PARTEC 2001
International Congress for Particle Technology

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Proceeding
Session: Poster
Internal Number: 083

A stochastic model for particle mixing and segregation in fluidized beds with baffles

1.Introduction

- The model concept

In chemical engineering, mathematical models are widely applied as an essential tool to model transport phenomena of particles in various systems. Mathematical models for physical transport processes can be categorized into two types, one is the standard deterministic model and the other is a stochastic model also known as a probabilistic model. The deterministic model has been used extensively and developed in every many branches of the physical sciences. Moreover it is a very successful approach. The method is based on formulating and solving differential conservation equations. Although there are so many advantages of the deterministic model, there are also some disadvantages. For instance, formulating the model when the process gets more sophisticated can be a problem. This kind of model can also consume plenty of time to evaluate. In these cases the stochastic model may be an attractive alternative way.

Another advantage of stochastic models is that they give more information than deterministic models about processes in which a strong random element is present, for instance when they involve movement of individual solid particles. For systems such as the transport of particles in fluidized beds, a stochastic model is in accordance with the inherent random nature of the process, and is intuitively appealing. A stochastic model is chosen here for modeling a baffled batch fluidized bed containing a binary mixture system. Since stochastic models focus on a single particle and models its path through the fluidized bed reactor the approach can also be referred to as a “microscopic” approach.

- Fluidized beds with baffles

There are many different applications of fluidization in industry nowadays, for instance for granulation, coating, mixing, drying, catalytic cracking and recycling.

Hartholt *et al.* (1996) found that using internal baffles enhanced particle segregation in fluidized beds, although the bed at low fluidization velocities retained its coherence with little influence of the baffles on the bubble behavior. They proposed that a baffled fluidized bed might be used for dry particle classification, with possible industrial applications, for instance in recycling, granulation and purification of powders.

The key mixing process in bubbling fluidized beds is the upward transport of jetsam (particles naturally tending to sink) in the wakes of rising bubbles. The baffles decrease mixing, and thus enhance segregation, by knocking out part of the bubble wakes (Figure 1). Research using baffles in binary mixtures has already proven that such baffles boost segregation.

- A stochastic model for fluidized beds with baffles

Dehling *et al.* (1999) and Hoffmann *et al.* (1998) first proposed a stochastic model for particle transport in continuous fluidized beds containing uniform particles and no internals. The attractive features of probabilistic models are for instance that they are simple to formulate based on the physical phenomena and computationally easy to cope with using a matrix-oriented package such as MATLAB. Formulating a stochastic model to batch fluidized beds with a binary mixture and internal baffles is another challenge to make a mathematical model retaining the simplicity of the stochastic approach yet describing the process sufficiently accurately.

2. Description of the model

In bubbling fluidized beds, both jetsam and flotsam (particles tending to float) are carried in bubble wakes (Figure 1), and fluidization bubbles cause a stirring action referred to as “dispersion”. The shearing of the bed material due to this stirring action also allows individual jetsam particles to segregate towards the bottom of the bed. Gibilaro and Rowe (1974) first introduced these particle transport concepts. Gibilaro and Rowe also operated with a rate of material exchange between the wakes of the fluidization bubbles and the surrounding bulk; we neglect this here.

The particle motion is modeled as a convection-diffusion process with segregation, modified by allowing jumps upward due to transport in bubble wakes based on Dehling and Hoffmann's concepts. The motion of one particle is considered, and the transport processes are converted to transition probabilities between cells in a discretized bed, see Figure 2. The probability distribution for the particle's position as a function of time reflects the behavior of a pulse of marked particles. The model based on a Markov chain, such that the probability distribution of a single particle is independent of the past history of the system.

