© Strojniški vestnik 48(2002)10,520-527
ISSN 0039-2480
UDK 628.16.04/.09:004.94
Izvirni znanstveni članek (1.01)

© Journal of Mechanical Engineering 48(2002)10,520-527
ISSN 0039-2480
UDC 628.16.04/.09:004.94
Original scientific paper (1.01)

Simuliranje nastajanja gruč dispergiranih delcev pod vplivom zunanjega magnetnega polja

A Simulation of the Cluster-Formation Process in a Dispersion of Fine Particles Under the Influence of an External Magnetic Field

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Naprave za magnetno obdelavo vode (MOV) so učinkovita, gospodarna in dobra ekološka rešitev za preprečevanje izločanja vodnega kamna. Na podlagi laboratorijskih preskusov so ugotovili, da je učinkovitost MOV odvisna od sestave obdelovanega disperznega sistema in obratovalnih razmer naprave. Na temelju teorije Derjagin-Landau in Verway-Overbeek (DLVO) in statistične metode Monte Carlo Metropolis smo razvili teoretični model nastajanja gruč dispergiranih delcev pod vplivom zunanjega magnetnega polja. Nadalje smo po načelu "odprtega vira" na podlagi omenjenega modela razvili računalniški program za simulacijo in grafično predstavitev nastajanja gruč pod vplivom zunanjega magnetnega polja. Rezultate izračunov smo analizirali z metodo delitve in metodo stopenjske porazdelitve.

(Ključne besede: obdelava vode magnetna, vodni kamen, metode Monte Carlo Metropolis, analize gruč)

Magnetic water-treatment (MWT) devices for scale control can be used with good economic and ecological benefits. From experimental results under well-controlled laboratory conditions we have established that the effects of MWT devices are very dependent on the composition of the treated dispersion system and their working conditions. To investigate the effects of magnetic field on the process of cluster formation in a fine-particle dispersion under the influence of the external magnetic field of a MWT device a theoretical model based on the Derjagin-Landau and Verway-Overbeek (DVLO) theory and the statistical Monte Carlo Metropolis method was used. The open-source computer programs for the simulation and the graphical presentation of clustering under the influence of an external magnetic field were developed. The results were analysed by cluster analysis, based on the partitioning and hierarchical methods.

(Keywords: magnetic water treatment, scale prevention, Metropolis Monte Carlo, cluster analysis)

0 UVOD

Magnetna obdelava vode je pogosto uporabljana metoda nekemične obdelave vode za nadzor izločanja vodnega kamna. Nadzor vodnega kamna se dosega z vodenjem napajane vode skozi magnetno polje. Je gospodarna metoda, vendar še vedno daje nezanesljive rezultate. Kljub več desetletnim proučevanjem na tem področju še ni izdelana dokončna znanstvena teorija, kako te naprave natančno delujejo in kakšni so pogoji za njihovo optimalno delovanje.

Naravne vode so bogati disperzni sistemi, ki vsebujejo različne koloide, ione in druge sestavine. Zaradi naravne prenasičenosti ali pa vzpostavitve prenasičenja ob spremembah med predelavo vode (npr. sprememba temperature, tlaka ali *pH*) lahko na stenah cevovodov in naprav pride do izločanja nekaterih izmed teh snovi v obliki težko odstranljivih

0 INTRODUCTION

Magnetic water-treatment is a frequently used non-chemical method for scale control. The scale prevention is achieved by passing the water through the magnetic field. It is an economically favorable technique, but it still gives unreliable results. Despite several decades of intensive research done in this area, no scientifically confirmed theoretical explanation exists yet that adequately describes how MWT devices work and the conditions for their effective and optimum operation.

Natural waters are rich dispersion systems that contain many colloids, ions, etc. Due to the natural supersaturating of water supplied to various systems or the supersaturating as a result of changed conditions during water processing (such as pressure drop, temperature and *pH*) a hard scale precipitates on the pipeline and the walls of the equipment. The

oblog vodnega kamna. MOV je še posebej obetavna metoda za uravnavanje interakcij med koloidnimi delci v vodnih disperzijah [1].

