JOURNAL OF COMPUTATIONAL PHYSICS 9, 290–302 (1972)

The Numerical Simulation of Particle Motion in a Homogeneous Field of Turbulence

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Received April 6, 1971

A technique is described for simulating the motion of individual particles in a homogeneous stationary field of turbulence by the use of numbers drawn at random from a normally distributed set. The turbulence is approximated by a Brownian motion Markov process and the scales of motion are assumed to lie in the inertial subrange.

An application of the technique in the study of the growth of droplets in a turbulent cloud is also described.

INTRODUCTION

A substantial literature exists describing the use of simulation techniques to solve a range of problems involving essentially random processes (e.g. [1, 2]). The work described in this paper was motivated by a desire to study the effects of turbulence on the size distributions of droplets growing in clouds. Several workers (e.g. [3–6]) have obtained analytical solutions to the droplet-growth equations in such conditions, but found it necessary to make rather severe assumptions. Their restrictions can be removed by simulating the fluctuating updraughts associated with the turbulent motion and obtaining a numerical solution of the full droplet growth equations.

Obukov [7] suggested that some problems of atmospheric diffusion could be solved by approximating turbulence in the atmosphere to a Brownian motion Markov process. Simulation techniques using this approximation have been derived by several workers (e.g. [8, 9]). In particular, Kraichnan [9] developed a technique to simulate the motion of a particle through a field of turbulence with an arbitrary energy spectrum. For many purposes, however, it is only necessary to consider scales of motion which lie in the inertial subrange and in these circumstances the simpler simulation technique described in this paper can be used.

In this work it is assumed, firstly, that the turbulence is stationary in time and homogeneous in space and, secondly, that the velocities in any given direction of a large number of particles are normally distributed about the mean velocity in that direction. It is also assumed that particles having the same velocity component at a given instant will have a distribution of velocity components some time later which preserves the assumptions of stationarity and homogeneity. The assumption that the scales of motion are in the inertial subrange (i.e., that the effects of viscosity can be neglected) implies that the distribution of velocity components depends only on the time interval and the initial velocity. Warner [10] has also attempted to simulate the growth of cloud droplets but the velocity-simulation technique he used did not preserve the stationarity of the turbulence and is therefore not accurate over long integration periods.

THE SIMULATION TECHNIQUE

The assumption that the components of the velocities of particles in a given direction are normally distributed about the mean velocity component in the same direction, $\bar{u}$, means that the probability that a particular particle will have a velocity component in the range u–$(u + du)$ is given by

$$P(u)\,du = \frac{1}{(2\pi)^{1/2}\,\sigma_u} \exp\left[-\frac{1}{2}\left(\frac{u-\bar{u}}{\sigma_u}\right)^2\right] du, \tag{1}$$

where σ_u is the standard deviation of the velocity components of all particles in the turbulent field.

The *initial* velocity component of a typical particle, u_0, can be selected by the following relationship

$$u_0 = \bar{u} + n_0\sigma_u\,, \tag{2}$$

where n_0 is a number drawn at random from a set of numbers which form a normal distribution with unit standard deviation and zero mean.

Now let the probability that a particle which has an initial velocity[1] between u_0 and $u_0 + du_0$ will have a velocity between u_τ and $u_\tau + du_\tau$ at time τ be $P(u_\tau\,, u_0)\,du_\tau\,du_0$. Then the probability, $P(u_\tau)\,du_\tau$, that *any* particle will have a velocity between u_τ and $u_\tau + du_\tau$ at time τ, is given by

$$P(u_\tau)\,du_\tau = \left[\int_{-\infty}^{+\infty} P(u_0)\,P(u_\tau\,, u_0)\,du_0\right] du_\tau\,. \tag{3}$$

The assumption that the field of turbulence is homogeneous and stationary will clearly be satisfied if the distribution of velocities at time τ is also a normal distri-

[1] Strictly "the velocity component in a given direction," but since it is implicit in the treatment that each component of the velocity is independent, this expression is abbreviated here and subsequently to "the velocity" of the particle.

bution with a mean of $\bar{u}$ and a standard deviation, σ_u. It is not difficult to show by substitution into Eq. (3) that this condition is satisfied if

$$P(u_\tau, u_0) = \frac{1}{(2\pi)^{1/2}\,\sigma_\tau} \exp\left[-\frac{1}{2}\left(\frac{u_\tau - \{p_\tau(u_0 - \bar{u}) + \bar{u}\}}{\sigma_\tau}\right)^2\right], \tag{4}$$

where

$$p_\tau^2 = (\sigma_u^2 - \sigma_\tau^2)/\sigma_u^2, \tag{5}$$

i.e., the velocities of particles with initial velocity u_0 are normally distributed about $\{p_\tau(u_0 - \bar{u}) + \bar{u}\}$ with a standard deviation σ_τ after time τ.

