RRB-88-86

MODELING OF SETTLING AND FLOCCULATION OF FINE SEDIMENTS IN STILL WATER

by

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November 1988
NWRI Contribution #89-143

ABSTRACT

A numerical model to predict settling behaviour of fine sediment mixtures in a stagnant water column is described. Both single grain settling mode and the floc settling mode are considered. The single-grain settling mode is analyzed by solving the unsteady, one-dimensional diffusion-advection equation numerically and the floc settling mode is examined by solving a coagulation equation expressed as a discrete equation in logarithmic radius space considering the differential settling as the only collision mechanism.

The model results are compared with the laboratory experimental data of K. Kranck for both modes of sediment settling. The agreement between the model predictions and the experimental data is good. The model can be used for such practical applications as predicting sedimentation rates in reservoirs and settling basins.

Keywords: sediment mixtures, settling, flocculation, advection, diffusion, floc size distribution, primary particles.

RÉSUMÉ

Le présent ouvrage décrit un modèle numérique visant à prévoir la décantation des mélanges de sédiments fins dans une colonne d'eau stagnante. On y étudie à la fois le mode de décantation par grain et le mode de décantation par floc. Le premier mode est analysé en solutionnant numériquement l'équation instable de diffusion-advection unidimentionnelle, et le mode de décantation par floc est étudié en solutionnant l'équation de coagulation exprimée sous forme d'équation discrète dans l'espace logarithmique des rayons en considérant la décantation différencielle comme étant le seul mécanisme de collision.

Les résultats du modèle sont comparés avec les données d'expériences en laboratoire de K. Kranck pour les deux modes de décantation des sédiments. La concordance entre les prévisions du modèle et les données expérimentales est bonne. Le modèle peut être utilisé pour des applications pratiques comme la prévision de la vitesse de sédimentation dans les réservoirs et les bassins de décantation.

Mots-clés : mélanges de sédiments, décantation, floculation, advection, diffusion, granulométrie du floc, particules primaires.

MANAGEMENT PERSPECTIVE

The fine-grained sediments play an important role in the transport of contaminants in aquatic environments. For proper modelling of contaminant transport, modelling of fine grained sediment transport becomes an essential prerequisite. In this paper, a numerical modelling of settling and flocculation of fine sediments in still water is developed and compared with existing experimental data. The close agreement between model predictions and measured data observed in this paper is a hopeful sign for further developments in modelling of fine grained sediment transport processes in natural river systems.

PERSPECTIVE-GESTION

Les sédiments à grains fins jouent un rôle important dans le transport des contaminants en milieu aquatique. La modélisation du transport des sédiments à grains fins devient un élément essentiel pour la modélisation adéquate du transport des contaminants. Le présent article décrit l'élaboration d'un modèle numérique de décantation et de floculation des sédiments fins en eau calme et le compare avec les données expérimentales existantes. La concordance entre les prévisions du modèle et les données mesurées, observée dans ce rapport, est un signe prometteur pour les développements futurs en modélisation des processus de transport des sédiments à grains fins dans des réseaux fluviaux naturels.

Modeling of Settling and Flocculation of Fine Sediments in Still Water

by

Bommanna Gounder Krishnappan[1]

Introduction

The role of fine grained sediments in the transport of pollutants in rivers, estuaries and other water bodies has been widely recognized by a number of investigators (e.g., Allan, 1986; Frostner and Wittmann, 1981; Frank, 1981; Kuntz and Wary, 1983; Blackford and Ongley, 1984). As a result, a number of mathematical models has been developed to predict the transport of fine-grained sediments in a variety of flow environments. Among the models, the notable ones are:

1) SERATRA and FETRA by Yasuo Onishi, 1979, 1984
2) University of California model by K. Ziegler and W. Lick, 1986
3) Finite Element Hydrodynamic and cohesive sediment transport modelling system by E.J. Hayter, 1987
4) TABS-2 by U.S. Army Corps of Engineers, 1985
5) WASP-4 by U.S. EPA, 1988

In most of these models, the sediment is considered in different size fractions, and each size fraction is assumed to behave independent of the other fractions, i.e., the interaction between the size

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fractions (flocculation) is neglected. But in reality, the fine sediments do interact and flocculate. In fact, the flocculation has been found to be a dominant mechanism in the transport of fine sediments as it affects the sediment settling characteristics in the water column as well as the depositional and erosional characteristics at the sediment water interface (Krishnappan and Ongley, 1988). Hence, the inclusion of an explicit treatment of flocculation process in sediment transport model is necessary to make realistic predictions of fine-grained sediment transport.

Attempts have already been made to include the explicit treatment of flocculation process in the sediment transport models (see Valioulis _et_ _al_., 1984 a,b). In the work of Valioulis _et_ _al_. in which a sedimentation basin was modelled numerically, the flocculation of settling sediment was analyzed using a coagulation equation with three collision mechanisms, namely, Brownian motion, turbulent shear and the differential sedimentation. But the model of Valioulis _et_ _al_. lacks experimental verification.

In the present work, a computer model of flocculation process was developed for a simpler case of sediment settling in a stagnant water column for which laboratory experimental data are readily available in the literature. It was possible, therefore, in the present study to make a comparison of model results with experimental data and draw conclusions regarding the adequacy of the model for the treatment of the flocculation process.

Model Formulation

The approach used in the development of the present model is to consider the motion of sediment particles in two stages, namely, a settling stage and a flocculation stage. These two stages are assumed to occur alternately over a fixed time interval. The details of the formulation of each of the two components of the model are given in the following two sections.

a) Settling component

The settling stage is analyzed using the one-dimensional unsteady diffusion-advection equation which can be expressed as follows:

$$\frac{\partial C_k}{\partial t} + W_k \frac{\partial C_k}{\partial z} = \frac{\partial}{\partial z} \left(D \frac{\partial C_k}{\partial z}\right) \qquad (1)$$

where C_k is the volumetric concentration of sediment of kth size fraction, W_k is the fall velocity. D is the molecular diffusion coefficient, t is time and z is the vertical distance from the water surface (see Fig. 1 for the definition of the co-ordinate system).