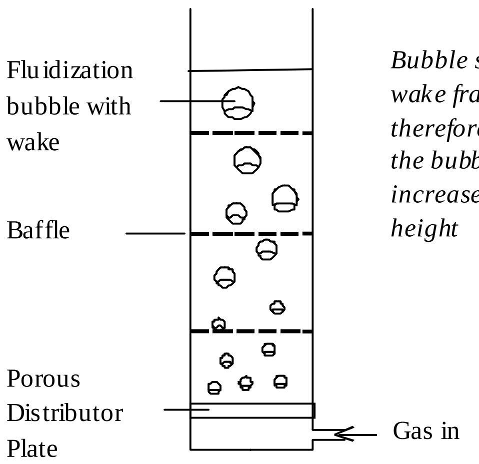

Fig 1. Sketch of a bubbling fluidized bed with baffles

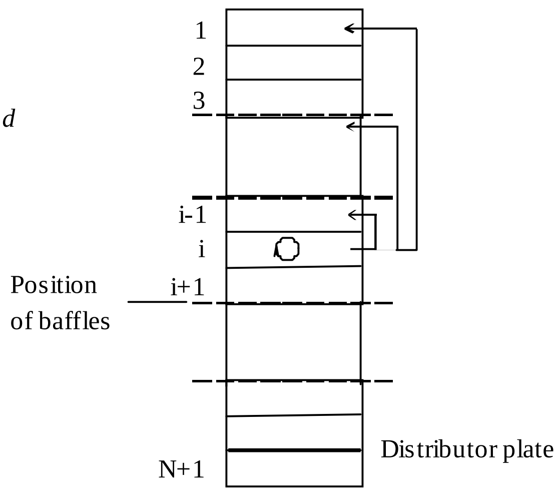

Fig 2. The discretized fluidized bed with baffles

In our discrete Markov model, the reactor is divided into N horizontal cells, and we model the particle's position at discrete times only. The cells are numbered as shown in Figure 2. The model calculates the probability distribution of the axial position of one particle as a function of time. The possible transitions are:

a) staying in the same cell
b) moving to the next cell
c) moving back to the previous cell
d) being caught up in a bubble wake and deposited under one of the baffles passed by the rising bubble, or at the top of the bed. We assume that only part of the wake is retained by a baffle

We introduce parameters α_i, β_i and δ_i, with sum equal to 1, for the first three probabilities, conditionally on the particle not being caught up in a bubble wake, the latter probability being given by λ_i. θ denotes the fraction wake retained by a baffle.

The transfer probabilities from cell i to cell j form a matrix, $\boldsymbol{Q}$, with the elements $q_{i,j}$. The transition probabilities for the interior of the reactor, *i.e.* for $2 \le i \le N$, are:

$$
\begin{aligned}
q_{i,i} &= \alpha_i (1-\lambda_i) \\
q_{i,i+1} &= \beta_i (1-\lambda_i) \\
q_{i,i-1} &= \delta_i (1-\lambda_i) \\
q_{i,1} &= \lambda_i (1-\theta)^{\left[\frac{i-1}{S}\right]} \\
q_{i,mS+1} &= \lambda_i \theta (1-\theta)^{\left[\frac{i-1}{S}\right]-m}; \qquad m = 1,2,\ldots,\left[\frac{i-1}{S}\right]
\end{aligned}
\tag{1}
$$

Note that $\lambda_i = \lambda_i\theta + \lambda_i\theta(1-\theta)^1 + \ldots + \lambda_i\theta(1-\theta)^{\left[\frac{i-1}{S}\right]-m} + \ldots + \lambda_i(1-\theta)^{\left[\frac{i-1}{S}\right]}$. m is the index of the baffles and S is number of cells between two baffles. The square brackets indicates "the integer part of...".

Regarding the boundaries, i.e., i = 1 and $i = N$;

$$q_{1,1} = 1 - \beta_1(1-\lambda_1),$$
$$q_{1,2} = \beta_1(1-\lambda_1), \qquad (2)$$
$$q_{N,N} = 1 - \delta_N(1-\lambda_N) - \lambda_N .$$

The position of the particle at the n'th time step is given by the probability vector $\boldsymbol{p}(n)$, with elements $p(n,i)$.

Knowing $\boldsymbol{p}(n-1)$, one can find $\boldsymbol{p}(n)$ from:

$$p(n,j) = \sum_{i=1}^{N+1} p(n-1,i) q_{i,j} \quad \text{or in matrix notation:} \quad \boldsymbol{p}(n) = \boldsymbol{p}(n-1)\boldsymbol{Q} \qquad (3)$$

After n time steps, we obtain the formula for the probability distribution of position of the particle at time n in terms of its initial probability distribution:

$$\boldsymbol{p}(n) = \boldsymbol{p}(0)\boldsymbol{Q}^n \qquad (4)$$

which $\boldsymbol{p}(0)$ is the initial condition of particle distribution in the reactor at time $t=0$.