It follows from Eq. (4) that the velocity at time τ of a typical particle having an initial velocity u_0 can be selected by the relationship

$$u_\tau = \{(1 - p_\tau)\bar{u} + p_\tau u_0\} + n_1\sigma_\tau, \tag{6}$$

where n_1 is another number drawn at random from the normally distributed set with zero mean and unit standard deviation.

The complete velocity record of a typical particle can be simulated by noting that in general

$$u_{i\tau} = \{(1 - p_\tau)\bar{u} + p_\tau u_{(i-1)\tau}\} + n_i\sigma_\tau, \tag{7}$$

where $u_{i\tau}$ and $u_{(i-1)\tau}$ are the velocities of the particle at times $i\tau$ and $(i-1)\tau$, respectively, and n_i is a number drawn at random from the normally distributed set.

Now it is clear that if the probability that a particle will have a given velocity after a certain time depends only on the time interval and its initial velocity, then the following relationship must be valid

$$P(u_{2\tau}, u_0) = \int_{-\infty}^{+\infty} P(u_{2\tau}, u_\tau)\, P(u_\tau, u_0)\, du_\tau. \tag{8}$$

By substituting expressions of the type given by Eq. (4) for $P(u_\tau, u_0)$, etc., it can be shown that this condition is satisfied provided that

$$p_{2\tau} = p_\tau^2. \tag{9}$$

Equation (9) will, in general, be satisfied if

$$p_\tau = A\exp(-\tau/T), \tag{10}$$

where T is a characteristic time.

However, when $\tau \to 0$, it is clear that the mean velocity of a group of particles with initial velocity u_0 will tend to u_0, i.e., $\lim_{\tau\to 0}\{(1 - p_\tau)\bar{u} + u_0\} = u_0$. This is true if $\lim_{\tau\to 0} p_\tau = 1$, which in turn requires that $A = 1$.

Further, if τ is short, but long enough for viscous forces to be unimportant, then according to the Kolmogoroff hypothesis, σ_τ will be a function of ϵ and τ only, where ϵ is the energy dissipated in unit mass of the turbulent fluid in unit time. It then follows from the dimensions of the quantities involved that

$$\sigma_\tau^2 = k\epsilon\tau \tag{11}$$

where k is a dimensionless constant, which for the purposes of simulation can be assumed to have a value of unity.

Now from Eqs. (5) and (10) we have

$$\sigma_\tau^2 = \sigma_u^2\{1 - \exp(-2\tau/T)\} \tag{12}$$

so that the requirement for short times is that $\sigma_u^2\{1 - \exp(-2\tau/T)\} \approx \epsilon\tau$. Expanding the exponential in the usual way, and neglecting second and higher powers of τ/T, gives $T = 2\sigma_u^2/\epsilon$.

On the other hand, when $\tau \to \infty$ the distribution of particles with initial velocity u_0 must tend to become identical with the distribution of all particles, i.e., $\lim_{\tau\to\infty} P(u_\tau, u_0) = P(u_\tau)$. This is true if $\lim_{\tau\to\infty} p_\tau = 0$ and $\lim_{\tau\to\infty} \sigma_\tau = \sigma_u$ and it will be seen that both of these conditions are also satisfied since the exponent is negative in Eqs. (10) and (12).

Finally, it may be noted that the full expression for σ_τ^2 derived above, namely $\sigma_u^2\{1 - \exp(-\epsilon\tau/\sigma_u^2)\}$, may be replaced by the simpler expression $\sigma_\tau^2 = \epsilon\tau$ provided that $\sigma_\tau^2/\sigma_u^2 \ll 1$. This approximation is equivalent to underestimating the true value of the energy dissipated by an amount $\delta\epsilon$ which is approximately equal to $(\epsilon/2)(\sigma_\tau^2/\sigma_u^2)$. Taking typical values for turbulence in a cumulus cloud, $\epsilon = 10^{-2}$ m^2 s^{-3}, $\sigma_u = 1.0$ m s^{-1}, then if τ is chosen to be 1 s, the error in the assumed value of ϵ is only 0.5%.

