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BRIEF COMMUNICATION

A SIMPLE EQUATION FOR THE DIFFUSION COEFFICIENT OF LARGE PARTICLES IN A TURBULENT GAS FLOW

A. H. GOVAN
Thermal Hydraulics Division, Harwell Laboratory, Didcot,
Oxon. OX11 0RA, England

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Abstract—Published models for particle diffusion coefficients are usually only applicable for small particles because they make assumptions that are not valid for larger particles, e.g. that Stokes law is valid, that gravity may be neglected or that the particle response time is less than the timescale of the turbulence. Nevertheless, there are situations where the dispersion of particles $>100\ \mu$m dia by a turbulent flow can be an important effect. In this paper it is shown that for particles $\gtrsim 100\ \mu$m the equations for the particle diffusion coefficient reduce to a very simple form. It is also shown that the resulting equation gives good agreement with the results of numerical simulations.

Key Words: turbulent flow, particles, diffusion, numerical simulation

1. INTRODUCTION

The motion of solid particles or liquid droplets in a turbulent gas flow is a problem which has many practical applications, e.g. pneumatic conveying, spray drying and annular mist flow in pipelines and boiler tubes. Although the physics of the particle–turbulence interaction is reasonably well understood, it has not yet proved possible to formulate a general theory describing the dispersion of a particulate phase under the influence of a turbulent flow field, even for the relatively simple case of dilute suspensions where the influence of the particles on the gas phase may be neglected.

Numerical simulations of the dispersion of an ensemble of particles, in which the trajectory of each particle is calculated as a series of interactions with discrete pseudo-random turbulent eddies ("random walks") are relatively easy to implement, but are often costly and time-consuming because a large number of particles must be modelled. Nevertheless, this "Lagrangian" approach can be a very valuable research tool. Examples of its use are the studies of Brown & Hutchinson (1979), James *et al.* (1980), Boysan *et al.* (1982), Weber *et al.* (1984) and Gouesbet *et al.* (1987).

The alternative ("Eulerian") approach, which has received much more attention in the literature, is to consider the particle dispersion as a diffusion process with an appropriate particle diffusion coefficient. In situations with a simple geometry and a constant diffusion coefficient the diffusion equation may be solved analytically. In more complex situations the diffusion coefficient will be a function of position and the solution will usually be obtained by incorporating the diffusion coefficient in a two-fluid model. However, in spite of the extensive literature on the subject, no general method exists for predicting particle diffusion coefficients.

Taylor (1921) showed that for a stationary process in a homogeneous turbulence, the long-time particle diffusion coefficient may be expressed as

$$\epsilon_{\mathrm{p}} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\langle X_{\mathrm{p}}(t)^2\rangle = \langle u_{\mathrm{p}}^2\rangle \tau_{\mathrm{p}}, \qquad [1]$$

where $X_p(t)$ is the total displacement of the particle, $\langle u_p^2 \rangle$is the mean square particle fluctuating velocity and τ_p is the integral timescale of the particle motion, given by

$$\tau_p = \int_0^\infty R_p(\theta)\,d\theta, \qquad [2]$$

where $R_p(\theta)$ is the particle autocorrelation, given by

$$R_p(\theta) = \frac{\langle u_p(t) u_p(t+\theta) \rangle}{\langle u_p^2 \rangle}.$$

In general, both $\langle u_p^2 \rangle$ and τ_p are unknown but by making some simplifying assumptions several authors have derived methods for calculating ϵ_p. For example, Ganic & Mastanaiah (1981) assumed a linear (Stokes) drag law (strictly applicable only for particle Reynolds numbers $\mathrm{Re}_p < 1$) and were able to calculate the ratio $\overline{u_p^2}/\overline{u_G^2}$. This ratio was assumed equal to the ratio of the particle diffusivity to the gas diffusivity, and so the model is valid only for diffusion times much less than the gas integral timescale τ_G. The analysis was later extended by El-Kassaby & Ganic (1986) to $\mathrm{Re}_p < 5$. A recent model by Lee & Wiesler (1987) made the same assumptions but calculated the amplitude ratio $\eta = \overline{u_p^2}/\overline{u_G^2}$ in a different way. McCoy & Hanratty (1978) also used Stokes law but extended the analysis to nonstationary dispersion.

