



CERENKOV RADIATION SIMULATION IN THE AUGER WATER GROUND DETECTOR

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ABSTRACT: The simulation of response of the Auger water Cerenkov ground detector to atmospheric shower muons is practically needed for the experimental research of cosmic rays at extreme energies. We consider here a simulation model for the process of emission and diffusion of Cerenkov photons concerned with muons moving through the detector volume with the velocity greater than the phase velocity of light in the water on purpose to define photons producing signal in the detector.

INTRODUCTION

In 1962 one observed cosmic rays with energy approximate to 10^{20} eV. In 30 subsequent years 8 extensive atmospheric showers with energy exceeding 10^{20} eV were observed. How is it possible to explain the existence of these extraordinarily energetic cosmic rays. This is a scientific mistery which there have not been reliable schemes for explaining. If understood the source and nature of extremely high energy cosmic rays are, we will lead to new discoveries or in the fundamental physics or in the astrophysics.

In recent years the interest in cosmic rays at extreme energies has increased rapidly. The experimental study of such cosmic rays will be carried out within the framework of the international Pierre Auger project with Auger observatories of a hybrid design including fluorescence detectors used to observe the longitudinal development of showers in the atmosphere and water Cerenkov ground detector arrays to sample the lateral density distribution on the ground level [1, 2].

The simulation of response of the water Cerenkov ground detector to atmospheric shower muons is practically needed for the experimental research of extremely high energy cosmic rays. In this paper we have developed a simulation model for the process of emission and diffusion of Cerenkov photons concerned with muons passing through the detector volume with the velocity greater than the phase velocity of light in the water on purpose to define photons producing signal in the detector.

SIMULATION MODEL FOR GENERATION AND RAY-TRACE OF CERENKOV PHOTONS IN THE AUGER WATER GROUND DETECTOR

The Auger water Cerenkov ground detector considered in our model is a $10\text{m}^2 \times 1.2\text{m}$ deep cylindrical volume of water, lined with a diffusely reflective white material, and viewed vertically from above by 3 photomultiplier tubes (pmts) $\approx 200\text{mm}$ in diameter. The detector geometry is illustrated on figure 1.

For simulation, the pmts are approximated as circular areas in the plane of the detector top surface with area equal to the effective area of 200mm pmts (530cm^2).

When an atmospheric shower muon strikes the top surface of the detector and moves through its volume with the velocity greater than the phase velocity of light in the water the Cerenkov photons are emitted. These Cerenkov photons are the optical photons. Passing through the water they undergo three kinds of interaction: Rayleigh scattering, absorption, and water boundary interaction (absorption and reflection).

However, as the water contained in the detector volume is purified, it may be considered as an optically homogenous medium and therefore the Rayleigh scattering is negligible.

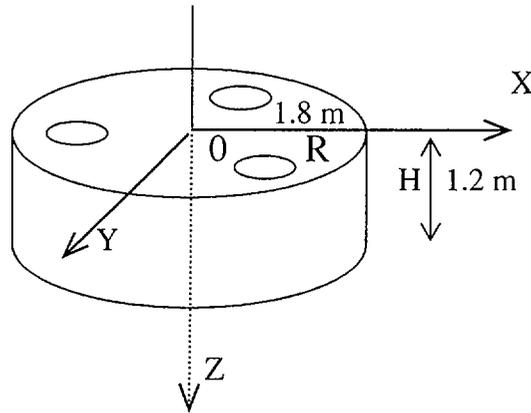


Figure 1. Illustration of the Auger water ground detector geometry

The motion of the atmospheric shower muon through the detector volume accompanied by the processes: the energy loss for ionization and atomic excitation, the bremsstrahlung, the direct pair $e^+ e^-$ production. The Monte-Carlo algorithms for simulation of the bremsstrahlung and direct pair $e^+ e^-$ production processes have been analyzed in detail by us in [3]. However, at energies smaller than 2 TeV (the energies which most of atmospheric shower muons have on the ground level) the ionization and excitation of atoms are the main mechanism and both the bremsstrahlung and direct pair $e^+ e^-$ production processes may be neglected. The simulation of the generation and diffusion of Cerenkov photons concerned with the muon moving in the detector volume can be carried out then based on the simulation algorithms developed by us as follows :

1. Calculating the characteristics of the considered muon: coordinates of its position $(X_{0\mu}, Y_{0\mu}, Z_{0\mu})$, the moving direction $(\varphi_\mu, \theta_\mu)$, energy (E_μ) .