Čeprav mnogi postopki vplivajo na koloidni sistem, pomeni ravnotežje med interakcijami privlakov in odbojev (pri določeni termični dejavnosti) kriterij za stabilnost koloidnih disperzij v naravnih vodah. Natančnejše razumevanje tega vzajemnega delovanja podaja teorija DLVO [2]. Težnji delcev, da bi se združili zaradi delovanja van der Waals–Londonovih sil kratkega dosega, nasprotuje električni naboj na trdni površini, ki deluje tudi na večjih razdaljah med delci. Tako je celotna interakcijska energija med dvema koloidnima delcema (E_t) vsota energije elektrostatskega odboja (E_r; ko se električni dvojni plasti delcev prekrivata) in energije medmolekularnega privlaka (E_a; delovanje van der Waals–Londonovih sil) [2]:

MOV is a particularly promising technique for controlling the interactions among colloidal particles in water dispersions [1].

Although many processes affect colloidal behavior, the balance between attraction and repulsion interactions (for a particular level of thermal activity) is a criterion for the stability in colloid dispersions. A detailed understanding of this interplay is the basis of the DLVO theory [2]. The tendency of particles to aggregate as a result of the short-range van der Waals–London forces is counter acted by the electrically charged layer on the particles' surfaces. Thus, the total interaction energy (E_t) between two colloidal particles is the sum of the repulsion energy (E_r; electric repulsion, when double layers of two particles overlap) and the attraction energy (E_a; the particles' interaction as a result of the van der Waals–London forces) [2]:

$$E_t = E_r + E_a \tag{1}.$$

Energija elektrostatskega odboja (E_r) med delcema je odvisna od polmera teh delcev (a), razdalje med njunima centroma (R), elektrokinetskega potenciala (φ_δ) in dielektrične konstante disperznega medija (ε_r). Med enakima, okroglima, razmeroma majhnima delcema s široko električno dvojno plastjo (majhen $\kappa\alpha$) je energija odboja:

The repulsion energy (E_r) between two particles depends on the radius (a), the distance between the centres of the particles (R), the electrokinetic potential (φ_δ) and the dielectric constant (ε_r) of the dispersion medium. For identical, spherical and relatively small particles with a wide electric double layer ($\kappa\alpha$ is small) the repulsion energy is:

$$E_r = \frac{\varepsilon_r \varepsilon_0 a \varphi_\delta^2}{s} \exp(-\kappa a(s-2)) \tag{2},$$

kjer sta: s razmerje med razdaljo med središčem in premerom delca ($s=R/a$) in κ Debye-Hückelov parameter (njegova obratna vrednost je v prvem približku enaka debelini električne dvojne plasti):

where parameter s is the ratio between the distance and the radius ($s=R/a$) and κ is the Debye-Hückel parameter (its reciprocal value is considered as a first approximation for the length of the electric double layer):

$$\kappa = \sqrt{\frac{2e_0^2 N_A \sum_i z_i^2 c_i}{\varepsilon_r \varepsilon_0 k_B T}} \tag{3}.$$

Za okside, dispergirane v vodi, je električni potencial na trdni površini (φ_δ) določen s pH disperzije ([2] in [3]). Energija medmolekularnega privlaka (E_a) med dvema enako velikima, okroglima delcema je določena z enačbo:

For oxide minerals in water, the surface potential (φ_δ) of the particles is determined by the pH of the dispersion ([2] and [3]). The energy of attraction (E_a) between two spherical particles with an identical radius is defined by the equation:

$$E_a = -\frac{k_H}{6}\left(\frac{2}{s^2-4} + \frac{2}{s^2} + \ln\frac{s^2-4}{s^2}\right) \tag{4},$$

kjer je k_H Hamakerjeva konstanta.

Magnetostatične interakcije med delci spreminjajo obnašanje tekočine in lahko destabilizirajo koloidni sistem. Ko je disperzija koloidnih delcev izpostavljena zunanjemu magnetnemu polju, se pojavijo magnetne sile, ki zmanjšujejo stabilnost koloidnega sistema. Energija magnetnega privlaka (E_m) med dvema okroglima delcema na razdalji R_{ij} je odvisna od gostote (B) in smeri delovanja zunanjega magnetnega polja, velikosti delcev (a) in magnetnih lastnosti minerala. Pri vzporedni usmeritvi magnetnih

where the parameter k_H is the Hamaker constant.