Equation (1) expresses the mass balance of settling particles by accounting for the settling flux and the diffusive flux induced by Brownian motion in the vertical direction.

The boundary and initial conditions used are as follows:

At water surface (z=0). At the water surface, it is assumed that there is no transfer of sediment across the boundary. Therefore, the diffusive flux is equal to the settling flux, i.e.,

$$W_k C_k = D \frac{\partial C_k}{\partial z} \qquad (2)$$

At the bed (z=h). At the bed, it is assumed that sediment settling to the bed remains at the bed. Therefore, the diffusive flux at this boundary becomes zero, i.e.,

$$D \frac{\partial C_k}{\partial z} = 0 \qquad (3)$$

Initial condition (at t=0). At time t=0, it is assumed that the sediment concentration is uniform throughout the water column.

i.e., At t=0. $C_k = C_k^{IN}$ for $0 \leq z \leq h$ (4)

where C_k^{IN} is a constant.

Equation (1) can be solved analytically for some special cases (W, D and initial concentration distributions are constants or simple functions of z). In the present model, since the settling component has to be linked with a flocculation component, a numerical solution of the equation is sought. A number of numerical schemes have been developed for solving the unsteady diffusion-advection equations (see Damotharan _et al._, 1981). In this work, a numerical scheme proposed by Stone and Brain (1963) and described in Lau and Krishnappan (1981) was adopted.

To test the accuracy of the numerical scheme comparisons of the numerical solution with the analytical solution for the case where both W and D are constants were carried out. Fig. 2 shows the comparison for two different values of the bulk peclet number, $P_e = (Wh/D)$ which is the controlling parameter for the one dimensional settling of the sediment particles. From Fig. 2, it can be seen that there is no detectable difference between the two solutions. It is also evident from this figure that the concentration is fairly uniform over the depth and the solution is independent of the peclet number for the range of the peclet numbers tested which is 0.2 to 0.0002. This peclet number range would adequately cover the settling of fine sediments in the range of 1 μm to 40 μm.

b) Flocculation component

The flocculation stage of settling sediment was analyzed using the coagulation equation which expresses the rate of change of number of particles per unit fluid volume in a particular size class i as:

$$\frac{\partial N(i,t)}{\partial t} = - N(i,t) \sum_{j=1}^{\infty} K(i,j)\, N(j,t) +$$

$$\frac{1}{2} \sum_{j=1}^{\infty} K(i-j,j)\ N(i-j,t)\ N(j,t) \tag{5}$$

where N(i,t) and N(j,t) are the number concentrations of size classes i and j respectively at time t and K(i,j) is the collision frequency function which is a measure of the probability that a particle of size i collides with a particle of size j in unit time (see Valioulis _et_ _al_., 1984c). The first term on the right hand side of the above coagulation equation describes the reduction in number of particles in size class i by the flocculation between particles of class i and all other particles. The second term on the right-hand side gives the generation of new particles in size class i by the flocculation of pairs of particles in smaller size classes. In this process, it is assumed that the volume of the sediment particles is conserved. In other words, if r_i and r_j are the radii of particles of size classes i and j, then the radius r of the particle formed by flocculation of i and j class particles are given by:

$$r_i^3 + r_j^3 = r^3 \tag{6}$$

The flocculation formulation as described by equation (12) is based on the binary or two-body collision process; the probability that three or more particles colliding simultaneously and forming a single new particle is assumed to be negligible. Furthermore, the coagulation factor defined as the probability that a pair of collided particles coalesce and form a new particle is assumed to be unity. In the general form of the coagulation equation, the coagulation factor will figure as a multiplier along with the collision frequency function.

The collision frequency function K(i,j) takes different functional forms depending on the collision mechanism which is responsible for bringing particles to close proximity. Various collision mechanisms for which the collision frequency functions have already been derived are:

1) Brownian motion
2) Laminar or turbulent fluid shear
3) Particle inertia in turbulent flows
4) Differential settling of sediment mixtures.

The forms of the functions are tabulated in Pearson _et_ _al_. (1984).

For the present problem, only the first and the last mechanisms are relevant as there is no flow involved. Between these two mechanisms the Brownian motion is considerably less significant for particles larger than 1.0 μm (Hunt, 1980). Therefore, for the present model, only the differential settling mechanism is considered. The collision frequency function for the differential settling mechanism has been derived by Findheisen as early as in 1939 (see Pearson _et_ _al_., 1984). The form of the function is:

$$K(i,j) = \frac{2\pi G}{9\nu} \left(\frac{\rho_s - \rho_w}{\rho_w}\right) (r_i + r_j)^2 \mid r_i^2 - r_j^2 \mid \tag{7}$$

where G is acceleration due to gravity, ν is the kinematic viscosity of the fluid, ρ_s is the density of settling particles and ρ_w is the density of the fluid medium.

The solution of equation (5) in continuous radius space is tedious because of the wide range of particle sizes normally found in natural systems. To simplify the solution procedure, a discrete equation in logarithmic radius space was developed. Following Yue and Deepak (1979), the continuous radius space was discretized into a set of discrete ranges:

$$r_i = r_1 2^{\frac{1}{3}(i-1)} \qquad i=2,3,\ldots M \tag{8}$$

Each range can be treated as a bin containing particles of certain size range. r_1 is the geometric mean radius of particles in the first bin and M is the total number of bins. Above transformation implies that the volume of one particle in bin i is twice that of a particle in the preceding bin (particles are assumed to be spherical). Each bin is assumed to contain particles with volumes ranging from $(v_i - 1/2\Delta v_i)$ to $(v_i + 1/2\Delta v_i)$ where $v_i = (4/3)\pi r_i^3$ and Δv_i equals $2^{1-1} v_1$.

