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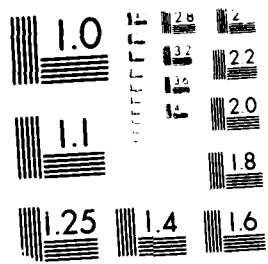
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**A diffusion model for large particles
in a turbulent gas flow**

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A DIFFUSION MODEL FOR LARGE PARTICLES

IN A TURBULENT GAS FLOW

A H Govan

Abstract

The diffusion model of Hutchinson et al (1971) for small particles has been extended to large particles in a vertical pipe. Allowance has been made for the slippage in the vertical direction and for the fact that successive particle displacements are no longer entirely independent. It is shown that the equations can be simplified to give a simple expression for the diffusion coefficient, and that this expression gives values which are in good agreement with the values obtained using a full 2D simulation of the particle trajectories. A criterion is given for determining when a particle may be considered to be "large".

Thermal Hydraulics Division
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1. INTRODUCTION

The motion of solid particles or liquid droplets in a turbulent gas flow is a problem which has many practical applications, eg in pneumatic conveying and spray drying. It is often necessary to account for particle dispersion due to turbulence, as a simple Newtonian calculation will usually underestimate the degree of dispersion. Hutchinson et al (1971) reviewed the available information and presented a model which treats the particle motion as a diffusive process. This model was shown to give good predictions for small particles (up to 110 microns) but it was suggested that the model may not be applicable to large particles.

The present work investigates the behaviour of large particles (greater than 1 mm) in a vertical pipe and shows how the Hutchinson model may be adapted to allow for slippage between the particles and the mean gas flow. This report also shows that for large particles there is a considerable degree of correlation between successive particle displacements. A method is presented for calculating the magnitude of the correlation terms, and this results in a simple expression for the diffusion coefficient. The predicted values are compared with those obtained from a 2D simulation of the particle trajectories.

2. DIFFUSION MODEL

2.1 Diffusion coefficient for small particles

The model of Hutchinson et al considers the particle motion in two parts (i) constant velocity parallel to the axis of the pipe and (ii) a radial motion consisting of a large number of displacements due to particle-eddy interactions. This radial motion is treated as a diffusive process and, assuming cylindrical symmetry, the density distribution $W(r,t)$ is given by the solution of the diffusion equation

$$K \nabla^2 W(r,t) = \frac{\partial}{\partial t} W(r,t) + S(r,t)$$

where $S(r,t)$ is the source term and K is the diffusion coefficient given by

$$K = v \frac{\langle l_p^2 \rangle}{4}$$

where $\langle l_p^2 \rangle$ is the mean square displacement per interaction and v is the interaction frequency. This expression for K assumes that the directions of individual displacements are uncorrelated; ie at any given time the particle has an equal probability of moving in any direction.

Assuming the turbulence is homogeneous ie has no preferred direction, then

$$\langle i_p^2 \rangle = 2 \langle i_{pr}^2 \rangle$$

where i_{pr} is the component of i_p in the radial direction. Thus we need only calculate the displacements for a one-dimensional problem. We obtain values for v and $\langle i_{pr}^2 \rangle$ by simulating the interactions between a particle and a large number of randomly-oriented one-dimensional eddies.

For a straight circular pipe the eddies were found by Hutchinson to be approximately uniform in size and velocity, and given by

$$l_e = 0.22 R$$

$$\text{and } U_e = U_t = U_G \sqrt{f/f_t} \quad (3)$$

where U_t is the characteristic friction velocity and f is a single-phase friction factor. The eddy lifetime was also assumed constant and given by

$$T_e = 1.6 l_e / U_e$$

Since the particles are small their mean velocity will be close to the mean gas velocity and so there will be negligible slip in the axial direction. The interaction time for each eddy is therefore given by

$$T = \min (T_e, T_x) \quad (4)$$

where T_x is the time taken for the particle to cross the eddy in the radial direction.

