0.9993	3.4457

A topology with a single hidden layer with 10 neurons was obtained, having a good performance in the training phase: MSE = 0.000475, r = 0.999 and E_p = 3.05 % (table 2). Figure 1 presents the topology of MLP(2:10:1), chosen for the process modelling.

The model MLP(2:5:1) can also be a good choice for our purpose because it represents a combination between simplicity and good performance in the training phase (MSE = 0.000586, r = 0.999 and E_p = 3.41 %, in table 2). The real test for the two neural networks will be the validation phase, described in the next section of the paper.

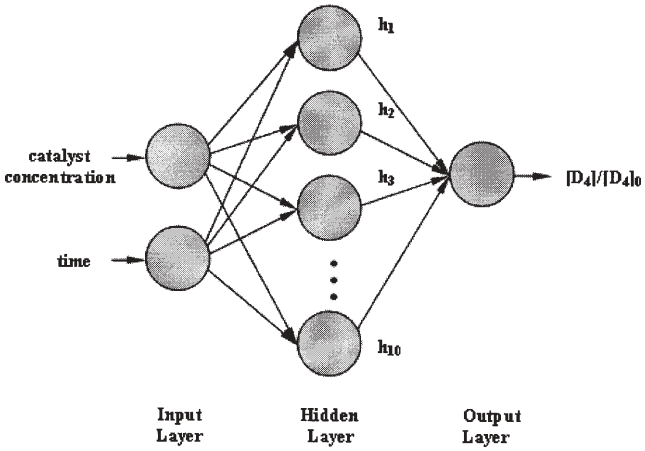


Fig. 1. Representation of MLP(2:10:1).

In order to compare the rate of disappearance of D_4 with that of DSX, another neural model was developed, having time as input and two outputs – the concentrations of D_4 and DSX reported to initial concentrations, $[D_4]/[D_4]_0$ and $[DSX]/[DSX]_0$. A MLP(1:10:2) was chosen from a set of trained network, with MSE = 0.000654, r = 0.998 and E_p = 2.485 %.

Another type of application of neural networks consists of the operating condition definition, starting from the end properties of the polymer. This way we can also solve an inverse problem such as: what is the catalyst concentration which leads to an imposed value of $[D_4]/[D_4]_0$, working in a pre-established time interval? The inverse neural model has two inputs: $[D_4]/[D_4]_0$ and time and one output – the catalyst concentration. Several tests in inverse neural network modeling (table 3) led to an optimal topology MLP (2:9:3:1) with MSE = 0.009131, r = 0.9909 and E_p = 3.75 % for the training phase.

In this paper, a special software application - NeuroSolutions - was used in order to project and obtain predictions of neural networks.

Results and Discussion

The neural networks' predictions were compared with experimental data in order to verify how the direct neural model learned the behaviour of the process.

The values of r being over 0.99, the MSE less than 0.0004 and E_p less than 3.4 % (table 2) prove the possibility of making a good choice. In this sense, there were chosen two network types: MLP(2:5:1) and MLP(2:10:1).

Table 3

DIFFERENT TOPOLOGIES OF NEURAL NETWORKS IN INVERSE MODELING

	Neural network topology	MSE	r	E_p
1	MLP(2:5:1)	0.012691	0.9883	14.8295
2	MLP(2:10:1)	0.013971	0.9875	17.0803
3	MLP(2:9:3:1)	0.009131	0.9909	3.7538
4	MLP(2:12:3:1)	0.009322	0.9907	4.3275

Good predictions are obtained with the two neural models at the comparison between experimental training data and network results: average relative errors of 3.1530 % and r = 0.9995 for MLP(2:5:1) and E_p = 2.6904 % and r = 0.9996 for MLP(2:10:1) (table 4). This fact is also emphasized in figure 2, which present the MLP(2:5:1) predictions of the three catalyst concentrations chosen. Relative errors were calculated using the following formula:

Table 4

PREDICTIONS OF MLP(2:5:1) AND MLP(2:10:1) COMPARED WITH EXPERIMENTAL TRAINING DATA IN DIRECT MODELING

			MLP(2:5:1)			MLP(2:10:1)		
Catalyst conc. [mole %]	**time [min]**	**Experim. $[D_4]/[D_4]_0$**	**Network $[D_4]/[D_4]_0$**	**E_r**	**r**	**Network $[D_4]/[D_4]_0$**	**E_r**	**r**
0.012	0.0	1.00	1.03	3.1185	**0.9995**	1.02	2.0018	**0.9996**
0.012	9.0	0.93	0.94	0.1343		0.93	0.4763	
0.012	15.0	0.91	0.90	1.4771		0.90	1.4771	
0.012	30.0	0.85	0.85	0.4215		0.85	0.4215	
0.012	61.0	0.79	0.79	0.3714		0.79	0.3714	
0.012	77.0	0.76	0.76	0.3410		0.76	0.3410	
0.012	99.0	0.72	0.72	0.4164		0.72	0.4164	
0.012	120.0	0.68	0.68	0.5158		0.68	0.5158	
0.012	142.0	0.64	0.64	0.6140		0.65	0.9388	
0.012	154.0	0.62	0.62	0.4303		0.62	0.4303	
0.012	165.0	0.60	0.60	0.7365		0.60	0.7365	
0.012	180.0	0.57	0.57	0.7094		0.57	0.7094	
0.062	1.0	0.95	0.95	0.2610		0.95	0.2610	
0.062	5.0	0.72	0.71	1.0934		0.71	1.0934	
0.062	10.0	0.45	0.45	0.7722		0.45	0.7722	
0.062	22.0	0.29	0.29	0.0631		0.29	0.0631	
0.062	31.0	0.28	0.27	3.7220		0.27	3.7220	
0.062	41.0	0.28	0.27	2.5682		0.27	2.5682	
0.062	51.0	0.27	0.27	0.2475		0.27	0.2475	
0.062	61.0	0.26	0.27	2.2820		0.27	2.2820	
0.062	71.0	0.26	0.26	0.2310		0.26	0.2310	
0.062	81.0	0.25	0.26	2.2213		0.25	1.7102	
0.062	91.0	0.25	0.25	0.4099		0.25	0.4099	
0.062	101.0	0.24	0.24	1.8236		0.24	1.8236	
0.062	111.0	0.24	0.23	5.7987		0.23	5.7987	
0.062	121.0	0.23	0.22	6.2313		0.23	1.9691	
0.126	0.0	1.00	0.97	3		0.96	4	
0.126	10.0	0.13	0.16	23.0088		0.15	15.320	
0.126	20.0	0.09	0.08	14.8326		0.08	14.8326	
0.126	30.0	0.09	0.08	14.3332		0.09	3.6248	
0.126	41.0	0.09	0.09	3.3140		0.10	7.4288	
0.126	51.0	0.09	0.09	3.0749		0.09	3.0749	
0.126	61.0	0.09	0.09	2.8161		0.09	2.8161	
0.126	71.0	0.09	0.09	2.5372		0.09	2.5372	
0.126	81.0	0.09	0.09	2.3317		0.09	2.3317	
0.126	90.0	0.09	0.09	2.8324		0.09	2.8324	
			MLP(2:5:1)			**MLP(2:10:1)**		
Catalyst conc. [mole %]	**time [min]**	**Experim. $[D_4]/[D_4]_0$**	**Network $[D_4]/[D_4]_0$**	**E_r**	**r**	**Network $[D_4]/[D_4]_0$**	**E_r**	**r**
0.126	100.0	0.09	0.09	2.9571		0.09	2.9571	
0.126	120.0	0.08	0.09	8.3195		0.09	8.3195	
0.126	140.0	0.08	0.08	3.4902		0.08	3.4902	
0.126	155.0	0.08	0.08	2.2615		0.08	2.2615	
			average E_r	**3.1530**		**average E_r**	**2.6904**	

$$E_r = \frac{p_{exp} - p_{net}}{p_{exp}} \cdot 100 \qquad (2)$$

where p represents the parameter under study ($[D_4]/[D_4]_0$), indexes exp and net denote experimental and network values.

As can be seen in figure 2, the rate of disappearance of D_4 increased with KOH concentration increasing . One can notice that equilibrium concentration of D_4 from the reaction containing 0.126 mole % KOH, with respect to the initial D_4 concentration, is attained in about 15 min. The D_4 concentration has not reached equilibrium after 180 min at lower catalyst level.

A key issue in neural network based process modelling is the robustness or generalization capability of the developed models, i.e. how well the model performs on unseen data. Thus, a serious examination of the accuracy of the neural network results requires the comparison with experimental data, which were not used in the training phase (previously unseen data). The predictions of the networks on validation data are given in table 5.