When particles in bin i collide and flocculate with particles of bin j ($j < i$), the newly formed particles will fit into bin i and bin i+1. The proportion in which the new particles are allocated to bin i and bin i+1 is calculated by the equation of conservation of mass before and after flocculation. For example, if N_{ij} is the total number of newly formed particles and N_x and N_y are the numbers of new particles going to bins i and i+1 respectively, then applying the conservation of mass principle, we get:

$$\rho_s N_{ij} v_i + \rho_s N_{ij} v_j = \rho_s N_x v_i + \rho_s N_y v_{i+1} \tag{9}$$

$$\text{i.e.,} \quad v_i + v_j = v_i \frac{N_x}{N_{ij}} + v_{i+1} \frac{N_y}{N_{ij}}$$

$$= v_i f_{ij} + v_{i+1} (1 - f_{ij}) \tag{10}$$

where f_{ij} is the fraction going to bin i and $(1 - f_{ij})$ is the fraction going to bin (i+1). Therefore, by knowing the particle volumes in bins i, i+1 and j, the particle allocation function f_{ij} can be computed as:

$$f_{ij} = (v_i + v_j - v_{i+1})/(v_i - v_{i+1}) \tag{11}$$

Under these conditions Eqn. (52) can be rewritten as:

$$\frac{\Delta N_i}{\Delta t} = - \sum_{j \neq i} K(i,j)\, N_i N_j + \sum_{j<i} f_{ij}\, K(i,j)\, N_i N_j + \sum_{j<i-1} (1 - f_{i-1,j})\, K(i-1,j)\, N_{i-1}\, N_j \qquad (12)$$

Applying the above equation to each of the bins, the change in the particle size distribution can be computed over a time interval of Δt.

Model Application and the Results

Laboratory experiments of Kranck (1980) were selected to test the predictions of the models. Kranck measured settling of sediment mixtures in still water under flocculated and unflocculated states. She used a glacial marine clay collected from a bank by the Miramichi River at Sillikers, New Brunswick as the settling material and 3% salt solution and 2% $(NaPO_3)_6$ dispersant solution as settling media. In salt solution, the sediment settled in a flocculated state whereas in $(NaPO_3)_6$ solution, the sediment settled as individual grains. Six tests were selected: three for flocculated state and three for single grain settling without flocculation.

The experimental procedure of Kranck was as follows: The sediment was suspended in a 15 cm diameter, 3 L glass bottle which served as the settling column. The suspension solution was filtered through a 0.45 μm millipore filter and was kept overnight at 10°C in a constant temperature bath.

The sediment was mixed evenly in the settling bottle by turning the bottle end over end a few times and the bottles were returned to the constant temperature bath. During the test, sediment samples were drawn at a distance of 15 cm from the surface at different times over a period of five days. The samples were analyzed for size distribution using a Coulter counter.

The results of the experiments and the model predictions are shown in Figs. 3 to 6. In these figures, experimental data are plotted as points and the model predictions are plotted as solid or dotted lines. In Fig. 3, the total concentration of sediment at the sampling level was plotted as a function of time for the three tests in which single grain settling was simulated. Model predictions corresponding to these three runs were carried by employing the settling component of the model only. The measured size distributions at an elapsed time of around 10 minutes were used as initial conditions for the model. During the initial 10 minute period, the settling was suspected to be influenced by the turbulence generated by the initial shaking of the settling bottles. Therefore, model predictions were not carried out for this initial period.

In performing the model simulations, for each time interval which is 10 secs, the governing equation (Eqn. 1) was solved for each size fraction to determine the concentration distribution of that size fraction over the depth. The fall velocity for the size fraction was computed using Stokes' equation with geometric mean size as particle diameter. A diffusion coefficient of 3.4×10^{-4} m^2/s was used. It was noticed that the results were not sensitive to the value of the diffusion coefficient as the fall velocities of the sediment fractions were very small (0.899×10^{-6} m/s to 0.92×10^{-3} m/s). A tenfold increase or decrease in the values of the diffusion coefficient did not alter the final results. The value of the fall velocity, on the other hand, had a significant effect on the results. In fact, it was necessary to apply a correction factor to the Stokes' fall velocity to bring the computed curves in Fig. 3 to match the experimental data. The correction factor used was 0.50. This is reasonable because the Stokes' equation assumes that the particle are spherical. Nonspherical particles such as clay particles can have significantly lower fall velocities (see Brun-Cottan, 1976).

From the simulation of the concentration distribution over the depth of all the size fractions, the total concentration of the sediment mixture at the sampling depth was computed as the sum of the concentration of the individual size fractions at the sampling height. The changes in total concentrations at the sampling level with time as predicted by the model compare favourably with the experimental data for the three tests in which the particles settle as individual particles without flocculation.

Fig. 4 shows the changes in particle size distribution as a function of time for these three tests and the agreement between the measured size distributions and the predicted distributions is also reasonable.

Fig. 5 shows the changes in total local sediment concentration as a function of time for sediment settling in salt solutions. The settling behaviour as depicted in these figures are drastically different from that of the previous tests. In these tests, the drop in total local concentration is more pronounced in the beginning and then gradually slows down. This is especially so for the test with the highest initial concentration. To simulate these tests in the model, the flocculation component of the model was coupled with the settling component. Starting from an initial size distribution and consequently an initial total concentration, the settling component of the model was employed to predict the size distribution after a time step, i.e., 10 secs. Then using this size distribution, the flocculation model was employed to calculate the change in the size distribution due to flocculation during the same 10 sec time interval. Using new size distribution as calculated from the flocculation component of the model as initial distribution to the settling component the size distribution for the next time step was computed. The procedure was repeated until the required settling time of 5 days is reached.