2.2 Equations of motion for small particles

To calculate the mean square displacement we must integrate the equation of motion of the particle, over the time T given by equation (4). For small particles gravity may be neglected and the equation of motion is

$$m \frac{dU_p}{dt} = C_D \frac{1}{2} \rho_g \frac{U_p^2}{4} (U_G - U_p) |U_G - U_p|$$

For small particles, the slip in the axial direction is usually much smaller than the eddy velocity. For example, for $U_G = 6 \text{ m/s}$ and $R = 0.165 \text{ m}$, a typical eddy velocity is about 0.25 m/s . The terminal velocity of a particle with density 1600 kg/m^3 and diameter $20 \text{ }\mu\text{m}$ is about 0.02 m/s . Thus, for small particles, we can write

$$m \frac{dU_{px}}{dt} = C_D \frac{1}{2} \rho_g \frac{v_d^2}{4} (U_{Gx} - U_{px}) |U_{Gx} - U_{px}| \quad (6)$$

for the velocity component in the radial direction. The mean gas flow has no horizontal component and so $U_{Gx} = (-1)^q U_g$ where q is a random number. Hutchinson used the following equation for the drag coefficient

$$C_D = \frac{10^C}{Re_p} \text{ where } C = 0.116 (\log_{10} Re_p)^2 + 0.0544 \log_{10} Re_p + 1.443.$$

Equation (6) was integrated by Hutchinson et al to give the particle velocity and displacement after each interaction, and hence the mean square displacement per interaction.

2.3 Equations of motion for large particles

For large particles the slip in the axial direction will usually be much greater than in the radial direction. For example, the terminal velocity of a 1 mm particle with a density of 1600 kg/m³ is 6 m/s. Equation (5) thus becomes

$$m \frac{dU_z}{dt} = C_D \frac{1}{2} \rho_g \frac{v_d^2}{4} (U_g - U_z) \Delta U_z$$

where ΔU_z is the velocity difference in the axial direction, assumed constant.

For the radial component, this gives

$$m \frac{dU_{px}}{dt} = C_D \frac{1}{2} \rho_g \frac{v_d^2}{4} ((-1)^q U_g - U_{px}) \Delta U_z$$

Integrating over time T gives

$$-m \log((-1)^q U_g - U_{px}) = C_D \frac{1}{2} \rho_g \frac{v_d^2}{4} \Delta U_z T$$

Rearranging and using dimensionless variables $V = \frac{U_{px}}{U_g}$,

$$x_1 = T/(l_g/U_g), S = \pm 1, h = l_{pr}/l_g, \text{ gives}$$

$$V = S - (S - V_0) e^{-x_1 h \Delta U_z / U_g}$$

$$\text{where } A = \frac{C_D \rho_p l}{d \rho_f \mu}$$

Integrating again gives

$$h = Sx_1 - \frac{(S-v_0)}{A \Delta U_z / U_0} (1 - e^{-x_1 A \Delta U_z / U_0}) \quad (8)$$

Because the slip is large in the axial direction, the interaction time will always be the time taken to cross the eddy in that direction

ie $T = l_0 / \Delta U_z$. Thus $x_1 = \frac{U_0}{\Delta U_z}$. Thus equation (7) becomes

$$v = S - (S - v_0) e^{-A} \quad (9)$$

and equation (8) becomes

$$h = \frac{U_0}{\Delta U_z} \left[S - \frac{(S - v_0)}{A} (1 - e^{-A}) \right] \quad (10)$$

If $A \ll 1$, then $1 - e^{-A} = A$, so

$$h = \frac{v_0 U_0}{\Delta U_z} \quad (11)$$

2.4 Diffusion coefficient for large particles

Equation (2) may be written

$$K_0 = \frac{v_0}{4} \cdot 2 \langle h^2 \rangle l_0^{-1}$$

$$= \frac{v_0}{2} l_0^{-1} \frac{1}{N} \sum_{i=1}^N h_i^2$$

where the h_i 's are the dimensionless displacements calculated from the simulation. It has already been pointed out that this equation applies only when individual displacements are uncorrelated. For large particles this is unlikely to be the case since a particle moving in a particular direction will have too great a momentum to be immediately diverted to any other direction. In general

$$\begin{aligned}
K &= \frac{v}{2} \frac{1}{e} \frac{1}{N} \left(\sum_{i=1}^N h_i \right)^2 \\
&= \frac{K_0}{\langle \bar{h}^2 \rangle} \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N h_i h_j \\
&= \frac{K_0}{\langle \bar{h}^2 \rangle} \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N h_i h_{i-j}
\end{aligned}$$

where the summation over j is understood to "wrap around" the value of 1.