Reeks (1977) also assumed a linear drag law but allowed that $\tau_p \neq \tau_G$ and obtained analytic solutions for the diffusion coefficient with and without the effect of gravity. In the zero-gravity case it was shown that ϵ_p may be greater than ϵ_G [in agreement with the findings of Brown & Hutchinson (1979) from a simulation], but it was also shown that the effect of gravity (known as the "crossing-trajectories" effect) is to greatly reduce ϵ_p.

In the model of Hutchinson *et al.* (1971) the diffusion coefficient was calculated using a 1-D random-walk, in which case

$$\langle X_p^2 \rangle = \left\langle \left(\sum_i x_i \right)^2 \right\rangle, \qquad [3]$$

where the x_i are the individual displacements in the random-walk. Assuming $\langle x_i x_j \rangle = 0$ if $i \neq j$ (equivalent to saying that $\tau_p = \tau_G$), this gives

$$\begin{aligned} \langle X_p^2 \rangle &= \left\langle \sum_i x_i^2 \right\rangle \\ &= \nu t \langle x_i^2 \rangle, \end{aligned}$$

where ν is the interaction frequency.

Thus,

$$\epsilon_p = \frac{1}{2}\frac{d}{dt}\langle X_p^2 \rangle = \frac{1}{2}\nu \langle x_i^2 \rangle \qquad [4]$$

which is the equation given by Hutchinson *et al.* In this model a non-linear drag law was used but the crossing-trajectories effect was neglected.

The purpose of the work described in this paper is to present a method of calculating the diffusion coefficient for larger particles ($\gtrsim 100\ \mu$m) which do not obey Stokes drag, have a long relaxation time (so $\tau_p > \tau_G$) and are strongly influenced by gravity. The analysis presented here is restricted to vertical flow. Particles of this size may occur in practice in annular-mist flow in pipes, spray drying, prilling and the motion of raindrops. The work described here is concerned mainly with long-time behaviour. In some real systems the residence time of the particles may be less than the time necessary for these large particles to achieve long-time behaviour, but it is felt that an understanding of such behaviour is a necessary prerequisite to understanding the behaviour in developing systems.

It is shown that for such particles the equation for the diffusion coefficient can be reduced to a very simple form. The predictions of this equation are compared with a numerical simulation and with the methods of Reeks (1977) and Hutchinson *et al.* (1971).

2. THEORY

2.1. Equation of motion

For particles which are sufficiently heavy that virtual mass and Basset history forces may be neglected, the drag equation may be written as

$$m_p \frac{d\mathbf{U}_p}{dt} = C_D \frac{1}{2} \rho_G \frac{\pi d_p^2}{4} (\mathbf{U}_G - \mathbf{U}_p) |\mathbf{U}_G - \mathbf{U}_p|, \quad [5]$$

where $\mathbf{U}_G = (u_G, v_G, w_G)$ and $\mathbf{U}_p = (u_p, v_p, w_p)$ are the gas and particle velocities, m_p and d_p are the particle mass and diameter, ρ_G is the gas density and C_D is the drag coefficient. In this work C_D is calculated using the equation suggested by Brown (1978):

$$C_D = \frac{24}{\mathrm{Re}_p} + 0.44 \quad [6]$$

In figure 1 this equation is compared with the standard curve given by Clift *et al.* (1978) and shown to give reasonable results. However, the use of this drag equation is not essential and in fact any suitable equation could be used.

For large particles in a vertical gas flow the settling velocity Δw_T is generally greater than the gas turbulence velocity u_e and thus,

$$|\mathbf{U}_G - \mathbf{U}_p| \simeq \Delta w_T$$

for particles which have reached long-time behaviour. Equation [5] thus gives, for motion in the horizontal plane,

$$m_p \frac{du_p}{dt} = C_D \frac{1}{2} \rho_G \frac{\pi d_p^2}{4} (u_G - u_p)\, \Delta w_T, \quad [7]$$

where $C_D = C_D(\mathrm{Re}_p)$ with $\mathrm{Re}_p = \rho_G \, \Delta w_T d_p / \mu_G$. According to the model of Hutchinson *et al.* (1971), u_G may be taken as $\pm u_e$ and [7] may be integrated to give the dimensionless particle velocity

$$V = \pm 1 - (\pm 1 - V_0)\exp(-\beta t), \quad [8]$$

where $V = u_p/u_e$ and β, the inverse particle relaxation time, is given by

$$\beta = \frac{3}{4} \frac{C_D}{d_p} \frac{\rho_G}{\rho_p} \Delta w_T.$$

In a random-walk model, u_G is assumed constant during each particle–eddy interaction. For large particles, the interaction time t_i is always the crossing due to gravity, i.e.

$$t_i = l_e / \Delta w_T,$$

where l_e is the eddy lengthscale.