Magnetostatic particle interactions modify the behavior of the fluid and can affect the colloidal stability. When a dispersion of colloid particles is placed in an external magnetic field an additional magnetic force arises, which decreases the stability of the colloid system. The energy of the magnetic attraction (E_m) between two spherical particles separated by a distance R_{ij} depends on the magnetic density (B) and the angle of the external magnetic field, the radius of the particles (a) and the magnetic properties of the particles. For the

momentov dveh enakih, okroglih delcev je energija magnetnega privlaka:

parallel-orientated magnetic moments of two identical particles, the energy of the magnetic interaction is:

$$E_m = -\frac{32\pi^2 a^6 \chi^2 B^2}{9\mu_0 R_{ij}^3} \quad (5).$$

Celotna energija (E_t) interakcij med koloidnima delcema v sistemu, izpostavljenemu zunanjemu magnetnemu polju, je tako:

Thus, the total energy of the interaction (E_t) for colloid particles in an external magnetic field is:

$$E_t = E_r + E_a + E_m \quad (6).$$

Statistične numerične metode, znane kot metode Monte Carlo, za simulacijo uporabljajo zaporedja naključnih števil. Model za proučevanje lastnosti koloidnih vodnih disperzij pod vplivom magnetnega polja ([2] do [8]) temelji na metodi Monte Carlo Metropolis ([4] in [13]).

Osnova modela je dvorazsežna kvadratna celica z dolžino stranice A , z N-timi naključno razporejenimi delci (sl.1). Vsi delci so okrogli in enaki. Lega slehernega delca je znana in označena s koordinatami (x, y,θ), kjer je θ kot med magnetnim momentom delca in zunanjim magnetnim poljem [6] (sl.2).

Celotna energija sistema (E_S) je enaka vsoti vseh energij interakcij med koloidnimi delci v prostoru:

Statistical numerical methods, known as Monte Carlo methods, are methods that utilize sequences of random numbers to perform the simulation. The presented model is based on the Monte Carlo Metropolis ([4] and [13]) method and has been used to investigate the properties of colloid particle dispersions in water under the influence of a magnetic field ([2] to [8]).

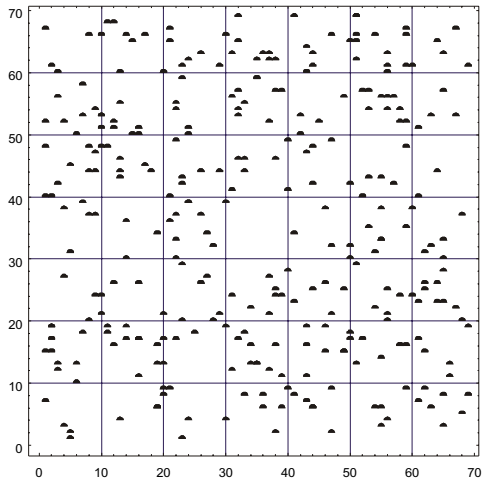
The model is based on a two-dimensional square cell with a side of length A, containing N randomly distributed particles (Fig. 1). All the particles are spherical and identical. The position of any particle is known and can be specified with coordinates (x, y,θ), where θ is the angle between the magnetic moment of the particle and the applied magnetic field [6] (Fig. 2).

The total energy of the system (E_S) is the sum of the total energies of the interactions amongst all the colloid particles:

$$E_S = \sum_{i=1}^{N} E_{t(i)} \quad (7).$$

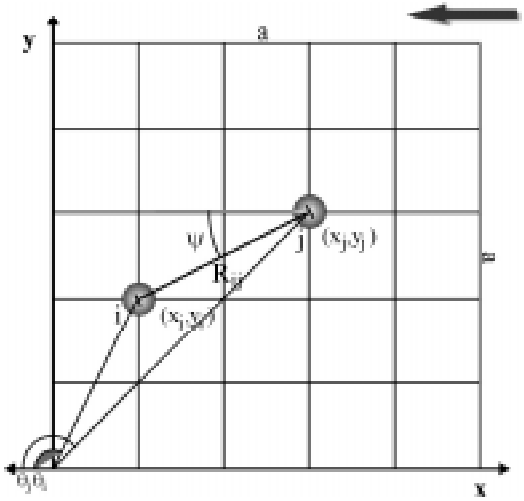
Metoda vsebuje izračunavanje energijskih sprememb (ΔE), medtem ko se koordinate enega delca v analizirani celici naključno spremenijo za majhne