In the same way, the exponential expression for p_τ can be replaced by $(1 - \epsilon\tau/2\sigma_u^2)$ when τ is small.

To sum up, we conclude that any component of the velocity of a typical particle moving in a field of turbulence having the assumed characteristics can be simulated by means of the following relationships.

$$u_0 = \bar{u} + n_0\sigma_u\,,$$

$$u_{i\tau} = \{(1 - p_\tau)\bar{u} + p_\tau u_{(i-1)\tau}\} + n_i\sigma_\tau\,,$$

where

$$\begin{aligned}\sigma_\tau^2 &= \sigma_u^2\{1 - \exp(-\epsilon\tau/\sigma_u^2)\},\\ &\approx \epsilon\tau \qquad \text{for small } \tau,\end{aligned} \tag{13}$$

and

$$\begin{aligned}p_\tau &= \exp(-\epsilon\tau/2\sigma_u^2),\\ &\approx 1 - \epsilon\tau/2\sigma_u^2 \qquad \text{for small } \tau.\end{aligned}$$

The simulation technique requires a sequence of numbers drawn at random from a normally distributed set of numbers with a mean of zero and unit standard deviation. A suitable pseudorandom sequence of numbers was generated by adding together N successive terms of another pseudorandom sequence in which the numbers were evenly distributed in the range 0–1. The resultant sequence is easily transformed into the required set with zero mean and unit standard deviation. The evenly distributed numbers were themselves generated by the Lehmer congruence method [1] in which the $(i+1)$-th number is obtained by the relation

$$n_{i+1} = kn_i \bmod m. \tag{14}$$

The computations were carried out on a computer having 48 bit words. It was therefore convenient to choose $m = 2^{48}$. With this value of m, the maximum length of the cycle of 2^{46} is obtained if $k \equiv -3 \bmod 8$, a condition which is conveniently satisfied by choosing k to be the largest odd power of 5 which can be contained in one word of the computer store—in this case 5^{19}. The starting value, n_0, can be any convenient odd number. Numbers generated in this way were subjected to several statistical tests and the performance was satisfactory with $N \geqslant 8$. However, the true test of a sequence of pseudorandom numbers is to test them in the situation in which they are to be used and this was achieved by analyzing the velocity traces which were simulated.

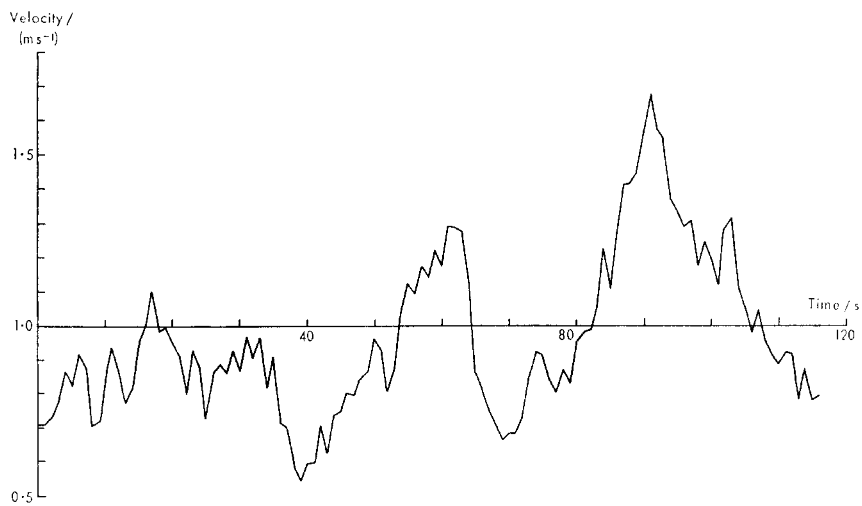

Fig. 1. Simulated-velocity trace of a typical particle in a field of turbulence with a mean energy dissipation of 0.01 m^2 s^{-3}. The mean and standard deviation of the particle velocities are 1 m s^{-1}.

Simulated Velocity Traces

Figure 1 shows part of a typical simulated-velocity trace for a particle with a mean velocity, $\bar{u}$, of 1 m s^{-1}. The standard deviation of the velocities was 1 m s^{-1} and the turbulent energy dissipation, ϵ, was 0.01 m^2 s^{-3}, these values being typical of small cumulus clouds. The velocities were calculated at 1 s intervals. The similarity between this trace and the fluctuations observed in turbulent air is obvious.