3. Markov chain model

The model introduced above is a discrete one, but the transfer probabilities will be related to physical parameters describing the particle transport as continuous processes, following Dehling *et al.* (1999). We call the time step ε and the cell width Δ. Letting ε and Δ go to 0, we obtain a discrete Markov chain approximation to the continuous process.

The vertical distance from the top of the reactor is denoted by x, i.e., $x = 0$ corresponds to the top and $x = 1$ to the bottom, and the convective axial velocity due to circulation by $v_{cir}(x)$. The dispersion due to the disturbance by bubbles is denoted by a dispersion coefficient, $D(x)$. The rate of returns to the top of the bed is described by λ_x. The parameters in the transition matrix are defined as follows:

$$\delta_i = \frac{\varepsilon}{2\Delta^2} D(i\Delta) - \frac{\varepsilon}{2\Delta} v_{cir}(i\Delta), \qquad (5)$$

$$\beta_i = \frac{\varepsilon}{2\Delta^2} D(i\Delta) + \frac{\varepsilon}{2\Delta} v_{cir}(i\Delta), \qquad (6)$$

$$\alpha_i = 1 - \delta_i - \beta_i , \qquad (7)$$

4. Modeling of segregation and the effect of the baffles

The model outlined so far does not account for segregation. We model only the jetsam fraction. Since segregation adds an extra convective downwards velocity, a simple way of modeling this is to modify the above probabilities as follows:

$$\delta_i{*} = \delta_i , \qquad (5*)$$

$$\beta_i{*} = \beta_i + \frac{\varepsilon}{\Delta} v_{seg}(i\Delta) , \qquad (6*)$$

$$\alpha_i{*} = 1 - \delta_i{*} - \beta_i{*} , \qquad (7*)$$

where λ_i^* equals to λ_i and v_{seg} is a velocity of jetsam segregation. This, then, are the final transition probabilities in the interior, *i.e.* for i = 1 , . . ., N.

5. Quantification of the physical parameters

The parameters v_{cir}, v_{seg}, λ and D can be quantified from the empirical relationship in the literature. A full account of this is given in Dehling *et al*.(1999). The essential empirical formulae, which have been used are:

- the wake angle (Hoffmann *et al.*, 1990)

$$\theta_w = 160 - 160 e^{-55 D_b} \qquad (8)$$

- the bubble size as a function of height in the bed (Geldart, 1972)

$$D_b = \frac{1.3}{g^{0.2}} \left(\frac{U - U_{mf}}{1000} \right)^{0.4} \left(\frac{1}{1 - f_w} \right)^{0.33} + 2.05 h \left(U - U_{mf} \right)^{0.94} \qquad (9)$$

- the total flow of empty bubble volume (two-phase theory)

$$Q_b = A(U - U_{mf}) \tag{10}$$

- the dispersion coefficient derived by particle drift measurements caused by one fluidization bubble by.

$$D = \frac{0.19 D_b (U - U_{mf})}{1 - f_w} \tag{11}$$

- the dimensionless segregation distance of jetsam particles associated with the passage of one fluidization bubble (Tanimoto *et al.*, 1981; Hoffmann *et al.*, 1991)

$$Y_s = 0.8\left[\frac{\rho_j d_j^{\,0.33}}{c_f(\rho_f d_f^{\,0.33}) + (1 - c_f)(\rho_j d_j^{\,0.33})} - 1\right] \tag{12}$$

6. Numerical simulations and comparison with experiments

The experiments were carried out in a glass column of 15 cm diameter. In these experiments the mixing of two solids in a bubbling fluidized bed with baffles is studied. The initial bed height was approximately 30 cm and 50/50 mixtures by volume of glass beads (83 µm) and painted glass beads (221 µm). Properties of the solids used for these experiments are shown in Table 1.

Table 1 Properties of the solids used in the experiments

Particles	d_p(µm)	σ^*(-)	ρ (kg/m^3)	U_{mf} (cm/s)	ε_{mf} (-)
Glass beads	83	0.11	2500	0.595	0.416
Painted glass beads	221	0.09	2480	5.290	0.427

*The standard deviation obtained by fitting the particle size distribution with the normal distribution of the natural logarithm of the particle size

The relative humidity of fluidizing air was kept at approximately 30%. The baffles used consist of woven wires of 0.65 mm diameter with stitch of 0.42 cm giving 71.1% open area. The baffles were attached to three bars as shown in Figure 3. The spacing between the baffles varied between 0.43 and 7.40 cm.