Table 5

THE VALIDATION OF MLP(2:5:1) AND MLP(2:10:1) FOR THE D_4 DISAPPEARANCE

			MLP(2:5:1)			MLP(2:10:1)		
Catalyst conc. [mole %]	time [min]	Experim. $[D_4]/[D_4]_0$	Network $[D_4]/[D_4]_0$	E_r	r	Network $[D_4]/[D_4]_0$	E_r	r
0.012	5.0	0.96	0.98	1.8447	0.9989	0.97	1.1528	0.9992
0.012	44.0	0.82	0.83	0.2916		0.83	0.3941	
0.012	170.0	0.59	0.59	0.4173		0.59	0.5369	
0.062	4.0	0.76	0.78	2.1324		0.78	2.4228	
0.062	12.0	0.36	0.39	8.8959		0.39	8.0788	
0.062	89.0	0.25	0.25	0.2764		0.25	1.2322	
0.062	117.0	0.23	0.23	3.8864		0.23	1.4904	
0.126	8.0	0.20	0.23	13.4488		0.23	11.8104	
0.126	27.0	0.09	0.08	13.7575		0.09	9.1007	
0.126	135.0	0.08	0.08	1.5670		0.08	2.2747	
				average E_r	4.6518		average E_r	3.8494

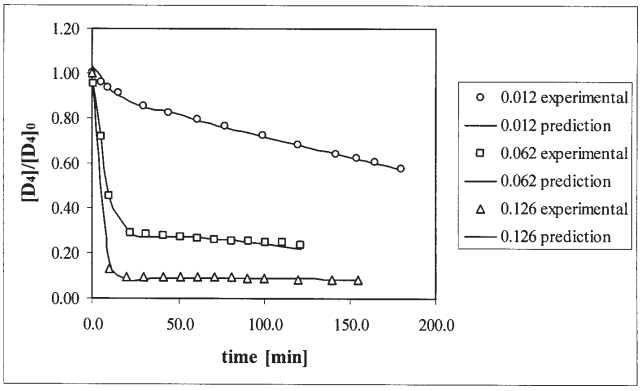


Fig. 2. The neural network predictions vs. experimental training data using MLP(2:5:1) model for the variation in time of D_4 concentration at 160°C and different catalyst concentrations

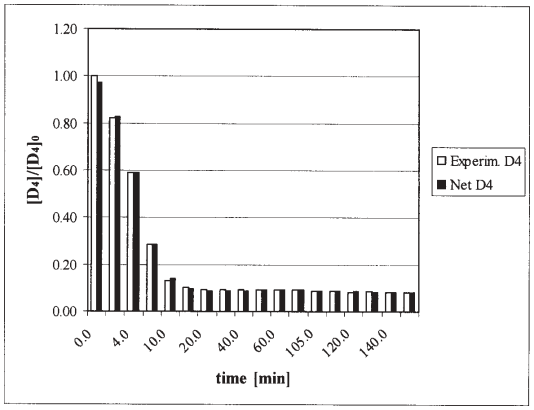


Fig. 3. The neural network predictions vs. experimental training data using MLP(2:10:1) model for the variation in time of D_4 concentration at 160°C and 0.126 mole % KOH

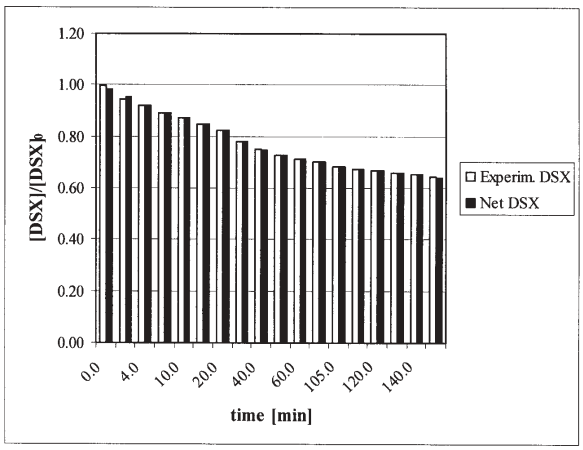


Fig. 4. The neural network predictions vs. experimental training data using MLP(2:10:1) model for the variation in time of DSX concentration at 160°C and 0.126 mole % KOH

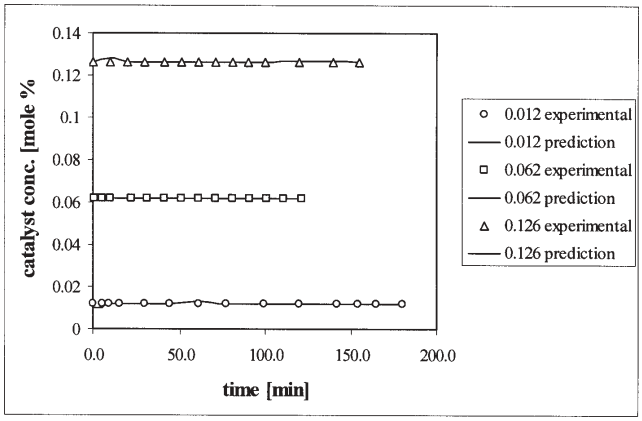


Fig. 5. The neural network predictions vs. experimental training data using MLP(2:9:3:1) model for the amount of catalyst which leads to an imposed D_4 concentration in a fixed time interval