The changes in total local concentration with time predicted by the model are shown in Fig. 5 as solid lines. It can be seen from this figure that the model predictions agree reasonably well with the measured data: especially for the test with highest initial concentration, the sudden drop in total local concentration around the settling time of 1000 to 2000 sec is properly predicted by the model. The agreement around the settling period of 1 day to 5 days is also reasonable.

During the intervening period, the model tends to over predict the drop in the total concentration. It may be due to the schematization of the settling velocity of a floc in the model. It is assumed in the model that when two spherical particles collide and form a floc, it forms a new <u>spherical</u> particle whose volume is equal to the volumes of the individual particles and the settling velocity of the floc is computed using the Stokes' equation. Such schematization may not be completely valid especially if the flocculating particles are of comparable sizes. The effective density of the flocs is also likely to be less than the density of the primary particles. No attempt was made to correct for the fall velocity and bring the curves closer to the measured data since the measured data itself show a considerable scatter.

The size distributions of the flocs as predicted by the model for different time intervals are shown in Fig. 6. The size distributions measured by Kranck for these tests <u>should not be</u> compared with these predicted distributions because the Coulter counter used for the size analysis would break up the flocs and give the size distribution of primary particles only. Nevertheless, the experimental data of Kranck are plotted in Fig. 6 to highlight the difference between the floc size distribution and the primary particle size distribution. It can be seen from Fig. 6 that the predicted floc size distributions differ significantly from the primary particle size distributions during the initial periods of sediment settling (within the first hour). During this initial period, the flocs form and settle out. After that the flocculation process slows down and the settling is more dominated by single grain settling than the floc settling. The distribution of the sediment during the later stages of sediment settling resemble that of the primary particle. It is also clear from Fig. 6 that the floc settling behaviour is drastically different from the single-grain settling as is evidenced by the dramatic changes in the size distribution of the sediment mixtures. The measurement of size distribution of flocs (without disturbing the structure of flocs) will be useful to make a comparison with the predicted size distributions as an additional verification of the model results. But such measurements are very difficult to obtain at the present time, as the conventional sampling techniques are likely to disrupt the floc-structure (Gibbs, 1981). Only recently, some progress has been made in this area. Bale _et al_. (1987) have modified a laser particle size analyser manufactured by Malvern Instruments Ltd., and have used it to measure the floc size distribution in-situ in Tamar Estuary near Plymouth, England. They compared the size distributions measured with this instrument to those measured using conventional sampling technique and found that there are significant differences between the two distributions. Attempts are underway at the National Water Research Institute (Canada) to measure the floc size distributions using the Malvern Particle size analyzer and to verify the distributions predicted by the present model (Krishnappan and Ongley, 1988).

Summary and Conclusions

A numerical model capable of predicting the settling behaviour of sediment mixtures in a water column is described. Both single-grain settling mode and floc settling mode are considered. The model consists of two components: 1) a settling component and 2) a flocculation component. The settling component consists of a numerical scheme to solve the unsteady, one dimensional diffusion-advection transport equation and the flocculation component solves a coagulation equation expressed as a discrete equation in logarithmic radius space with the differential settling as the only collision mechanism.

Comparison of the model results with the experimental data of Kranck suggests that the model is capable of predicting both the single grain settling and floc settling behaviour of sediment mixtures in stagnant water columns. The model can be used for such practical applications as predicting the sedimentation rates in reservoirs and settling basins.

Acknowledgements

I wish to express my gratitude to:

1) Dr. Kate Kranck of Bedford Institute of Oceanography at Dartmouth, Nova Scotia, Canada, for providing the raw data for model comparison.

2) Dr. Y.L. Lau of National Water Research Institute for providing an analytical solution of the diffusion-advection equation for testing the accuracy of the numerical scheme.

3) Dr. S. Beltaos, Chief, River Modelling Project and Dr. E.D Ongley, Director, Rivers Research Branch, both at National Water Research Institute, for useful discussions and critical review of the manuscript.

4) Mr. Richard Frenette for assisting in the development of computer code for the settling component of the model.

5) Prof. John List and the other anonymous reviewers for their constructive criticisms and suggestions for the improvement of the manuscript.

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Appendix II. Notation

The following symbols are used in this paper:

a = weighting coefficient

b = weighting coefficient

C = volumetric concentration of sediment

d = weighting coefficient

D = vertical turbulent diffusion coefficient

f = particle allocation function

g = weighting coefficient

G = acceleration due to gravity

h = depth of water column

i = grid location along time axis

j = grid location along depth axis

K = collision frequency function

k = subscript referring to size fractions

m = weighting coefficient

N = number of particles in a given size range

p = element of the tri-diagonal matrix

P_e = Peclet number = wh/D

q = element of the tri-diagonal matrix

r = radius of sediment particles

S = elements of R.H.S. of matrix equation

t = time

u = element of the tri-diagonal matrix

v = volume of particles

w = fall velocity of sediment particles

z = vertical co-ordinate

Δ = operator denoting change

ϵ = weighting coefficient

θ = weighting coefficient

ν = kinematic viscosity of fluid

ρ_s = density of sediment particles

ρ_w = density of fluid

$\sum$ = summation sign

List of Figure Captions

Fig. 1. Schematic representation of sediment settling column

Fig. 2. Comparison between analytical solution and numerical prediction of single grain settling phase

Fig. 3 Changes in total local sediment concentration as a function of time (single grain settling)