2. Calculating the threshold energy for Cerenkov radiation emission according to the coherent condition: $n\beta > 1$

$$E_{thres} = \frac{E_0}{\left(1 - \frac{1}{n^2}\right)^{\frac{1}{2}}} \quad (1)$$

where E_0 - the muon energy at rest, n - the refractive index of the water, $\beta = v/c$.

3. Checking whether the muon's energy E_μ is greater than the threshold energy for Cerenkov radiation emission E_{thres} or not. If $E_\mu \leq E_{thres}$, the calculation with the considered muon is ceased and then the operations are passed to performing with a new muon (when a number of given muons, N_μ , remains in the memory of the computer) by returning to 1. Otherwise, go to 4.

4. Advancing the muon a rather small step, Δl , along its moving direction

5. Verifying whether the final point of Δl is inside the detector volume or not by calculating its coordinates :

$$\begin{aligned}
 X_{\mu} &= X_{0\mu} + \Delta l \sin \theta_{\mu} \cos \varphi_{\mu} \\
 Y_{\mu} &= Y_{0\mu} + \Delta l \sin \theta_{\mu} \sin \varphi_{\mu} \\
 Z_{\mu} &= Z_{0\mu} + \Delta l \cos \varphi_{\mu}
 \end{aligned}
 \tag{2}$$

If the final point of Δl is outside the detector volume, the calculation is finished with the given muon. Otherwise, go to 6.

6. Calculating Cerenkov radiation energy on Δl

$$\Delta E_c = \frac{dE_c}{dl} \times \Delta l \tag{3}$$

Here

$$\frac{dE_c}{dl} = \frac{4\pi^2 z^2 e^2}{c^2} \int_{v_{\min}}^{v_{\max}} v \left(1 - \frac{1}{n^2 \beta^2} \right) dv = \frac{2\pi^2 z^2 e^2}{c^2} \left(1 - \frac{1}{n^2 \beta^2} \right) (v_{\max}^2 - v_{\min}^2)$$

and $v_{\min} \div v_{\max}$ is the frequency band within which the detector is sensitive.

7. Calculating the number of Cerenkov photons emitted on Δl . The average number of Cerenkov photons produced on Δl is defined by:

$$N_c = \frac{dN_c}{dl} \times \Delta l \tag{4}$$

Here

$$\frac{dN_c}{dl} = \frac{z^2 e^2}{\hbar^2 c^2} \int_{E_{c \min}}^{E_{c \max}} \left(1 - \frac{1}{n^2 \beta^2} \right) dE_c \approx 370 z^2 \left(1 - \frac{1}{n^2 \beta^2} \right) (E_{c \max} - E_{c \min})$$

Then the number of Cerenkov photons given off on Δl is calculated according to the Poisson distribution

$$P(n) = e^{-N_c} \times \frac{N_c^n}{n!} \tag{5}$$

by the simulating formula $n = k$, here k is the least whole number taken so as to satisfy the in-equality:

$$\sum_{i=1}^{k+1} \frac{1}{N_c} \ln(1 - \alpha_i) > 1$$

with the random numbers α_i uniformly distributed on $(0,1)$.

