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COMPARTMENTAL MODELLING FOR FLOCCULATION IN STIRRED TANKS

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SUMMARY A kinetic model in terms of total particle numbers for flocculation in a baffled stirred tank is presented. The tank is compartmentalised into regions of uniform shear. By using experimental data of energy dissipation rate from the literature, flocculation rate is predicted from a volume average shear rate. The use of this average collapses the results of a number of models onto a single curve under realistic conditions.

When the volume average shear rate is applied to experimental measurements of flocculation rate in stirred tanks, the results are brought into coincidence with measurements in a Couette geometry, in which the shear field is better defined. This lends support to the use of this average.

1. INTRODUCTION

Flocculation can be promoted by shear, such as exists in a stirred tank. The flow field in a baffled stirred tank is very complex and the shear is far from uniform. The flow condition in a stirred tank and its effect on the flocculation process can be approximated by compartmentalizing the tank into regions of relatively uniform shear. Experimental results of the flocculation process in a Couette geometry, which provides nearly uniform shear, can be applied to a stirred tank once the shear rate and flow rate distributions within the tank are known. These distributions are available in the literature.

For a dilute suspension of monosized spheres, the rate of decrease of the local number concentration N at time t owing to orthokinetic flocculation in a laminar shear field is described approximately by the well known relation, following Smoluchowski $dN/dt = -(4/\pi)\alpha\phi GN$ where G is the local shear rate, α is a collision efficiency to account for the fraction of collisions which result in permanent aggregates, and ϕ is the particle volume fraction which remains constant for a batch system. This equation can be integrated with respect to time to give

$$N/N_o = \exp\,(-\,4\alpha\phi Gt/\pi) \qquad (1)$$

where N_o is the initial particle number concentration.

2. SHEAR RATE IN STIRRED TANK

According to Camp and Stein (1943), for homogeneous isotropic turbulent flow, the mean shear rate over a volume V is $\bar{G}$ which can be calculated from the power input P to the volume:

$$\bar{G} = \sqrt{P/(\mu V)} \qquad (2)$$

where μ is the viscosity. The application of Eqn. 2 to practical flocculators has been reviewed by Polasek (1979). The mean shear rate calculated from Eqn. 2 is usually inserted in Eqn. 1 in place of the uniform or local value G. This approach of using a single value of $\bar{G}$ for calculating flocculation in stirred tanks is not always satisfactory in cases where values of the shear rate are distributed over a wide range throughout the volume. For example, Tambo and Hozumi (1979) reported that only 10-20% of the mean rate of energy dissipation is effective for flocculation in a paddle blade mixer; while for laminar tube flow, Gregory (1981) observed that the mean shear rate as defined in Eqn. 2 and calculated from pressure drop is 6% higher than the effective mean shear rate calculated from the velocity profile. Gregory further suggested that a flow-weighted shear rate is the appropriate mean value for prediction of flocculation rate using Eqn. 1.

Patterson (1974) divided the stirred tank into thirty compartments which are concentric about the tank axis (Fig. 1) and calculated the energy dissipation rate for each compartment from data reported by Cutter (1966). Volumetric flow rates between compartments are also given by Patterson. For compartmental modelling in general, the energy dissipation rate ε_i in compartment i of volume V_i is related to the mean dissipation rate $\bar{\varepsilon}$ for the whole tank $\sum_i v_i\varepsilon_i = \bar{\varepsilon}$ where $v_i = V_i/V$, and $\sum_i v_i = 1$. The mean energy dissipation rate is obtained from the total power input by $\bar{\varepsilon} = P/(\rho V)$ where ρ is the fluid density. By analogy with Eqn. 2, the shear rate G_i in compartment i is taken as $G_i = \sqrt{\varepsilon_i\rho/\mu}$. Now, dividing G_i by $\bar{G}$ and defining a dimensionless shear rate g_i as

$$g_i = G_i/\bar{G} = \sqrt{\varepsilon_i/\bar{\varepsilon}} \qquad (3)$$

the average shear rate in compartment i can be calculated from the energy dissipation rate of the compartment. It is also proposed that the dimensionless volume average shear rate represented by parameter s is defined by