2.2. Particle autocorrelation

By writing [8] as a recurrence relation,

$$V_n = \pm 1 - (\pm 1 - V_{n-1})\exp(-A),$$

where $A = \beta l_e / \Delta w_T$, Govan (1986) showed that, provided $A \ll 1$ (i.e. the particle relaxation time $1/\beta$ is much greater than the interaction time $l_e/\Delta w_T$), then

$$\langle V_n V_{n-r} \rangle = \frac{A}{2} \exp(-rA)$$
$$= \langle V^2 \rangle \exp(-rA)$$

and

$$\langle x_n x_{n-r} \rangle = \left(\frac{u_e l_e}{\Delta w_T} \right)^2 \frac{A}{2} \exp(-rA) \quad [9]$$
$$= \langle x^2 \rangle \exp(-rA), \quad [10]$$

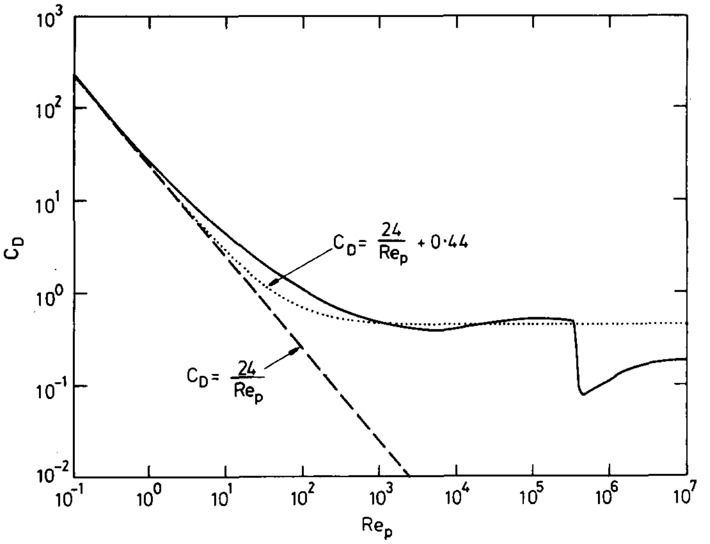

Figure 1. Comparison of the drag coefficient with the standard curve.

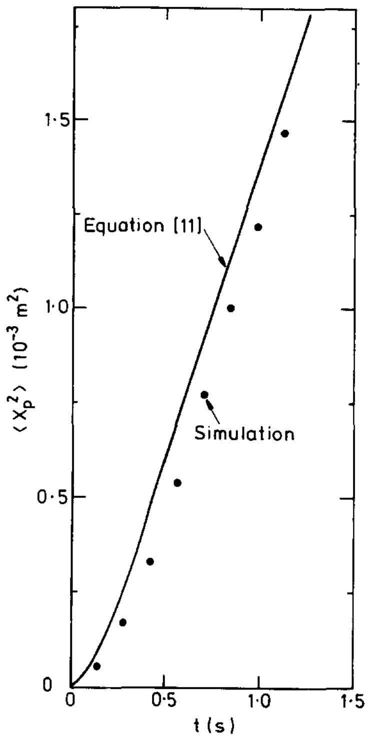

Figure 2. Particle dispersion rates (250 μm glass, $l_e = 3.5$ mm).

where x_n is the particle displacement during the nth interaction. Setting $\theta = rt_i = rl_e/\Delta w_T$ gives the autocorrelation $R_p(\theta) = \exp(-\beta\theta)$ and $\tau_p = 1/\beta$ which is consistent with the idea that large particles are in an essentially Eulerian frame of reference.