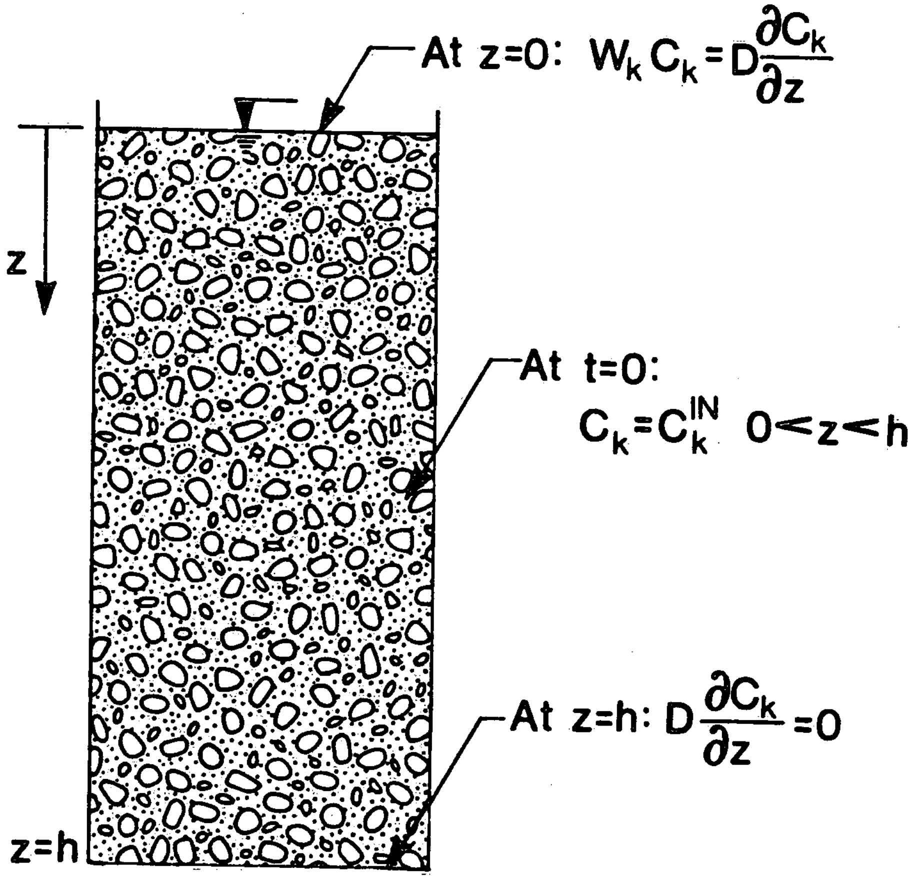
Fig. 4. Changes in grain-size distribution as a function of time (single grain settling)

Fig. 5. Changes in total local sediment concentration as a function of time (floc settling)

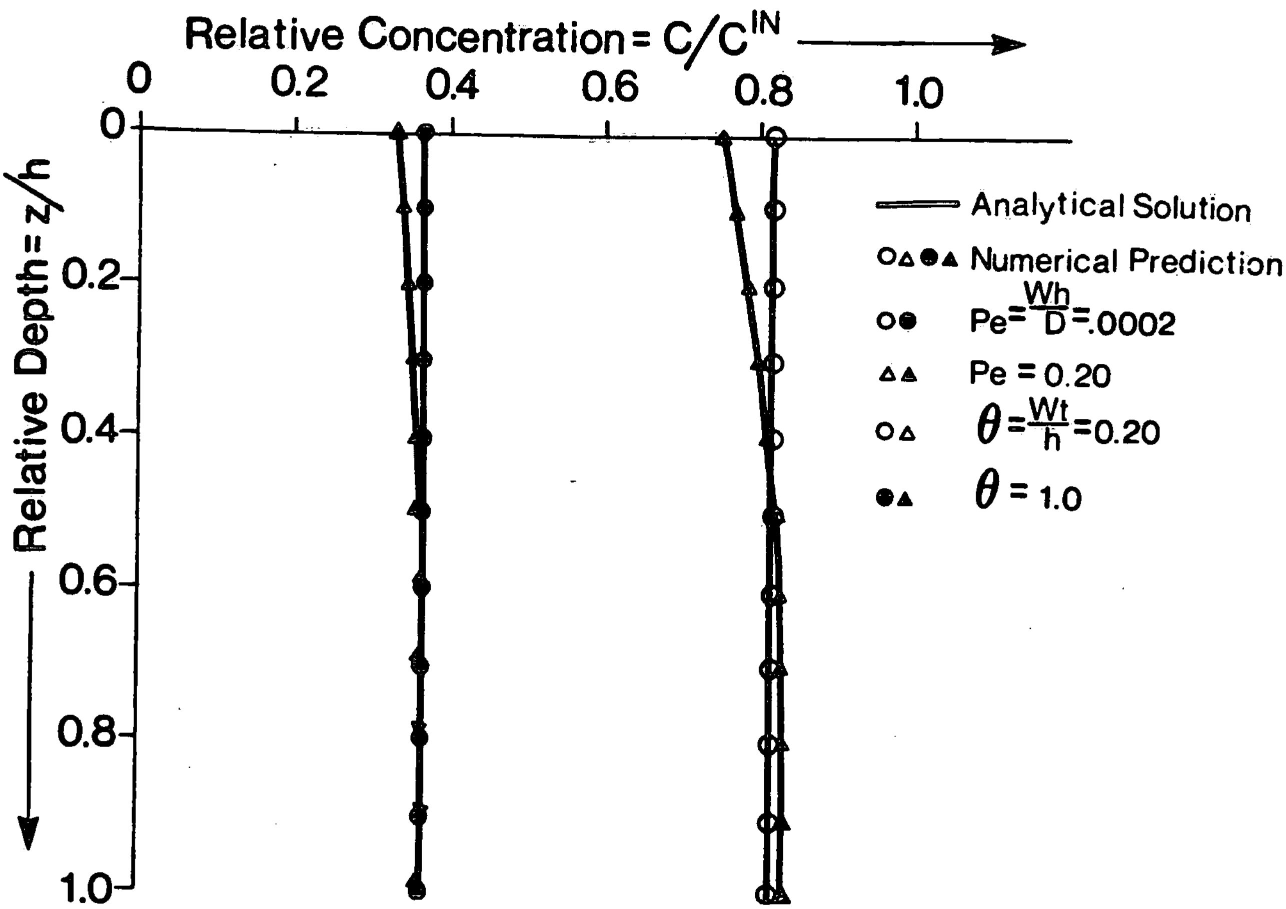
Fig. 6. Changes in grain size distribution as a function of time (floc settling)

Summary

A numerical model of settling of flocculated fine grained sediments is presented. The model consists of two components: a single grain settling component and a flocculation module. The model is verified using laboratory experimental data available in the literature.