$$sV\bar{G} = \sum_i V_i G_i \qquad (4)$$

or in dimensionless form by $s = \sum_i v_i g_i$. For a simple two-compartment model, the impeller zone (approximating to compartments 13 - 18 in Fig. 1) and the bulk zone (remaining compartments) are both assumed to contain uniform shear (Okamoto et al, 1981). For a three-compartment model, an impeller tip zone (compartment 15) of intense shear may be separated from the general impeller zone (Tomi and Bagster, 1978). The fractional volumes and the energy dissipation rates reported in the literature for two- and three-compartment models given in Table 1 are quite different because the criteria for partitioning the total volume into compartments as used by the workers quoted is arbitrary, and different fractional volumes are obtained. Table 1 includes the dimensionless shear rates in the compartments and parameter s calculated from the energy dissipation rates using Eqns. 3 and 4. The parameter s is highly dependent on geometry and this is shown in a plot of s against D/T in Fig. 2.

A continuous shear rate distribution can be calculated from energy dissipation rate data at seventy-six locations in a baffled tank of D/T = 0.50 reported by Okamoto et al. The cumulative distribution in terms of fractional volume is plotted against the dimensionless shear rate in Fig. 3 which also includes the plot of a four-parameter log-normal probability function with $\mu = 0.16$, $\sigma = 4.8$, $g_{min} = 0.39$ and $g_{max} = 2.7$ defined as

$$\frac{dv}{d(\ell nx)} = \frac{1}{\sqrt{2\pi}(\ell n\sigma)} \exp[- \frac{(\ell nx - \ell n\mu)^2}{2(\ell n\sigma)^2}] \qquad (5)$$

where $x = (g - g_{min})/(g_{max} - g)$. The necessity for upper and lower limits in fitting the shear rate distribution in a stirred tank is not surprising as g cannot approach infinity nor is it likely to approach zero in a real stirred tank, even in very small localised zones. For the continuous shear rate distribution, the parameter s may be obtained by integration, $s = \int_0^1 g.dv$. A value of s = 0.86 is obtained numerically for the shear rate distribution in Fig. 3 with D/T = 0.50. The parameter s is the first moment of the volumetric shear rate distribution, while the mean shear rate $\bar{G}$ calculated from power dissipation per unit mass is the second moment of this distribution, since

$$\bar{G}^2 = \bar{\varepsilon}\rho/\mu = \int_0^1 (\varepsilon\rho/\mu).dv = \int_0^1 G^2.dv.$$

In modelling, the impeller pumping rate Q can be calculated from the impeller pumping coefficient $N_Q = Q/ND^3$ where N is the impeller speed. For six-pladed turbine impellers, a value of N_Q of approximately 1.0 is recommended (Bertrand et al, 1980).

3. COMPARTMENTAL MODELLING FOR FLOCCULATION

For flocculation of monosized particles in a compartmentalized stirred-tank model such as the one shown in Fig. 1, the particle number balances are:

$$\frac{dn_i}{dt} = \sum_j \frac{Q_{ji}\, n_j}{V_j} - \frac{n_i}{V_i} \sum_j Q_{ij} - \frac{4\alpha\phi G_i n_i}{\pi} \qquad (6)$$

where n_i is the number of particles in compartment i and the summations are over all values of j the counter for neighbouring compartments. Q_{ij} and Q_{ji} are the flow rates from compartment i to compartment j and back. These flow rates can be expressed as fractions of the impeller pumping rate Q such that $q_{ij} = Q_{ij}/Q$. Eqn. 6 may be written in dimensionless form by defining $k = 4\alpha\phi\bar{G}/\pi$, $t^* = kt$, $c = Q/(kV)$, $g_i = G_i/\bar{G}$ and $v_i = V_i/V$. Thus

$$\frac{dn_i}{dt^*} = c \sum_j \frac{q_{ij}\, n_j}{v_j} - \frac{cn_i}{v_i} \sum_j q_{ij} - g_i n_i \qquad (7)$$