A typical experiment was started at a high gas velocity at which the bed was well mixed. Then the baffles were inserted and the gas velocity was reduced to the required velocity. The segregation layer built up from the bottom and its height was monitored visually until the system reached steady state. The air supply was then cut off suddenly to freeze the powder distribution in the bed, and the baffles were pulled out gently, disturbing the system as little as possible. The bed was sectioned in layers of 2 cm thickness using a vacuum technique. The powders were analyzed by sieving.

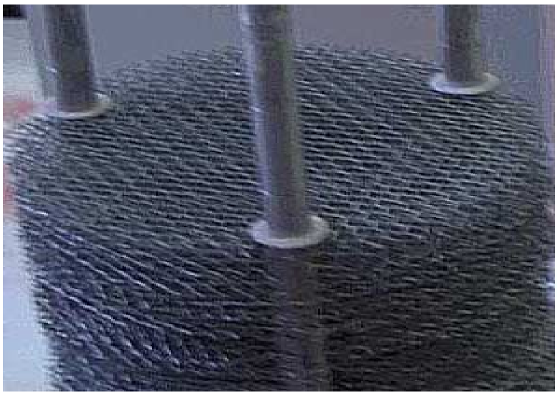

Fig 3. Baffle construction with 0.43 cm separation between the baffles

To compare the experimental data with the model the probabilities *p(n,i)* were converted to jetsam concentration *c(n,i)* using: *c(n,i)* = *N* C_j *p(n,i)*, where C_j is the volumetric jetsam concentration in the entire bed. Obviously the physics imposes a maximum concentration of *c(n,i)* = 1. This is not yet accounted for in the model, and was imposed in the numerical evaluation of the model.

All of the experimental results used for comparison were obtained using a superficial fluidization velocity *U* higher than the U_{mf} of the jetsam to avoid defluidization in the bottom of the bed. The more baffles used, the better the segregation of jetsam.

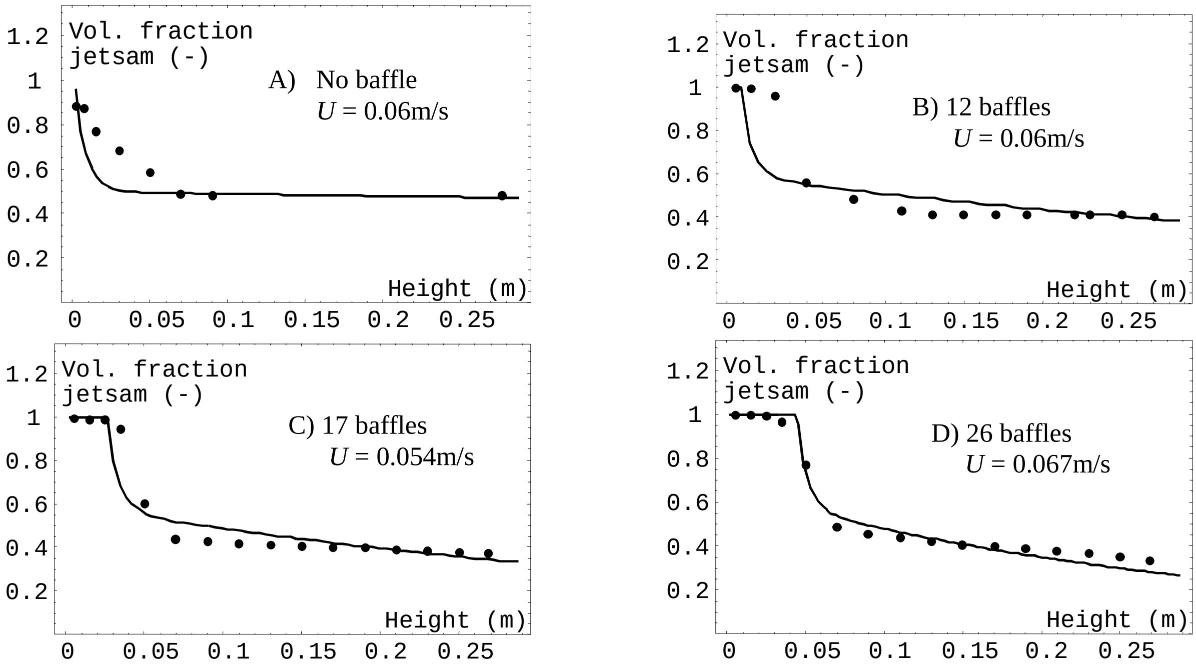

Fig. 4 Comparison between experimental data (points) and our stochastic model (lines). Baffle separations are: A) No baffles, B) 2.40 cm, C) 1.72 cm and D) 1.13 cm