$$\begin{aligned}
\text{Thus } K &= \frac{K_0}{\langle \bar{h}^2 \rangle} \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N \langle h_i h_{i-j} \rangle \\
&= \frac{K_0}{N} \sum_{i=1}^N \sum_{j=1}^N e^{-A(j-1)} \text{ using equation (A5)} \\
&= K_0 \sum_{j=1}^N e^{-A(j-1)}
\end{aligned}$$

Converting the summation to an integral,

$$\begin{aligned}
K &= K_0 \int_1^N e^{-A(j-1)} dj \\
&= \frac{K_0}{A} (1 - e^{-(N-1)A}) \quad (12)
\end{aligned}$$

If N is sufficiently large, this gives $K = K_0/A$. Otherwise, equation (12)

must be evaluated, with N given by $N = \frac{Z \cdot \Delta U_z}{1 \cdot U_{pz}}$. The value of K_0 may be obtained from the 1D simulation discussed in Section 2.1. However, equation (A4) shows that it can be approximated by

$$\begin{aligned}
K_0 &= \frac{v}{4} \frac{1}{e} \frac{1}{2} \frac{A}{\Delta U_z} \frac{U_e}{\Delta U_z} \cdot 2 \\
\text{Putting } v &= \frac{\Delta U_z}{1 \cdot e} \text{ gives } K_0 = \frac{1 \cdot U_e^2 A}{4 \Delta U_z} \quad (13)
\end{aligned}$$

thus, for a sufficiently long pipe,

$$K = \frac{l_e U_e^2}{4AU_e^2}$$

3. TWO DIMENSIONAL SIMULATION OF PARTICLE TRAJECTORIES

To investigate the validity of the above mathematical treatment of the droplet motion, a technique has been devised in which the particle distribution is calculated by plotting the trajectories of a large number of particles as they interact with a succession of eddies of specified size and velocity.

The technique is described in more detail by James et al (1980) who applied it to the motion of small droplets flowing co-currently with a gas stream. They used the same description of the eddies as in section 2.1 of this report but they treated the eddies as two-dimensional and used a random number to describe the orientation of each eddy. They used the following approximation for the drag coefficient:

$$C_D = 24/Re_p + 0.44$$

because using this equation it is possible to resolve the drag law into components and integrate over the interaction time.

Boysan et al (1982) used a similar technique for the motion of droplets in a cyclone. However, instead of assuming constant eddy properties, they calculated local values from the following equations

$$l_e = 0.3 k^{3/2}/\epsilon$$

$$T_e = 0.37 k/\epsilon$$

$$U_{ex} = q_1 \sqrt{\frac{2}{3}} k$$

$$U_{ey} = q_2 \sqrt{\frac{2}{3}} k$$

where k and ϵ are the turbulent kinetic energy and dissipation rate predicted by a $k-\epsilon$ model for the single phase flow, and q_1, q_2 are pseudo-random numbers with a normal distribution. The drag coefficient was assumed constant during any interaction.

The techniques of James and Boysan may both be applied to countercurrent flow provided the equations describing the particle-eddy interactions are modified as shown in section 2.3 to allow for the large vertical slip. However, for particles flowing in a straight pipe (not close to the wall) the two approaches gave very similar results.

4. COMPARISON OF PREDICTIONS OF DIFFUSION MODEL AND TRAJECTORY SIMULATION

The diffusion model of Section 2 and trajectory simulation of Section 3 have been used to calculate the distribution of particles dropped vertically on the centre line of a 0.33 m diameter vertical column. The calculations were carried out for particles of diameter 2.4 mm and 1 mm, density 1600 kg/m³ and gas velocities of 6 m/s and 3 m/s.

Provided the particles do not reach the walls then the solution to the diffusion equation, equation (1), for these conditions, is a two-dimensional Gaussian.

$$W(x,y) = \frac{1}{2\pi\sigma^2} e^{-(x^2 + y^2)/2\sigma^2}$$

where $\sigma^2 = 2Kt$

Integrating over all values of y gives

$$W(x) = \frac{1}{\sqrt{2\pi} \sigma} e^{-x^2/2\sigma^2}$$

which is a Gaussian with rms displacement σ .