The number fraction of particles remaining in the tank at any time is $N/N_o = \sum_i n_i / \sum_i n_{io}$ where n_{io} is the initial number of particles in compartment i. The solution in terms of N/N_o for any value of c can be obtained numerically using energy dissipation rate data from the literature. For the thirty-compartment model, the values of N/N_o for c = 0 and for c = ∞ (taken as c = 1000, see below), are plotted against st* in Fig.4. For the simple two- and three-compartment models, where the fluid can be assumed to be discharged between compartments at a volumetric flow rate equal to the impeller pumping rate, that is $q_{ij} = 1$, the numerical solutions for c = 0 and for c = ∞ are also included in Fig.4 for comparison. Expressions for the analytical solution of the two-compartment model have been reported elsewhere (Koh et al, 1983). In stirred tanks with high pumping rates, a plug-flow model, which describes the kinetics more precisely, has been proposed by Koh et al (1983). In the plug-flow model, a stirred tank, may be viewed as a pipe consisting of sections with varying diameters, having uniform shear rate in each section. The analytical solution of the plug-flow model for c = ∞ and any number of compartments can be shown to be

$$N/N_o = \exp(- st^*) \qquad (8)$$

As shown in Fig. 4, the numerical solution for all models with c = ∞ is descfibed exactly by Eqn.8. The results for Poiseuille flow in pipes have been obtained by Gregory (1981) for the case of no radial mixing with c = 0, and are included in Fig.4. For the continuous shear rate distribution shown in Fig. 3, the stirred tank may be viewed as having an infinite number of compartments. Simple solutions may be obtained for c = 0 and c = ∞. c = 0 describes an unrealistic situation where there is no mixing in the tank, and the particles stay at the same locations at all times. The log-normal distribution given in Eqn.5 may replace G in Eqn.1 and by a change of variables for integration, numerical solutions can be obtained and these are included in Fig.4.

$$N/N_o = \int_0^\infty \frac{1}{x\sqrt{2\pi}(\ell n\sigma)} \exp\left[- \frac{(\ell n\, x - \ell n\mu)^2}{2(\ell n\sigma)^2} - \frac{4\alpha\phi\bar{G}t(x\, g_{max} + g_{min})}{\pi(x+1)} \right] dx \qquad (9)$$

When c = ∞ and the shear is continuously distributed, the plug-flow concept can also be applied, and the analytical solution of Eqn. 8 is again obtained. The results in Fig. 4 show that for c = ∞, the solution for all models is identical to that for a single-compartment model where the effective mean shear rate in Eqn. 8 is given by $G_{eff} = s\bar{G}$.

For c = 0, the solutions of the various models are slightly different. The difference between the models is possibly due to differences in treatment of the original energy dissipation rate data by the various authors whose compartmentalisation was adopted. In particular, the 30 compartment model of Patterson shows the greatest difference; Pattenon's results also give the largest value of s = 0.90, which appears to be unrealistic for a baffled stirred tank. Undoubtedly Patterson's partitioning of energy dissipation rate and flow rate data is the cause of the difference. However, the discrepancy is not serious since the case c = 0 is not likely to be of practical significance.

In the general compartment model, Eqn. 7, the case for c = ∞ is important even when α = 1, as shown in the following typical example. For a suspension with $\phi = 3.3 \times 10^{-4}$ in a tank of T = 176 mm with an impeller of D = 73 mm rotating at 200 rpm, producing a mean shear rate $\bar{G} = 250\ s^{-1}$ and pumping at a rate Q = 1.3 litre/s, a value of 0.11 s^{-1} is obtained for the rate constant $k = 4\alpha\phi\bar{G}/\pi$. The value of parameter c = Q/(kV) of 3.0 can also be obtained. The numerical solutions of Eqn. 7 for this value of c are very close to the results for c = ∞ in Fig. 4. For the range of experimental conditions encountered in flocculation, 2 < c < 9 is typical. In the presence of an energy barrier to flocculation owing to surface forces, and resulting in α << 1, the value of c would be increased and would approach c = ∞. It is thus possible to describe approximately the flocculation kinetics in stirred tanks for all values of α by a single line, that for c = ∞.