2.3. Particle diffusion coefficient

Following the random-walk approach of Hutchinson *et al.* (1971),

$$\langle X_p^2 \rangle = \left\langle \left(\sum_i x_i \right)^2 \right\rangle \qquad [3]$$

$$= 2\left\langle \sum_i \sum_{j>i} x_i x_j \right\rangle$$

$$= 2\left\langle \sum_{i=1}^{N} \sum_{r=0}^{N-i} x_i x_{i-r} \right\rangle$$

$$= 2N \sum_{r=0}^{N} \langle x_i x_{i-r} \rangle$$

(provided N is large and $\langle x_i^2 \rangle$ is constant)

$$= 2N \sum_{r=0}^{N} \langle x_i^2 \rangle \exp(-rA)$$

(using [10])

$$= 2N\langle x_i^2 \rangle \int_0^N \exp(-Ar)\,\mathrm{d}r$$

$$= 2\frac{\Delta w_T}{l_e}\frac{\langle x_i^2 \rangle}{A}\left[1 - \exp\left(-\frac{A\,\Delta w_T t}{l_e}\right)\right]$$

(since N, the total number of interactions, $= vt$)

$$= \frac{u_e^2 l_e t}{\Delta w_T}[1 - \exp(-\beta t)] \qquad [11]$$

since

$$\langle x_i^2 \rangle = \left(\frac{u_e l_e}{\Delta w_T}\right)^2 \frac{A}{2} \qquad ([10]).$$

Thus the long-time particle diffusion coefficient, ϵ_∞ is given by

$$\epsilon_\infty = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\langle X_p^2 \rangle = \frac{u_e^2 l_e}{2\,\Delta w_T}. \qquad [12]$$

Equation [12] may also be obtained directly from [1] using the results

$$\tau_p = \frac{1}{\beta}$$

and [9],

$$\langle u_p^2 \rangle = \langle V^2 \rangle u_e^2 = \frac{A}{2} u_e^2.$$

Equation [12] is also in agreement with the results derived by Friedlander (1957) for a linear drag law:

$$\epsilon_\infty = u_e^2 \int_0^\infty R_{Gp}(\theta)\,\mathrm{d}\theta = u_e^2 \tau_{Gp}, \qquad [13]$$

where the correlation $R_{Gp}(\theta)$ represents the correlation of the fluid velocity at one point with the fluid velocity experienced by the particle. Although a non-linear drag law is used in this paper, the drag coefficient is assumed to depend only on the particle settling velocity and is therefore constant for a given particle, so Friedlander's result applies. Equation [13] can be seen to agree with [12] when it is recognized that $\tau_{Gp} = l_e/2\,\Delta w_T$, i.e. the integral timescale is *one-half* of the interaction time.

It is also worth noting that using the above analysis the equation of Hutchinson *et al.* [4], gives, for large particles,

$$\epsilon_\infty = \frac{A}{4}\frac{u_e^2 l_e}{\Delta w_T}, \qquad [14]$$

which underpredicts the particle diffusion coefficient by a factor of $2/A$.

3. RESULTS AND DISCUSSION

3.1. Comparison with numerical simulation

The analysis given in section 2 contains several important assumptions and simplifications which are strictly valid only for "infinitely" heavy particles. To assess the accuracy for particle sizes of practical interest, the predictions have been compared with particle dispersion rates calculated from numerical simulations.

In the simulations the turbulence is 3-D, homogeneous and isotropic, with a single lengthscale l_e and a Gaussian distribution of velocities with an r.m.s. value u_e in each direction. Particle trajectories were calculated using [5] and [6]. The velocity difference $|\mathbf{U}_G - \mathbf{U}_p|$ was not set equal to Δw_T but was assumed constant during each interaction. This is reasonable since the interaction time [given by $t_i = l_e/(w_G - w_p)$] is small and the particle inertia is high. For each set of conditions 1000 particles were used and $\langle X_p^2 \rangle$ was calculated as a function of time (since the calculation was isotropic the same results would be obtained using $\langle Y_p^2 \rangle$.