At z=0: $W_k C_k = D\frac{\partial C_k}{\partial z}$
z
At t=0:
$C_k = C_k^{IN}$ $0 < z < h$
At z=h: $D\frac{\partial C_k}{\partial z} = 0$
z=h



Relative Concentration = C/C^IN
0
0.2
0.4
0.6
0.8
1.0
Relative Depth = z/h
0
0.2
0.4
0.6
0.8
1.0
Analytical Solution
Numerical Prediction
Pe = Wh/D = .0002
Pe = 0.20
θ = Wt/h = 0.20
θ = 1.0

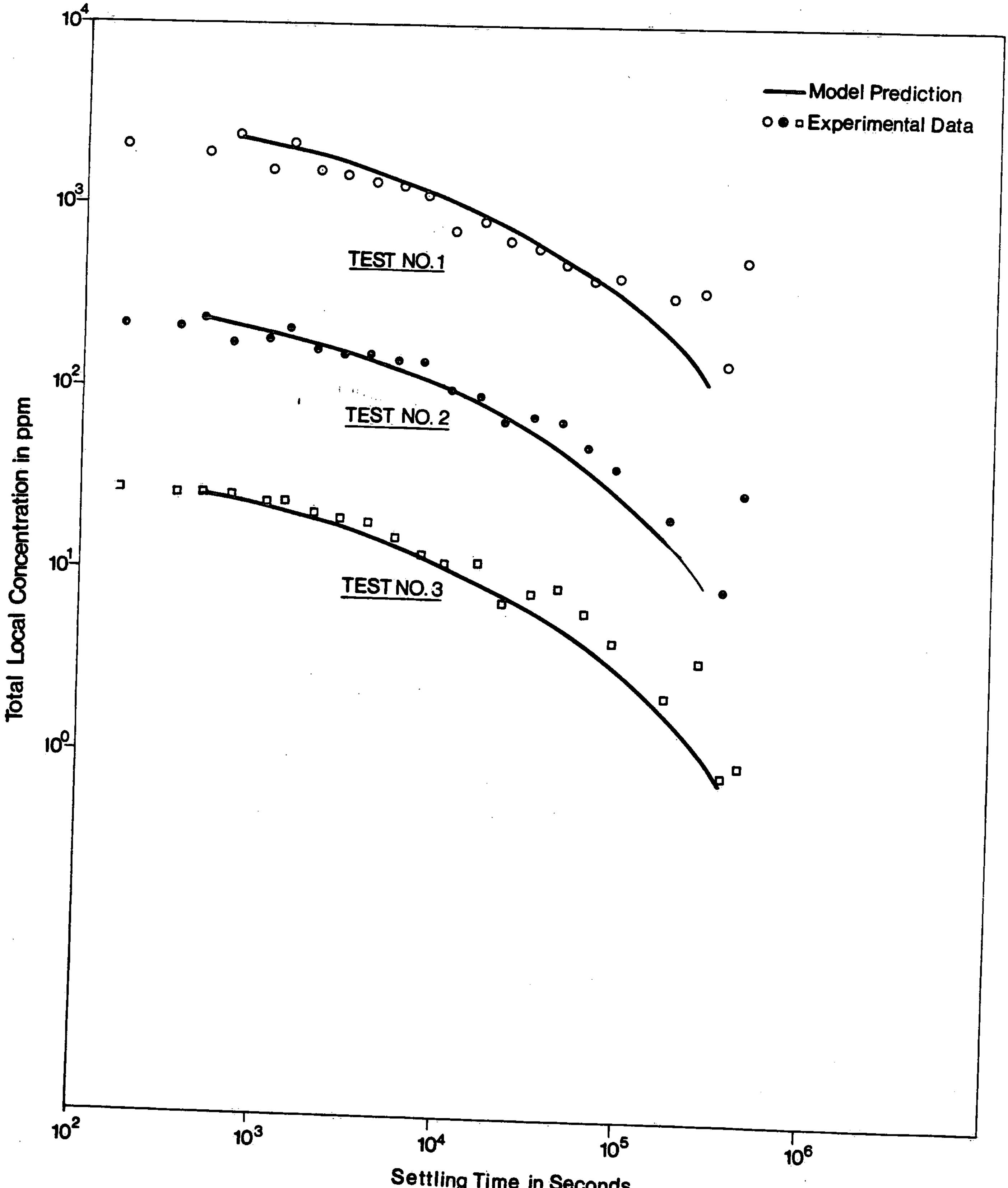
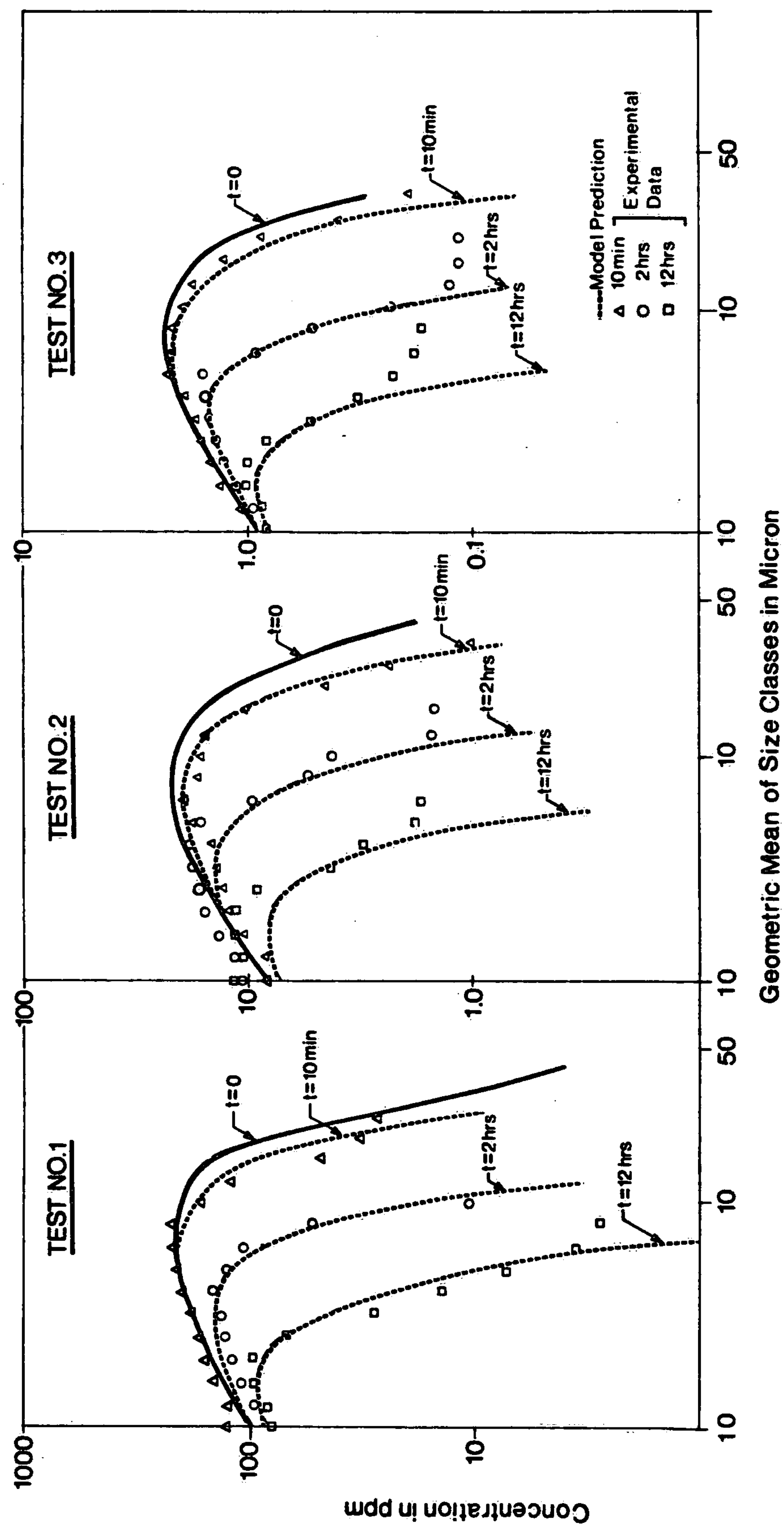