Each Cerenkov photon generated on Δl is simulated then, in turn, as follows:

a. Calculating the emission angle of photons produced on Δl

$$\cos \omega = \frac{1}{n\beta} \tag{6}$$

b. Calculating the azimuthal emission angle of a photon emitted on Δl . It is chosen at random from the uniform distribution on $(0,2\pi)$ according to the formula $\varphi = 2\pi\alpha$, α - a random number uniformly distributed on $(0,1)$.

c. Calculating the flight direction of a Cerenkov photon in the Cartesian perpendicular fixed coordinate system

$$\begin{aligned}
 u_c &= u_\mu \cos \omega - (v_\mu \sin \varphi + u_\mu w_\mu \cos \varphi) \left(\frac{1 - \cos^2 \omega}{1 - w_\mu^2} \right)^{\frac{1}{2}} \\
 v_c &= v_\mu \cos \omega + (u_\mu \sin \varphi - v_\mu w_\mu \cos \varphi) \left(\frac{1 - \cos^2 \omega}{1 - w_\mu^2} \right)^{\frac{1}{2}} \\
 w_c &= w_\mu \cos \omega + (1 - w_\mu^2) \cos \varphi \left(\frac{1 - \cos^2 \omega}{1 - w_\mu^2} \right)^{\frac{1}{2}}
 \end{aligned} \tag{7}$$

Here u_c, v_c, w_c , are the components of the unit vector directing the photon's flight. They are defined as follows:

$$u_c = \sin \theta_c \cos \varphi_c, \quad v_c = \sin \theta_c \sin \varphi_c, \quad w_c = \cos \theta_c \tag{8}$$

Also for the muon:

$$u_\mu = \sin \theta_\mu \cos \varphi_\mu, \quad v_\mu = \sin \theta_\mu \sin \varphi_\mu, \quad w_\mu = \cos \theta_\mu \tag{9}$$

d. Calculating the energy of an emitted photon. As the energy of generated photons has the distribution density function

$$f(E_c) = 1 - \frac{1}{n^2 \beta^2}$$

it may be simulated according to the formula $E_c = E_{c \min} + \alpha(E_{c \max} - E_{c \min})$, here α is a random number uniformly distributed on (0,1).

e. Calculating the absorption free pathlength of a Cerenkov photon.

Each generated Cerenkov photon may travel a free pathlength before it is absorbed. As this free pathlength has the probability distribution density function

$$P(l_a) = \frac{1}{l_A} e^{-\frac{l_a}{l_A}} \tag{10}$$

it may be selected at random by solving the equation

$$\int_0^{l_a} \frac{1}{l_A} e^{-l/l_A} dl = \alpha \tag{11}$$

or $l_a = -l_A \ln(1 - \alpha)$. Here l_A is the mean absorption free pathlength dependent on the energy of the photon, α is a random number uniformly distributed on (0,1).

After the random selection of the considered photon's absorption free pathlength it is needed to verify whether its final point is inside the detector volume or not by calculating the coordinates of this final point:

$$\begin{aligned}
 X &= X_\mu + l_a \sin \theta_c \cos \varphi_c \\
 Y &= Y_\mu + l_a \sin \theta_c \sin \varphi_c \\
 Z &= Z_\mu + l_a \cos \varphi_c
 \end{aligned} \tag{12}$$

If the final point of the absorption free pathlength is inside the detector volume, the photon is absorbed in the water. Otherwise, the photon hits a detector surface, we have to consider then, in turn, the following situations possible to occur :

- If $Z \leq 0$ and $X^2 + Y^2 < R^2$ the photon strikes the detector top surface.
- If $Z \leq 0$ and $X^2 + Y^2 > R^2$ then giving $Z_c = 0$ and calculating

$$X_c = X_0 + l_c \sin \theta_c \cos \varphi_c, \quad Y_c = Y_0 + l_c \sin \theta_c \sin \varphi_c$$

Here X_c, Y_c, Z_c are the coordinates of the intersecting point of the ray traced along the photon's direction with the plane including the detector top surface, l_c is the distance from the initial position of the photon to this intersecting point.

We need to verify the condition $X_c^2 + Y_c^2 < R^2$. If this condition is realized, the photon hits the detector top surface. Otherwise, the photon strikes the detector sideward surface.

