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APPLICATION OF NEURAL NETWORKS TO MATHEMATICAL MODELING OF SEDIMENTATION PROCESSES

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ZASTOSOWANIE SIECI NEURONOWYCH W MODELOWANIU MATEMATYCZNYM PROCESU SEDYMENTACJI

Urządzenia sedymentacyjne są powszechnie stosowane w oczyszczaniu zawiesin przemysłowych i w gospodarce komunalnej. Efektywność procesu sedymentacji ma ważne znaczenie w ochronie środowiska. Celem badań było rozpoznanie możliwości zastosowania sieci neuronowych do obliczania efektywności procesu sedymentacji. Jako dane wejściowe do przetwarzania wzięto wyniki obliczeń otrzymanych z symulacji komputerowych prowadzonych według modelu matematycznego uwzględniającego obciążenie powierzchniowe w urządzeniu sedymentacyjnym oraz parametry fizyczne zawiesiny, w tym gęstość rozkładu prawdopodobieństwa wielkości cząstek fazy stałej. Rozważano i porównywano dwa typy funkcji gęstości rozkładu wielkości cząstek fazy stałej zawiesiny: rozkład logarytmiczno-normalny i uogólniony rozkład gamma.

Badania zostały przeprowadzone za pomocą sieci typu *feed-forward* (bez sprzężenia zwrotnego o jednym kierunku przepływu informacji). Wybrano sposób uczenia z nauczycielem metodą wstecznej propagacji błędu (*backpropagation*) według algorytmu Levenberg-Marquardta. W przypadku, gdy sieci były uczone za pomocą zbiorów zawierających poniżej 400 zestawów danych wówczas popełniane błędy przekraczały wartość 1%. Sieci uczone za pomocą zbiorów zawierających około 500 zestawów danych dawały możliwe do zaakceptowania wyniki. Popełniany przez nie błąd był mniejszy niż 1%. Na tej podstawie można wnioskować, że najmniejszym uczącym zbiorem danych, jest zbiór zawierający około 500 zestawów. Najlepsze wyniki obliczeń uzyskano, gdy liczba zestawów wynosiła 5 tysięcy – różnice obliczeń efektywności sedymentacji wynosiły poniżej 0.5 %. Dalsze zwiększanie liczby zestawów danych powyżej 5 tysięcy obniżało dokładność obliczeń.

Summary

The sedimentation devices are commonly used in the clarifying of industrial suspensions and in the civil engineering. The sedimentation efficiency plays very important role in the environmental protection. The aim of the research was to investigate the possibilities of applying neural networks in computing the efficiency of sedimentation processes. Input data were the results of computer stimulation performed according to the mathematical model taking into account the overflow rate in the sedimentation facilities and physical parameters of the suspension, such as probability density function of solid particle size. Two probability density functions of solid particle size were compared: log-normal distribution and gamma distribution.

Feed-forward neural networks (with no feedback and with one- stream flow of information) were applied in research work. Teacher-supervised teaching, according to back-propagation method with the use of Levenberg-Marquardt algorithm, was chosen. When neural networks were taught with the use of sets including less than 400 data elements, the errors were more than 1%. Neural networks taught by means of series including more than 500 data sets would yield acceptable results and the error was less than 1%. Accordingly, one can presume that the smallest teaching set is the one composed of 500 data elements. The best results were obtained when the number of data sets was about 5 000 – the differences in computed sedimentation efficiency were then less than 0.5%. A further increase in the number of data elements – above 5 000 – would lead to lower accuracy of calculations.

INTRODUCTION

Water plays a very important role in interrelated natural processes. It has very special functions and has to be protected from pollution. Coal mines and steelworks are main sources of inland water pollution. Unfortunately, the usage of closed water circulation systems in technological processes still cannot eliminate solid contaminants, such as heavy metals and other toxic compounds.

In industry water is mainly treated in settling facilities – various types of settling tanks. The costs of settling tank operation and maintenance are low though the investment costs tend to be rather high. To ensure a long service life of settling tanks utmost care is given to settling tank modernisation to improve the efficiency of sedimentation processes and hence, to obtain better results of water purification. Lamella sedimentation is a method for more intense water purification, widely applied nowadays. Application of lamella sedimentation improves the efficiency of processes or machine capacity. Forecasting the sedimentation efficiency is the fundamental though most difficult problem in design of lamella sedimentation facilities.