Figure 1 shows the particle distribution at $z = 3.6$ m predicted by the simulation model using 500 particles. Clearly this is also Gaussian, with σ given by the rms value of x_p . Thus an effective diffusion coefficient K may be obtained from the calculated value of σ for this distribution.

Figure 2 shows average values of the correlation terms $\langle h_i h_{i-j} \rangle$ calculated by the simulation model. The magnitude of these terms decays very slowly, with several hundred interactions required before the correlation decays to a negligible value. The predictions of equation (16) are also shown and agree quite well with the simulation model.

Consider now the diffusion coefficients calculated with and without the correlation terms. In Table 1 K_0 is the diffusion coefficient obtained when correlation terms are neglected, and K is the value obtained when they are included. For the conditions used here, K is two orders of magnitude greater than K_0 . Table 1 also shows that the values of K and K_0 predicted by the simplified equations (17 and 18) agree with the values obtained from the 1D and 2D simulations, especially for the larger particles (which have a higher value of A). Here N , the total number of interactions, = 130 and 130 for the 2.4 mm and 1.0 mm particles respectively.

5. CONCLUSIONS

The diffusion model of Hutchinson et al (1971) for small particles in a turbulent gas flow has been extended to large particles in a vertical pipe, where the slip between the particles and the mean gas flow is large.

It was shown that under these circumstances the displacements resulting from successive particle-eddy interactions are correlated ie there is a high probability that successive displacements will be in the same direction. These correlation effects can result in diffusion coefficients which are two orders of magnitude higher than would be expected.

It was also shown that provided the parameter A , defined by

$$A = \frac{3}{4} \frac{C_D \rho_g l_e}{d_p \rho_p}$$

is small (ie $A \ll 1$) then the equations describing the particle eddy interactions can be greatly simplified and the following equation was derived for the diffusion coefficient, including the correlation effect just described.

$$K = \frac{1}{4} \frac{U^2}{\Delta U^2} (1 - e^{-(N-1)A})$$

$$\text{where } N = \frac{ZAU}{U^2}$$

Particle distributions calculated with this diffusion coefficient agreed well with the distributions predicted by a trajectory simulation, for a particular set of conditions. This shows that the mathematics of the process have been correctly described. However, since the physics of the particle-eddy interactions is the same in both models, this aspect has not yet been tested.

It is intended to carry out experiments in a perspex test section using photographic methods for determining particle position. A parametric study will also be carried out using the model to determine the limits of validity of the model.

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APPENDIX - Calculation of correlation terms

Equation (9) may be written as a recurrence relation

$$V_i = S_i - (S_i - V_{i-1}) e^{-A} \quad (A1)$$

Applying this relation n times gives

$$V_n = (1 - e^{-A}) \sum_{i=1}^n S_i e^{-(n-i)A} + e^{-nA} V_0 \quad (A2)$$

If n is sufficiently large the term $e^{-nA} V_0$ may be neglected.
 Applying equation (A1) to i=n, and i=n-r,

$$V_n = S_n (1 - e^{-A}) + V_{n-1} e^{-A}$$

$$\text{and } V_{n-r} = S_{n-r} (1 - e^{-A}) + V_{n-r-1} e^{-A}$$

Multiplying and summing over n,

$$\begin{aligned} \sum_{n=1}^N V_n V_{n-r} &= \sum_{n=1}^N e^{-2A} V_{n-1} V_{n-r-1} + e^{-A} (1 - e^{-A}) \sum_{n=1}^N V_{n-1} S_{n-r} \\ &+ (1 - e^{-A})^2 \sum_{n=1}^N S_n S_{n-r} + e^{-A} (1 - e^{-A}) \sum_{n=1}^N S_n V_{n-r-1} \end{aligned}$$