The variation of c with impeller speed can be predicted from the expression:

$$c = \frac{\pi Q}{4\alpha\phi\bar{G}V} = \frac{(\pi/4)^{1/2}(D/T)^{3/2} N_Q}{\alpha\phi\, N_{Re}^{1/2}\, N_{Po}^{1/2}} \qquad (10)$$

where $N_{Po} = P/(N^3D^5\rho)$ is the power number, $N_{Re} = ND^2\rho/\mu$ is the impeller Reynolds number. For a given geometry, N_Q and N_{Po} are constants under turbulent conditions; only N_{Re} varies directly with impeller speed. The value of c increases with decreasing impleller speed.

For the paddle-blade mixer where, according to Okamoto eta al (1981), the effective rate of energy dissipation ε_{eff} for flocculation is only 10-20% of the mean rate $\bar{\varepsilon}$, the corresponding values of 0.32-0.45 for parameter s can be calculated from $\varepsilon_{eff} = s^2\,\bar{\varepsilon}$. This is obtained by analogy with G_{eff} and Eqn. 3.

4. COUETTE FLOW

Flocculation in stirred tanks can be compared with that in a Couette apparatus provided the difference in shear rate distributions can be accounted for. For a Couette apparatus with a rotating inner cylinder, the critical shear rate at which Taylor vortices appear is quite low, as first observed by Taylor in 1923. It is common for some flocculation processes to require shear rates up to 1000 s^{-1} and flocculation tests must inevitably be carried out in the presence of Taylor vortices. The shear stresses generated in water in the Couette apparatus can be measured by a dynamometer. Values of the shear stress for ideal flow can be calculated from the viscosity of water. In the unstable regime, the shear rate calculated from the stable laminar flow assumption underestimates the shear condition in the Couette apparatus.

It is proposed that the effective shear rate G_{eff} may be obtained from the following equation:

$$G_{eff} = (G_{lam}{}^2 + G_{vor}{}^2)^{\frac{1}{2}} \qquad (11)$$

where G_{lam} is the shear rate of the tangential flow in the absence of any vortices and may be calculated in the usual way from

$$G_{lam} = 2\Omega R_1 R_2/(R_2{}^2 - R_1{}^2)$$

where Ω is the angular speed, R_1 and R_2 are the radii of the inner and outer cylinders. G_{vor} is the additional shear resulting from Taylor vortices and may be calculated by analogy with the fully turbulent stirred tank, from $G_{vor} = \sqrt{\varepsilon_{vor}\rho/\mu}$ where ε_{vor} is the energy dissipation rate due to Taylor vortices. ε_{vor} can be obtained by subtracting the laminar dissipation rate from the total measured dissipation rate. The basis for Eqn. 11 is the conservation of energy which has also been used by Camp and Stein (1943) for summing orthogonal components of shear rate, and by Polasek (1979) for summing contributions of shear rate induced by mechanical and hydraulic means. Although the energy dissipation rate due to Taylor votices is large by comparison, the shear calculated makes only a small contribution to the total effective shear rate. For example, in an apparatus with R_1 = 20.04 mm and R_2 = 21 mm at a rotational speed of 1000 rpm, a value of G_{eff} = 2496 s^{-1} is obtained, consisting of G_{lam} = 2340 s^{-1} and G_{vor} = 869 s^{-1}.

5. EXPERIMENTAL

Experiments to study the effect of shear rate on flocculation in stirred tanks of 0.5 and 1.0 litre capacity and in a Couette apparatus have been carried out. Suspensions of 2 g/ℓ of an ultrafine scheelite ($CaWO_4$) fraction with average size of 2 μm in 2 x 10^{-4}M sodium carbonate solution were used. Flocculation was achieved by shearing the suspension in the presence of 10^{-4}M sodium oleate at initial pH 10. Size distributions at various times up to 170 min were measured with a Leitz photosedimentometer. The observed size distributions of the flocculated suspensions were bimodal. The disappearance rate of the mass concentration of the original particles less than 2 μm in size can be described by a second-order rate equation. In Fig. 5 the rate constant k_2 is plotted against the effective shear rate calculated from $G_{eff} = s\bar{G}$ for stirred tanks and from Eqn. 11 for Couette flow. Fig. 5 shows that the effective shear rates calculated by the two methods for the two different geometries produce the same flocculation rate.