- If $Z \geq H$ and $X^2 + Y^2 < R^2$ the photon hits the detector bottom surface.
- If $Z \geq H$ and $X^2 + Y^2 > R^2$ the treatment is made then in such a similar way as for the case $Z \leq 0$ and $X^2 + Y^2 > R^2$
- If $0 < Z < H$ and $X^2 + Y^2 > R^2$, the photon strikes the detector sideward surface.

Now we shall consider the separate concrete cases where the photon hits a detector surface.

The first case is associated with the fact that the photon strikes the top detector surface. Then we must define the coordinates of the hitting point (X_c, Y_c, Z_c) and verify the following conditions :

$$\begin{aligned} (X_c - X_{pmt_1})^2 + (Y_c - Y_{pmt_1})^2 &< R_{pmt}^2 \\ (X_c - X_{pmt_2})^2 + (Y_c - Y_{pmt_2})^2 &< R_{pmt}^2 \\ (X_c - X_{pmt_3})^2 + (Y_c - Y_{pmt_3})^2 &< R_{pmt}^2 \end{aligned} \quad (13)$$

where $X_{pmt_1}, Y_{pmt_1}, X_{pmt_2}, Y_{pmt_2}, X_{pmt_3}, Y_{pmt_3}$ are the coordinates of the center of pmts, respectively, and R_{pmt} is their radius.

If one of three abovementioned conditions is realized, the photon hits a pmt and is absorbed here. Otherwise, it is necessary to verify the condition $P_a > \alpha$, here P_a is the probability that the photon is absorbed in the detector wall, α is a random number uniformly distributed on (0,1). When this condition is satisfied, the photon is absorbed in the detector top surface's wall and the operations are passed to performing with a new photon by returning b. or going to 8 if there is not any photon in the memory of the computer.

For the case where the photon is not absorbed, it will be reflected back into the detector volume. The photon's direction after the reflection may be defined by the perfect reflection condition: $\cos \theta_{\text{cref}} = -\cos \theta_c, \sin \theta_{\text{cref}} = \sin \theta_c, \varphi_{\text{cref}} = \varphi_c$

The second case corresponds to the fact that the photon hits the detector bottom surface. This case is treated in such a similar way as the first case.

The third case is related to the fact that the photon strikes the detector sideward surface. The photon's fate is treated here as well as in the first and second cases. However, the coordinates of the hitting point in this case are calculated by solving the system of equations :

$$\begin{aligned} X_c &= X_0 + l_c \sin \theta_c \cos \varphi_c \\ Y_c &= Y_0 + l_c \sin \theta_c \sin \varphi_c \\ Z_c &= Z_0 + l_c \cos \theta_c \\ X_c^2 + Y_c^2 &= R^2 \end{aligned} \quad (14)$$

The solution of the above mentioned system of equations gives

$$l_c = \frac{-c + \sqrt{c^2 + R^2 - X_0^2 - Y_0^2}}{\sin \theta_c} \quad (15)$$

where $c = X_0 \cos \varphi_c + Y_0 \sin \varphi_c$

As far as the photon's direction is concerned upon being reflected back into the detector volume at the hitting point, it may be calculated according to the perfect reflection condition:

$$\begin{aligned} \theta_{cref} &= \theta_c \\ \cos \varphi_{cref} &= -\frac{1}{R^2} \left[(X_c^2 - Y_c^2) \cos \varphi_c + 2X_c Y_c \sin \varphi_c \right] \\ \sin \varphi_{cref} &= \frac{1}{R^2} \left[(X_c^2 - Y_c^2) \sin \varphi_c - 2X_c Y_c \cos \varphi_c \right] \end{aligned} \quad (16)$$

Thus, passing through the detector volume of water the Cerenkov photon may hit the detector walls many a time and be reflected from them. The process of reflection proceeds until the photon will be absorbed or in the water or in the detector walls. The simulation is passed then to performing with subsequent photons.

