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RANDOM-WALK MODELLING OF TURBULENT IMPACTION TO A SMOOTH WALL

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Abstract—A recently-published random-walk model of particle deposition from turbulent pipe flow, which gave good agreement with measured deposition velocities over a wide range of dimensionless stopping time (τ^+), predicted a large build-up in particle concentration close to the wall for low values of τ^+ (< 10). The present work demonstrates that this effect is very likely to be an artefact of the failure of the random-walk prescription to satisfy the "well-mixed" condition (which requires that in the limit that particles follow the eddy motions of the carrier fluid exactly an initially uniform concentration should, on average, remain so). The consequences of this failure are shown first by analysing the transport equation underlying the random-walk process, in the course of which it is shown how a one-dimensional form of the transport process can be used to calculate deposition velocities, analogous to the one-dimensional eddy-diffusivity equation conventionally used. Secondly, the published random-walk procedure is reformulated to satisfy the "well-mixed" condition and applied to the problem of deposition from turbulent pipe flow (albeit with simplified flow characteristics and particle equation of motion). No concentration build-up is observed, whereas a build-up of similar magnitude to that observed in the earlier work returns if the unmodified prescription is applied to the same problem. The reformulated random-walk model itself gives results for deposition velocity vs τ^+ which are sufficiently encouraging to suggest the work could be carried further.

Key Words: particles, deposition velocity, turbulence, inertial impaction, interception, random-walk, pipe flow.

1. INTRODUCTION

The need to predict the deposition of aerosol particles or small droplets from a turbulent gas stream to a bounding surface arises in a wide variety of situations, e.g. in the design of air-cleaning systems, the estimation of plate-out in nuclear-reactor coolant circuits and the assessment of the hazard posed by toxic pollutants in the atmosphere. Many mechanisms may contribute to this deposition, including inertial impaction, Brownian diffusion, gravitational settling, electrostatic forces and thermophoresis. However, for electrically-neural particles, inertial impaction is often the dominant mechanism for particles above about 1 μm in diameter.

There have been many attempts to model inertial impaction to the smooth wall of a pipe carrying aerosol suspended in a turbulent flowing gas [see Kallio & Reeks (1989) for a list of earlier references]. Many useful data are available on the Eulerian properties of the turbulence in this situation. The most common modelling approach has assumed that particles follow the fluid motions until they are a certain distance from the surface, then make their final crossing to the surface in a "free flight" which short-circuits the resistance afforded by the near-surface fluid layers. The distance from the boundary at which the free flight is taken to commence is related to the stopping distance of the particle for a given projection velocity. However, in order to match experimental data, the required velocity turns out to be unreasonably high, whereas, if it is related self-consistently to local fluid velocities at one stopping distance from the wall, an underprediction in deposition by 1–2 orders-of-magnitude results (Davies 1966).

In addition, the "free-flight" notion suffers from a conceptual difficulty in that particles are assumed to faithfully follow the fluid motions until they are within one stopping distance of the boundary, whereas in reality the tendency to disentrain from eddies is present throughout the fluid. Liu & Ilori (1974) introduced a modified particle diffusivity to account for this effect, but the attempt was only partially successful, and the manner in which the diffusivity was modified also raises conceptual difficulties (Reeks 1982). A key feature of eddy-diffusivity models is that they deal with "local" gradients in the concentration, whereas there is experimental evidence that finite

lengthscales and timescales play a vital role in boundary-layer turbulence (Cleaver & Yates 1975). When the aim is to evaluate the effect of an additional timescale, namely the stopping time of a particle, it seems unlikely therefore that local models will provide the best approach.

Kallio & Reeks (1989), hereafter denoted by KR, took a major step forward by developing a Lagrangian trajectory model for calculating turbulent inertial deposition to a smooth pipe surface. In this type of model, the trajectories of individual suspended particles are followed as they interact with the turbulent flow field. Modelling the latter in terms of eddies that persist for a finite time before decay enables the timescales present in turbulent flow to be recognized. The stopping time of a particle enters the modelling via the response of a particle to the eddy in which it finds itself at any given time. In this way, the inability of particles to fully follow the eddy motions is represented throughout the flow. A stochastic element enters via the choice of eddy velocity for each eddy that the particle finds itself in: usually the velocity is sampled from a Gaussian distribution with standard deviation equal to the Eulerian r.m.s. turbulent velocity. The method thus involves tracking a large number of particle trajectories in order to obtain estimates of "mean" parameters—such as the deposition velocity—with acceptably low statistical error. Although conceptually appealing, application of the method does depend on the availability of information on *Lagrangian* timescales.

KR were by no means the first to treat the turbulent dispersion of suspended particles via a random-walk model [for some earlier references, see Underwood (1991a)], but their work had the virtue, *inter alia*, of recognizing that the time an eddy survives should be chosen randomly if the correct asymptotic behaviour is to be obtained in the limit of homogeneous turbulence. This introduces a second stochastic element into the model. Furthermore, their model is carefully formulated to ensure that, in the limit that particles are points following the eddy motions perfectly, zero deposition results. The model yielded good agreement with the experimental data of Liu & Agarwal (1974) on the variation of deposition velocity with particle stopping time, without the need for any adjustable fitting parameters.

A startling feature of the KR results, however, is the prediction of a build up in particle concentration in the region of very small eddy velocities close to the boundary, an effect which increases as particle inertia diminishes. The effect is not minor, amounting to nearly a 2 orders-of-magnitude increase in concentration near the wall compared to its value far from the wall, for particles around a few microns in diameter. Heuristically, the effect can be viewed as the result of particles being propelled by larger "kicks" from regions of relatively large turbulent velocities into regions where they receive smaller kicks and from which they therefore have difficulty escaping. However, in reality the situation is more complex in that the detailed prescription of KR leads to an acceleration/deceleration of particles which *partly* compensates for the above asymmetry (see later).

Such an effect, if real, would have important repercussions for other aspects of the modelling of mass and heat transfer from the bulk flow to the boundary. Similar behaviour was apparently observed in an earlier attempt at random-walk modelling of inertial deposition (Hutchinson *et al.* 1971) and also emerged from an eddy-diffusivity model (Reeks 1982) modified to include a "turbophoretic" drift velocity (which accounts for the influence of particle inertia within the framework of a "local" model). Experimentally, some authors have found a modest increase in particle concentration near the wall [e.g. Sun & Lin (1986) find a factor of 2–3 for particles of order 1 μm in size], whereas others have not; the role played by rebound and re-entrainment in the experiments is unclear.

A build-up in concentration similar to that observed by KR was also noted in another type of random-walk modelling that has been widely applied to turbulent dispersion in the atmosphere [the so-called "Langevin-equation" approach (Sawford 1985)]. The phenomenon has been the subject of much discussion and analysis (Wilson *et al.* 1981; Legg & Raupach 1982; Thomson 1984) and was found to be an artefact of an incorrect specification of the random-walk process in inhomogeneous conditions. To be physically consistent, the model should satisfy the constraint that in the limit that the pollutant follows the eddy motion of the carrier gas *exactly* there should be no build-up of concentration anywhere. This is equivalent to the requirement that if the random-walk process is applied to the elements of the carrier fluid itself (assumed incompressible) there should be no build up of fluid density anywhere. The criterion has been termed, for short,

the "well-mixed" condition (Thomson 1987) on the grounds that in this limiting case an initially uniform concentration should remain so (on average) as the elements are propagated by the random-walk process.