The method consists of calculating the energy change (ΔE) when the coordinates of one particle in the analyzed cell are changed, at random, by small



Sl. 1. *Naključna porazdelitev okroglih delcev v dvorazsežnem prostoru kvadratne oblike (A=70 μm, α=0,5 μm, N=300)*

Fig. 1. *Randomly distributed spherical particles in a two-dimensional square cell (A=70 μm, α=0.5 μm, N=300)*



Sl. 2. *Par delcev (i,j) - okrogle oblike v dvorazsežni celici ob delovanju zunanjega magnetnega polja pod kotom ψ [9]*

Fig. 2. *A pair of spherical particles (i,j) in a two-dimensional square cell under a magnetic field applied at an angle ψ[9]*

vrednosti. V primeru, da je nova vrednost celotne energije sistema nižja od predhodne, delec ostane v novi legi; v nasprotnem primeru se izračuna faktor P in primerja z naključno vrednostjo ξ, $\xi \in [0,1]$:

amounts. If the new total energy of the system is less than the previous one the particle stays in its new position; otherwise a factor P is calculated and compared with the random number ξ, $\xi \in [0,1]$.

$$P = \exp\left(-\Delta E / k_B T\right) \tag{8}.$$

Če je faktor P večji od naključnega števila, delec ohrani novo lego, sicer se vrne na prvotno lego. Opisani postopek se izvede za vseh N delcev v kvadratni celici.

If the P factor is greater than the random number the particle retains its new position, otherwise it is returned to its original position. This procedure is applied for all N particles in a square cell.

1 RAČUNALNIŠKI PROGRAM ZA SIMULACIJO NASTAJANJA GRUČ

Pri proučevanju magnetne obdelave vode smo uporabili teorijo koloidov, matematike in statistike. Računalniški program Open Source (MCM) [15] smo priredili za dvorazsežno simulacijo postopka nastajanja gruč v finih disperzijah pod vplivom zunanjega magnetnega polja. Do takšnega nastajanja naj bi namreč prišlo v napravah MOV, kot predvidevajo nekateri avtorji ([10] in [11]). Za grafično predstavitev smo uporabili sklop računalniških programov MCM View [9] in za analizo gruč Fanny in Twins [12].

Podatki so vneseni z dvema vhodnima datotekama. V prvi datoteki so podani: velikost celice, število in fizikalne lastnosti delcev; določena je tudi struktura vmesnih izhodnih datotek. V drugi vhodni datoteki je določena izhodiščna lega delcev.

Rezultati simulacije so zapisani v različnih oblikah in so lahko predstavljeni s programi, kakršna sta Microsoft Excel [15] ali Microcal Origin [15]. Za grafično predstavitev je razvit CM View program Compaq Array Visualizer [15]. Rezultati so bili nadalje ovrednoteni z metodo delitve in metodo stopenjske porazdelitve za analizo gruč po Kaufmanu in Rousseauwu [12]. V ta namen sta bila uporabljena programa Fanny in Twins.

1 A COMPUTER PROGRAM FOR THE SIMULATION OF CLUSTER FORMATION

Well-known theories from the field of colloid science, statistics and mathematics have been taken into consideration and applied in magnetic water-treatment research. An open-source computer program (MCM) [15] for the two-dimensional simulation of the cluster-formation process in a fine-particles dispersion under the influence of an external magnetic field was developed. According to some authors ([10] and [11]) such a cluster formation might occur in MWT devices. A set of computer programs, MCM View [9] and Fanny and Twins [12], were used for the graphical presentation and the cluster analysis, respectively.

The data are entered with two input files. In the first input file the size of the cell, the number and the physical properties of the particles are determined and the structure for the intermediate output files is defined. In the second input file the original position of the particles is determined.

The results of the simulation are written in various formats and can be presented with the programs such as Microsoft Excel [15] or Microcal Origin [15]. For the graphical presentation, the MCM View program was developed on the basis of the Compaq Array Visualizer [15]. The results were further analysed with the partitioning and hierarchical methods for cluster analysis of Kaufman and Rousseauw [12]. For this purpose we used the Fanny and Twins programs.