After all the photons emitted on a step Δl are simulated, the operations are passed to 8

8. Calculating the energy losses for ionization by the muon on Δl

$$\Delta E_{ion} = \frac{dE_\mu}{dl} \times \Delta l \quad (17)$$

Here $\frac{dE_\mu}{dl} = \rho Z^2 \frac{L}{\beta^2} (B_M + 0.69 + 2 \ln \beta\gamma - 2\beta^2 - \delta)$

$$B_M = \ln \left(\frac{m_e c^2 w_{max}}{I^2} \right) \quad (18)$$

$$W_{max} = \frac{2\beta^2 \gamma^2 m_e c^2}{1 + \frac{2\gamma m_e}{m_\mu} + \frac{m_e^2}{m_\mu^2}} \quad (19)$$

$$\gamma = \frac{E_{\mu}}{m_{\mu}} \quad (20)$$

$$\delta = \begin{cases} 0 & \text{if } y \leq y_0 \\ 2y \ln 10 + c + a(y_1 - y)^b & \text{if } y_0 < y \leq y_1 \\ 2y \ln 10 + c & \text{if } y > y_1 \end{cases}$$

where $Y = \lg \beta \gamma \quad (21)$

For the water we have [4]

$$\begin{aligned} I &= 74.1 \text{ eV}, & L &= 0.0853 \text{ MeV cm}^2/\text{g}, & -c &= 3.47 \\ a &= 0.519, & b &= 2.69, & y_1 &= 2, & y_0 &= 0.23 \end{aligned}$$

9. Calculating the remaining energy of the muon at the end of Δl

$$E_{\mu}' = E_{\mu} - \Delta E_c - \Delta E_{ion} \quad \text{and then return to 3.}$$

It should be noted that the calculation of Cerenkov photons has a cyclic character and leads to frequently repeating some basic blocks. After a photon is calculated, the operations are repeated for the other photons produced on the considered muon step, and then for photons generated at the subsequent muon steps until the final point of a muon step will be outside the detector volume or the muon's energy at the end of its step will fall below the threshold energy for Cerenkov radiation emission. This process of calculation can be repeated many a time with a number of muons for reducing the statistical fluctuations of the calculated quantities. Schematically, it is illustrated on figure 2.