The well-mixed condition applied to the "Langevin-equation" model in inhomogeneous conditions leads to a requirement that even when the actual suspended particles follow the flow exactly the "particles" tracked in the simulation are subject to an acceleration which is additional to the velocity changes introduced by the random "kicks" representing interaction with the turbulent flow. That such an acceleration has to be "imposed" stems from the extreme simplicity of the modelled turbulent flow field. The author has recently worked out the implications of the "well-mixed" condition for the type of random-walk process utilized by KR (Underwook 1991c) and found that it also requires an acceleration of the simulation "particles" quite separate from the changes in velocity that arise when one eddy is replaced by another (section 2).

This acceleration, the magnitude of which is related to the gradient in the r.m.s. turbulent velocity, achieves a neat balancing in the limiting case that the suspended particles exactly follow the flow: it precisely counteracts the asymmetry in "kicks" which would otherwise lead to an accumulation in regions of low r.m.s. turbulent velocity. This does not necessarily imply that there can be no build-up when the particles are no longer able to faithfully follow the flow, e.g. as a result of their inertia. McLaughlin (1989) and Brooke *et al.* (1992) found such an accumulation of larger particles when trajectories were computed in a directly-simulated three-dimensional time-dependent turbulent flow field (a procedure which should automatically satisfy the well-mixed condition). However, the effect was found to *increase* with particle inertia, contrary to that observed by KR.

Thus, the aim of the present work is to ascertain whether or not the build-up in concentration observed by KR is likely to be an artefact of a deficient formulation of the random-walk model or whether it might remain even if the model is modified to satisfy the well-mixed condition. This goal will be achieved by a combination of theoretical analysis and computer simulation of a somewhat simplified problem, which nevertheless contains all the elements of the KR calculation vital for the point at issue.

2. ANALYSIS

2.1. Reduction to a One-dimensional Problem

The simulation used by KR was two-dimensional: both the advection of a particle down the pipe (x-direction) and the turbulent transport perpendicular to the pipe walls (y-direction in KR's notation) was tracked. However, KR noted that the concentration profile in the y-direction became virtually independent of x sufficiently far down the pipe from where particles were "injected". In this "equilibrium" situation it is possible to define a *deposition velocity* (the ratio of flux to concentration) which is dependent on the characteristics of the fluid flow and the physico-chemical properties of the dispersed phase but not on the source configuration nor on x.

It would be very economical if the quasi-equilibrium y-profile could be generated directly by a one-dimensional simulation rather than as the asymptotic behaviour of a two-dimensional simulation. This turns out to be possible subject to certain provisos, as has been demonstrated elsewhere (Underwood 1991b).

In the present context, the one-dimensional random-walk can be formulated straightforwardly provided the effect of the Saffman lift force (Saffman 1965) is ignored, where the latter arises from the relative x-motion between a particle and the shear flow. This force creates a coupling between x- and y-motions that would complicate the one-dimensional treatment. However, its omission is not significant for the present purposes since KR found a similar build-up in concentration even in the absence of the lift force (and indeed the concentration profiles they present were calculated without it). In addition, the behaviour of the deposition velocity vs stopping time was qualitatively similar both with and without lift. Thus, the lift force will be ignored for the purposes of the present investigation.

It is assumed that the radius of the pipe is large enough that the net flux in the y-direction can be assumed constant across the y-regime of interest.

2.2. *One-dimensional Transport Equation*

Consider a steady-state situation in which the source releases a constant number of particles per unit time. Quantities below are normalized to a constant number of particles released from the source.

Let $n_+(y, v_+)\,\mathrm{d}v_+$ by the number of particles per unit range of x which cross level y upwards with vertical velocity in the range v_+ to $v_+ + \mathrm{d}v_+$ (and similarly n_- for downward-moving particles). In the "equilibrium", constant-flux limit, conservation of particles can be applied separately in the y-direction since the number of particles entering a unit "slice" of x from the left balances, on average, the number leaving from the right as a result of the negligible x-gradient. This enables an equation for n_+ to be derived (Underwood 1991b) which expresses the change in n_+ over a spatial interval δy in terms of the "scattering out" from the velocity interval v^+ to $v^+ + \mathrm{d}v_+$ (i.e. eddy changes which put particles outside this velocity range) and "scatterings in" (i.e. eddy changes which put particles into this velocity range). For homogeneous turbulence and in the limit that particles follow the flow exactly, this takes the following form:

$$T_\mathrm{L}\frac{\mathrm{d}n_+}{\mathrm{d}y} = -\frac{n_+(y, v_+)}{v_+} + p(v_+)c(y), \qquad [1]$$

where T_L is the Lagrangian timescale (i.e. the mean time between "scatterings"), $p(v_+)\,\mathrm{d}v_+$ is the probability of a particle emerging from a scattering with vertical velocity upwards in the range v_+ to $v_+ + \mathrm{d}v_+$ (taken to be given by the Eulerian distribution of turbulent y-velocities in the flow) and $c(y)$ is the concentration. To be precise, c is the across-flow (i.e. z-direction)-integrated, time-integrated particle number concentration, with dimensions $[\mathrm{T\,L^{-2}}]$.

A similar equation to [1] applies to downward-moving particles, and the two equations together are the counterpart in this random-walk model to the one-dimensional eddy-diffusivity equation which is conventionally used as a starting point for theoretical estimates of dry deposition velocity.

For this homogeneous case, and assuming particles are able to follow the eddy motions perfectly, the simulation keeps a particle's y-velocity fixed until it enters a new eddy. Satisfaction of the "well-mixed" condition in this case is ensured by the fact that when c (and n_+) are independent of y,

$$n_+(y, v_+) \propto v_+ p(v_+), \qquad [2]$$

as it should be, since $p(v_+)\,\mathrm{d}v_+$ is the relative number of eddies in the flow having y-velocities in the range v_+ to $v_+ + \mathrm{d}v_+$.

2.3. *Derivation of the Acceleration*

For the inhomogeneous situation, generally both T_L and $p(v)$ are dependent on y [the latter henceforth being written $p_y(v)$]. In this case, if v is held constant between "scatterings", then setting c constant and $n_+ \propto v_+ p_y(v_+)$ no longer constitutes a solution of [1], violating the well-mixed condition.

The situation can be recovered if v is allowed to vary between scatterings; the acceleration must be such as to satisfy

$$\frac{\mathrm{d}(n_+(y, v_+)\delta v^+)}{\mathrm{d}y} = 0 \qquad [3]$$

when $n_+(y, v_+) \propto v_+ p_y(v_+)$ where $\mathrm{d}/\mathrm{d}y$ is a *total* derivative (allowing for changes in v with y also) and the interval δv_+ has to be included since it changes with y also.

For a Gaussian distribution of turbulent y-velocities, with standard deviation $\sigma(y)$, the required variation in v turns out to be (Underwood 1991c):

$$\frac{\mathrm{d}v_+}{\mathrm{d}y} = \sigma'\left(\frac{v_+}{\sigma(y)} + \frac{\sigma(y)}{v_+}\right), \qquad [4]$$

where σ' is $\mathrm{d}\sigma/\mathrm{d}y$. Introducing $\eta = v/\sigma$, [4] can be re-written as

$$\frac{\mathrm{d}\eta}{\mathrm{d}\sigma} = \frac{1}{\eta\sigma}, \qquad [5]$$

which integrates to

$$\eta^2 - 2\ln(\sigma) = \text{const.} \qquad [6]$$

It is important to note that, for σ' positive, an initially negative η (i.e. negative v) may change sign between scatterings, i.e. the particle can change direction.

Expressed in terms of the change in velocity with time since the last scattering, t, [4] becomes

$$\frac{dv_+}{dt} = \sigma\sigma'\left(1 + \frac{v_+^2}{\sigma^2}\right), \qquad [7]$$

which, incidentally, shows that the singularity at $v_+ = 0$ in [4] is harmless. It is interesting to note that an acceleration of exactly this form has been obtained in a careful analysis of the "Langevin-equation" type of random-walk modelling with Gaussian forcing (Luhar & Britter 1989).