TABLE I

Results of Chi-Squared Test on a Comparison of the Distributions of Particle Velocities after Several Times, and the Theoretical Normal Distributions

t/T	χ^2 for 3 degrees of freedom	Probability that calculated value of χ^2 will be exceeded
0	1.22	0.78
0.05	2.26	0.52
0.01	0.19	0.98
0.5	2.84	0.42
1.0	0.88	0.83
5.0	8.07	0.05
10.0	2.81	0.43
50.0	9.23	0.01
100.0	3.47	0.33

In order to check that the technique had correctly simulated stationary turbulence, the velocities of 100 particles, initially having different velocities, were calculated at time t. For each time the distributions were split into four categories, $u_t \leqslant \bar{u} - \sigma_u$, $\bar{u} - \sigma_u < u_t \leqslant \bar{u}$, $\bar{u} < u_t \leqslant \bar{u} + \sigma_u$ and $u_t > \bar{u} + \sigma_u$ and the number in each category determined. A chi-squared test for three degrees of freedom was then applied at each time and the results are tabulated in Table I, together with the probability that the value of chi-squared found would be exceeded if the observed velocities were drawn at random from a distribution with a mean of $\bar{u}$ and standard deviation σ_u. The times in this table were expressed in nondimensional form by dividing by the characteristic time, $T\ (= 2\sigma_u^2/\epsilon)$. The values of chi-squared found in this test are consistent with the assumption of stationary turbulence.

The power spectrum is an important characteristic of a randomly fluctuating record. In order to correctly simulate turbulent motion in the inertial subrange, the energy per unit mass of the fluid in unit frequency range, $E(f)$, must be inversely proportional to the square of the frequency, f, a result obtained by dimensional analysis in this range where $E(f)$ depends only on ϵ and f.

The exact form of $E(f)$ can be derived as follows (see [11]). Since the turbulent

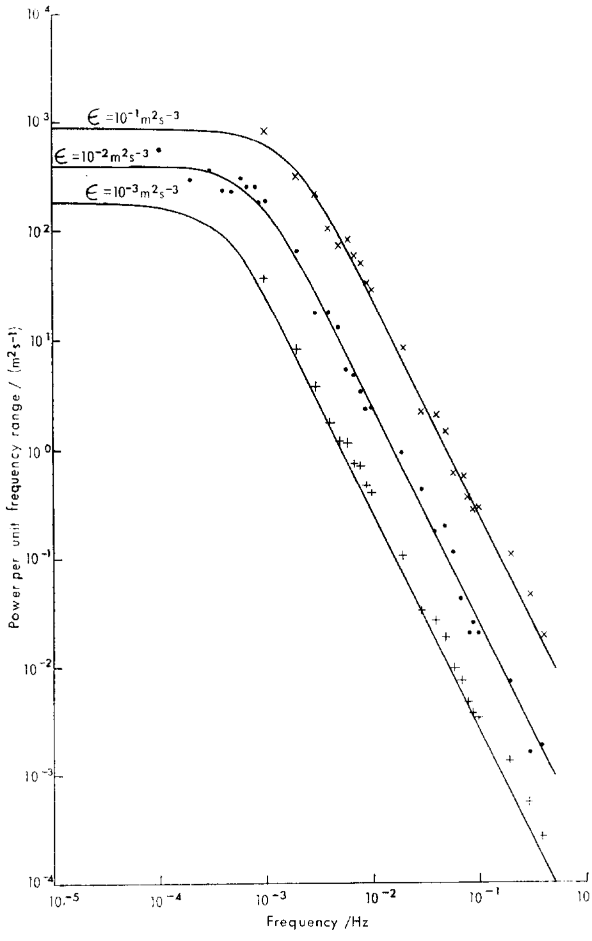

FIG. 2. Power spectra obtained from the motion of a particle for turbulent energy dissipation rates, ϵ, of 10^{-1}, 10^{-2} and 10^{-3} m^2 s^{-3}. The curves were obtained from Eq. (19).

