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RESEARCH ARTICLE

MODELLING AND NUMERICAL SIMULATION OF THE FLOCCULATION PROCESS

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Abstract:

The paper deals with a mathematical model and a numerical simulation procedure for the flocculation process, using usual parametrization solutions of the collision frequency and particle fragmentation rate. The results obtained through numerical simulation have shown a high sensitivity of the model with respect to the flocs strength that intervenes in the expression of the fragmentation rate. It has been illustrated the possibility of the flocculation process control through the fluid stirring, that determines the speed gradient that occurs in the expression of the collision frequency.

Keywords: Mathematical modelling, flocculation process, numerical simulation.

Introduction

The flocculation process is important in many fields as biotechnology, colloidal and polymer technologies etc (Han *et al.*, 2003). Liquid-solid separation processes are common in biotechnology where is the question of the separation cells from suspending medium. In all applications where the flocculation processes intervene, the synthetic polymeric flocculants are used. The synthetic polymeric flocculants are added in liquid medium in order to destabilize the suspension and promote flocculation. In the biotechnology field positively charged flocculants are commonly used, because the cells are negatively charged (Han *et al.*, 2003).

Flocculation process modelling issue is widely approached in literature (Ahmad *et al.*, 2008), (Coufort *et al.*, 2007), (Runkana *et al.*, 2006). Within these models the main phenomena that appear in the mentioned process are mathematically described: aggregation – which produces the increase of the flocculants dimension – and the flocculants fragmentation. The aggregation and fragmentation rates depend on the flocculants dimension and the permanent regime establishes to the balance of the two rates.

Within this paper the results obtained through numerical simulation of the flocculation process are presented. The objective followed in the present paper was to highlight the influence of physical measurements that affect the process efficiency, from the control point of view.

Materials and methods

The mathematical description of the flocculation process is based on the classic model PBM (Population Balance Model) introduced by Smoluchowski, that describes the aggregation-

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fragmentation processes of the suspensions. The two processes are incorporated into the PBM through the following integro-differential equation with partial derivatives:

$$\frac{\partial n(v,t)}{\partial t} = \frac{1}{2}\int_0^v n(v-u)n(u,t)Q(v-u,u)\mathrm{d}u - \\ - n(v,t)\int_0^\infty n(u,t)Q(v,u)\mathrm{d}u + \\ + \int_v^\infty \gamma(v,u)\Gamma(u)n(u,t)\mathrm{d}u - \Gamma(v)n(v,t) \tag{1}$$

In this equation n is the flocculants concentration [number/volume unit], v and u represent the particle volume, t is the current time in the flocculation process. The time evolution of the particle concentration with the volume v, $n(v,t)$, is obtained from the four sub-processes that are described by the four terms from the right side of equation (1). The first term expresses the occurrence rate of the particles of the volume v, obtained through the particle aggregation of the volume u and $v-u$. This yield rate depends on the function $Q(u,v)$, named aggregation core of the flocculants of volume u and v. The second term describes the decreasing rate of particles of volume v, as a consequence of the aggregation of these particles of volume v with other particles. This rate also depends on the aggregation rate of flocculants, $Q(u,v)$. The third term expresses the producing rate of particles of volume v, resulted from the particle fragmentation of volume greater then v. In the expression of this rate two functions intervene: $\Gamma(v)$ and $\gamma(v,u)$. The first function represents the fragmentation frequency of the flocculants of volume v, and $\gamma(v,u)\mathrm{d}v$ is the flocculants number that is created in the domain of volume [v, v + dv] through the flocculants fragmentation of volume u. The last term expresses the decreasing rate of the particles of volume v, following the events of fragmentation of these particles.

When the aggregation is generated by the speed gradients caused by the stirring (mixing), the general expression of the aggregation core, $Q(u,v)$, is (Coufort *et al.*, 2007):

$$Q(u,v) = 0.31\sqrt{\frac{\varepsilon}{\nu}}\left(u^{1/3}+v^{1/3}\right)^3 \tag{2}$$

where ε is the dissipation rate of turbulence kinetic energy, and ν is the kinematic viscosity of the liquid.