6. CONCLUSIONS

The various multi-compartment models appear to give very similar results and our calculations show that there is little advantage for modelling flocculation processes in compartmentalizing the stirred tank beyond two compartments. In fact, a single-compartment incorporating the effective mean shear rate is adequate.

The coincidence of results of flocculation rate from Couette experiments and from stirred tank experiments lends support to the use of the effective shear rate $s\bar{G}$ to describe conditions in stirred tanks.

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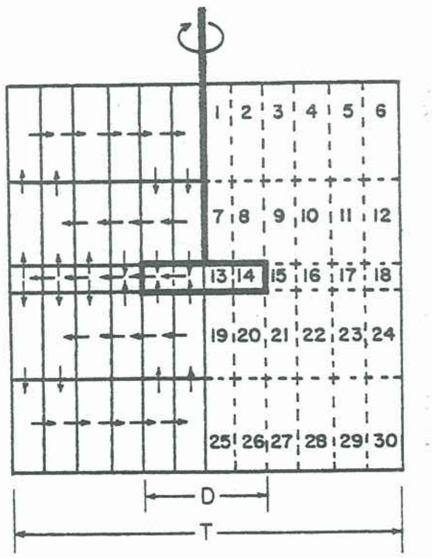

Figure 1 Thirty-compartment model for a stirred tank as partitioned by Patterson (1974).

TABLE I

FRACTIONAL VOLUMES, ENERGY DISSIPATION RATES, SHEAR RATES AND PARAMETER s FOR TWO- AND THREE- COMPARTMENT MODELS CALCULATED FROM LITERATURE DATA

D/T	v_1	v_2	v_3	$\varepsilon_1/\bar{\varepsilon}$	$\varepsilon_2/\bar{\varepsilon}$	$\varepsilon_3/\bar{\varepsilon}$	g_1	g_2	g_3	s
Okamoto et al (1981): Two-compartment										
0.25	0.03	0.97	-	28.5	0.20	-	5.34	0.45	-	0.60
0.33	0.05	0.95	-	16.0	0.27	-	4.00	0.52	-	0.69
0.50	0.11	0.89	-	5.9	0.42	-	2.43	0.65	-	0.85
0.70	0.24	0.76	-	2.3	0.61	-	1.52	0.78	-	0.96
Levins and Glastonbury (1972): Two-compartment										
0.33	0.10	0.90	-	7.7	0.26	-	2.77	0.51	-	0.74
Tomi and Bagster (1978): Three-compartment										
0.33	0.005	0.095	0.90	50	5.4	0.25	7.07	2.32	0.50	0.71

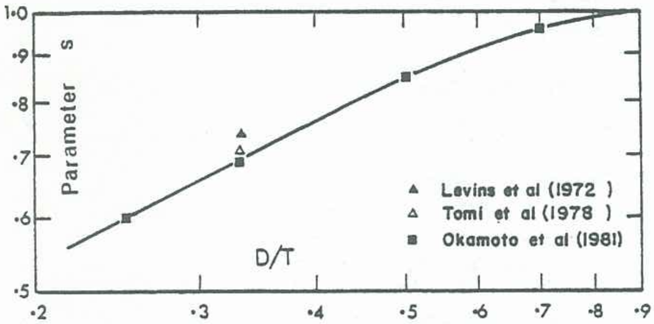

Figure 2 Dimensionless volume average shear rate (parameter s) as a function of impeller to tank diameter ratio, D/T, calculated from literature data.