field is stationary the covariance of the velocities of a particle at two times separated by an interval τ can be defined as

$$C(\tau) = \lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} u_t u_{t+\tau}\, dt = \mathrm{ave}(u_t u_{t+\tau}), \tag{15}$$

where u_t and $u_{t+\tau}$ are the velocities of the particle at times t and $t + \tau$ respectively. The average value of $u_t \cdot u_{t+\tau}$ is clearly given by

$$\iint_{-\infty}^{+\infty} u_t \cdot u_{t+\tau} P(u_t) \cdot P(u_{t+\tau}, u_t)\, du_t \cdot du_{t+\tau}\,.$$

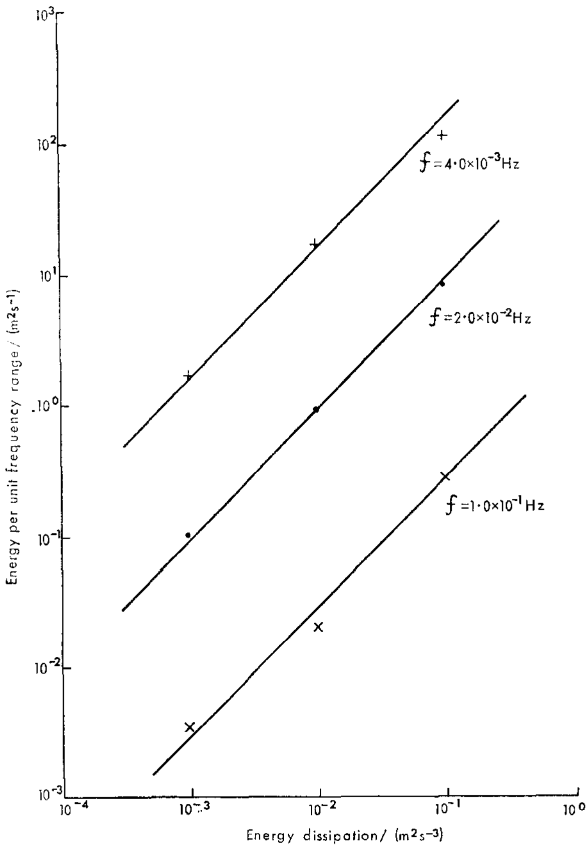

FIG. 3. Variation of the energy per unit frequency range as a function of the energy dissipation rate at three frequencies, f, higher than f_0.

Substituting for the variables and noting that $C(-\tau) = C(+\tau)$ we obtain

$$C(\tau) = \sigma_u^2 \exp(-\epsilon \mid \tau \mid /2\sigma_u^2) = \sigma_u^2 \exp(-\mid \tau \mid /T), \tag{16}$$

where T is the characteristic time. Then, as shown in [11]

$$E(f) = \int_{-\infty}^{+\infty} C(\tau) \cos(2\pi f \tau)\, d\tau, \tag{17}$$

which gives on integration

$$E(f) = \epsilon/(4\pi^2 f^2 + f_0^2), \tag{18}$$

where $f_0 = 1/T = \epsilon/2\sigma_u^2$. Clearly when $f \gg f_0$, $E(f) \propto f^{-2}$ the result expected on dimensional grounds.

A spectral analysis using a Fast Fourier Transform routine [12] was carried out on three separate records consisting of the simulated velocities of a particle at 1024 successive intervals of 1 or 5 s in turbulent fields with values of ϵ of 10^{-3}, 10^{-2} and 10^{-1} m^2 s^{-3}, respectively. The value of σ_u was chosen to correspond to a scale L, defined as σ_u^3/ϵ, of 100 m. The resultant spectra are shown in Fig. 2 which shows that $E(f)$ varies with f as predicted by Eq. (18). Fig. 3 shows that $E(f) \propto \epsilon$ when $f \gg f_0$.

These tests have indicated that the simulation technique is a valid approximation for the simulation of particle motion in a field of homogeneous turbulence to which the initial assumptions are applicable.

Application of the Simulation Technique

The simulation technique can be used to calculate the trajectories of individual particles moving in a field of homogeneous turbulence when the individual motion, rather than a statistical description, is required. The displacement $x_{t+\tau}$, can be obtained from that at a previous time, t, using the equation

$$x_{t+\tau} = x_t + u_t \cdot \tau. \tag{19}$$

The use of this equation implies that the time step, τ, is sufficiently short for the change in velocity to be neglected. This also implies that $\sigma_\tau \ll \sigma_u$.