PBM model is often written in a form different from (1) by expressing the aggregation core as a product of the following shape:

$$Q(v,u) = \alpha(v,u).\beta(v,u) \tag{3}$$

where $\alpha(v,u)$ is called efficiency factor of the collision, and $\beta(v,u)$ is the frequency factor of the collision. Based on these variables, the model is as follows:

$$\frac{\partial u(v,t)}{\partial t} = \frac{1}{2}\int_0^v n(v-u)n(u,t)\alpha(v-u,u)\beta(v-u,u)\mathrm{d}u \\ -n(v,t)\int_0^\infty n(u,t)\alpha(v-u,u).\beta(v-u,u)\mathrm{d}u + \\ + \int_v^\infty \gamma(v,u)\Gamma(u)n(u,t)\mathrm{d}u - \Gamma(v)n(v,t) \tag{4}$$

PBM model written in this form allows a more detailed approach of the aggregation process, through a variety of parameterization procedures of collision efficiency and collision frequency factors.

For numerical simulation of the flocculation process the discrete model of the process is used. It is assumed that the initial condition is known:

$$n(v,0) = n^{in}(v) \tag{5}$$

as is the dimension field [0,v_{max}] of the particle volume. In accordance with fixed pivot technique – FPT introduced by Kumar (Kumar and Ramkrishna, 1996), the continuous interval [0,v_{max}] is divided in a reduced number of cells:

$$\Lambda_i = \left[v_{i-1/2}, v_{i+1/2}\right], i = 1,\ldots,I \tag{6}$$

where

$$v_{1/2} = 0, \quad v_{I+1/2} = v_{\max}, \quad \Delta v_i = v_{i+1/2} - v_{i-1/2} \le \Delta v \tag{7}$$

and Δv is given. For every field is considered the center

$$v_i = (v_{i-1/2} - v_{i+1/2})/2 \tag{8}$$

which is called *pivot* or *grid point*. Such a partitioning of the spatial domain is known as a

cell-centered representation. Figure 1 illustrates a typical partitioning of the domain [0,v_{max}] through centered cells.

Based on this procedure of dimension discretization, the integro-differential equation with partial derivatives (1) is transformed into an ordinary differential equations system. From integro-differential equation with partial derivatives (4), through discretization, the model is obtained as ordinary differential equations:

$$\frac{dv_i}{dt} = \frac{1}{2}\sum_{j+k=i}\alpha_{jk}\beta_{jk}v_j v_k - v_i\sum_{k=1}^{max}\alpha_{ik}\beta_{ik}v_k + \sum_{j=i+1}^{max}\gamma_{ij}S_j v_j - S_i v_i \quad (9)$$

where v_i, v_j, v_k, represent the volume ratio of the particles of size *i, j and k respectively*; α_{jk} is the collision efficiency between two particles j and k ; β_{jk} is the collision frequency between the particles j and k; S_j is the fragmentation rate of the particles of size j; $\gamma_{i,j}$ is the function of size i fragment distribution that come from the particles of size j.

The equation (9) can be expresses with respect to the ratio of size i particle number:

$$\frac{dN_i}{dt} = \frac{1}{2}\sum_{j+k=i}\alpha'_{jk}\beta'_{jk}N_j N_k - N_i\sum_{k=1}^{max}\alpha'_{ik}\beta'_{ik}N_k + \sum_{j=i+1}^{max}\gamma'_{i,j}S'_j N_j - S'_i N_i \quad (10)$$

where notations are similar to the ones of the previous model, except that N_i is the concentration of the particle number from the section i [in no./cm^3].

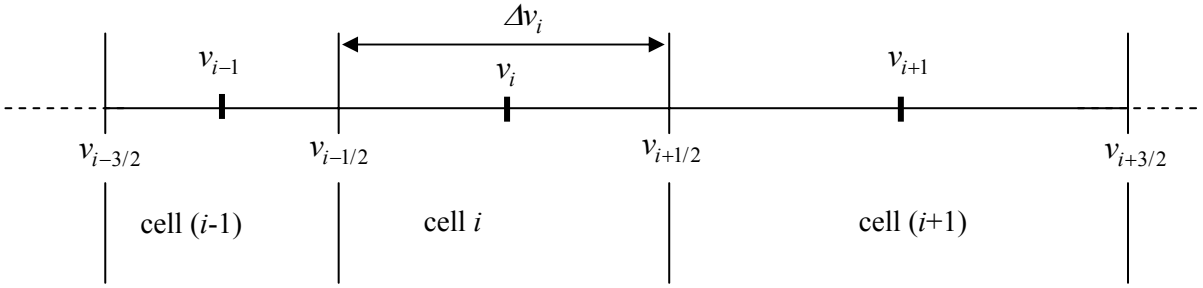

Figure 1. Discretization of the particle dimensions

Results and Discussions

For numerical simulation of the process in a given applicative context, it is necessary the parameterization of the collision efficiency, α_{jk}, collision frequency, β_{jk}, and fragment distribution, γ_{ij}. These variables depend on the particle nature but the nature and moving speed of the fluid too. In (Han *et al.*, 2003) is presented a survey regarding the expressions used for α_{jk}, β_{jk} and γ_{ij} in different applications. The variety of these parametrization expressions illustrates a very important idea: concretization of the discretized model, given by the equations (9) or (10) in numerical simulation purpose requires the selection of the parametrization type and the numerical coefficients that intervene in the selected functions in accordance with the physical properties of the simulated system. Further on a "nominal" version of the model, in which relatively simple assumptions and frequently cited in literature are allowed, is considered.