The results of theoretical and practical studies on modernisation of settling tanks with lamella packets [2, 6] include not only their application in mining and metallurgy but also the development of design methods based on mathematical models providing analytical results. At present the Department of Technological Device and Environmental Protection is engaged in new research on new lamella sedimentation technologies and new designs of sedimentation facilities. They include studies on cross-current sedimentation processes [7, 8], the efficiency of which will be much higher than that of counter-current sedimentation processes, and on sedimentation processes in a complex system including co-current and counter-current flows of suspension. Sedimentation facilities and processes are so complex that the possibility of formulating a proper analytic mathematical model is said to be minimal. To solve such difficult and complex non-linear mathematical problems the researchers often resort to neural networks. The research work presented in this study was undertaken with the aim to recognise the potentials of neural networks for forecasting the efficiency of the sedimentation processes and mechanisms.

Neural networks can be used in such applications thanks to some of their features [13, 14, 16]:

- the possibility of creating free, non-linear transformations without formulating proper mathematical models (i.e.: without showing the relationships between input and output data),
- the possibility of teaching a given neural network i.e. the process of developing proper non-parametric mapping of output data into input data in the net,
- the possibility of multidimensional data processing thanks to the parallel structure of the network, hence parallel data processing is possible.

Because of those features neural networks can be used in many branches of science and industry, e.g. in modelling of chemical engineering processes [4, 14], in modelling of metal plastic working [9, 10, 14] and in detection and location of structural defects [11].

The aim of the research is to determine the possibilities of neural networks application to forecasting the efficiency of sedimentation facilities when one of the most important factors influencing that efficiency, i.e. the solid particle size is a random variable with the log-normal or generalized gamma distribution.

CALCULATION OF SEDIMENTAION EFFICIENCY FOR LOG-NORMAL DISTRIBUTION OF SOLID PARTICLE SIZE

First studies on applications of neural network to calculations of the sedimentation efficiency are presented in [4]. The calculations provided there are based on the assumption that the distribution of solid particle size is the log-normal distribution with the density function $f(d;\, m,\sigma)$

$$f(d;m,\sigma)=\frac{1}{\sqrt{2\pi}d\sigma}\exp\left(-\frac{1}{2}\left(\frac{\ln d-m}{\sigma}\right)^2\right) \tag{1}$$

where

- d – solid particle size (particle diameter),
- m – parameter of distribution – the mean value of distribution function of particle diameters,
- σ – parameter of distribution – the standard deviation of the particle diameter distribution function.

The sedimentation efficiency is obtained from the formula:

$$\begin{aligned}\eta(d_g;m,\sigma)=1-\Phi_N\left(\frac{\ln d_g-m}{\sigma}\right)+\\ +\exp\{2\cdot[\sigma^2-(\ln d_g-m)]\}\cdot\Phi_N\left(\frac{\ln d_g-m}{\sigma}-2\cdot\sigma\right)\end{aligned} \tag{2}$$

where

- η – the efficiency of sedimentation,
- $\Phi_N(x)$ – the value of log-normal distribution function of x,
- d_g – diameter of the limiting particle, i.e. a particle whose rate of descent equals the overflow rate q.

The relationship between the diameter of limiting particles and the overflow rate q is derived from the Stokes equation applied on the basis of the generalized Hazen's sedimentation theory [5], that is:

$$d_g = \sqrt{\frac{18\mu_0}{(\rho - \rho_0)g} q} \tag{3}$$

where

μ_0 – dynamic viscosity coefficient,

ρ, ρ_0 – density of solid particles, density of the medium (liquid),

q – overflow rate,

g – gravitational acceleration.

The coefficient of dynamic viscosity μ_0 depends mainly on temperature t. For water this dependency may be obtained from an empirical equation (4)

$$\mu_0 = \frac{1.79 \cdot 10^{-3}}{1 + 0.0337\, t + 0.000222\, t^2} \tag{4}$$

The choice of log-normal distribution of particle size was justified by the fact that it is simple for calculations and it is frequently used in mathematical modelling of sedimentation processes. The log-normal distribution involves two parameters only and therefore the calculations are relatively simple. It is a well-known fact, however, that a smaller number of parameters leads to a lower precision of calculations.