Figure. 4 CHANGE IN TOTAL SEDIMENT CONCENTRATION AS A FUNCTION OF TIME (SINGLE GRAIN SETTLING)

Figure 4



TEST NO.1
TEST NO.2
TEST NO.3
t=0
t=10min
t=2hrs
t=12hrs
Model Prediction
10min
2hrs
12hrs
Experimental Data
Concentration in ppm
Geometric Mean of Size Classes in Micron
1000
100
10
1.0
0.1
50

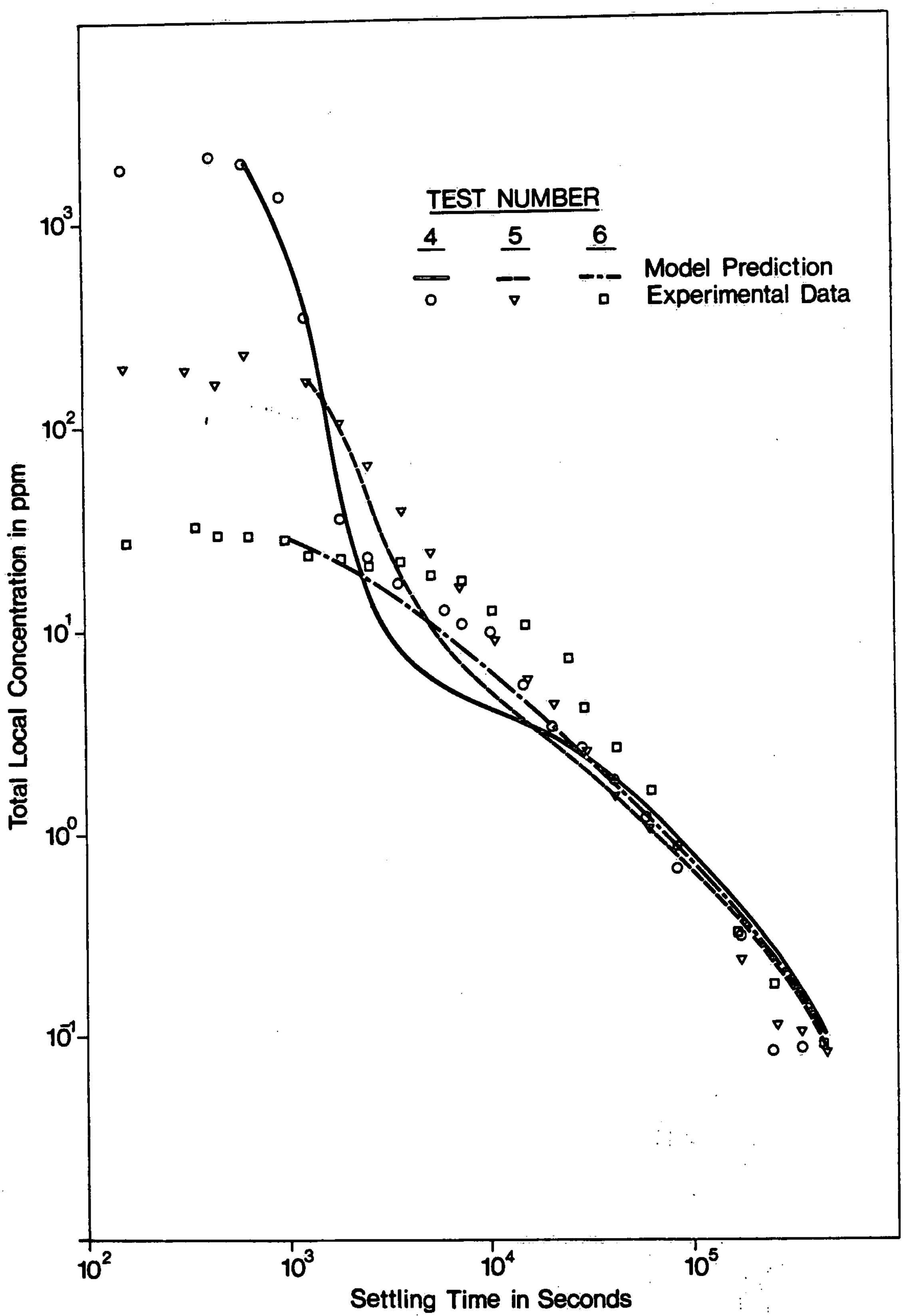