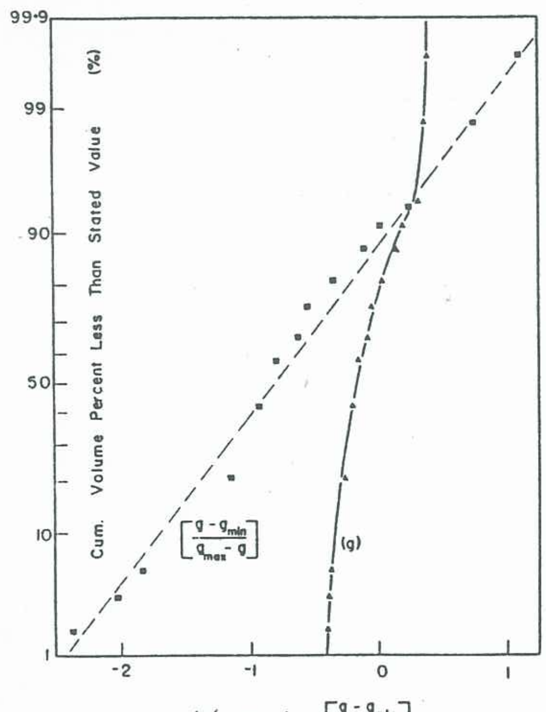

Figure 3 Log-probability distribution for shear rate in a baffled stirred tank with D/T = 0.5, calculated from seventy-six energy dissipation rates of Okamoto et al (1981).

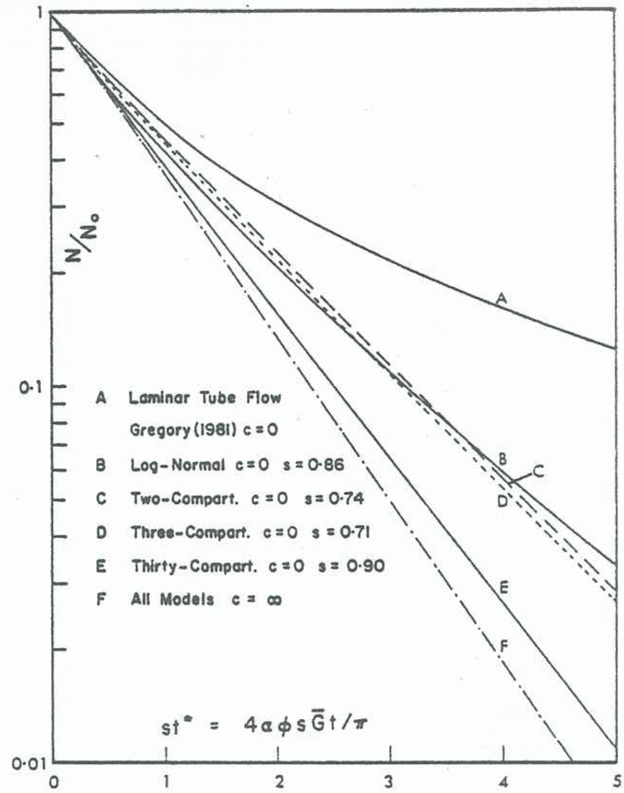

Figure 4 Theoretical flocculation rates for various models. Values of s are dependent on D/T ratios used in the models.

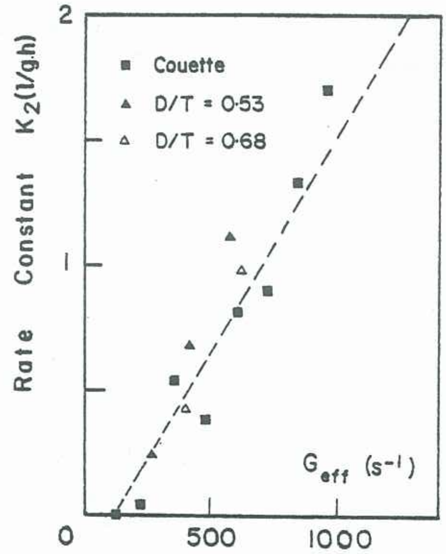

Figure 5 Experimental second order flocculation rate constant for Couette flow and for stirred tanks.