The gas is air ($\rho_G = 1.2\ \mathrm{kg/m^3}$, $\mu_G = 0.000018\ \mathrm{Ns/m^2}$) with $u_e = 1.05$ m/s. The simulations were carried out with particles of 100–500 μm dia, density 2600 kg/m^3 (glass) and 1000 kg/m^3 (water) and $l_e = 0.00352$ and 0.0352 m (which are typical of the eddy sizes found in pipes of 0.032 and 0.32 m dia, respectively). $\mathrm{Re_p}$ varied between 5 and 160.

Figure 2 shows the values of $\langle X_p^2 \rangle$ for 250 μm glass particles, calculated from [11] and compares them with those obtained from a simulation in which the particles initial velocities are close to their long-time values. It is clear that although $\langle u_p^2 \rangle$ has a constant value, the diffusion coefficient is initially low and reaches a constant value (corresponding to a linear relationship between $\langle X_p^2 \rangle$ and t) after about 0.3 s, suggesting that the timescale τ_p requires a "development time". Both the long-time behaviour and the developing region are quite well predicted by [11].

Figure 3 shows the long-time diffusion coefficients predicted by [12] as a function of particle size and compares them with values obtained from the simulation. The agreement is good except for the smaller particles ($d_p \sim 100\,\mu$m, i.e. Re < 10), indicated by the encircled symbols, where the assumption $\Delta w_T > u_e$ was no longer valid. The agreement with the results for the larger scale turbulence are also slightly poorer because the assumption $A \ll 1$ is a poorer approximation.

3.2. *Comparison with the model of Hutchinson et al. (1971)*

Figure 4 compares the results for the 250 μm glass particles with the values calculated using the model of Hutchinson *et al.* ([4]) with the drag coefficient given by [6]. The model as published, neglecting the crossing-trajectories effect, underpredicts ϵ_∞ by about an order of magnitude and predicts too rapid a decrease with increasing particle size (because the increase in τ_p is ignored). With the inclusion of the crossing-trajectories effect, the predictions are two orders of magnitude too low, in agreement with [14].

3.3. *Comparison with the calculations of Reeks (1977)*

Since Reeks (1977) used a Stokes drag law in his calculations they are not applicable to the large particles discussed in this paper. However, there is a small overlap in the range of conditions covered so some of Reeks results are shown here (in figure 5) for comparison. The results are

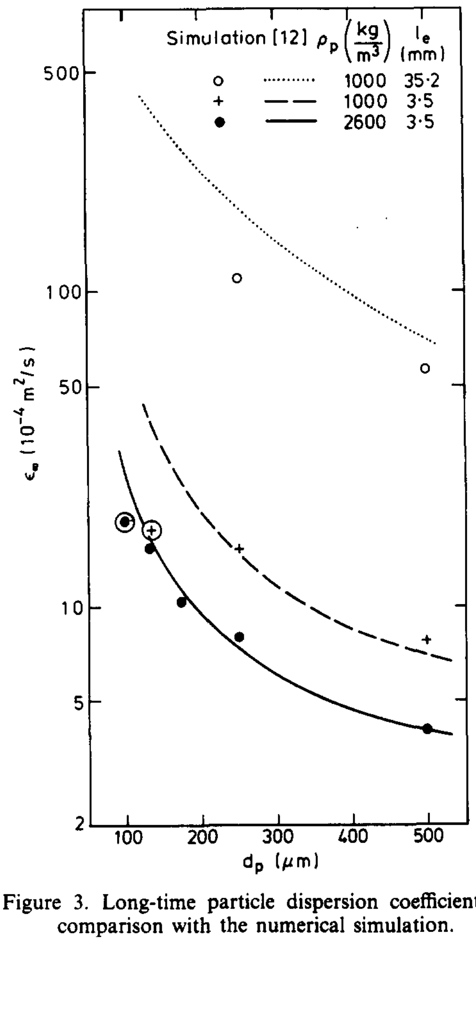

Figure 3. Long-time particle dispersion coefficients—comparison with the numerical simulation.