CALCULATION OF SEDIMENTATION EFFICIENCY IN THE CASE OF THE GENERALIZED GAMMA DISTRIBUTION OF PARTICLE SIZES

We can make an assumption that distribution of the solid phase in the suspension is a random variable with generalized Stacy gamma distribution. That generalized distribution has three parameters: d_0, p, n. The function of probability density $f(d; d_0, p, n)$ can be written as:

$$f(d; d_0, p, n) = \frac{n}{d_0 \Gamma(p)} \left(\frac{d}{d_0}\right)^{pn-1} \cdot \exp\left[-\left(\frac{d}{d_0}\right)^n\right] \tag{5}$$

where

d_0 – distribution parameter, called the scale parameter,

p, n – parameter of distribution, called shape parameter,

$\Gamma(p)$ – gamma Euler function defined by the equation:

$$\Gamma(p) = \int_0^\infty x^{p-1} e^{-x}\, dx \tag{6}$$

When the solid particle size follows the generalized gamma distribution, the efficiency of sedimentation η is defined by the equation (7):

$$\eta(d_g;d_0,p,n)=1-\frac{\Gamma\left[p,\left(\frac{d_g}{d_0}\right)^n\right]}{\Gamma(p)}+\left(\frac{d_0}{d_g}\right)^2\cdot\frac{\Gamma\left[p+\frac{2}{n},\left(\frac{d_g}{d_0}\right)^n\right]}{\Gamma(p)} \tag{7}$$

where

$\Gamma(a,b)$ – incomplete gamma function defined by the equation

$$\Gamma(a,b)=\frac{1}{\Gamma(a)}\int_0^b x^{a-1}\cdot e^{-t}\,dt \tag{8}$$

And in relation to (7):

$$a=p \text{ or } a=p+\frac{n}{2} \qquad b=\left(\frac{d_g}{d_0}\right)^n \tag{9}$$

STRUCTURE OF ANALYSED NEURAL NETWORKS

When studies on the applications of neural network to calculating the sedimentation efficiency were undertaken, an assumption was made that the created neural networks should have the structure of reversed pyramids and that they should have three layers plus the input one. It is the best configuration of a *feed–forward* network, taught by a teacher.

The structure of compared neural networks is presented in Fig. 1, for the log-normal distribution of particle size the structure is [5 20 11 1], which means that the number of inputs „*i*" is 5; input data included the following parameters:

- t – temperature – ranging from 10 to 40°C,
- ρ – density of solid particle material ranging from 1 500 to 4 500 kg/m^3
- m – the mean value of natural logarithms of solid phase particles ranging from 0.5 to 3.5,
- σ – standard deviation of natural logarithms of solid particles size ranging from 0.1 to 1.2,
- q – overflow rate ranging from of 0.1 to 2 $m^3/m^2/h$.

There are 20 neurons in the first hidden layer (j = 20) and 11 neurons (k = 11), in the hidden second layer while the output layer has only one neuron. The datum at the network output (i.e. the correct response of the neural network to input data) was the efficiency of sedimentation η obtained from the equation (2). The results of computer calculations are presented in [4].

To examine networks being taught on data generated from the mathematical model in which particle sizes followed the generalized gamma distribution, the network with the

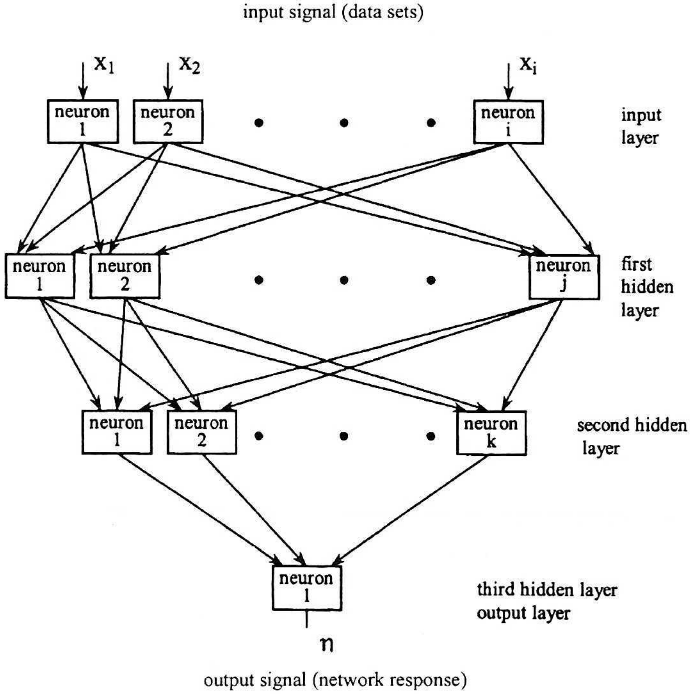

Fig. 1. Structure of studied neural networks

structure of [6 20 11 1] was created. It means that the index i for that network was 6, j was 20 and index k was 11. Input data include the following parameters:

- t – temperature – ranging from 10 to 40°C,
- ρ – density of solid particle material ranging from 1 500 to 4 500 kg/m^3
- d_0 – scale parameter of the generalized gamma distribution of particle size,
- p – shape parameter of generalized gamma distribution of particle size,
- n – shape parameter of generalized gamma distribution of particle size,
- q – overflow rate ranging from 0.1 to 2 m^3/m^2/h.

The parameter at the network output was the efficiency of sedimentation η obtained from the equation (7).

COMPUTER SIMMULATION USING THE GENERALIZED GAMMA DISTRIBUTION

Selection of appropriate data is of primary importance for neural network teaching. Input data in the present analysis are the simulation results obtained on the basis of mathematical models presented in the earlier sections.

Another important problem is the choice of adequate software affording the development and analysis of neural networks. MATLAB software package [1, 15] is considered to be the best and the most suitable one (mainly because it is easily available and has strong computing power). All calculations were done at the University Computer Centre CYFRONET-AGH, using the computer "Maria" having the computing power of 11.52 Gflops.

Several options of computer programs for generating and teaching neural networks were developed using the chosen mathematical model and the software package. Additionally, the programme for network testing was created. The aim of the final stage of research was to carry out numerous tests on different types of neural networks. The results help to answer the question whether neural networks taught from data sets generated by mathematical models based on gamma distribution of particle size can be applied in calculations of the sedimentation efficiency.

The method uses *feed–forward* neural networks (with no feedback, providing only one direction for information flow). A teacher-supervised method (*backpropagation* method, in accordance with the Levenberg–Marquardt algorithm) was selected.

In the first stage the approximated size of the neural network was defined. Accordingly, eight neural networks were created, with different numbers of neurons in the subsequent hidden layers. Networks were taught by means of data set including 5 000 data elements — generated at random, according to the mathematical model. It allowed for specifying the number of neurons in the subsequent hidden layers: 20, 11, 1 neurons, respectively.

These neural networks were taught with data sets of various size so as to obtain the neural network model where the approximation results would best agree with the input data. Data sets used in teaching were recorded in teaching sets of variable length, including data at the network input and correct answers at the output.

The teaching process was restricted to 100 periods only so as to prevent network overlearning and to limit the teaching time (it was found out that 100 periods were sufficient because after that the teaching process would stop). Besides, the minimal error made by the network was limited to 10^{-7}. It means that whichever restricting value is reached, the teaching process is interrupted.

DISCUSION OF RESULTS

The results of several computer simulations reveal that in situations when networks were taught with sets including 400 data sets the errors exceeded 1%. Only the networks taught with sets including 500 data sets would yield acceptable results and the error would be less than 1%. Accordingly, we can conclude that the smallest teaching set ought to include 500 elements. It should be mentioned here that when other neural networks are applied (different in size, structure or kind), the size of the required teaching set can slightly change. The relationship between the standard error value and the number of data sets in the teaching series for the neural network structure [6 20 11 1] is presented in Fig. 2. It can be clearly seen on the graph that the number of 5 000 data sets in the teaching series seems the most effective one in the light of standard error minimization. Further increase in the number of data sets (in excess of 5 000) leads to greater errors.

Thus we conclude that computations of the mean standard error and the smallest number of data sets in a teaching series seem to be most representative and valuable options for further analyses.