It is readily shown that [7] applies to negative values of v also. Thus, still in the limit that particles are following the carrier fluid exactly, the average acceleration, taken over the distribution of v at a given height, becomes $d(\sigma^2)/dy$, as it must from fluid-dynamic considerations (e.g. Legg & Raupach 1982).

It is worth noting that in the well-mixed limit, for which c is independent of y and $n_\pm(y, v_\pm) \propto |v_\pm| p_y(v_\pm)$,

$$N_\pm(y) \propto \sigma(y), \qquad [8]$$

where N_+ is the integral of n_+ over all values of v_+ and similarly for N_-. Also,

$$\left|\left\langle \frac{1}{v_\pm} \right\rangle\right| \propto \frac{1}{\sigma(y)}, \qquad [9]$$

where $\langle\ \rangle$ denotes the average over particles crossing a given level y.

Since c can be written as

$$c(y) = N_+(y)\left\langle \frac{1}{v_+} \right\rangle - N_-(y)\left\langle \frac{1}{v_-} \right\rangle, \qquad [10]$$

it can be seen that a constant value of c is preserved in the well-mixed case by a cancelling of the opposing variations of $N_\pm$ and $\langle 1/v_\pm \rangle$ with σ.

2.4. Implications for the KR Simulation

In the KR simulation, the ratio v/σ is maintained constant between scatterings. The superficially-plausible alternative of keeping v itself constant between scatterings would have led to far-too-high a probability of reaching the boundary in a single flight from relatively far away. With v/σ held constant, the eddy velocity approaches zero as the boundary is approached since σ itself approaches zero.

Thus, simulation particles in the KR random walk accelerate (or decelerate) between scatterings even in the limit that they are following the eddy motions perfectly, since σ is function of y. However, the magnitude of the acceleration is not the same as that required to satisfy the well-mixed condition. In fact, it turns out that the KR prescription is such as to ensure that

$$\frac{dn_\pm(y, v_\pm)}{dy} = 0 \qquad [11]$$

(see the appendix).

In this case, it is readily shown that, in the limit of point particles following the eddy motions exactly, $N_\pm$ satisfy

$$N_\pm(y) = \text{const}, \qquad [12]$$

rather than [8], whereas $\langle 1/v_\pm \rangle$ continues to satisfy [9]. Thus, as y decreases, the concentration increases in direct proportion to the increase in $1/\sigma(y)$, a result also found for the "Langevin-equation" type of random-walk modelling when v/σ is held constant (Wilson *et al.* 1981).

This could readily account for the magnitude of the concentration increase observed by KR: for the smaller value of dimensionless stopping time (see section 3.1), τ^+, for which the concentration

profile is presented (i.e. $\tau^+ = 1$), the concentration at y^+ (the dimensionless y-coordinate) = 1 is around 30 times its value at $y^+ = 100$, whereas σ has decreased by a factor of 180. The fact that the calculated concentration does not continue to rise as y^+ approaches zero—and indeed that the concentration rises less rapidly than the decrease in σ would imply—can be attributed to departures from the idealized case of point particles exactly following the eddies. Thus, even for $\tau^+ = 1$, there *is* some deposition: no particle which reaches within one particle radius of the boundary returns, which significantly cuts down the concentration in the vicinity of the boundary. At $\tau^+ = 100$, where the effect of loss at the wall is very much higher, this effect has apparently cancelled any concentration increase in the KR results.

This evidence suggests that at least a part of the concentration build-up observed by KR is a consequence of the failure of their random-walk prescription to satisfy the well-mixed condition. However, it remains a possibility that, even if the well-mixed condition were to be satisfied, such a build-up may arise when the particles have an inertial lag compared to the surrounding fluid. In section 3 below, a random-walk prescription which satisfies the well-mixed condition is defined for the case of inertial deposition to a smooth pipe surface. The specification of the turbulent-flow parameters differs from that given in KR in that the dependence of σ on y is linearized (whereas in KR it is near quadratic close to the boundary); this modification leads to a major saving in computation, as explained in section 3.1. However, it does not represent a vital simplification from the viewpoint of the concentration build-up issue, although there will be differences in detail in the resulting concentrations and deposition velocities compared to those that would have been obtained using the more complex $\sigma(y)$ prescription.

3. SIMULATION

3.1. Specification of $\sigma(y)$

As in KR, dimensionless variables are defined by normalizing distances by ν/u_* (where ν is the kinematic viscosity of the carrier fluid and u_* is the friction velocity), velocities by u_* and times by ν/u_*^2. Normalized variables have a superscript "+".

The variation of σ^+ and y^+ is simplified to

$$\sigma^+(y^+) = \begin{cases} y^+/30 & y^+ < 30 \\ 1 & y^+ \geqslant 30. \end{cases} \qquad [13]$$

It is readily shown from [5] that η (i.e. v/σ—or alternatively v^+/σ^+) satisfies

$$\frac{d\eta}{dt^+} = \frac{d\sigma^+}{dy^+}, \qquad [14]$$

which is constant for a linear variation of σ with y. Thus, in the non-uniform $\sigma(y)$ regime, η increases linearly with time-since-last-scattering, t. The position at time t of a particle which is following the eddy motion exactly can therefore be determined analytically, whereas, for the variation of σ used by KR, numerical integration would be required, thereby considerably slowing down the simulation. Utilizing this simplification, the tracking of an adequate number of particles through their one-dimensional random walk comes within the range of a desk-top microcomputer.

It is worth noting that the simulation must account for the fact that particles following the eddy motion exactly and which enter the non-uniform σ region may change direction (see section 2.3) and may even re-emerge from the non-uniform region before their next scattering.

3.2. Random Walk for Particles with Inertia

The simulation "particle" now represents a real suspended particle which is unable to follow exactly the eddy in which it sits. A basic premise adopted is that the eddy velocity and time-to-decay are not affected by whether or not it contains suspended particles—i.e. the pollutant is "passive". The eddy velocity changes discontinuously at a scattering (i.e. when one eddy is replaced by another), but the particle velocity is now assumed continuous (although its acceleration is

discontinuous). When the eddy changes, the particle starts to adjust to the new eddy velocity according to the following equation of motion:

$$\frac{dv_p}{dt} = \frac{v - v_p(t)}{\tau}, \qquad [15]$$

where $v_p(t)$ is the velocity of the particle and τ is the particle stopping time, given by

$$\tau = \frac{2\left(\frac{\rho_p}{\rho_f}\right)a^2}{9\nu}; \qquad [16]$$

ρ_p is the particle density, ρ_f is the fluid density, ν is the kinematic viscosity of the fluid and a is the particle radius. It is assumed that no body forces (including the effect of gravity) are operative. The eddy velocity v is a function of time in the non-uniform region but not in the uniform region. Equation [15] is a very simplified equation of motion, omitting such terms as the Basset history integral and modifications to Stokes' law. However, the omissions were considered justifiable by KR, and the above equation is the one they used, apart from the additional omission of the Saffman lift force, discussed earlier.

According to the basic premise given above, the time-to-next-scattering is not governed by the values of y^+ that the *particle* passes through between scatterings (labelled y_p^+) but by the values that the *eddy* passes through (i.e. the locations that a reference simulation particle following the eddy motion exactly would pass through). When the eddy decays, the particle passes into a new eddy with velocity *representative of the eddies found at the location of the particle*. Thus, the particle is envisaged as staying within the influence of the current eddy until the latter decays, even though it may stray some distance from a reference particle following the eddy motions exactly. When the current eddy decays, the simulation particle "picks up" an eddy which is representative of the local environment in which it has been "dumped". This prescription is easily extended to include the "trajectory-crossing" effect (whereby particles lose the "memory" of turbulent velocity more rapidly because of their relative motion to the fluid) by defining a lengthscale for the range of influence of an eddy (potentially a function of y)—i.e. an eddy "size"—such that, if the particle strays further than this distance from the reference position before the current eddy decays, a new eddy is chosen prematurely. Trajectory-crossing will be omitted here since KR did not include it, but remains a possibility for future work.