The displacements of six typical particles were computed at 5 s intervals using Eq. (19) for a case in which the mean velocity, $\bar{u}$, was zero, the energy dissipation, ϵ, was 10^{-2} m^2 s^{-3} and the characteristic time, T, was 100 s. The initial velocities were chosen at random from the distribution given by Eq. (2). The results, which were output as a function of time using a special graphing program, are shown in Fig. 4.

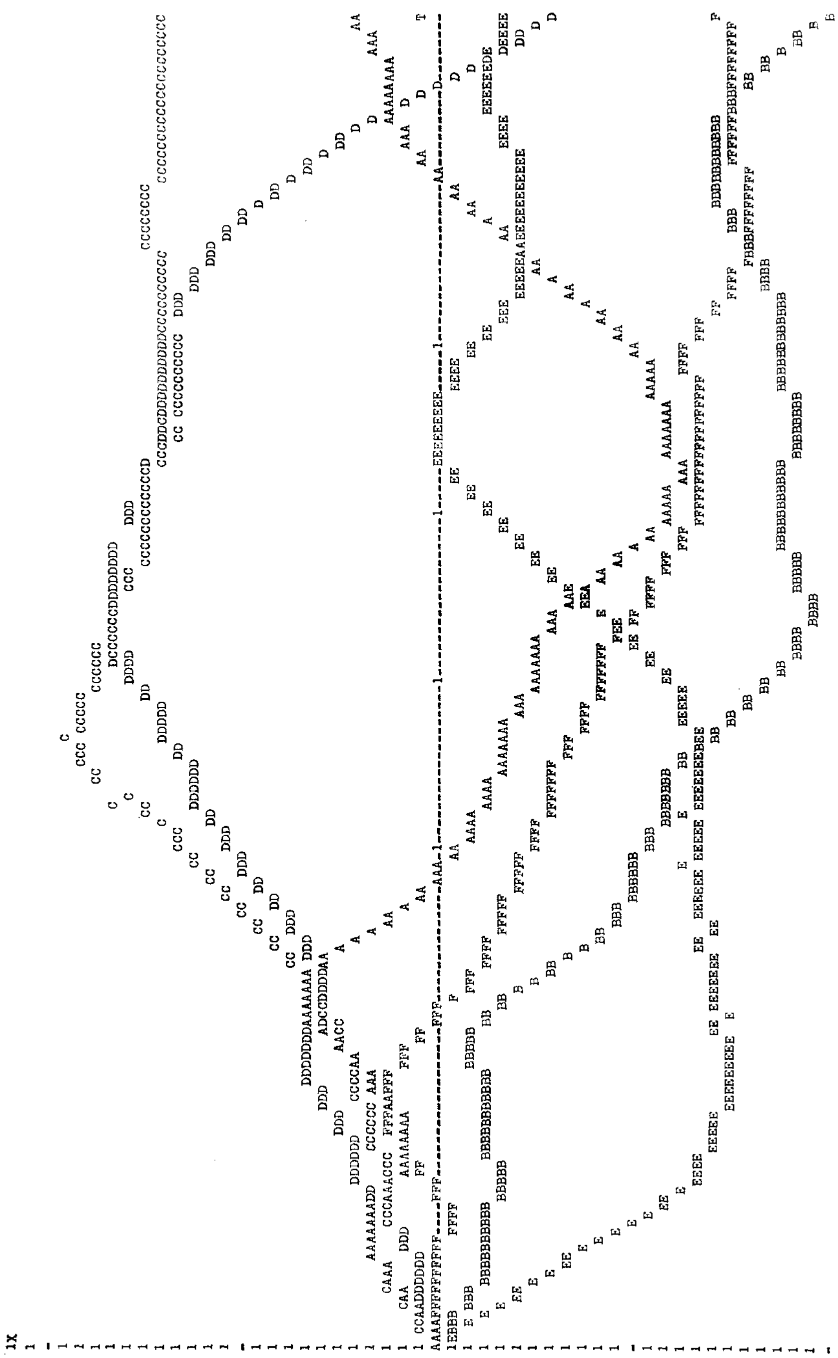

FIG. 4. Diagram showing the displacements of six typical particles (denoted by the letters *A* to *F*) as functions of time, for one-dimensional motion in a field of turbulence. The mean of the initial velocities of the particles is zero, the turbulent energy dissipation, 0.01 $m^2 s^{-3}$ and the characteristic time, 100 s. The scale markers on the horizontal axis are at intervals of 100 s and on the vertical axis at intervals of 100 m.