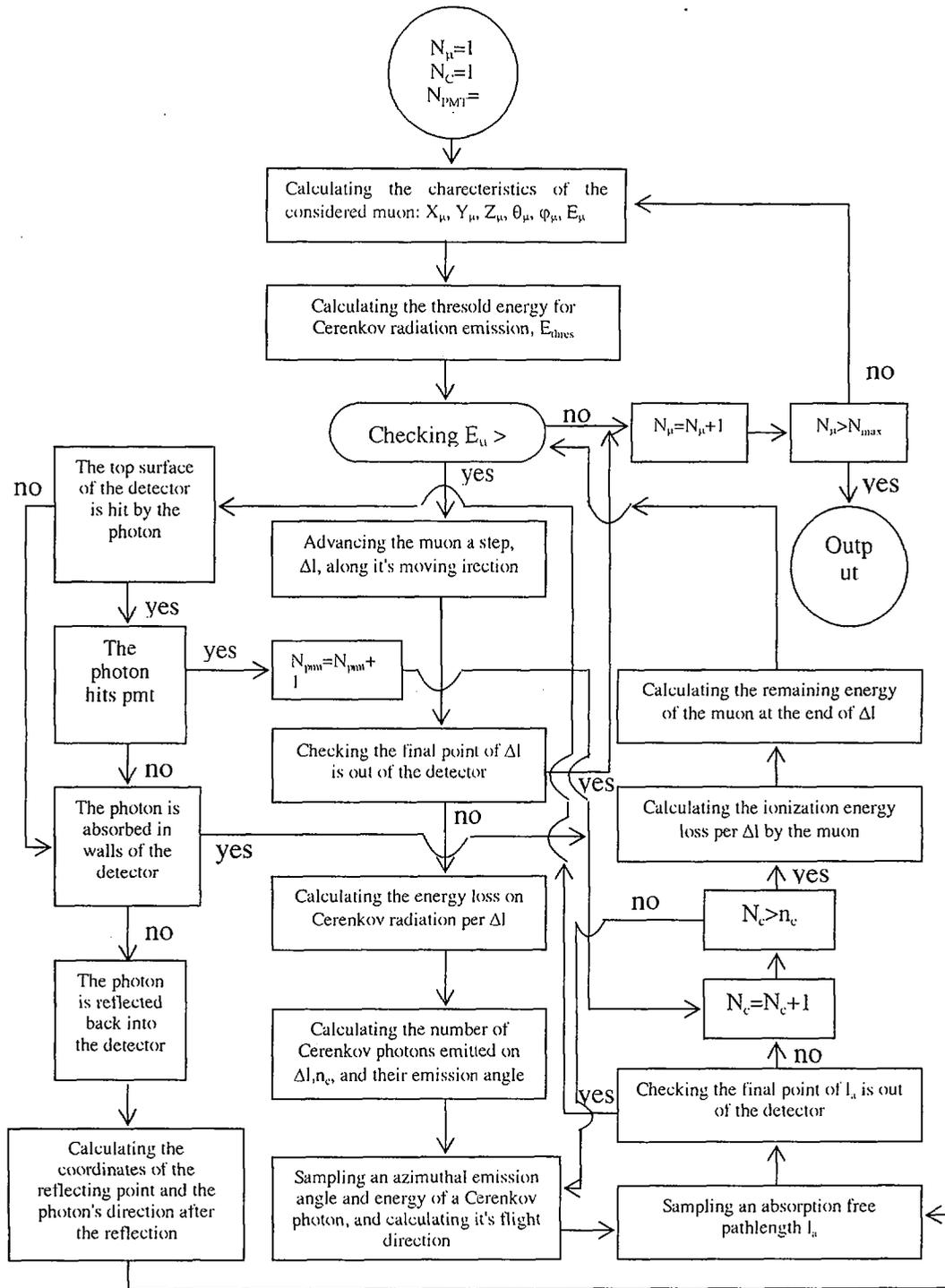


Figure 2. Illustration of the simulation process of Cerenkov radiation in the Auger water ground detector concerned with the motion of muons.

CONCLUSION

In this paper a simulation model for the process of emission and diffusion of Cerenkov photons concerned with muons moving through the volume of the Auger water ground detector with the velocity greater than the phase velocity of light in the

water is developed. In the considered model the motion of each muon is tracked, the number of Cerenkov photons generated on a muon step at an angle with the muon's moving direction is selected at random from the Poisson distribution. Each photon is ray-traced as it passing through the water, and reflected from the detector walls. When photons strike the photomultiplier tubes, their arrival times are recorded. The developed model is applicable to calculating photons producing signal in the detector and their characteristics of diffusion. Based on this model we have designed the computer software to carry out theoretical simulations. The results of numerical calculations will be analyzed in comparison with the experimental data collected on the water Cerenkov detector installation of the Auger training laboratory at INST and published in a separated paper.

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MATHEMATICAL MODEL FOR CRYSTALIZATION OF INORGANIC COMPOUNDS IN PRACTICAL CONDITIONS OF VIETNAM

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ABSTRACT: By experiments and calculations it has been proved that precipitation of ammonium di-uranate begins at the reagent input point in the reactor before the over-saturation occurs in the bulk of solution.

The level of local over-saturation depends on the following parameters:

- Structure of the equipment;
- Flow-rate of reagent;
- Kinetics of precipitation process.

Utilizing the behavior of over-saturation in the system it is possible to improve the precipitation process in terms of decrease or increase the finess of the products.

CONTENT

Precipitation process in all equipment, from laboratory to industrial scales, obeys the laws of macro-kinetics. Besides physical parameters of the system, the macro-model also contains parameters of the equipment. Equipment of lab. or industrial scales are objects for modeling and optimization. Values of parameters of macro-models obtained from the simulation of batch precipitation are not consistent by time and space. Macro-models are built on basis of micro-models.