For each section is defined a characteristic volume, v_i, which is the average volume of the particles contained in the section. The volume v_i is

$$v_i = \frac{b_{i-1} + b_i}{2} \quad (11)$$

where b_i represents the superior limit volume of the section i. On the other hand, the volume v_i is a function of previous volume, v_{i-1}:

$$v_i = f\, v_{i-1} \quad (12)$$

Accordingly to the data that can be found in many works [4,5,6] (Kumar and Ramkrishna, 1996), (Runkana *et al.*, 2006), (Spicer and Pratsinis, 1996), it was considered f = 2. Moreover, if it is admitted that α_{ij}=α, it could be shown that the model (10), that offers the distribution of the

particle number of size i, can be written as equation (5):

$$\frac{dN_i}{dt} = \sum_{j=1}^{i-2} 2^{j-i+1} \alpha\beta_{i-1,j} N_{i-1} N_j + \\ + \frac{1}{2} \alpha\beta_{i-1,i-1} N_{i-1}^2 - N_i \sum_{j=1}^{i-1} 2^{j-i} \alpha\beta_{i,j} N_j - \\ - N_i \sum_{j=i}^{i_{max}} \alpha\beta_{i,j} N_j - S_i N_i + \sum_{j=i}^{i_{max}} \gamma_{i,j} S_j N_j \quad (13)$$

The number of differential equations of the model is equal to the number of sections. In the following the numerical simulation has been achieved using 30 sections, for i = 1,.., i_{max} , where i_{max} = 30. In the assumptions considered in the paper, the volume v_i is

$$v_i = v_1 2^{i-1} \quad (14)$$

where v_1 is the volume of the primary particle.

Since it was adopted the collision efficiency $\alpha_{ij} = \alpha$, it results that the collision frequency, β_{ij}, reflect, to the constant α, the aggregation core. Having in view the equation (2) of the aggregation core, a similar equation for the collision frequency from the discretized model of form (5) is obtained:

$$\beta(v_i, v_j) = 0.31G(v_i^{1/3} + v_j^{1/3})^3 \quad (15)$$

where G is the spatial average speed gradient. Obviously the variable G can be adopted as a parameter, because it can be also modified (in real time) through physical implementation of the system in which the flocculation process is achieved.

The fragmentation rate in section i is a function of the particle volume, v_i:

$$S_i = A v_i^a \quad (16)$$

where a = 1/3 (Spicer and Pratsinis, 1996). The parameter A is a coefficient of the burst rate for the fragmentation induced by the fluid movement. This parameter is calculated using equation (5):

$$A = A' G^y \quad (17)$$

where y is a constant inversely proportional with flocs strength and A' is a constant that is experimentally determined.

For the distribution function of the fragments, γ_{ij}, the parametrization solution can be adopted from a large number of variants, depending on the dominant fragmentation mechanism. Usually two mechanisms can be admitted: a) *primary particle erosion*, when small fragments detaches from the flocs surface, and b) *flocculants breakage*. The erosion results when the fluid turbulences are comparable with the flocculants dimension. The breakage mechanisms occur as a consequence of the differential pressure that is applied on the opposite sides of the flocculants. In (Spicer and Pratsinis, 1996) three distinct expressions of the fragment distribution function have been admitted: binary, ternary and normal breakage. Further on the binary breakage was considered, when from the initial flocculants two fragments with the same volume are obtained. In this case,

$$\gamma_{i,j} = \frac{v_j}{v_i} \quad (18)$$

and in (13) it can be considered $i_{max} = i+1$.

In numerical simulation of the flocculation process the discretized mathematical model (13) was adopted, in which the following parameters were used: A'= 0.0047; y = 1.6; α = 1 ; G = 150 s^{-1}; the primary particle size d_1 = 2.17μm, the maximum number of pivots i_{max} = 30. The initial values of the state vector N_i were established as following: N_1 = 9.3x10^6 [no./cm^{-3}], N_i = 20/1.2^i [no./cm^{-3}], i = 2,..., i_{max} . Therefore a hypothetical situation was considered, in which the particle concentration is large at the primary particle level, and for the rest of sections, i = 2,..., i_{max}, the considered concentration is significantly less.