It can be noticed a satisfactory agreement between the two categories of data: experimental and neural network predictions. For this reason, the projected neural model MLP (2:10:1) with a value of average error of 3.849 can be used to make predictions under different reaction conditions, substituting the experiments that are time and material consuming.

A second neural model, MLP(1:10:2) was developed in order to appreciate comparatively the rates of disappearance of D_4 and DSX at 160°C in the presence of catalyst. First of all, good agreement between experimental training data and model predictions are registered (figs. 3 and 4).

As expected, the attack of potassium siloxanolate catalyst on aminopropyl disiloxane proceeds much more slowly than attack on D_4. After 15 min, only 10 mole % of the initial D_4 was present, while 80 mole % of the initial disiloxane remained.

The validation phase, which emphasizes the generalization performance of the neural model, is given in table 6.

Table 6
THE VALIDATION PHASE FOR THE MODEL MLP(1:10:2) WHICH COMPARES THE RATES OF DISAPPEARANCE OF D_4 AND DSX.

time [min]	Experim. $[D_4]/[D_4]_0$	Experim. $[DSX]/[DSX]_0$	Network $[D_4]/[D_4]_0$	Network $[DSX]/[DSX]_0$	E_r D_4	r D_4	E_r DSX	r DSX
5.0	0.49	0.91	0.47	0.91	4.4238	**0.9988**	0.5279	**0.9995**
11.0	0.12	0.86	0.14	0.86	9.7098		0.2673	
23.0	0.09	0.81	0.09	0.81	9.0607		0.5279	
37.0	0.09	0.76	0.09	0.76	1.1858		0.5121	
67.0	0.09	0.71	0.09	0.71	4.4099		0.0107	
100.0	0.09	0.68	0.09	0.68	1.6507		0.1533	
145.0	0.09	0.65	0.08	0.65	1.44398		0.07262	
			average error		**4.55499**		**0.29601**	

Table 7
THE VALIDATION DATA SET OF MLP(2:9:3:1) IN INVERSE NEURAL NETWORK MODELLING

Experim. KOH conc. [mole %]	time [min]	$[D_4]/[D_4]_0$	Net KOH conc. [mole %]	E_r	r
0.012	5.0	0.96	0.011	12.4833	**0.9997**
0.012	44.0	0.82	0.013	4.8083	
0.012	170.0	0.59	0.012	1.6250	
0.062	4.0	0.76	0.064	3.0774	
0.062	12.0	0.36	0.063	1.2338	
0.062	89.0	0.25	0.062	0.6129	
0.062	117.0	0.23	0.063	0.8145	
0.126	8.0	0.20	0.125	0.6777	
0.126	27.0	0.09	0.126	0.1873	
0.126	135.0	0.08	0.127	0.8809	
			average E_r	**2.6401**	

Supplementary information is obtained by inverse neural modeling, that is an optimization problem representing the identification of reaction conditions (amount of catalyst), which lead to an imposed final concentration of D_4 in a pre-established time interval. Table 3 shows MLP(2:9:3:1) as the best topology for inverse neural network model.

The comparison between the predictions on training data and experimental data (fig. 5) put in evidence the similarities that exist between them.

The validation stage with data presented in table 7 emphasizes the capacity of this network type to make good predictions with an average error value of 2.64.

Conclusions

Simple architecture neural networks and simple methods of establishing the networks' structure are proposed for kinetics modeling of the equilibrium anionic polymerization of cyclic siloxanes. MLP(2:10:1) and MLP(1:10:2) are proposed for direct modeling which appreciates the rates of disappearance of D_4 and DSX in the presence of KOH as catalyst. An inverse neural modelling is performed with MLP (2:9:3:1) and represents the identification of reaction conditions (amount of catalyst), which leads to an imposed concentration of D_4 in a pre-established time interval.

Good predictions are obtained with neural models in validation phase, so these neural networks give a very good representation for the kinetics modelling of the equilibrium anionic polymerization of cyclic siloxanes and they are able to provide useful information for experimental practice.

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