The last two summations may be neglected since the S_n 's are uncorrelated and there is no correlation between S_n and V_{n-r-1} , provided $r > 0$. Thus

$$\begin{aligned} \sum_{n=1}^N V_n V_{n-r} &\approx e^{-A} (1 - e^{-A}) \sum_{n=1}^N V_{n-1} S_{n-r} \\ &= e^{-A} (1 - e^{-A}) \sum_{n=1}^N S_{n-r} \sum_{i=1}^{n-1} (1 - e^{-A}) S_i e^{-(n-1-i)A} \\ &\quad \text{using equation (A2)} \\ &= e^{-A} (1 - e^{-A})^2 \sum_{n=1}^N e^{-(n-1)A} \end{aligned}$$

since the S_n 's are uncorrelated

$$\text{Hence } \langle v_n v_{n-r} \rangle = \frac{e^{-A}(1-e^{-A})^2}{1-e^{-2A}} e^{-(r-1)A}$$

Putting $e^{-A} = 1-A$ gives

$$\langle v_n v_{n-r} \rangle = \frac{A}{2} e^{-(r-1)A} \quad (\text{A3})$$

In particular $\langle v_n^2 \rangle = \frac{A}{2} e^A \approx \frac{A}{2}$ since A is small

Thus, equation (11) gives

$$\langle h^2 \rangle = \frac{U^2}{\Delta U^2} \cdot \frac{A}{2} \quad (\text{A4})$$

$$\begin{aligned} \text{and } \langle h_n h_{n-r} \rangle &= \frac{U^2}{\Delta U^2} \langle v_n v_{n-r} \rangle \\ &= \langle h^2 \rangle e^{-(r-1)A} \end{aligned} \quad (\text{A5})$$

NOMENCLATURE

A	constant defined in equation (7)
C_D	drag coefficient
d_p	particle diameter
h^p	dimensionless particle displacement
k	turbulent kinetic energy
K	diffusion coefficient
K_0	diffusion coefficient, neglecting correlation terms
l_e	eddy lengthscale
l_p	particle displacement
l_{pr}	particle displacement in plane perpendicular to gas flow
m	particle mass
N	total number of particle-eddy interactions
q	random number
q_1, q_2	normally distributed pseudo-random numbers
R	pipe radius
Re_p	particle Reynolds number
S^p	dimensionless eddy velocity
T	interaction time
T_e	eddy lifetime
U	eddy velocity
U_C	mean gas velocity
U_p	particle velocity
V^p	dimensionless particle velocity
V_0	dimensionless particle velocity at start of interaction
W	particle density distribution
x, y	co-ordinates in plane perpendicular to tube axis.
Z	length of tube
ΔU_z	particle slip velocity in axial direction
c	turbulent dissipation rate
v	interaction frequency
ρ_g	gas density
σ_g	standard deviation of particle distribution
x_i	dimensionless interaction time

Subscripts

x, y	directions perpendicular to tube axis
i, j, n, r	ith, jth, nth, rth interaction

TABLE 1

COMPARISON OF DIFFUSION COEFFICIENTS

d_p (mm)	2.4	1.0
U_G (m/s)	6	3
ΔU_z (m/s)	9.5	5.9
Re_p	1500	390
C_D	0.41	0.59
A	0.005	0.0174
N (for Z = 3.6 m)	180	130
K_0 (mm^2/s) predicted by 1D simulation	0.37	0.57
K_0 predicted by equation (13)	0.42	0.73
K (mm^2/s) predicted by equations (12) and (13)	50	38
K evaluated from predictions of 2D simulation model at Z = 3.6 m.	43	46