The above prescription for the random-walk of particles with inertia is not unique but it is intuitively appealing and does satisfy the broad physical constraints of the problem, in particular the well-mixed condition in the limit that τ approaches zero.

3.3. *Time-to-next-scattering*

The variation of the Lagrangian timescale with y is taken to be exactly that used by KR over the range $0 < y^+ < 200$, namely

$$T_L^+ = \begin{cases} 10 & y^+ \leqslant 5 \\ b_0 + b_1 y^+ + b_2 (y^+)^2 & 5 < y^+ < 200, \end{cases} \qquad [17]$$

with $b_0 = 7.122$, $b_1 = 0.5731$ and $b_2 = -0.00129$.

Particle trajectories are actually initiated some distance above $y^+ = 200$ (see section 3.5); for $y^+ > 200$, T_L^+ is held fixed at the $y^+ = 200$ value given by [17], defining a third, "core" region of constant Lagrangian timescale.

In KR, the time-to-next-scattering is chosen by "randomizing the integral scale from an exponential probability density distribution"; i.e. if an eddy change occurs at y_0^+, the dimensionless time to the next change is given by

$$\exp\left[\frac{-t^+}{T_L^+(y_0^+)}\right] = r, \qquad [18]$$

where r is a random deviate chosen uniformly on the range 0–1.

However, the analysis in section 2 assumes that the probability that a particle (which is following the eddy exactly) at y^+ scatters in the next dt^+ is given by $dt^+/T_L^+(y)$, in keeping with the Markov nature of the process envisaged. On this view, T_L is no longer interpreted as an *integral* timescale

but rather as a timescale representing the (local) rate at which the turbulent velocity is losing its correlation (Durbin & Hunt 1980). When T_L^+ is not constant, this does not result in an exponential probability distribution for the time-to-next-scattering. Thus, even when the "correct" acceleration is being used, if t^+ is chosen according to [18] the well-mixed condition ceases to be satisfied and spurious concentration build-up can arise.

Here, therefore, t^+ is chosen via the following:

$$\exp\left[-\int_0^{t^+} \frac{dt'}{T_L^+(y^+(t'))}\right] = r, \qquad [19]$$

given that the LHS of [19] approaches zero for large enough t^+.

Alternatively, the integral on the LHS of [19], denoted I, can be written as

$$I = \int_{y_0^+}^{y^+} \frac{dy'}{v^+ T_L^+(y')}, \qquad [20]$$

where y_0^+ is the value of y^+ at the site of the last scattering.

Generally, [19] is much harder to invert than [18], particularly if the particle can enter the non-uniform region of σ, where v^+ varies with y^+. In the region of constant σ (i.e. $y^+ > 30$), T_L^+ is either a constant or a quadratic function of y^+, and the integral can be performed analytically. For the non-uniform region ($y^+ \leqslant 30$), a simple numerical scheme was introduced.

3.4. *Particle Velocity*

At each scattering, a new eddy velocity is sampled from a Gaussian distribution with standard deviation given by $\sigma(y)$.

In the uniform region of σ, [15] is analytically solvable for v_p as a function of time-since-last-scattering. In the non-uniform region, the eddy velocity between collisions is governed by [14], and the formal solution of [15] can be written as

$$v_p(t) = v_p(0)\exp\left(\frac{-t}{\tau}\right) + \frac{1}{\tau}\int_0^t \exp\left[\frac{-(t-t')}{\tau}\right] v(t')\,dt'; \qquad [21]$$

$v_p(0)$, the particle velocity at entry into the current eddy, is simply taken to equal its velocity at the time that the last eddy decayed.

Even for a linear variation of $\sigma(y)$, the solution to [21] cannot be given in terms of simple functions, since it is v/σ which has a straightforward dependence on t, rather than v itself. However, the need for numerical integration during the course of the simulation was kept to a minimum by a procedure which made use of linear interpolation on a pre-calculated table of values.

3.5. *Termination and Injection*

The solution of the equation for n_+ (the equivalent of [1] for the problem under consideration) requires a lower boundary condition: it is assumed that particles are always lost when they reach the wall (i.e. no rebound). Allowing for the finite size of particles, the condition is that

$$n_+(a, v_+) = 0, \qquad [22]$$

where a is the physical radius of the particle (related to τ via [16]). In the simulation, this implies that a particle trajectory terminates if the particle reaches a distance a of the boundary (i.e. y_p^+ drops below a^+).

The corresponding equation for n_- requires an upper boundary condition. In principle, to obtain the exact one-dimensional profile in the present case, the upper boundary should be extended to infinity, but in practice it only need be taken sufficiently high that the profile up to the height of interest has converged sufficiently close to the "true" profile.

The procedure can be illustrated for the simple case of homogeneous turbulence (with particles exactly following eddies) referred to in section 2.1. The solution for n_- then becomes (see [1])

$$n_-(y, v_-) = \int_y^\infty \frac{c(y')}{T_L} p(v_-)\exp\left[-\frac{(y-y')}{v_- T_L}\right] dy'. \qquad [23]$$

Formally, the upper limit can be replaced by a finite one as follows:

$$n_-(y, v_-) = n_-(y_i, v_-)\exp\left[-\frac{(y-y_i)}{v_- T_L}\right] + \int_y^{y_i} \frac{c(y')}{T_L} p(v_-)\exp\left[-\frac{(y-y')}{v_- T_L}\right] dy', \qquad [24]$$

where y_i is any value greater than y, but this just throws the difficulty onto specifying $n_-(y_i, v_-)$. However, as y_i becomes large compared to y, n_- and c at y become insensitive to inaccuracies in the specification of $n_-(y_i, v_-)$ and so it is only necessary to specify it approximately.

To continue the illustration, in the limiting case of particles following the eddy motions exactly (with no loss at the wall therefore), it has already been shown that

$$n_-(y_i, v_-) = C|v_-|p(v_-), \qquad [25]$$

where C is the (constant) concentration. If, now, particles follow the eddy motions except for when they reach the wall, where they are lost (rather than being reflected), $c(y)$ will no longer be constant (in fact it is close to being a linearly increasing function of y), but a satisfactory procedure, when information is being sought only up to a value of y_1, is to choose a value of y_i sufficiently greater than y_1 and set $n_-(y_i, v_-)$ equal to its asymptotic form [25]. (The term "asymptotic" is used since the LHS of [1] becomes small compared to either term on the RHS as y becomes large in the present example.) In terms of the simulation, particles are "injected" at y_i with a downward velocity chosen randomly from a distribution which satisfies [25], achieved by choosing

$$v_- = -\sigma[2\ln(r)]^{1/2}. \qquad [26]$$

The first value of the time-to-next-scattering can be chosen as if a scattering had just occurred at y_i.

To find what constitutes "sufficiently" high for y_i in order to achieve a specified degree of convergence below y_1 will generally require the simulation to be repeated for a few trial values of y_i, but this is not very onerous, given that the simulation is only one-dimensional.

Returning now to the case of particles with inertial lag, initiation of a trajectory at y_i requires the specification of both the eddy velocity and the particle velocity (and the time-to-first-scattering). In principle, a particle can be travelling downwards across the level y_i in an eddy which is travelling upwards; in any case, particle and eddy speeds may be quite different. Nevertheless, a simple, approximate specification is to choose the eddy velocity according to [26] and to assume that the particle velocity is perfectly correlated with the eddy velocity.