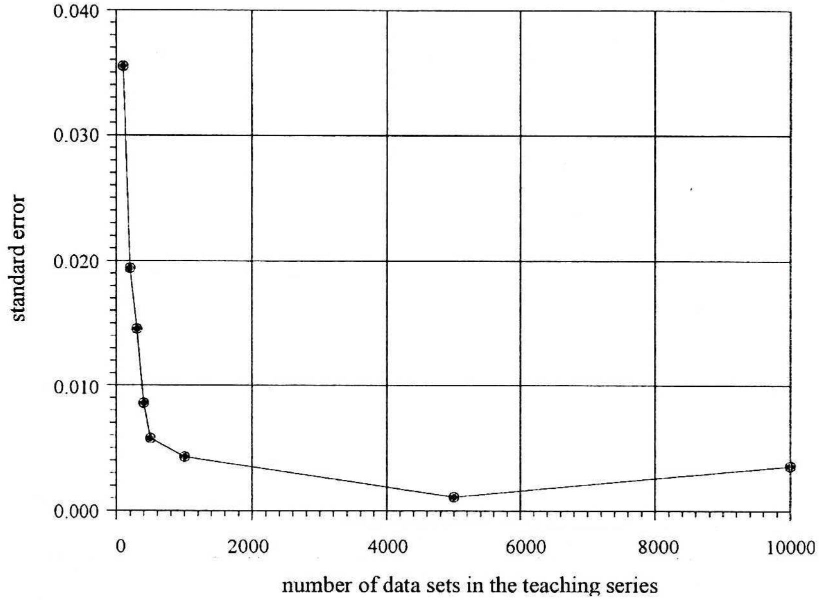

Fig. 2. Standard error value for networks with the structure [6 20 11 1] vs. number of data sets in the teaching series

Results obtained for 5 000 data sets are presented in Fig. 3 and 4. Fig. 3 shows the differences in calculated values of sedimentation efficiency, while Fig. 4 presents the relationship between the efficiency obtained at the network output and the corresponding value calculated from the mathematical model. It follows from Fig 3 that the differences in calculated values fall into the interval (-0.005, 0.005). The maximum error was 0.003616 while the standard error was 0.001092, which may be considered very good results.

Analogous relationships for networks taught with data sets composed of 500 data elements are presented in Fig. 5 and 6. Here, the maximum error was 0.021953 while the standard error was 0.005765. These results are worse than the previous one, yet the data set had only 500 elements. However, taking into consideration the accuracy of sedimentation efficiency measurements in industrial conditions, the results can be regarded as satisfactory.

COMPARISON OF CALCULATION RESULTS OBTAINED FOR TWO TYPES OF SOLID PARTICLE SIZE DISTRIBUTIONS

The standard error for neural networks with the structure [5 20 11 1] (log-normal distribution) and neural networks with the structure [6 20 11 1] (generalized gamma distribution) are presented in Fig. 7. A data set containing 108 testing series was used to extensively test the networks.

Graphs representing the errors made by the two neural networks are presented. It can be clearly seen that for teaching series including more than 500 data sets the error would remain on the same level (0.5%). Major differences are found when we deal with smaller data sets (about 300 elements).

Network teaching using the data generated by generalized gamma distribution leads to much smaller errors. That is related to the number of neurons in the input layer which

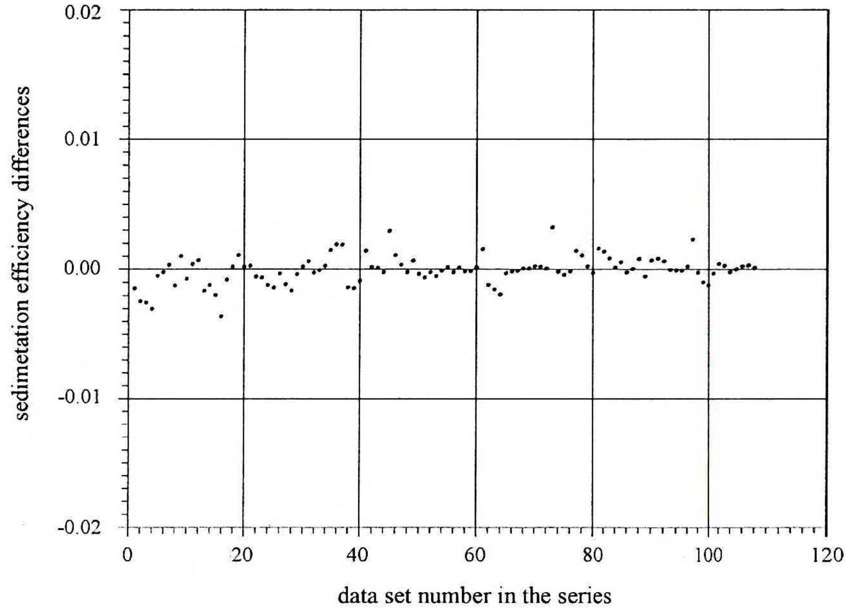

Fig. 3. Differences between sedimentation efficiency at the output of networks taught with series including 5 000 data sets and sedimentation efficiency computed in accordance with the mathematical model