The numerical simulation technique was used to solve the equations for the growth of droplets by condensation in a turbulent cloud. Detailed results of this investigation will be published elsewhere [13] but an outline of the solution of the problem is given below.

The set of equations describing the changes in pressure, p, temperature, T, supersaturation, σ, and liquid water content, w, in a moving parcel of air are

$$(dp/dt) = -(gm_a p/RT)(dz/dt), \tag{20}$$

$$(dT/dt) = (L/c_{pa})(dw/dt) - (g/c_{pa})(dz/dt), \tag{21}$$

$$(d\sigma/dt) = (m_a g/RT)\{(\epsilon L/Tc_{pa}) - 1\} - (dw/dt)\{(m_v/Rc_{pa})(L/T)^2 + (p/\epsilon p_s)\}, \tag{22}$$

$$(dw/dt) = 4\pi r^2 \rho N(dr/dt), \tag{23}$$

where

- z is the height of the parcel,
- R is the universal gas constant,
- g is the acceleration due to gravity,
- m_a is the molecular weight of dry air,
- m_v is the molecular weight of water vapour,
- ϵ is the ratio m_v/m_a,
- L is the latent heat of vaporization of water,
- c_{pa} is the specific heat of dry air at constant pressure,
- p_s is the saturation vapour pressure of water,

and we have assumed that the parcel contains N drops/unit mass of radius r and density ρ. The relation between dr/dt and r, σ, p, T has been given by Mason and Ghosh [14].

These equations can be integrated numerically if the variation of dz/dt, the vertical velocity of the parcel, with time, is obtained by the simulation technique. Analytical solutions of these equations, using a distribution of velocities consistent with the turbulence, are not possible without considerable simplifying assumptions. A large number of parcels were considered, each initially containing droplets of the same radius. At various heights above the starting level the droplet sizes were compared. It was found that at a particular height the spread in radii was very small, the small spread being due to the close correlation between the supersaturation and the vertical velocity which is indicated in Fig. 5 for a typical particle.

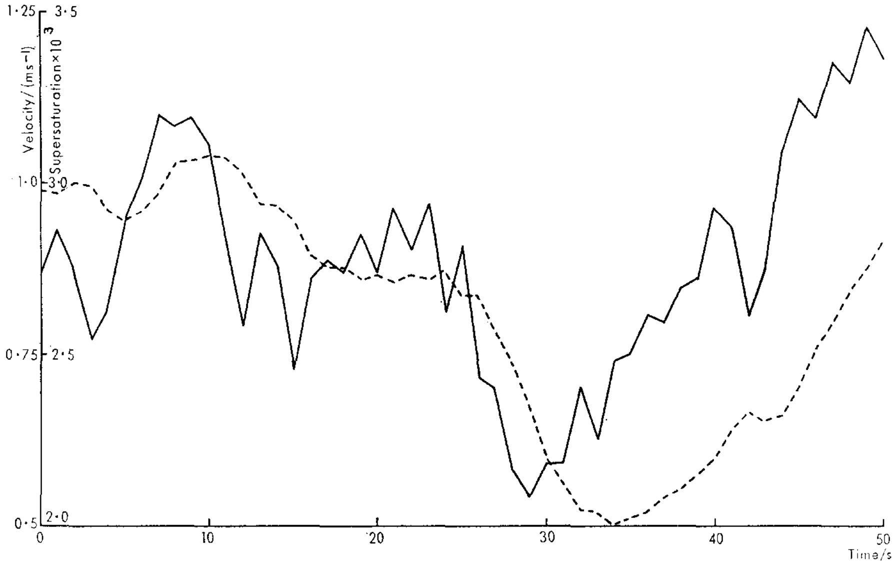

FIG. 5. The variation with time of the velocity (solid line) and supersaturation (dashed line) of a typical parcel of air. The mean updraught is 1 m s^{-1} and the turbulent energy dissipation 0.01 m^2 s^{-3}.

CONCLUSIONS

A simple method of simulating the velocity of a particle moving in a field of uniform homogeneous turbulence involving only the generation of a set of random numbers with a Gaussian distribution has been established. The velocities calculated using this method have been shown to be consistent with the assumptions made about the turbulence. An application of the model has been made to the problem of droplet growth in turbulent clouds.

ACKNOWLEDGMENT

This paper is published with the permission of the Director-General of the Meteorological Office.

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