Although the correlation is assumed to be unity, the mean value of v_p on injection is not assumed equal to the mean value of v but is reduced—to account for inertia—to the local "equilibrium" value (i.e. reduced by a factor $[1 + (\tau/T_L)]^{1/2}$).

Once a particle is injected, it is tracked until it is either lost at the wall or it emerges above y_i.

3.6. Scoring

During the random-walk, various data on the particle trajectory need to be recorded at the values of y^+ of interest, in order to form estimates of concentration, flux, deposition velocity etc. This is achieved by defining a series of "scoring" levels y_k, $k = 1, 2, \ldots n$, with associated scoring arrays, and recording the values of v_p, $1/v_p$, $1/|v_p|$ etc. at each crossing of any level.

The process of scoring must allow for the fact that between scatterings a particle may change its direction of travel and thus cross a given level more than once. When the eddy is travelling in the constant-σ region, for which the eddy velocity is constant, at most one reversal can occur between scatterings, but when the eddy is travelling in the non-uniform region up to two reversals are possible between scatterings.

The key quantities of interest for comparison with the work of KR are the concentration profile and the deposition velocity (labelled K by KR). In the present work, the latter is defined, conventionally, as the ratio of the net downward flux at a given level to the concentration at the same level. (N.B. In the one-dimensional simulation, the net downward flux is a constant by definition but the concentration is not when there is loss at the boundary.) The principal level of interest for K is $y^+ = 200$ in line with the work of KR, and so y_1^+, introduced in section 3.5, is taken to be 200.

The definition of K used here differs somewhat from that introduced by KR, who appear to use the mean concentration over $0 < y^+ < 200$. They justify this on the grounds that it corresponds more closely to what is actually measured in experiments, but this argument is open to question: if the flux is measured via the attenuation per unit length of pipe, as they envisage, the appropriate mean concentration should include the core of the flow and not just the thin layer near the wall,

which would weight the pertinent concentration more towards the "core" value. In practice, in the current work, the concentration is not a strong function of y^+ across the region 0–200 and so there is not a large difference between the two estimates.

3.7. Checks

A valuable check on the computer program implementing the random-walk model defined above is provided by the well-mixed condition. In the limit that the simulation particles coincide with the reference particles (which follow eddy motions exactly), the concentration should become uniform. Figure 1 shows the dimensionless normalized concentration $(c/N_-(y_i))^+$—denoted by c_N^+—vs y^+ resulting from such a simulation using 10^5 particles in 10 batches of 10^4 in order to estimate the statistical error shown, which is $<1\%$ for $y^+ > 10$, rising to about 4% at $y^+ = 1$. The dashed line on the figure denotes the expectation value of c_N^+, readily shown to equal $\sqrt{2\pi}$ in this case.

3.8. Results

3.8.1. Deposition velocity

A series of simulations for increasing values of y_i and for various τ^+ values established that a choice of $y_i^+ = 600$ was adequate to achieve convergence on the deposition velocity at $y^+ = 200$ to within an accuracy comparable to the target statistical accuracy of around 1%. Figure 2 shows the dimensionless deposition velocity K^+ (200) as a function of τ^+, obtained in each case using a sample of 10^5 trajectories in 10 batches of 10^4; the statistical-error bars are too small to be shown for the larger values of K^+. The solid curve is merely an eye guide. The results show the principal features of the experimentally-observed dependence of K^+ on y^+, including the rapid rise over the

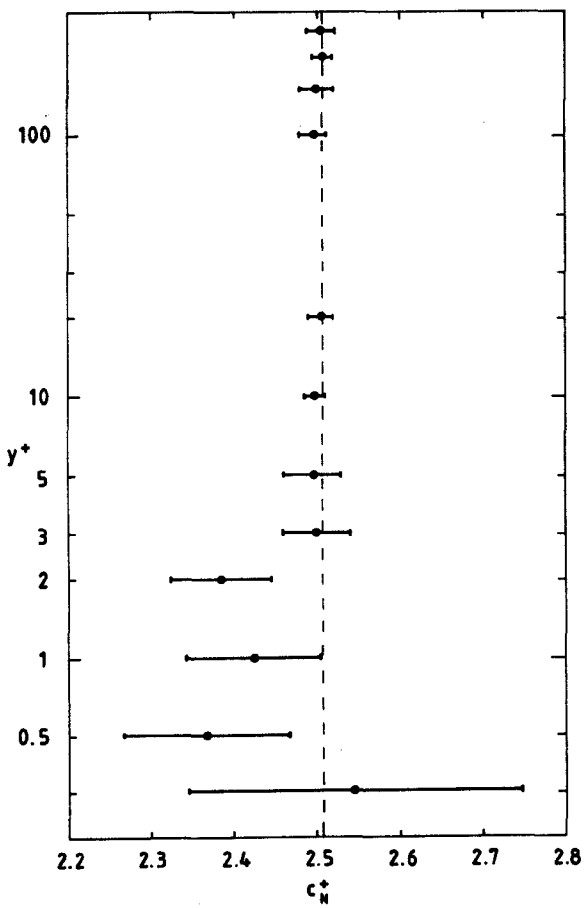

Figure 1. Dimensionless normalized concentration vs dimensionless distance from the wall, for the case where the particles follow the eddy motions exactly.

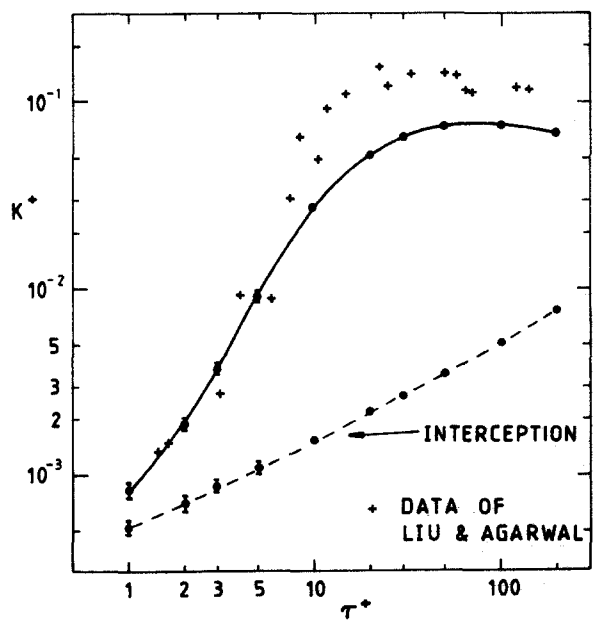

Figure 2. Dimensionless deposition velocity vs dimensionless particle stopping time: model predictions compared with the data of Liu & Agarwal (1974).