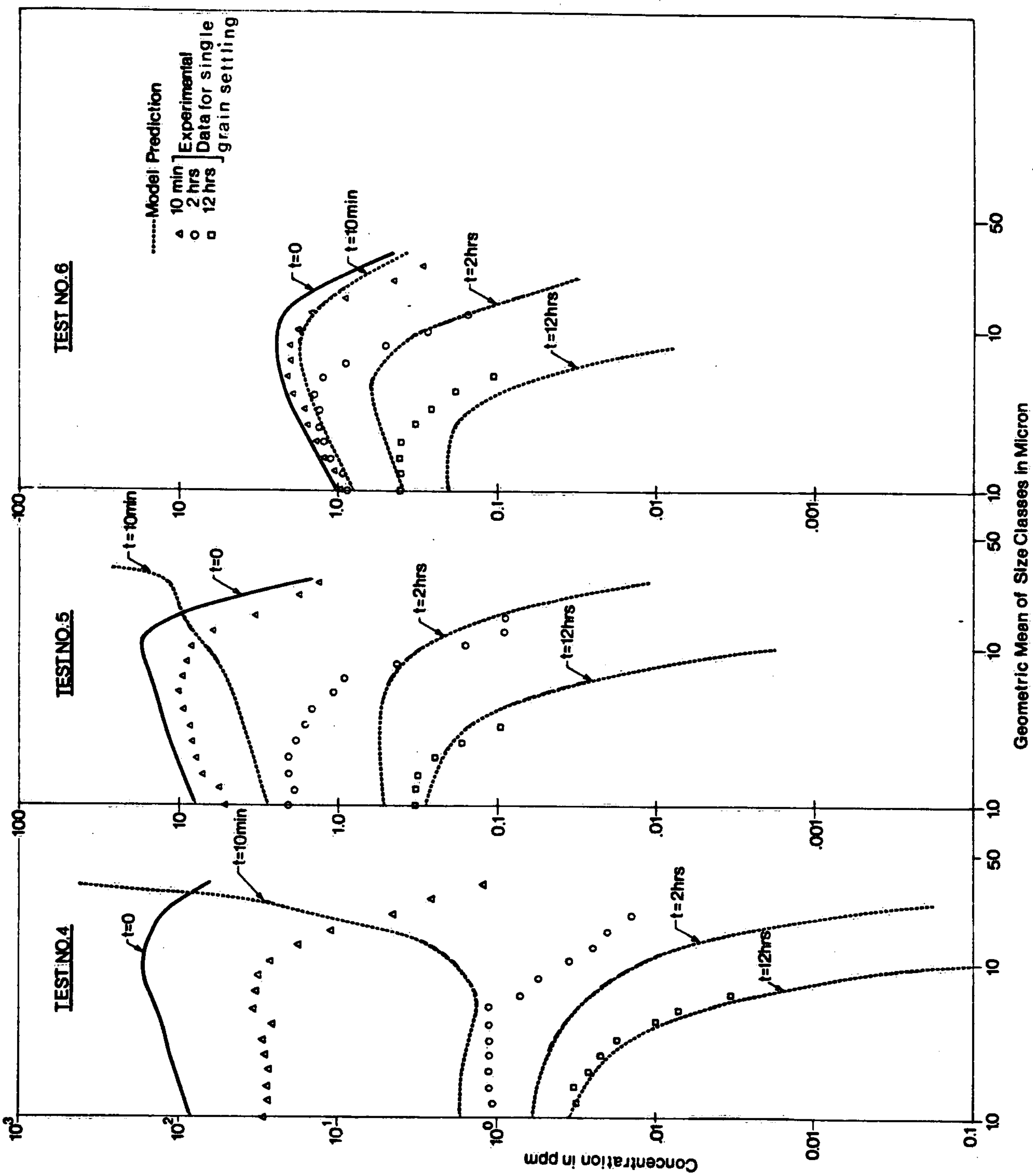


Fig. Change in Total Concentration as a Function of Time (Floc Settling)

Figure 6



TEST NO.4
TEST NO.5
TEST NO.6
Model Prediction
10 min
2 hrs
12 hrs
Experimental Data for single grain settling
t=0
t=10min
t=2hrs
t=12hrs
Concentration in ppm
Geometric Mean of Size Classes in Micron