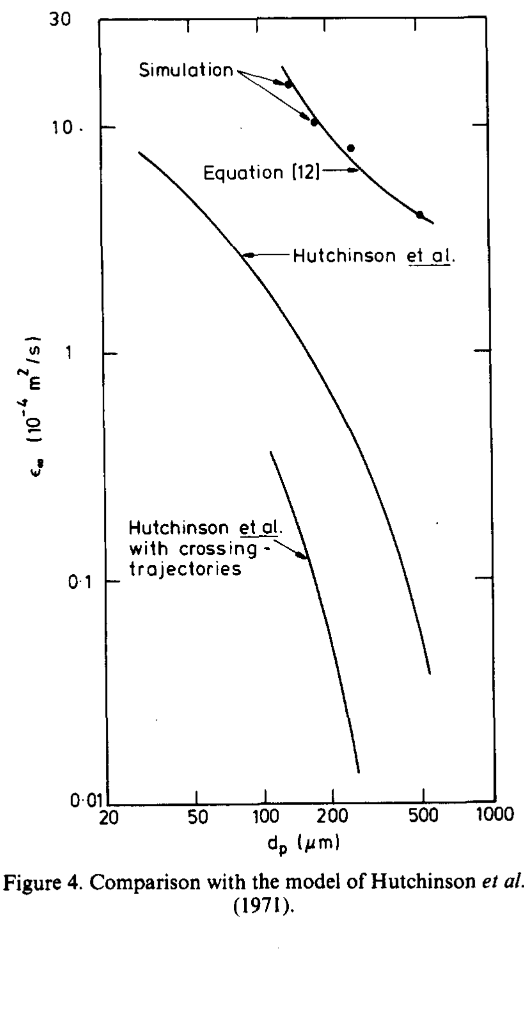

Figure 4. Comparison with the model of Hutchinson *et al.* (1971).

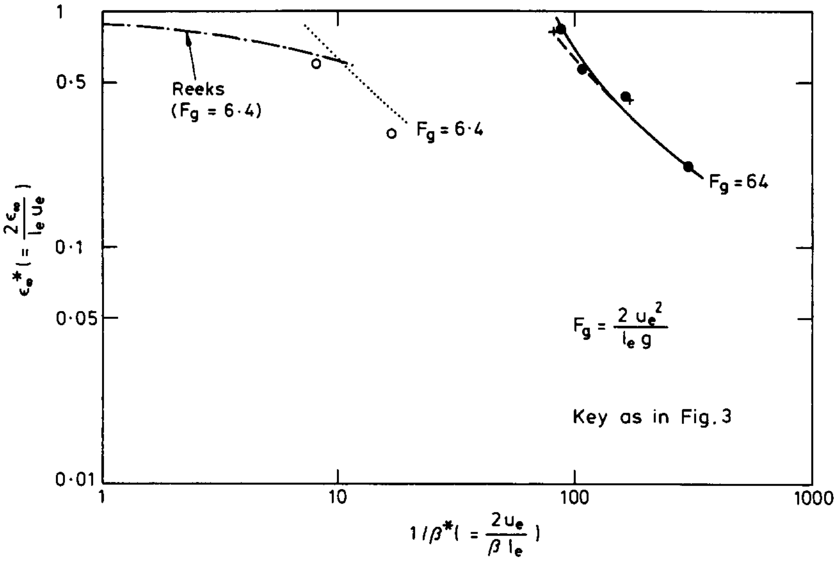

Figure 5. Comparison with the calculations of Reeks (1977).

presented in dimensionless form and the line representing Reeks calculations was estimated by interpolating Reeks results. Rather surprisingly, the Reeks model agrees quite well with the simulation and with [12] over a limited range of conditions. It appears, however, that for $1/\beta^* > 10$ the Reeks model predicts that ϵ_∞^* falls too slowly with increasing $1/\beta^*$.

4. CONCLUSIONS

It was shown that for large particles ($d_p > 100\,\mu$m, $\mathrm{Re}_p > 10$) in a vertically flowing turbulent gas, the equations for the particle diffusion coefficient reduce to a very simple form [12], consistent with a Eulerian frame of reference. It was also shown that provided the assumptions

$$(\Delta w_T)^2 \gg u_e^2$$

and

$$\beta l_e / \Delta w_T \ll 1$$

are valid, this simple equation is in good agreement with the results of numerical simulations of the dispersion of glass particles and water droplets.

Published models such as those of Reeks (1977) and Hutchinson *et al.* (1971) are usually derived from small particles, and were found to underpredict the particle diffusion coefficient for larger particles by orders of magnitude because their inherent assumptions that $\tau_p = \tau_G$ or that Stokes law is valid introduce gross errors.

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