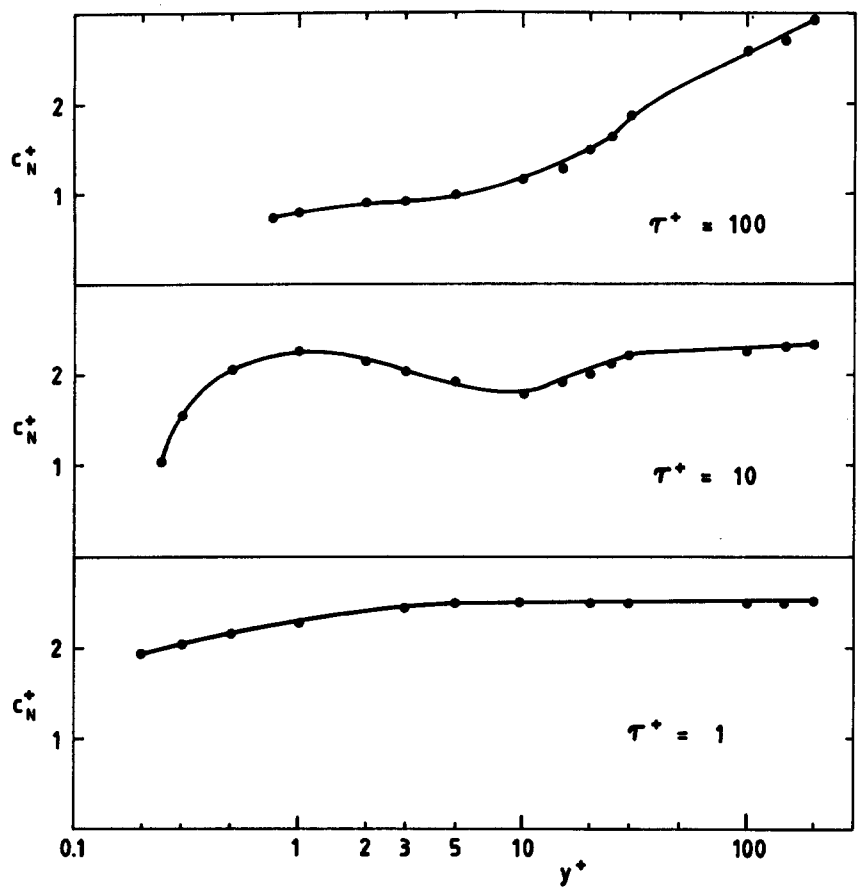

Figure 3. Dimensionless normalized concentration vs dimensionless distance from the wall for three values of the stopping time.

range $1 < \tau^+ < 10$ and the "roll-off" in K^+ values above about $\tau^+ = 30$. The latter arises from the reduction in the velocity that a particle is able to attain during the life of an eddy and from the limit on the time available for the particle to "stray" from its reference particle, set by eddy decay.

It is conventional to distinguish two contributions to K^+: impaction and interception. The former, arising from the inability of particles to follow the eddy motion precisely, would contribute even if a were set to zero in the boundary conditions [22] (but τ^+ left unchanged). Interception, due to the finite size of particles, would arise even if particles did follow the motion of the eddies exactly but were deposited when the "eddy" reached a dimensionless distance a^+ from the wall. Figure 2 also shows the "pure" interception contribution, obtained by repeating the simulation for each τ^+ value with a particle forced to coincide with the reference particle representing the eddy, except if it reaches a dimensionless distance a^+ from the wall, when it is deposited. At $\tau^+ = 1$, interception contributes a sizeable fraction of the total deposition, but rapidly becomes negligible at larger τ^+. It is likely that the interception contribution is sensitive to the precise manner in which σ approaches zero as y approaches zero, and appreciable differences can be expected if the KR behaviour (near quadratic at small y) were to be used.

In view of the simplifications adopted, the aim of the current work is not to provide the best possible model for inertial deposition to a smooth wall. Nevertheless, it is interesting to compare the results from the model with the well-known data of Liu & Agarwal (1974), denoted on the figure by the crosses. The overall agreement is remarkably good. Although this may result from a cancellation of omitted effects, it is sufficiently encouraging to suggest proceeding further with this type of modelling.

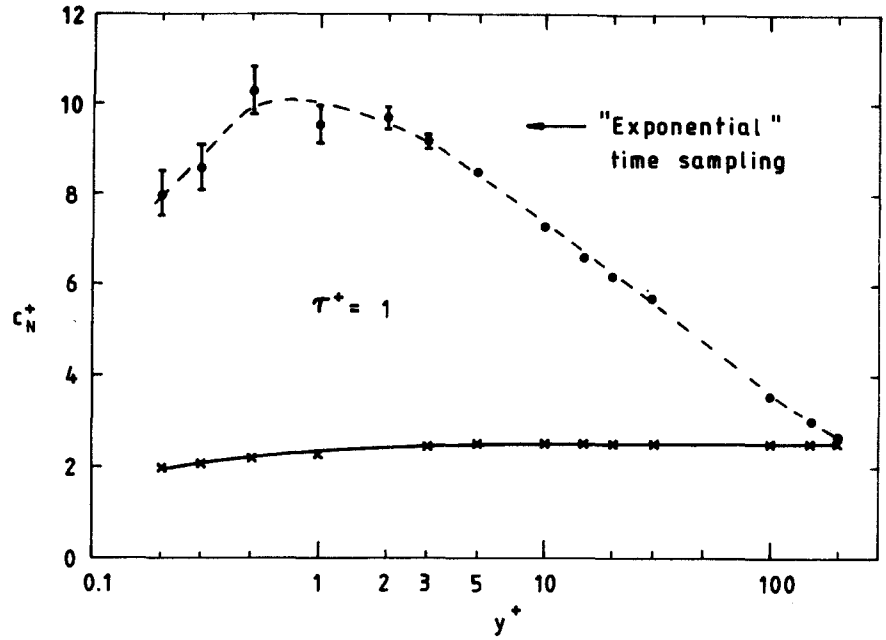

Figure 4. Effect on the concentration profile of assuming an exponential distribution of time-to-next-scattering, for a dimensionless stopping time of $\tau^+ = 1$.

3.8.2. Concentration profiles

Figure 3 shows the dimensionless normalized concentration for $y^+ \leqslant 200$, for $\tau^+ = 1$, 10 and 100. The solid lines are merely eye-guides through the results; the 1 SD statistical-error bars lie within the plotted points. At $\tau^+ = 1$, where the concentration build-up for $y^+ < 10$ was most pronounced in the KR results, no build-up is observed. In fact, the concentration is constant (within the

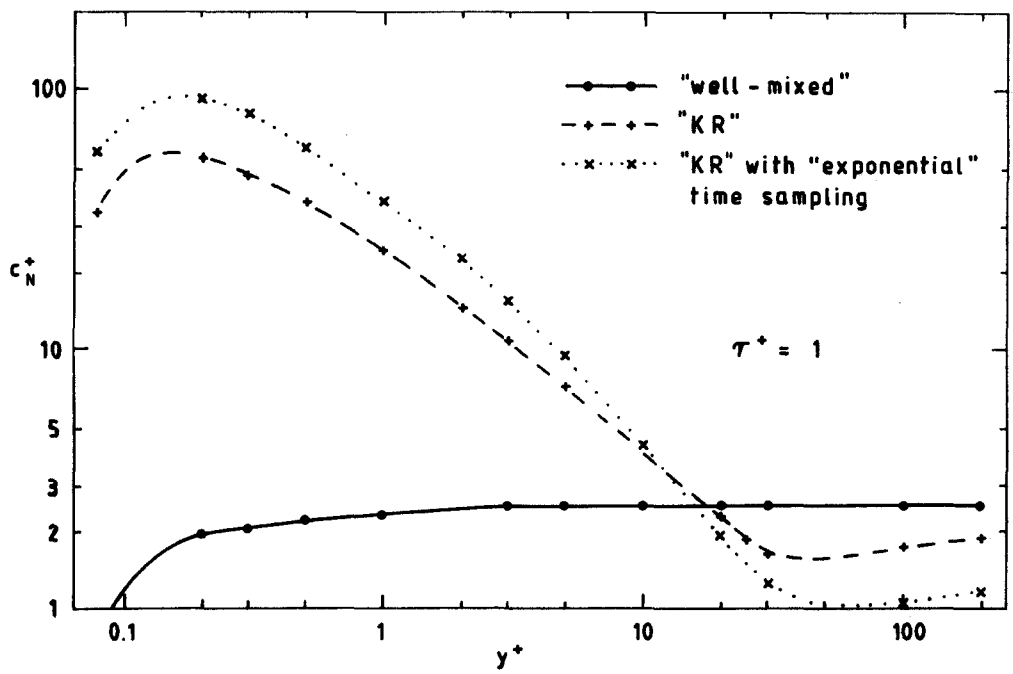

Figure 5. Concentration profile for a dimensionless stopping time of $\tau^+ = 1$, obtained by applying the KR random-walk formulation to the simplified boundary layer. Results are given for two methods of time sampling.