2 REZULTATI SIMULACIJE

Kot primerjalni podatki za primarne numerične izračune so bile uporabljene fizikalne lastnosti hematitnih delcev (Fe_2O_3) v vodni disperziji. Na podlagi tega so bili izvedeni numerični izračuni za nekatere minerale, ki ustvarjajo vodni kamen v vodi: diamagnetni kalcijev karbonat ($CaCO_3$), kalcijev sulfat ($CaSO_4$), silicijev dioksid (SiO_2), antiferomagnetna hematit (Fe_2O_3), getit (FeOOH) in feromagnetni magnetit (Fe_3O_4).

Za vse naštete minerale je bila simulacija nastajanja gruč izvedena v naslednjih razmerah:

- različno število delcev v kvadratni celici in različni polmer a,

2 RESULTS OF THE SIMULATION

As the reference data for the primary numerical calculations, the physical properties of hematite particles (Fe_2O_3) in an aqueous dispersion were used. On this basis, the numerical calculations for some of the scale-forming minerals in the water, such as diamagnetic calcium carbonate ($CaCO_3$), calcium sulfate ($CaSO_4$), silicon dioxide (SiO_2), antiferromagnetic hematite (Fe_2O_3), goethite (FeOOH) and ferromagnetic magnetite (Fe_3O_4), were carried out.

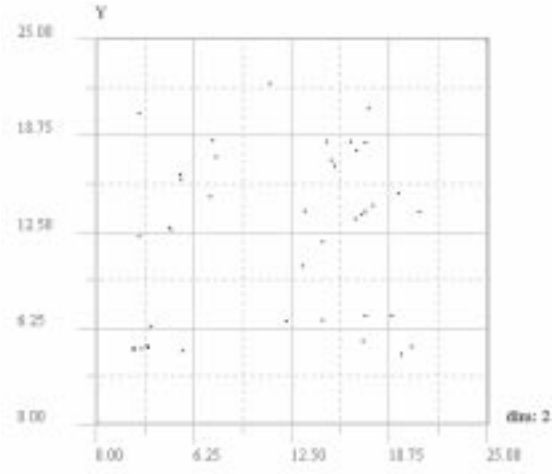
For all these minerals a simulation of cluster formation was carried out for the following conditions:

- a different number of particles in the square cell and a different radius a

- različni kot ψ uporabljenega magnetnega polja (0, 30, 60 in 90^0),
- različni elektrokinetski potencial φ_δ (10, 20 in 30 mV),
- različna gostota *B* uporabljenega magnetnega polja (od 0 do 1T) in
- različne *pH* vrednosti vodnih disperzij in drugo [9].

Celotna energija interakcije je bila izračunana za delce hematita (*N*=40 do 300) s polmerom *a*=0,5 do 5 μm, volumsko magnetno susceptibilnostjo χ=0,02 in Hamakerjevo konstanto k_H=5·10^{-20} J v kvadratni celici z dolžino stranice *A*=25 do 70 μm. Absolutna temperatura disperzije je bila nastavljena na 300 K in *pH* na 7,0.

Konvergenca je glede na prejšnje raziskave [6] naravnana na 600 premikov na delec. Izhodiščna lega delcev je bila naravnana z matriko 5 × 8. Slika 3 prikazuje lego delcev pri 10 in 600 premikih pod vplivom magnetnega polja z gostoto 0,5 T in kotom 30°.



Sl. 3.a. *Porazdelitev delcev po 10 premikih [9]*
Fig. 3.a. *Position of the particles after 10 shifts [9]*

Na sliki 3.b je razvidno nastajanje ene večje in dveh manjših gruč, ki so razporejene v smeri magnetnega polja. Iz slike ni moč neposredno ovrednotiti intenzivnosti in velikosti gruč, zato je treba rezultate analizirati z ustrezno matematično metodo. V računalniškem programu Fanny je bila uporabljena metoda logično mehke tvorbe gruč, ki je posplošitev metode delitve. Intenzivnost postopka nastajanja gruč je bila ovrednotena z normalizirano vrednostjo razdelitvenega koeficienta ($\bar{s}_{k=5}$).