Figure 2 presents the time evolution of the cell number $N_i(t)$, i=2,...i_{max}, for the mentioned numerical values of the model parameters. In Figure 3 the distributions N_i at different moments within the interval [0 6000s] were represented. The distribution was represented as a function of the ratio d_i/d_1, where d_i, $i=\overline{2,i_{max}}$ is the particle diameter from section i. The ratio between the average diameter of the particle and d_1 is d_{mean}/d_1=25.37.

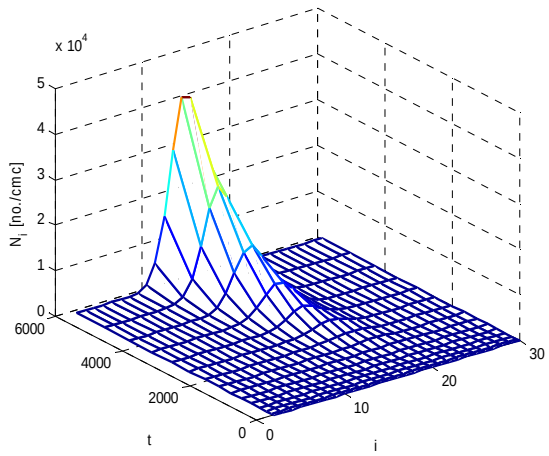

Figure 2. *Distribution $N_i(t)$, $i=2,...i_{max}$*

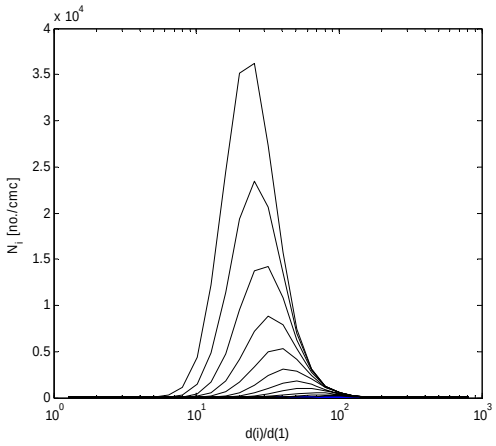

Figure 3. *Distribution N_i as a function of d_i/d_1 at different moments (G=150)*

In the flocculation process model, the collision frequency influence both aggregation and fragmentation of flocculants. It has a dominant influence at beginning of the flocculation process, when the aggregation subprocess is dominant. Analysing the equation (15), which gives the collision frequency, it results that the speed gradient G, caused by the fluid movement, has an important influence on the aggregation. This fact is illustrated in Figure 4, where the distribution N_i as a function of d_i/d_1 at different moments, when G=100 is presented. Unlike the situation when G = 150 (Figure 3), it can be noticed a reduction of the number of the formed particles, but their diameter increases: d_{mean}/d_1=46. For G=50 the results presented in Figure 5 are obtained and d_{mean}/d_1=90.66. The results presented in Figures 3, 4 and 5 illustrate the usefulness of adopting a time variable regime for the liquid stirring, so that a large value of the gradient G results at the process beginning, in order to facilitate the aggregation process. Then will result a lower value of the gradient G to avoid the excessive increasing of the fragmentation process rate. Figure 6 presents the distribution N_i as a function of d_i/d_1 at different moments, when G(t)=200, t=[0,1600) and G(t)=50, t=[1600,6000]. In this case is obtained d_{mean}/d_1=44.23, so a similar process with the one in which G=100 in all the time interval [0 6000] is obtained.

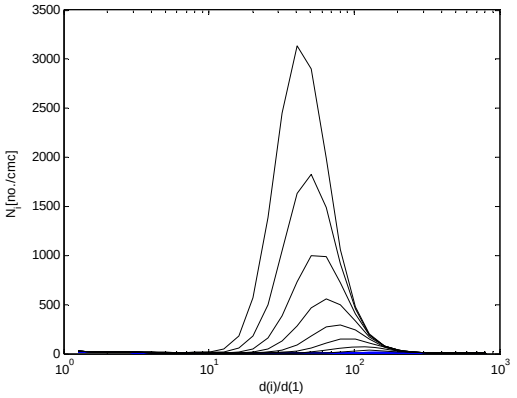

Figure 4. *Distribution N_i as a function of d_i/d_1 at different moments (G=100)*