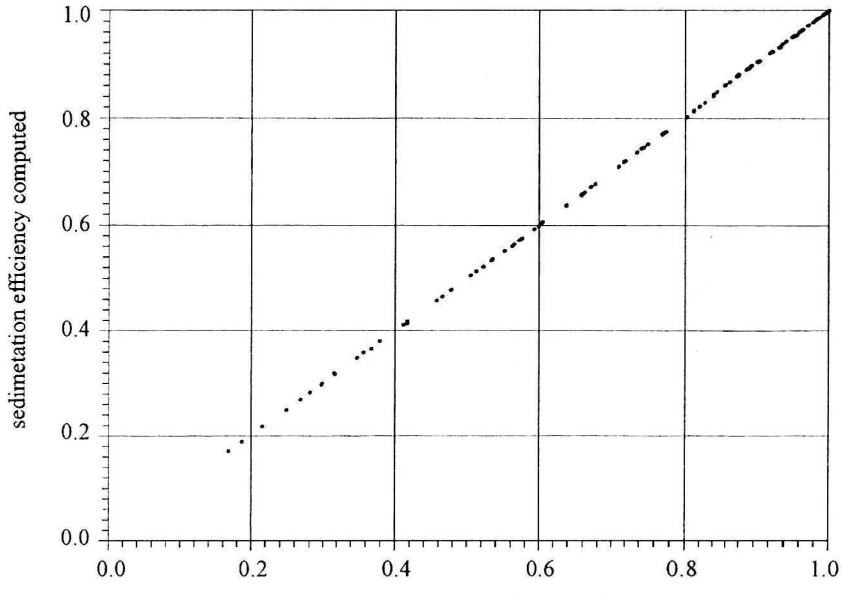

Fig. 4. Sedimentation efficiency at the output of networks taught with series including 5 000 data sets vs. sedimentation efficiency computed in accordance with the mathematical model

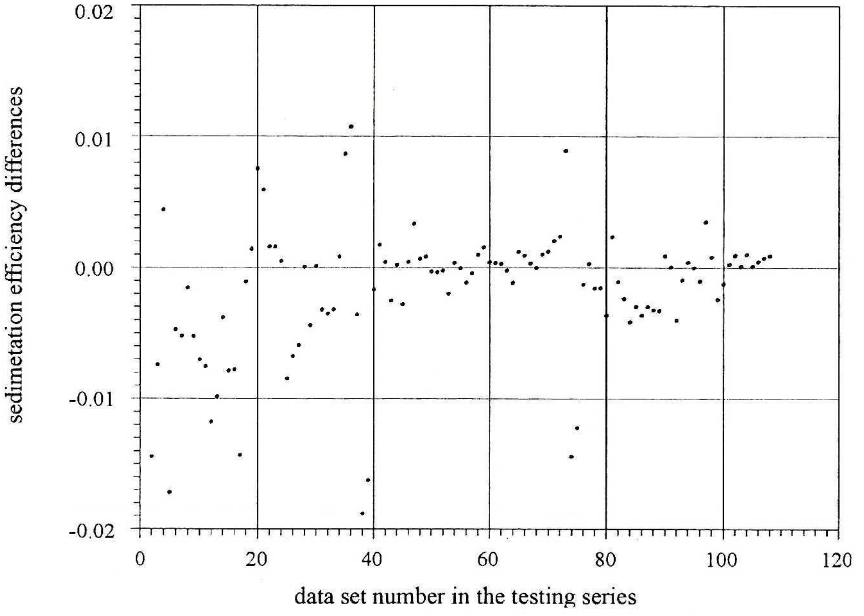

Fig. 5. Differences between sedimentation efficiency at the output of networks taught with series including 500 data sets and sedimentation efficiency computed in accordance with the mathematical model