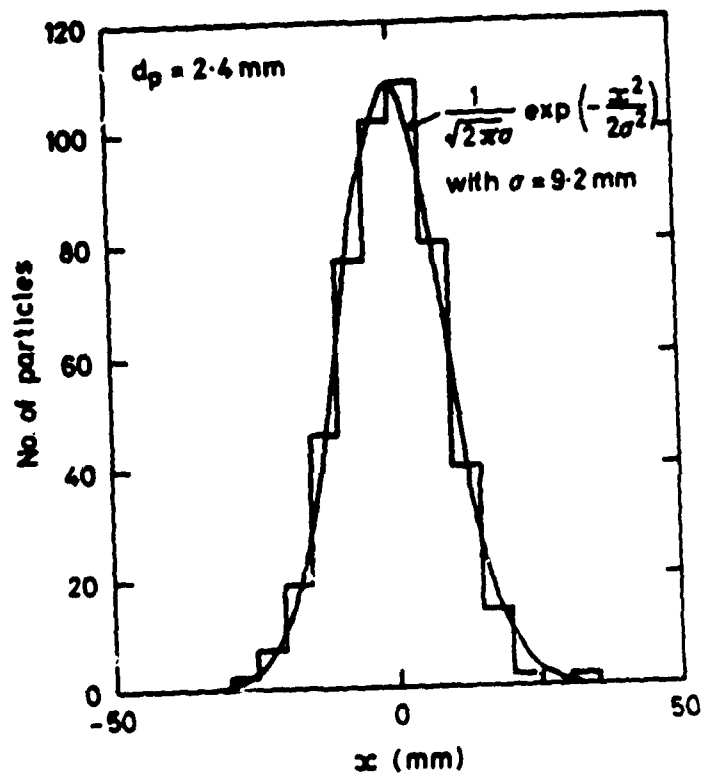


FIG. 1. PARTICLE DISTRIBUTION PREDICTED BY SIMULATION MODEL

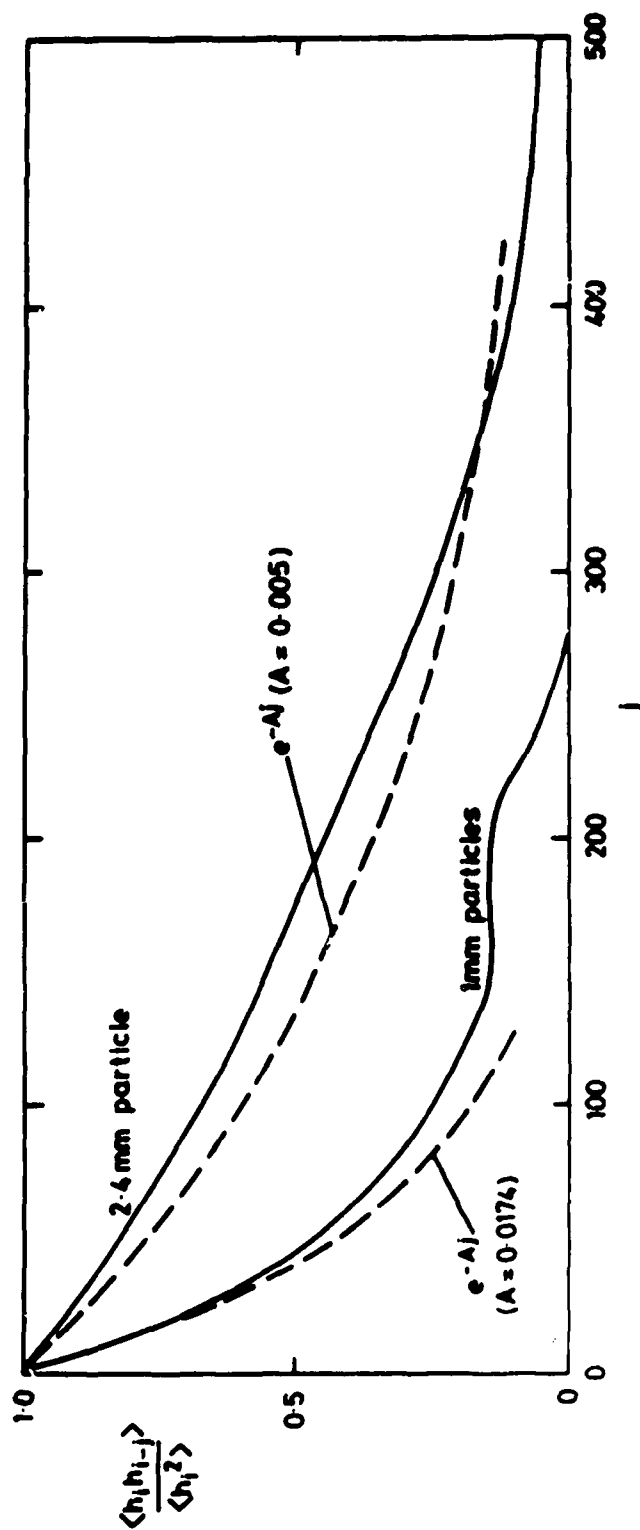


FIG 2 RATE OF DECAY OF CORRELATION TERMS

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