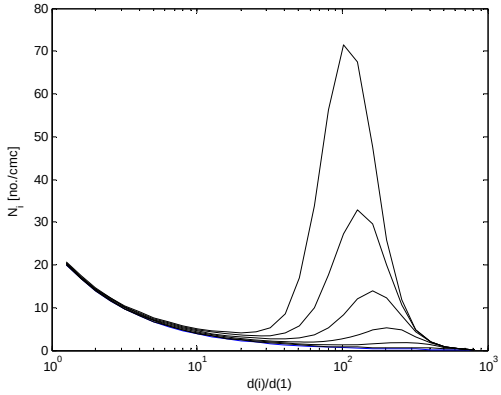

Figure 5. *Distribution N_i as a function of d_i/d_1 at different moments (G=50)*

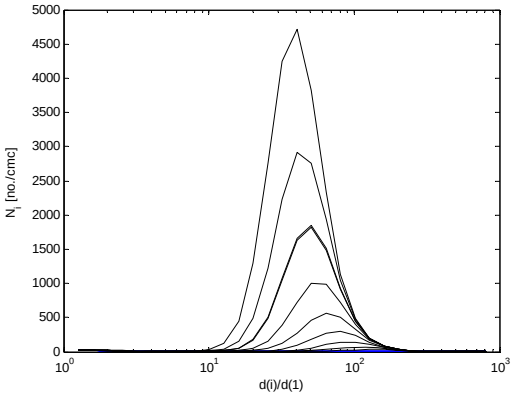

Figure 6. *Distribution N_i as a function of d_i/d_1 at different moments G(t)=200, t=[0,1600); G(t)=50, t=[1600,6000]*

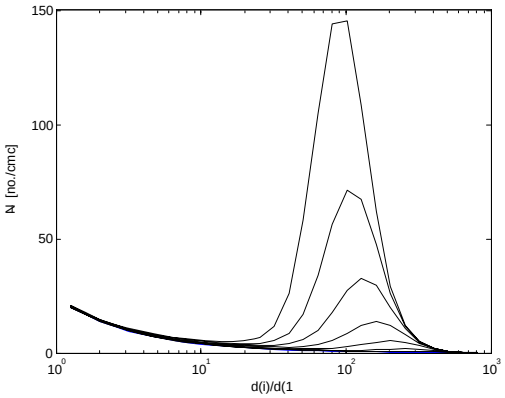

Figure 7. *Distribution N_i as a function of d_i/d_1 at different moments G=100, y=1.42*

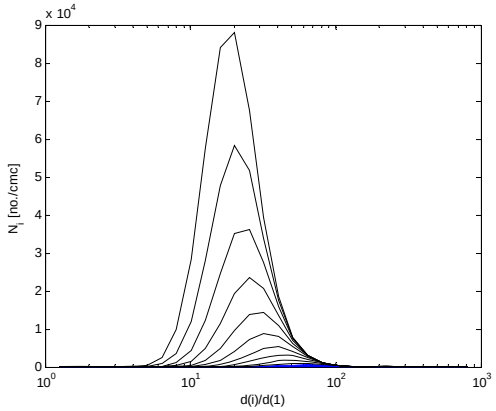

Figure 8. *Distribution N_i as a function of d_i/d_1 at different moments G=100, y=1.78*

The fragmentation rate has an important weight in the flocculation process dynamics. This is influenced by parameters *A'* and *y*, that depends – for the most part – on the nature of the particles in suspension. Accordingly to equation (5), the variation domain of the parameter *y* is [1.42...1.78]. In order to illustrate the model sensitivity with respect to parameter *y*, Figures 7 and 8 presents the distributions N_i for *y*=1.42 and *y*=1.78 respectively. It can be noticed that in this time the flocs strength is large, that means *y* is small, the flocculants concentration is reduced and their dimension is large: d_{mean}/d_1=83.7. When *y*=1.78, the fragmentation rate is large, the particle number is also large, but it results d_{mean}/d_1=21.37.

Conclusions

The flocculation process dynamics is dependent on the parametrization modality of the collision frequency, β_{ij}, and the fragmentation rate of particles. The simulation results have shown high sensitivity of the model with respect to parameter *y*, that intervenes in the expression of the fragmentation rate. Since this parameter mostly depends on the nature of the particles in suspension, for the control of the flocculation process can be used, besides the flocculants dosing, the stirring speed of the fluid, which determines the variable *G* from the collision frequency expression. The results of the numerical simulation have shown the usefulness of adopting a control strategy in order impose a large stirring speed in the initial period and a lower speed in the final part of the process. The numerical simulation of the process could be a useful tool for establishing this strategy.

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