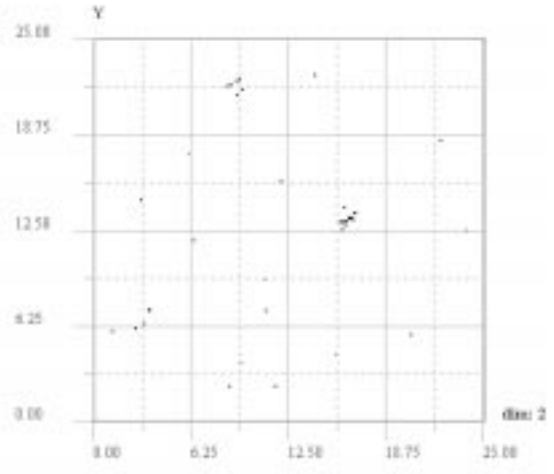
Slika 5 prikazuje intenzivnost postopka nastajanja gruč delcev hematita pri različnih elektrokinetskih potencialih in različnih kotih uporabljenega magnetnega polja.

V skladu z eksperimentalnimi rezultati [13] so učinki naprav za magnetno obdelavo vode močno odvisni od sestave obdelovanega disperznega sistema in obratovalnih razmer. Vrednost *pH* v sistemu

- a different angle ψ of the applied magnetic field (0, 30, 60 and 90^0)
- a different electrokinetic potential φ_δ (10, 20 and 30 mV)
- a different density *B* of the applied magnetic field (from 0 to 1T)
- different *pH* values of the aqueous dispersions and others [9].

The total interaction energy for the hematite particles (*N* = 40 to 300) with the radius *a*=0.5 to 5 μm the volume magnetic susceptibility χ=0.02 and the Hamaker constant k_H=5·10^{-20} J in a square unit cell with side length *A*=25 to 70 μm was computed. The absolute temperature was set to 300 K and the *pH* was set to 7.0.

According to earlier research [6], the recommended rate of convergence is up to 600 shifts per particle. The original position of the particles was set up as a 5×8 matrix. Figure 3 shows the positions of the particles after 10 and 600 shifts under a magnetic field of 0.5 T, applied at an angle of 30°.

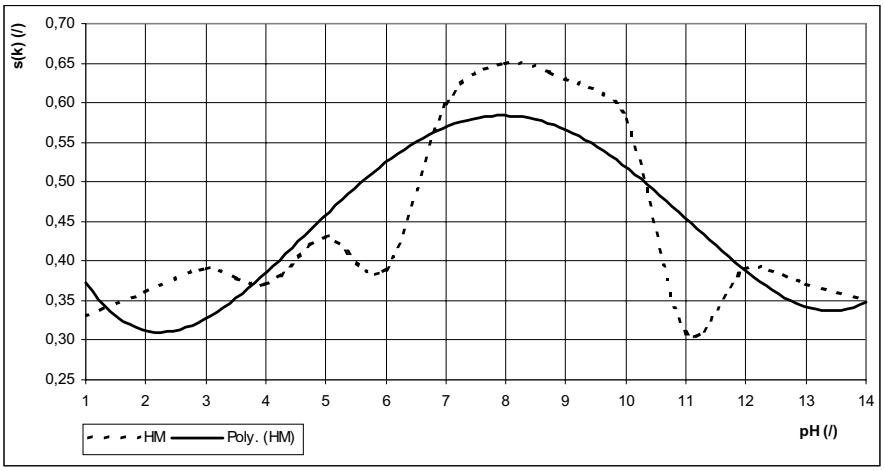


b. *Porazdelitev delcev po 600 premikih[9]*
b. *Position of the particles after 600 shifts [9]*

In Figure 3.b the formation of one major and two minor clusters is very clear, these are well aligned in the direction of the applied magnetic field. From the same figure the intensity and the size of the cluster cannot be evaluated directly, thus the results have to be analyzed with an appropriate mathematical method. The fuzzy clustering method, as a generalization of partitioning, was used in the Fanny computer program. The intensity of the cluster-formation process was measured with the value of the normalized version of the partition coefficient ($\bar{s}_{k=5}$).