Micro-model: Precipitation process is a model describing a system with dimensions of all representative parameters of the system and with identical concentrations in each phases.

Let ω over-saturation concentration of the solution; its effect on the rate of crystal generation (N) is by the equation: $N = k \cdot \omega^n$ where k and n depend on the nature of the system.

On the other side, ω also has an effect on process of crystal growth and agglomerat (λ_g) by the equation:

$$\lambda_g = hsD \cdot \varepsilon^{3/8} \cdot \omega \cdot r^{0,5}$$

where hsD : diffusion coefficient which is determined by experiments; ε : specific mixing energy, r : radius of single crystal or agglomerate.

Value of ω can also affect the rate of agglomeration (λ_a) by equation:

$$\lambda_a = \frac{hsA}{R^2} \int_{r^*}^R r^3 \cdot f(r) dr \cdot \int_{r^*}^R (R+r)^2 \cdot (R^2 - r^2) \cdot f(r) dr$$

$$r^* = \sqrt{R^2 - Z}$$

where: value of hsA is determined by experiments from analysis of spectrum of grain-size, and value of hsA is characteristic for ability of agglomeration, it depends on the nature of substance to be precipitated; r^* minimal radius of a crystal that are able adhere itself to an agglomeration with a radius of R .

Let $f(R)$: function of agglomerate size distribution, and it has a form of:

$$f(R) = \frac{\tau(R)}{\lambda_l} \quad \lambda_l = \lambda_a + \lambda_g$$

$$\tau(R) = 1 / \exp(-a) \quad a = 1 / (\tau(r) \cdot |r - 2T_{ib}| - hsP)$$

Where: T_{ib} : mean resident time of crystals during the crystallization process; hsP : value of hsP is determined by experiments from the data of size spectrum analysis, value of hsP is characteristic for the process and depends on the equipment and natures of substances to be precipitated. We call $f(h)$ the *mixed size distribution function* and it has the form of: $f(h) = hsF \cdot f(R) + (1 - hsF) \cdot f(r)$, where hsF is an experimental coefficient and it is determined by the experimental curve of mixed size distribution. Mass transfer rate (λ_{ck}) for the whole system is calculated by formula:

$$\lambda_{ck} = TgS \cdot \omega \cdot hsD$$

Total area (TgS) of solid-liquid interface of the system can be determined by formula:

$$TgS = c \cdot \int_0^R R \cdot R \cdot f(h) dR$$

The above set of equations is the micro-model of the changes in the size distribution spectrum.

Besides physical parameters, there are parameters of equipment in the macro-model. The task of modeling and optimization real processes needs to take into account actual equipment, either of laboratory or industrial scales. Values of those parameters are not the same in both time and space.

The macro-model of precipitation is the model which includes all parameters and size of the system.

Parameters of macro-model include:

1. Physical parameters (in micro-model)
2. Technological parameters: chemical reaction of precipitation, method of precipitation, number of stages of precipitation, flowrate, resident time, concentrations of components taking parts in precipitation.

Simulation by macro-model includes separate simulations of chemical reaction of precipitation; method of precipitation, number of stages of precipitation, flowrates, resident time in each stages.

Through observations in laboratory for the process of ADU precipitation it is revealed that at the value of $\text{pH} > 3$ precipitation occurs in neighbourhood of reagent input point (supplying NH_4OH), when the newly formed precipitates move further from the reagent input point they are dissolved. It can be concluded that the phenomena of precipitation occurring before the bulk solution reaches over-saturated concentration has been simulated in the model.

CONCLUSION

- Observation of ADU precipitation in a laboratory equipment (made of glass) revealed that solid precipitates appear before the bulk solution reaches saturation.
- From experimental data (ADU grain size distribution), simulation for precipitation has been made; it is determined that the local over-saturation is higher than the concentration in the bulk solution.
- For ADU precipitation in laboratory equipment with pre-determined parameters when the over saturation is of 0.4 of the saturation in the bulk solution ADU begins to precipitates.

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