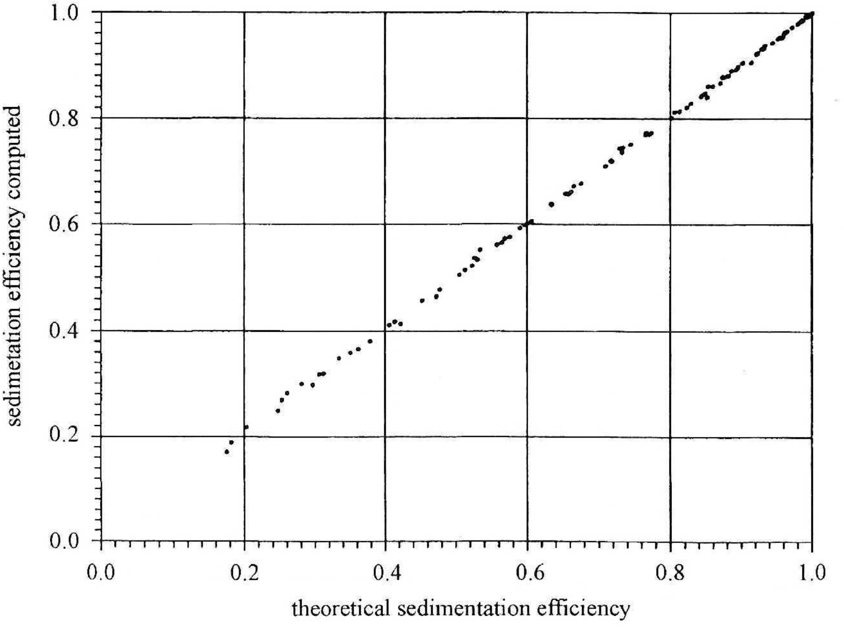

Fig. 6. Sedimentation efficiency at the output of networks taught with series including 500 data sets vs. sedimentation efficiency computed in accordance with the mathematical model

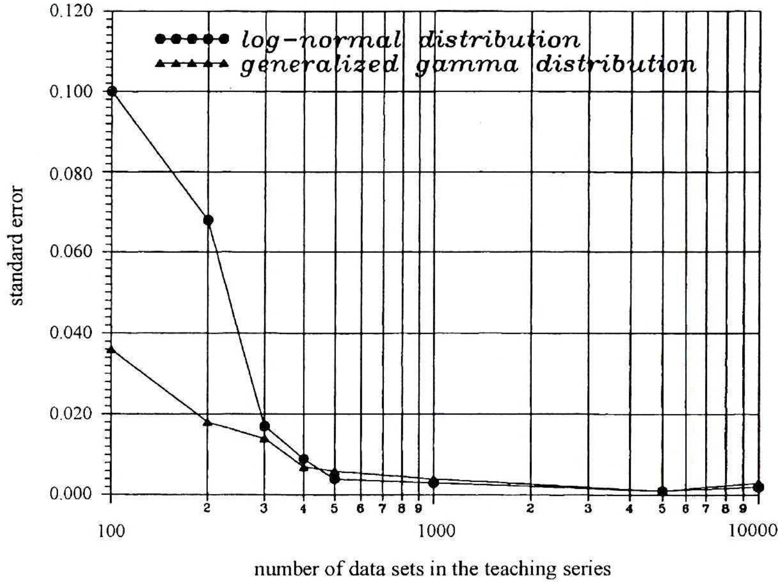

Fig. 7. Standard error value in calculations for neural networks having the structure [6 20 11 1] (generalized gamma distribution) or [5 20 11 1] (log-normal distribution) and being taught using series with variable number of data sets

involves the greater number of data in the teaching series, even though the number of data sets remains the same. It can be concluded, therefore, that both the number of data in the teaching series and the number of network inputs (i.e. the number of neurons in the input layer) are most important. When the number of inputs is very small but the number of data sets is significant, the network can make major errors. The results of the research work reveal that there is a certain optimal number of neurons for which the network gives the best results, hence there might also be a certain optimal number of data sets at the input (the number of network inputs) which ensure the best results.

When analysing the graphs, we notice that apart from mathematical model used to generate teaching sets, the smallest errors are found in networks taught by means of series including 5 000 data sets. We have to bear in mind that the difference in quality of network answers appears only when the error made by the network is considerable, beyond the acceptable range. In earlier studies the acceptable error was found to be the one involved in network teaching with the series including 500 or more data sets.

CONCLUSIONS

The analysis and discussions of results leads us to the conclusion that application of neural networks as the „tool" for evaluating the efficiency of sedimentation processes is justified. It follows from the comparison of the two methods that better results are achieved for neural networks taught with data sets generated on the basis of mathematical model assuming tri-parameter generalized gamma distribution of particle size. However, better results are obtained throughout the range where neural networks cannot be used to calculate the sedimentation efficiency. In the light of these conclusions, both mathematical models seem to have an equal value for practical applications. The differences in quality of calculations can be explained by the architecture and number of data at the network input, and not by quality of data generated by the two mathematical models.

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