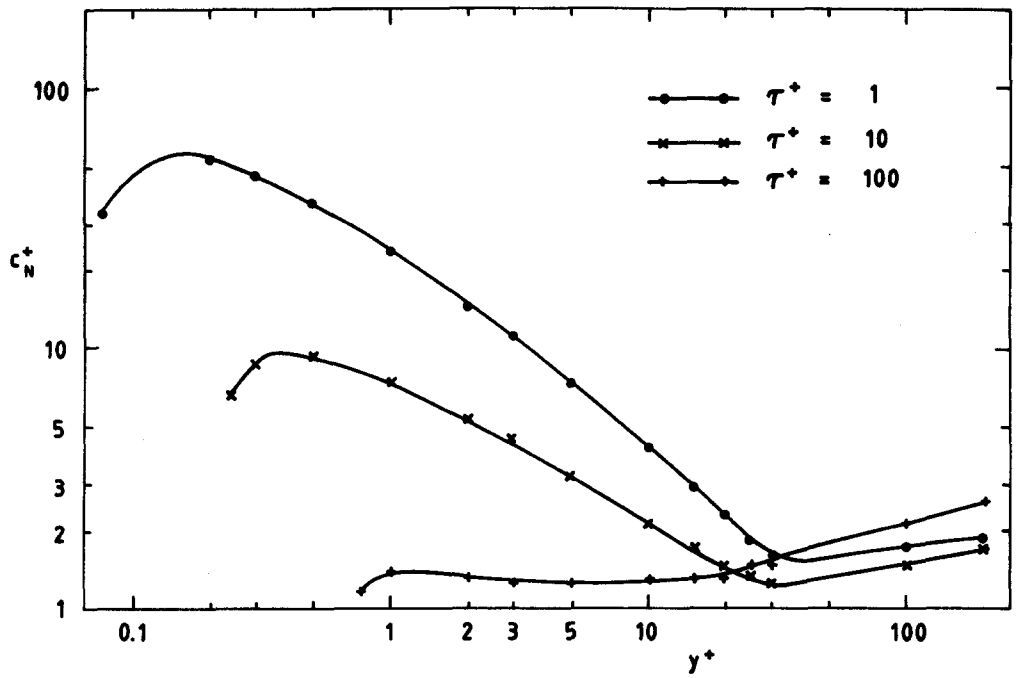

Figure 6. Concentration profiles for three values of the dimensionless stopping time, obtained using the KR random-walk formulation.

statistical accuracy) until $y^+ < 3$ where the effect of loss at the wall generates a decreasing concentration as y^+ decreases.

For $\tau^+ = 10$, there *is* a modest peak in concentration around $y^+ = 1$, but this arises more as a result of a dip in concentration just below the transition into the region of varying σ, with the concentration recovering at smaller y^+ to a value close to that found in the uniform-σ region, before again falling off due to loss at the wall. A check was made that this effect was not an artefact of the injection procedure both by increasing y_i for the given injection prescription and by adopting a different prescription: the feature was preserved in each case. The dip can be understood as arising from particles which are "thrown" into the non-uniform region from above, bringing with them higher velocities on average than the local eddy velocities. This is not balanced by a similar effect arising from particles moving up from regions of low σ since, *inter alia*, there is an inequality in the number of upward- and downward-moving particles at any point (due to the deposition at the wall).

The spatial extent of the "dip" is consistent with this explanation, being of order $\tau^+\sigma_u^+$—where σ_u^+ is the (dimensionless) σ value in the uniform region—i.e. of order 10. An approximate estimate of the relative magnitude of the dip is $(\Delta y\, \mathrm{d}\sigma/\mathrm{d}y)/\sigma$, where Δy is the typical distance a particle could stray from the reference particle in a single flight between scatterings. Taking the latter to be of order $\tau\sigma$ gives a fractional effect of $\tau\, \mathrm{d}\sigma/\mathrm{d}y$, i.e. $\tau\alpha$ in the present case. For $\tau^+ = 10$, this implies about a 30% effect at most, which is consistent with that observed.

This argument is also consistent with the observation of no dip for $\tau^+ = 1$, since the above estimate would be reduced by a factor of 10 for this case, bringing the effect down to the level of the noise. On the other hand, at $\tau^+ = 100$, one does not expect an order-of-magnitude increase in the effect since the lifetime of the eddy sets a limit on how far a particle can stray from the reference particle, with T_L^+ of order 10 in the region of interest. For $\tau^+ = 100$, the positive concentration gradient due to the loss at the wall is dominant and leads to a monotonic decrease in concentration with decreasing y^+. However, the tendency for the concentration to "dip" just below $y^+ = 30$ can still be detected in a marked change in slope there. Thus, there is only a fairly narrow "window" of τ^+ values for which even this modest peak at low y^+ can be observed.

The effect observed here at $\tau^+ = 10$ is certainly not large enough to explain the orders-of-magnitude build-up observed by KR at $\tau^+ = 1$. At the pertinent values of y^+, the value of $\mathrm{d}\sigma^+/\mathrm{d}y^+$

in their work is smaller than in the present work and, as noted above, the effect is expected to diminish with diminishing τ^+ to become negligible at $\tau^+ = 1$. On the other hand, the spurious build-up due to violation of the well-mixed condition will become more noticeable as τ^+ diminishes, since the effect on concentration profile of loss at the wall decreases.

Figure 4 shows the effect on the concentration profile (for $\tau^+ = 1$) of using the "exponential" method of choosing the time-to-next-scattering ([18]) rather than that represented by [19]. At its peak, the concentration is about 5 times higher than that obtained with the "well-mixed" formulation. Thus, the acceleration of simulation particles between collisions and the time-to-next-collision jointly have to be modelled correctly if spurious non-uniformities in the concentration profile are to be avoided. The deposition velocity is about a factor of 6 higher when [18] is used rather than [19].

3.9. Application of the KR Prescription

To confirm the conclusions reached in section 2 concerning the random-walk formulation of KR, it is of interest to apply their prescription to the present simplified boundary layer.

The basic requirement in their model is that in the non-uniform region of σ, (v/σ) should be held constant between scatterings, i.e.

$$\eta = \eta_0, \qquad [27]$$

where the subsrcipt 0 refers to the value immediately after the last scattering. For the linearized dependence of σ on y, this yields

$$\frac{dv}{dt} = \eta_0 \alpha v, \qquad [28]$$

giving an exponential variation of v with t between scatterings.

Conveniently, this also leads to an analytic solution for the velocity and position of a particle with inertia (see [21]), as follows:

$$v_p(t) = \left[v_p(0) - \frac{v_0}{(1+\alpha\eta_0\tau)}\right]\exp(-t/\tau) + \left[\frac{v_0}{(1+\alpha\eta_0\tau)}\right]\exp(\alpha\eta_0 t), \qquad [29]$$

which is readily integrated once more to give $y_p(t)$.

The resulting concentration profiles for $\tau^+ = 1$ are shown in figure 5 compared to the profile presented in figure 3. A marked concentration build-up is observed for both methods of time sampling, peaking around $y^+ = 0.1$ to 0.2. The peak is nearly a factor of 2 higher with "exponential" time sampling than that obtained using [19], i.e. around 40 times the concentration at large y^+ is the "well-mixed" case. This peak value is not much less than that observed by KR using the more complex $\sigma(y)$ behaviour, even though the σ values at these small y^+ are several times larger here than in their work. However, the precise peak magnitude depends on how the profile is affected at small y^+ by loss at the wall, and this could be quite different for the two $\sigma(y)$ functions.