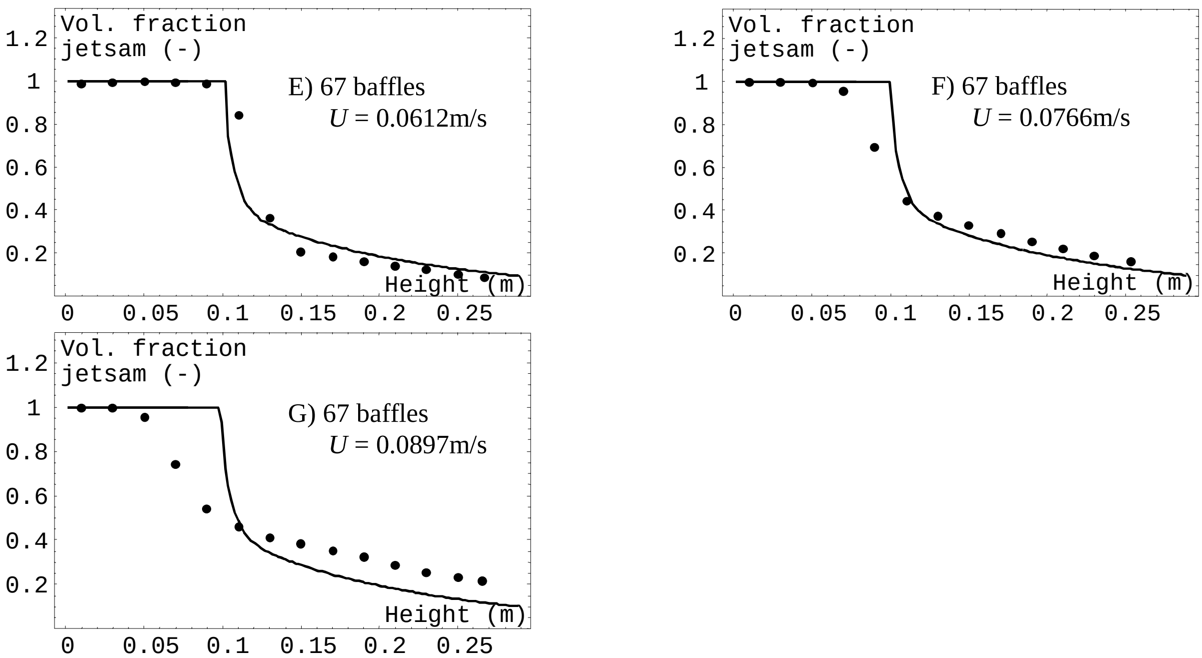

Fig. 5 Comparison between experimental data (points) and our stochastic model (lines) for the same number of baffles (baffle distance = 0.43 cm) but three different superficial fluidization velocities.