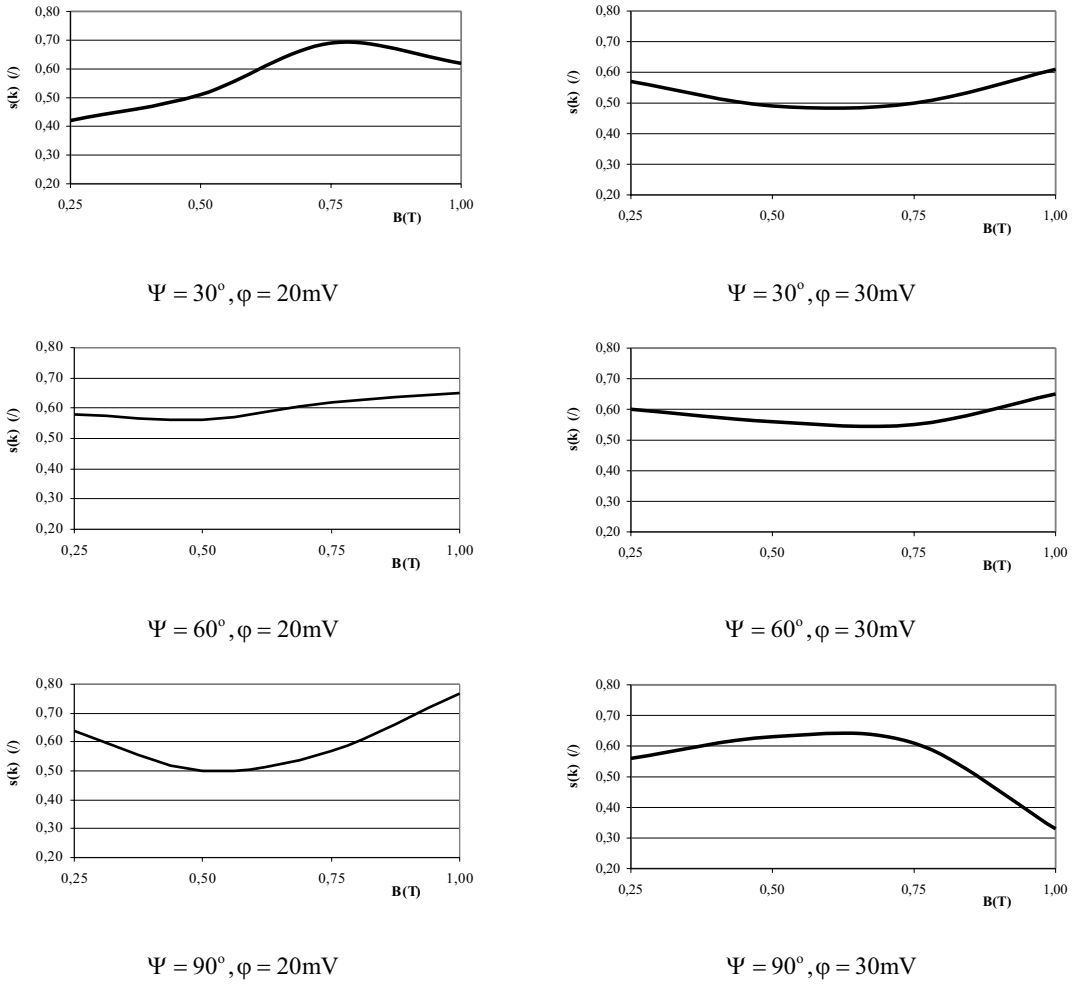
Figure 5 shows the intensity of the cluster-formation process of the hematite particles at the different electrokinetic potentials and under a magnetic field applied at different angles.

According to the experimental results [13], the effects of magnetic water-treatment devices are very dependent on the composition of the treated dispersion system and working conditions. The *pH* value of



Sl. 4. *Intenzivnost nastajanja gruč v odvisnosti od pH obdelovanega sistema in aproksimacija krivulje s polinomom druge stopnje [9]*

Fig. 4. *The intensity of the cluster-formation process versus pH and a graphical approximation with a polynomial of the second order [9]*



Sl. 5. *Intenzivnost nastajanja gruč (normalizirana vrednost Dunnovega koeficienta $\bar{s}_{k=5}$) pod vplivom zunanjega magnetnega polja gostote 0,5 T pri različnih kotih in različnih vrednostih elektrokinetskega potenciala [9]*

Fig. 5. *The intensity of the cluster-formation process (normalized version of Dunn's partition coefficient, $\bar{s}_{k=5}$) under a magnetic field of 0.5 T applied at different angles and different retardation potentials [9]*

je eden najbolj vplivnih parametrov v postopku nastajanja gruč. Za uspešno nastajanje gruč delcev hematita je optimalni *pH* v obdelovani disperziji 5,6 do 10,3 (sl. 4).