Figure 6 shows the results for $\tau^+ = 10$ and 100 (using [19] time sampling). As τ^+ increases, the build-up becomes less pronounced, and is barely noticeable at $\tau^+ = 100$, as was found by KR. The solid lines are merely an eye-guide through the points.

At small values of τ^+, use of the linearized σ variation leads to much higher values of K^+ compared to those of KR (and compared to experiment) due to an overestimation of the interception contribution. The latter, in turn, results from the slower fall off in σ as y^+ approaches zero. However, at large τ^+, the values of K^+ are quite close to those of KR (and to the experimental results).

4. CONCLUSIONS

The foregoing analysis and simulation results indicate that the large build-up in concentration near the wall observed by Kallio & Reeks (1989) at low τ^+ values is very likely to be a consequence of the failure of their random-walk prescription to satisfy the "well-mixed" condition [which

requires that, in the limit that the pollutant follows the eddy motions of carrier fluid everywhere *exactly*, an initially spatially uniform concentration should (on average) remain so].

The work highlights the fact that in constructing random-walk simulations for turbulent dispersion, in which simplified models of the turbulent flow-field are used, care must be taken to satisfy certain fundamental constraints if spurious concentration trends are to be avoided.

The work illustrates how it is possible in some circumstances to construct a one-dimensional random-walk process for calculating deposition velocities, analogous to the one-dimensional eddy-diffusivity equation which is conventionally used as a starting point for this purpose.

The results for deposition velocity vs stopping time obtained from the model developed here, albeit using a simplified boundary-layer specification, are sufficiently encouraging to suggest that it would be worth extending the treatment to handle a more realistic boundary-layer prescription and equation of motion for particles. The indications are that the modelling captures enough of the physics to enable a number of other questions concerning inertial deposition to be addressed, such as the effect of trajectory-crossing and the influence of body forces such as gravity.

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REFERENCES

BROOKE, J. W., KONTOMARIS, K., HANRATTY, T. J. & MCLAUGHLIN, J. B. 1992 Turbulent deposition and trapping of aerosols at a wall. *Phys. Fluids* **A4,** 825–834.

CLEAVER, J. W. & YATES, B. 1975 A sub layer model for the deposition of particles from a turbulent flow. *Chem. Engng Sci.* **30,** 983–992.

DAVIES, C. N. (Ed.) 1966 Deposition from moving aerosols. In *Aerosol Science*. Academic Press, London.

DURBIN, P. A. & HUNT, J. C. R. 1980 Dispersion from elevated sources in turbulent boundary layers. *J. Mec.* **19,** 679–695.

HUTCHINSON, P., HEWITT, G. F. & DUKLER, A. E. 1971 Deposition of liquid or solid dispersions from turbulent gas streams: a stochastic model. *Chem. Engng Sci.* **26,** 419–439.

KALLIO, G. A. & REEKS, M. W. 1989 A numerical simulation of particle deposition in turbulent boundary layers. *Int. J. Multiphase Flow* **15,** 433–446.

LEGG, B. J. & RAUPACH, M. R. 1982 Markov-chain simulation of particle dispersion in inhomogeneous flows: the mean drift velocity induced by a gradient in Eulerian velocity variance. *Boundary-layer Met.* **24,** 3–13.

LIU, B. Y. H. & AGARWAL, J. K. 1974 Experimental observation of aerosol deposition in turbulent flow. *Aerosol Sci.* **5,** 145–155.

LIU, B. Y. H. & ILORI, T. A. 1974 Aerosol deposition in turbulent flow. *Envir. Sci. Technol.* **8,** 351–356.

LUHAR, A. K. & BRITTER, R. E. 1989 A random walk model for dispersion in inhomogeneous turbulence in a convective boundary layer. *Atmos. Envir.* **23,** 1911–1924.

MCLAUGHLIN, J. B. 1989 Aerosol particle deposition in numerically simulated channel flow. *Phys. Fluids* **A1,** 1211–1224.

REEKS, M. W. 1982 Calculation of particle deposition in reactor coolants. CEGB Report TRPD/B/0016/N82.

SAFFMAN, P. G. 1965 The lift on a small sphere in a slow shear flow. *J. Fluid Mech.* **22,** 385–400.

SAWFORD, B. L. 1985 Lagrangian statistical simulation of concentration mean and fluctuation fields. *J. Climat. Appl. Met.* **24,** 1152–1166.

SUN, Y. F. & LIN, S. P. 1986 Aerosol concentration in a turbulent flow. *J. Colloid Interface Sci.* **113,** 315–320.

THOMSON, D. J. 1984 Random walk modelling of diffusion in inhomogeneous turbulence. *Q. Jl R. Met Soc.* **110,** 1107–1120.

THOMSON, D. J. 1987 Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *J. Fluid. Mech.* **180,** 529–556.

UNDERWOOD, B. Y. 1991a Discussion on "An interpretation of Taylor's statistical analysis of particle dispersion". *Atmos. Envir.* **25A,** 1129–1130.

UNDERWOOD, B. Y. 1991b Deposition velocity and the collision model of atmosphere dispersion: I. Framework and application to cases with constant turbulent velocity scale. *Atmos. Envir.* **25A,** 2749–2759.

UNDERWOOD, B. Y. 1991c Deposition velocity and the collision model of atmospheric dispersion: II. Extension to cases with variable turbulent velocity scale. *Atmos. Envir.* **25A,** 2761–2770.

WILSON, J. D., THURTELL, G. W. & KIDD, G. E. 1981 Numerical simulation of particle trajectories in inhomogeneous turbulence, II: Systems with variable turbulent velocity scale. *Boundary-layer Met.* **21,** 423–441.

APPENDIX

Implication of v/σ Constant

It is convenient to work back from the condition that

$$\frac{dn_+(y, v_+)}{dy} = 0, \tag{A.1}$$

when

$$n_+(y, v_+) \propto v_+ p_y(v_+), \tag{A.2}$$

where d/dy is a total derivative as before. This implies

$$\frac{\partial n_+(y, v_+)}{\partial y} + \frac{\partial n_+(y, v_+)}{\partial v_+}\frac{dv_+}{dy} = 0 \tag{A.3}$$

and thus that

$$\frac{dv_+}{dy} = -\frac{\left(\frac{\partial n_+}{\partial y}\right)}{\left(\frac{\partial n_+}{\partial v_+}\right)} \tag{A.4}$$

when n_+ is given by [A.2]. Focusing on the case that $p_y(y, v_+)$ is governed by a single scaling velocity at each y, $\sigma(y)$ say—as is certainly the case for a Gaussian distribution—then

$$v_+ p_y(y, v_+) = f(\eta), \tag{A.5}$$

where f is a (so far unspecified) function and $\eta = n_+/\sigma(y)$. Thus,

$$\frac{dv_+}{dy} = -\frac{\left[\frac{df}{d\eta}\left(-\frac{v_+}{\sigma^2}\right)\frac{d\sigma}{dy}\right]}{\frac{df}{d\eta}\left(\frac{1}{\sigma}\right)}. \tag{A.6}$$

Therefore,

$$\frac{dv}{d\sigma} = \frac{v_+}{\sigma}, \tag{A.7}$$

with solution

$$\frac{v_+}{\sigma} = \text{const.} \tag{A.8}$$

The same applies to negative values of v. This implies that holding v/σ constant between scatterings, as in the KR simulation, would lead to the condition that $dn_+/dy = 0$ in the limit that the particles are following the eddy motions exactly. This, in turn, implies that in the same limit

$$\frac{dN_\pm}{dy} = 0, \tag{A.9}$$

where N_+ is the integral of n_+ over all values of v_+ (and similarly for N_-).