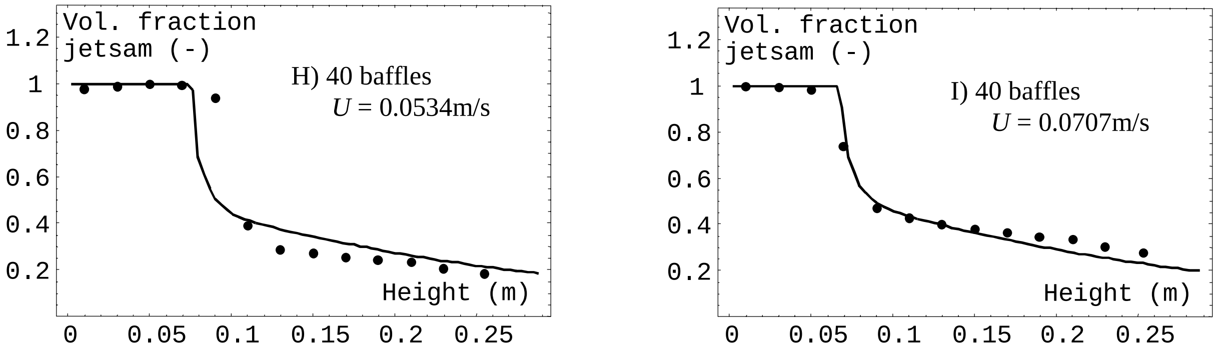

Fig. 6 Comparison between experimental data (points) and our stochastic model (lines) for the same number of baffles (baffle distance = 0.72 cm) and two different superficial fluidization velocities

There is one adjustable parameter in the model, θ, the fraction of wake left under the baffle. In all of the plots in Figures 4, 5 and 6 the same value of θ has been used, namely 0.03. Even so, the agreement between model and experiment is clearly good. The only effect not well accounted for is that of the fluidization velocity. The model correctly reflects:

1) the effect of the number of baffles on the separation without having to adjust θ
2) the effect of the baffles in causing an effective bulk/wake "exchange", which gives rise to a gradient in the jetsam concentration in the upper part of the bed.

As mentioned, the model underestimates the effect of the fluidization velocity, which may indicate that the fraction of wake retained by the baffles, θ, decreases with increasing fluidization velocity. The numerical value of 0.03 of θ is very low, especially in view of the X-ray pictures of van Dijk *et al.*, which showed most of the wake material left under a baffle by a single fluidization bubble. In the work of van Dijk *et al.*, however, the wake material had a significantly higher density than the surrounding bulk material, and it is possible that the wake therefore was more loosely associated with the bubble, and more easily left under the baffle. The relative size of the fluidization bubble and the baffle aperture may also play a role in determining the baffle retention efficiency.

7. Conclusions

The agreement between model and experiment seen in Figures 4, 5 and 6 show that our stochastic model, which can be evaluated in a PC within some seconds using packages such as Matlab or Mathematica, is capable of predicting the profile of segregation in baffled batch fluidized bed with a binary mixture as discussed above.

Further study is required to develop this model by relating θ to the baffle physical properties i.e. the baffle aperture and relative size of fluidization bubble and to the fluidization velocity. More work is also required to include particle/particle interference and the response of the mixing and segregation parameters to the local jetsam concentration, which changes the local U_{mf}. When this is achieved the maximum concentration no longer has to be imposed in the numerical evaluation. This would also automatically make the model account for defluidization of the bottom part of the bed for fluidization velocities below the U_{mf} of the jetsam.

The stochastic model is a simple and intuitive model. The approach offers great advantages above deterministic models for this type of process, it is easier to formulate, it gives more information about the statistics of the physical processes, and it is simpler and faster to evaluate. Due to its advantages, this type of model can be applied to a variety of particle behaviors in other fluidized bed systems.

8. Acknowledgement

The authors would like to thank the **NOVEM** for financial support within the framework of an EET project.

9. Nomenclature

A = cross sectional area of bed
C_j = volume fraction jetsam in entire bed
$c(n,i)$ = volume fraction jetsam in cell i
D = dispersion coefficient
D_b = diameter of bubble
d_f = diameter of flotsam particle
d_j = diameter of jetsam particle

f_w = wake fraction
g = gravitational acceleration
h = height in the bed from the distributor plate
i, j = indices denoting the number of cell
m = number of baffles
N = number of cells internal to the discretized beds
n = index denoting the time step
$\boldsymbol{p}$ = probability vector
p = elements of $\boldsymbol{p}$
Q_b = volumetric flow of gas in the bubble phase
$\boldsymbol{Q}$ = transition probability matrix
$q_{i,i}$ = elements of $\boldsymbol{Q}$
S = cells between two baffles
U = fluidization velocity (superficial)
U_{mf} = minimum fluidization velocity (superficial)
v_{cir} = circulation velocity
v_{seg} = segregation velocity
Y_s = dimensionless segregation distance

Greek:
ε = time step
Δ = width of the cells
α, β, δ = parameters in the transition probabilities
λ = removal rate
θ = baffle removal rate
θ_w = wake angle
ρ_f = density of flotsam
ρ_j = density of jetsam

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