3 SKLEP

V zadnjih desetletjih je bilo opravljenih veliko raziskav na področju magnetne obdelave vode, a je še vedno vprašljiv sam mehanizem delovanja naprav za MOV. Mehanizem je zapleten in neposredno odvisen od kemične sestave vode in obratovalnih razmer naprave MOV. Zaradi slabega poznavanja mehanizma delovanja ostaja tako njihova učinkovitost naključna.

Model simulacije nastajanja gruč smo priredili za področje magnetne obdelave. Začetni izračuni so temeljili na delcih hematita. Model je utemeljen na teoriji DLVO, statistični metodi Monte Carlo Metropolis in na teoriji analize gruč. Na temelju predstavljenega modela smo z računalniškim programom simulirali in analizirali nastajanje gruč za večino snovi, ki ustvarjajo vodni kamen. Predstavljeni rezultati dobro ponazarjajo pogoje delovanja naprav za MOV ob znani kemični sestavi vode.

the system is one of the most influential parameters for the cluster-formation process. For the successful clustering of hematite particles, the optimum *pH* range of the treated dispersion is from 5.6 to 10.3 (Fig. 4).

3 CONCLUSION

Despite the large amount of research work over past decades a theoretical understanding of the MWT mechanism is still incomplete. This is the main problem when it comes to the design of efficient MWT devices. The MWT mechanism is complex and directly depends on the chemical composition of the water and the working conditions.

A theoretical model for the simulation of cluster formation with hematite particles as reference data was supplemented to the region of magnetic water-treatment. The model is based on the DLVO theory, the Monte Carlo Metropolis method and the cluster-analysis theory. Numerical calculations for most of the scale-forming minerals were done with computer programs based on the presented model. The obtained results show that the model predicts well the operational conditions for the effective use of MWT devices, providing the chemical composition of the supplied water is known.

4 OZNAČBE
4 SYMBOLS

polmer delca	a	m	radius of interacting spheres
gostota magnetnega polja	B	Vs/m^2	magnetic field density
molarna koncentracija ionov i v raztopini	c_i	mol/L	molar concentration of ions i in the solution
osnovni električni naboj (1,6·10^{-19} As)	e_o	As	electron charge (1,6·10^{-19} As)
energija medmolekularnega privlaka	E_a	J	inter-molecular attraction energy
energija elektrostatskega odboja	E_r	J	electrostatic repulsion energy
energija magnetnega privlaka	E_m	J	magnetic attraction energy
celotna energija interakcij	E_t	J	total interaction energy)
Boltzmannova konstanta (1,38·10^{-23} J/K)	k_B	J/K	Boltzmann constant (1,38·10^{-23} J/K)
Hamakerjeva konstanta	k_H	J	Hamaker constant
število delcev	N		number of particles
Avogadrovo število delcev (6,022·10^{23}/mol)	N_A	1/mol	Avogadro number of particles (6,022·10^{23}/mol)
faktor po enačbi (8)	P		factor by equation (8)
razdalja med središčema delcev	R	m	distance between centers of particles
razmerje med razdaljo R in polmerom a	s		ratio between distance R and radius a
absolutna temperatura	T	K	absolute temperature
koordinati lege delca	x,y	m	coordinates of particle's position
valenca iona	z_i		valence of ion i
magnetna susceptibilnost minerala	χ	m	magnetic susceptibility of the mineral
dielektrična konstanta vakuuma (8,85·10^{-12} As/Vm)	ε_0	As/Vm	dielectric constant of vacuum (8,85·10^{-12} As/Vm)
relativna dielektrična konstanta vode	ε_r		relative dielectric constant of water
elektrokinetski potencial na trdni površini	φ_δ	V	electrokinetic potential at a solid surface
Debye-Hückelov parameter	κ	1/m	Debye-Hűckel parameter
magnetna permeabilnost vakuuma (4π·10^{-7} Vs/Am)	μ_0	Vs/Am	magnetic permeability of vacuum (4π·10^{-7} Vs/Am)
kot med magnetnim momentom delca in uporabljenim magnetnim poljem	θ	rad	angle between the magnetic moment of the particle and the applied magnetic field
naključna vrednost med 0 in 1	ξ		random number from 0 to 1
kot delovanja zunanjega magnetnega polja	ψ	rad	angle of the external magnetic field

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Prejeto: 6.3.2002
Received:

Sprejeto: 22.11.2002
Accepted: