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A MONTE CARLO METHOD  
FOR THE PDF EQUATIONS OF TURBULENT FLOW

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ABSTRACT

A Monte Carlo method is presented which simulates the transport equations of joint probability density functions (pdf's) in turbulent flows. (Finite-difference solutions of the equations are impracticable, mainly because of the large dimensionality of the pdf's.) Attention is focused on an equation for the joint pdf of chemical and thermodynamic properties in turbulent reactive flows. It is shown that the Monte Carlo method provides a true simulation of this equation, and that the amount of computation required increases only linearly with the number of properties considered. Consequently, the method can be used to solve the pdf equation for turbulent flows involving many chemical species and complex reaction kinetics. Monte Carlo calculations of the pdf of temperature in a turbulent mixing layer are reported. These calculations are in good agreement with the measurements of Batt (1977).

## 1. INTRODUCTION

The closure problem associated with non-linearities in the equations governing turbulent flow is avoided by considering the joint probability density function (pdf) of the flow variables. The joint pdf of velocity  $p(\underline{v}; \underline{x}, t)$  provides a complete statistical description of the turbulent velocity fluctuations, and, in reacting flows, a complete statistical description of the chemical and thermodynamic properties is provided by their joint pdf,  $p(\underline{\psi}; \underline{x}, t)$ .

These favorable attributes have led several authors to base turbulence closures on the transport equations for the joint pdf's. Lundgren (1969) and Ribeiro (1977) have suggested closure approximations for the transport equation for  $p(\underline{v}; \underline{x}, t)$ . For reacting flows, the transport equation for  $p(\underline{\psi}; \underline{x}, t)$  is particularly attractive since the effects of reaction appear in closed form, irrespective of the complexity and non-linearity of the reaction scheme. Closure approximations for other terms in the equation have been suggested by Dopazo (1975), by Pope (1976) and by Janicka, Kolbe and Kollmann (1979).

The attraction of the pdf approach appears to diminish when solving the transport equations is considered. Analytic solutions have been obtained in a few simple cases, but in general numerical methods are required. Such methods have to cope with the integro-differential nature of the equations and with the large dimensionality of  $p(\underline{v}; \underline{x}, t)$  and  $p(\underline{\psi}; \underline{x}, t)$ . For example, in a steady, two-dimensional flow, the joint pdf of velocity is  $p(v_1, v_2, v_3; x_1, x_2)$ --a five-dimensional quantity. Consequently, no numerical solutions of the transport equation for  $p(\underline{v}; \underline{x}, t)$  have been obtained. Janicka, Kolbe and Kollmann (1978) used a finite-difference method to solve the

transport equation for a single scalar -- that is, for  $p(\psi; x_1, x_2)$ . This is the most general solution that has been obtained so far.

Reactive flows of practical interest usually involve many species. Consequently the dimensionality of the pdf  $p(\psi_1, \psi_2 \dots \psi_\sigma; \underline{x}, t)$  is large because  $\sigma$  is large. An order-of-magnitude analysis (section 3.5) shows that the finite-difference solution of the pdf transport equation is impracticable for  $\sigma$  greater than 3. (This is a generous estimate.) More importantly, the computational expense is found to rise exponentially with  $\sigma$ . Therefore no conceivable improvement in computational ability can make possible finite-difference solutions for  $\sigma = 10$ , say.

In this paper, a Monte Carlo method is presented which makes possible the solution of the pdf transport equation for the general case. The computational expense of the method rises only linearly with  $\sigma$  which is the best that can be achieved by any algorithm. Consequently, the solution of the pdf transport equation by the Monte Carlo method can be envisaged for turbulent flows involving many reactive species. Although it is specific to the transport equation for  $p(\psi; \underline{x}, t)$ , the method contains the ingredients essential to simulating other joint pdf equations. Thus, solutions to the equations for  $p(\underline{v}; \underline{x}, t)$  and  $p(\underline{v}, \psi; \underline{x}, t)$  can be obtained.

In general, for simple problems Monte Carlo methods are inefficient compared with standard numerical techniques; but for multi-dimensional problems Monte Carlo methods remain practicable while other methods demand prohibitive amounts of computation. The works of Shreider (1966) and Handscomb and Hammersley (1965) describe various applications of the Monte Carlo method.

In the next section the transport equation for the joint pdf  $p(\psi; \underline{x}, t)$  is presented and the modelling assumptions are discussed briefly. The Monte Carlo method is described and analysed in section 3. Test calculations (reported in section 4) demonstrate the method and are used to check the error estimates obtained in section 3. The method was used to calculate pdf's of temperature in a turbulent mixing layer: the results, reported in section 5, are in good agreement with the measurements of Batt (1977). In the final section the method is discussed starting with a summary of the more important findings.

## 2. THE JOINT PDF EQUATION

The equations presented here are taken from Pope (1979). A detailed description of the formulation and a discussion of the equations can be found in that work.

In a low Mach number flow, the mean pressure, the species concentrations and the enthalpy provide a complete description of the chemical and thermodynamic properties of the fluid at each point. Let  $\phi_\alpha(\underline{x}, t)$  ( $\alpha=1, 2, \dots, \sigma$ ) denote one of the species mass fractions or the enthalpy at the location  $\underline{x}$  and time  $t$ . Then, from conservation principles, the following equation for  $\phi_\alpha$  is obtained:

$$\rho \frac{\partial \phi_\alpha}{\partial t} + \rho U_i \frac{\partial \phi_\alpha}{\partial x_i} + \frac{\partial}{\partial x_i} J_i^\alpha = \rho S_\alpha. \quad (2.1)$$

$U_i(\underline{x}, t)$  is the velocity in the  $x_i$ -direction;  $J_i^\alpha$  is the flux of  $\phi_\alpha$  in the  $x_i$ -direction due to molecular transport;  $\rho$  is the density; and  $S_\alpha$  is the rate of creation of  $\phi_\alpha$ . The set of quantities  $\phi_1, \phi_2, \dots, \phi_\sigma$  is denoted by  $\underline{\phi}$ , and  $\rho$  and  $S_\alpha$  can be expressed as functions of  $\underline{\phi}$ : thus,

$$\rho = \rho(\underline{\phi}) \quad \text{and} \quad S_\alpha = S_\alpha(\underline{\phi}). \quad (2.2)$$

The joint pdf of  $\underline{\phi}$  is  $p(\underline{\psi}; \underline{x}, t)$ .  $\underline{\psi}$  ( $= \psi_1, \psi_2, \dots, \psi_\sigma$ ) is the  $\sigma$ -dimensional composition space corresponding to  $\underline{\phi}$  -- a given location in composition space,  $\underline{\psi} = \underline{\psi}'$  say, corresponds to fluid of properties  $\underline{\phi} = \underline{\phi}'$ . If  $Q(\underline{\phi})$  is any function of  $\underline{\phi}$  then its expected value (denoted by angled brackets) is

$$\langle Q(\underline{\phi}(\underline{x}, t)) \rangle = \int p(\underline{\psi}; \underline{x}, t) Q(\underline{\psi}) d\underline{\psi}. \quad (2.3)$$

$d\underline{\psi}$  is written for  $d\psi_1 d\psi_2 \dots d\psi_\sigma$  indicating that integration is over the whole of  $\underline{\psi}$ -space. In order to simplify the notation,  $q(\underline{x}, t)$  will also be used for the expected value of  $Q$ :

$$q(\underline{x}, t) \equiv \langle Q(\phi(\underline{x}, t)) \rangle. \quad (2.4)$$

(The expected value of  $Q$  is sometimes called the ensemble average of  $Q$ : however, that term is reserved for a different use below.)

In variable-density flows the use of density-weighted averages has advantages both theoretically and practically. Density-weighted averages, denoted by a tilde, are defined by

$$\tilde{q}(\underline{x}, t) \equiv \tilde{Q}(\phi(\underline{x}, t)) \equiv \langle \rho(\underline{x}, t) Q(\phi(\underline{x}, t)) \rangle / \langle \rho \rangle. \quad (2.5)$$

And from the definition of the density-weighted joint pdf

$$\tilde{p}(\underline{\psi}; \underline{x}, t) \equiv \rho(\underline{\psi}) p(\underline{\psi}; \underline{x}, t) / \langle \rho \rangle \quad (2.6)$$

it follows

$$\tilde{q}(\underline{x}, t) = \int \tilde{p}(\underline{\psi}; \underline{x}, t) Q(\underline{\psi}) d\underline{\psi}. \quad (2.7)$$

Henceforth,  $\tilde{p}(\underline{\psi}; \underline{x}, t)$  is written  $\tilde{p}(\underline{\psi})$ , the dependence upon  $\underline{x}$  and  $t$  being implied.

A transport equation for  $\tilde{p}(\underline{\psi})$  can be obtained from the conservation equation for  $\phi_\alpha$ , equation (2.1). If the turbulent transport is modelled by simple gradient diffusion (with the turbulent diffusion coefficient being  $\Gamma_T(\underline{x}, t)$ ), the equation for  $\tilde{p}(\underline{\psi})$  is



$$\frac{\partial \tilde{p}(\underline{\psi})}{\partial t} + \tilde{U}_i \frac{\partial \tilde{p}(\underline{\psi})}{\partial x_i} + \frac{\partial}{\partial \psi_\alpha} (\tilde{p}(\underline{\psi}) S_\alpha(\underline{\psi})) =$$

$$\frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_i} \Gamma_T \frac{\partial \tilde{p}(\underline{\psi})}{\partial x_i} + E(\underline{\psi}; \underline{x}, t). \quad (2.8)$$

Summation is over repeated indices ( $i$  and  $\alpha$ ) and  $E(\underline{\psi}; \underline{x}, t)$  represents the effect of molecular mixing. The terms on the left-hand side are exact whereas those on the right are modelled or (in the case  $E$ ) need to be modelled. The two leading terms represent the rate of change of  $\tilde{p}(\underline{\psi})$  along a density-weighted streamline; the third term represents the transport of  $\tilde{p}(\underline{\psi})$  in composition space due to reaction. It is noteworthy that, in this formulation, reaction -- however complicated the scheme -- can be treated without approximation.

Models for the molecular mixing term  $E$  have been proposed by Curl (1963), Dopazo (1975), Pope (1976) and Janicka et al. (1979), but none is entirely satisfactory. Here, Curl's model is employed since it alone is applicable to an arbitrary number of quantities (i.e., any  $\sigma$ ) and can be expected to produce qualitatively correct results. Accordingly, we take

$$E(\underline{\psi}; \underline{x}, t) = 2^\sigma \omega \int \tilde{p}(\underline{\psi} + \underline{\psi}') \tilde{p}(\underline{\psi} - \underline{\psi}') d\underline{\psi}' - \omega \tilde{p}(\underline{\psi}) \quad (2.9)$$

where  $\omega(\underline{x}, t)$  is the appropriate turbulent frequency. A more complete discussion of the modelling of the turbulent transport and of  $E$  is given by Pope (1979).

### 3. THE MONTE CARLO METHOD

The Monte Carlo method described in this section provides a simulation of the density-weighted joint pdf equation (2.8). The usefulness of the method depends on three results obtained below: the simulation converges to the solution of equation (2.8); the numerical error is independent of  $\sigma$  (the dimensionality of  $\underline{\psi}$ ); and, the computational effort is proportional to  $\sigma$ . Consequently, for given accuracy, the amount of computation rises only linearly with  $\sigma$ .

#### 3.1 Dependent Variables

The simulation is performed on a finite-difference grid, of uniform spacing  $h$ , which extends over the region of interest,  $0 \leq \underline{x} \leq h\underline{L}$ , say. The node denoted by  $\underline{l}$  is located at  $\underline{x} = \underline{l}h$ . If  $\underline{x}$ -space is  $m$ -dimensional (in general  $m=3$ ), then  $\underline{L}$  and  $\underline{l}$  are  $m$ -vectors of integers and  $0 \leq l_i \leq L_i$ ,  $i=1,2,\dots,m$ . Each cycle of operations in the simulation advances time by an interval  $k$ . Hence, if initial conditions are supplied at  $t=0$ , after  $\lambda$  cycles the time is  $t = k\lambda$ .

Rather than considering  $\tilde{p}(\underline{\psi};\underline{x},t)$  explicitly, the dependent variables in the simulation are representative values of  $\underline{\phi}$ . An ensemble of  $N$  such representative values is located at each grid node. The ensemble at  $(\underline{x},t) = (h\underline{l},k\lambda)$  is denoted by  $\Phi(h\underline{l},k\lambda)$  and one of the  $N$  members of the ensemble is denoted by  $\underline{\phi}^{(n)}(h\underline{l},k\lambda)$ . Although each member of the ensemble (or element) is ascribed a unique number,  $1 \leq n \leq N$ , no ordering is implied. In fact, operations are performed either on all members of the ensemble or on some selected at random. Thus, the numbering is a convenience that has no effect upon the outcome. Recalling that  $\underline{\phi}$  represents  $\sigma$  quantities, we may write the ensemble as,

$$\begin{aligned}
\Phi(\underline{h}\ell, \underline{k}\lambda) &= \underline{\phi}^{(1)}(\underline{h}\ell, \underline{k}\lambda) = \phi_1^{(1)}, \phi_2^{(1)} \dots \phi_\alpha^{(1)} \dots \phi_\sigma^{(1)} \\
&\quad \underline{\phi}^{(2)}(\underline{h}\ell, \underline{k}\lambda) = \phi_1^{(2)}, \phi_2^{(2)} \dots \phi_\alpha^{(2)} \dots \phi_\sigma^{(2)} \\
&\quad \vdots \\
&\quad \underline{\phi}^{(n)}(\underline{h}\ell, \underline{k}\lambda) = \phi_1^{(n)}, \phi_2^{(n)} \dots \phi_\alpha^{(n)} \dots \phi_\sigma^{(n)} \\
&\quad \vdots \\
&\quad \underline{\phi}^{(N)}(\underline{h}\ell, \underline{k}\lambda) = \phi_1^{(N)}, \phi_2^{(N)} \dots \phi_\alpha^{(N)} \dots \phi_\sigma^{(N)}.
\end{aligned}$$

The general element is  $\underline{\phi}^{(n)}(\underline{h}\ell, \underline{k}\lambda)$ .

The ensemble average of any function  $Q(\underline{\phi})$  is defined by

$$\hat{q}(\underline{h}\ell, \underline{k}\lambda) = Q(\Phi(\underline{h}\ell, \underline{k}\lambda)) \equiv \frac{1}{N} \sum_{n=1}^N Q(\underline{\phi}^{(n)}(\underline{h}\ell, \underline{k}\lambda)). \quad (3.1)$$

The ensemble average  $\hat{q}$  is intended to simulate the density-weighted average  $\tilde{q}$ .

### 3.2 Initial Conditions

In most applications the initial conditions are likely to be simple -- a uniform composition for example. Consequently the task of specifying the initial ensembles is also likely to be simple. However, a consideration of the general case is informative.

At the node  $\underline{h}\ell$ , the initial values of the elements are chosen to be

$$\underline{\phi}^{(n)}(\underline{h}\ell, 0) = \underline{\xi}^{(n)}. \quad (3.2)$$

$\underline{\xi}^{(n)}$  is the value (on the  $n^{\text{th}}$  trial) of a random vector  $\underline{\xi}$  which is distributed identically to  $\underline{\phi}(\underline{h}\ell, 0)$  -- that is,

$$p(\underline{\xi}) d\underline{\xi} = \tilde{p}(\underline{\psi}; \underline{h}\ell, 0) d\underline{\psi}. \quad (3.3)$$

For any function  $Q(\underline{\psi})$ , the expected value of  $Q(\underline{\phi}^{(n)})$  is

$$\begin{aligned}
 E Q(\underline{\phi}^{(n)}(\underline{h}, 0)) &= \int Q(\underline{\xi}) p(\underline{\xi}) d\underline{\xi} \\
 &= \int Q(\underline{\psi}) \tilde{p}(\underline{\psi}; \underline{h}, 0) d\underline{\psi} \\
 &= \tilde{q}(\underline{h}, 0) .
 \end{aligned} \tag{3.4}$$

It clearly follows that the expected value of the ensemble average of  $Q$  is also  $\tilde{q}$ :

$$E \hat{q}(\underline{h}, 0) = \tilde{q}(\underline{h}, 0) . \tag{3.5}$$

The above shows that  $\hat{q}(\underline{h}, 0)$  is an unbiased estimate of  $\tilde{q}(\underline{h}, 0)$ . The error in this estimate can be determined from the Central Limit Theorem (Gnedenko 1962): since  $\hat{q}$  is the average of  $N$  independent random samples,

$$Q(\underline{\phi}^{(n)}(\underline{h}, 0)), \quad n = 1, 2, \dots, N,$$

as  $N$  tends to infinity the inequality

$$| \hat{q}(h\underline{\ell}, 0) - \tilde{q}(h\underline{\ell}, 0) | < \beta q' N^{-1/2} \quad (3.6)$$

holds with probability  $\text{erf}(\beta/\sqrt{2})$ , for  $\beta > 0$ .  $q'$  is the standard deviation

$$(q')^2 = \int Q(\underline{\psi})^2 \tilde{p}(\underline{\psi}) d\underline{\psi} = \int \tilde{p}(\underline{\psi}) (Q(\underline{\psi}) - \tilde{q})^2 d\underline{\psi} . \quad (3.7)$$

Two important conclusions can be drawn. As  $N$  tends to infinity, with probability one, the error tends to zero: the standard error is  $q' N^{-1/2}$  (with 68% probability the error is less than the standard error).

The expression for the standard error --  $q' N^{-1/2}$  -- is common to most Monte Carlo methods. The factor  $N^{-1/2}$  indicates that the error decreases slowly with increasing  $N$  which, clearly, is a disadvantage. The great advantage of the method is that the error is independent of  $\sigma$  -- the dimensionality of  $\underline{\psi}$ -space. Consequently, for given accuracy, the number of elements that are needed does not increase with  $\sigma$ . While this

argument applies only to the initial conditions, it is shown in sections 3.6 and 3.7 that the conclusions are true in general.

In the subsequent analysis, ensembles are related to the joint pdf through the following definition of equivalence. If, for all functions  $Q$ , the ensemble average  $\hat{q}(\underline{h}, t)$  converges\* in probability to the expected value  $\tilde{q}(\underline{h}, t)$ , then  $\Phi(\underline{h}, t)$  and  $\tilde{p}(\underline{\psi}; \underline{h}, t)$  are equivalent. Equivalence is denoted by an arrow:

$$\Phi(\underline{h}, t) \rightarrow \tilde{p}(\underline{\psi}; \underline{h}, t)$$

or

$$\hat{q}(\underline{h}, t) \rightarrow \tilde{q}(\underline{h}, t) .$$

Clearly, the initial ensembles are equivalent to the initial pdf's.

### 3.3 Operator Splitting

At successive time steps the ensembles are altered in such a way that they remain equivalent to the joint pdf. The ensembles change both by shifting elements from node to node (simulating transport in physical space) and by changing the values of  $\underline{\phi}^{(n)}$  (simulating transport in composition space). The precise manner in which these processes are to be performed can be determined by examining the governing transport equation.

Equation (2.8) shows that  $\tilde{p}(\underline{\psi}; \underline{x}, t)$  changes due to the simultaneous action of convection, reaction, diffusion and mixing. These four processes can be simulated sequentially by using the technique of operator splitting. Hence the following operators are defined:

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\*That is, converges as  $N$  tends to infinity for fixed  $h$ .

$$C_{(i)} \equiv \tilde{U}_{(i)} \frac{\partial}{\partial x_{(i)}} , \quad (3.8)$$

$$S \equiv S_{\alpha}(\underline{\psi}) \frac{\partial}{\partial \psi_{\alpha}} + \left( \frac{\partial S_{\alpha}}{\partial \psi_{\alpha}} \right) I , \quad (3.9)$$

and

$$D_{(i)} \equiv \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_{(i)}} \Gamma_T \frac{\partial}{\partial x_{(i)}} . \quad (3.10)$$

$I$  is the identity operator and the summation convention is suspended for bracketed suffices. The operator  $E$  is defined by

$$E \tilde{p}(\underline{\psi}; \underline{x}, t) \equiv E(\underline{\psi}; \underline{x}, t) , \quad (3.11)$$

$E$  being given by equation (2.9). For an  $m$ -dimensional flow (in general  $m=3$ ) the transport equation for  $\tilde{p}$  can be written,

$$\frac{\partial \tilde{p}(\underline{\psi})}{\partial t} = \{E - S - \sum_{i=1}^m C_{(i)} + \sum_{i=1}^m D_{(i)}\} \tilde{p}(\underline{\psi}) . \quad (3.12)$$

By approximating the time derivative by the forward difference

$$\frac{1}{k} (\tilde{p}(\underline{\psi}; \underline{x}, t+k) - \tilde{p}(\underline{\psi}; \underline{x}, t)) = \frac{\partial \tilde{p}(\underline{\psi}; \underline{x}, t)}{\partial t} + O(k) \quad (3.13)$$

we obtain

$$\tilde{p}(\underline{\psi}; \underline{x}, t+k) = \{I+kE-kS - k \sum_{i=1}^m C_{(i)} + k \sum_{i=1}^m D_{(i)}\} \tilde{p}(\underline{\psi}; \underline{x}, t) + O(k^2) . \quad (3.14)$$

The term in braces is the sum of operators which can be factored into products of operators plus terms of order  $k^2$ . For example, the first three operators can be factored as,

$$\begin{aligned}
(I+kE-kS) &= (I+kE)(I-kS) + k^2ES \\
&= (I+kE)(I-kS) + O(k^2) .
\end{aligned} \tag{3.15}$$

The sum of operators in equation (3.14) is factored similarly to produce,

$$\tilde{p}(\underline{\psi}; \underline{x}, t+k) = (I+kE)(I-kS) \prod_{i=1}^m (I-kC_{(i)}) \prod_{j=1}^m (I+kD_{(j)}) \tilde{p}(\underline{\psi}; \underline{x}, t) + O(k^2) . \tag{3.16}$$

The operator product that acts on  $\tilde{p}(\underline{\psi}; \underline{x}, t)$  can be split into a sequence of operators acting on the intermediate values  $\tilde{p}(\underline{\psi}; \underline{x}, t')$ , where  $t \leq t' < t+k$ . (This is a device that aids the notation:  $t'$  is not intended to correspond to any particular time.) The notional times  $t_{d(i)}$  and  $t_{c(i)}$  refer to the pdf's after diffusion and convection in the  $x_i$ -direction. After reaction and mixing the notional times are  $t_r$  and  $t_m$ . These times are related by

$$t = t_{d(0)} < t_{d(1)} \cdots < t_{d(m)} = t_{c(0)} < t_{c(1)} \cdots < t_r < t_m < t+k .$$

(This relation also defines  $t_{d(0)}$  and  $t_{c(0)}$ .) In terms of these intermediate times, the sequence of operations is

$$\tilde{p}(\underline{\psi}; \underline{x}, t_{d(i)}) = (I+kD_{(i)}) \tilde{p}(\underline{\psi}; \underline{x}, t_{d(i-1)}), \quad i = 1, \dots, m, \tag{3.17}$$

$$\tilde{p}(\underline{\psi}; \underline{x}, t_{c(i)}) = (I-kC_{(i)}) \tilde{p}(\underline{\psi}; \underline{x}, t_{c(i-1)}), \quad i = 1, \dots, m, \tag{3.18}$$

$$\tilde{p}(\underline{\psi}; \underline{x}, t_r) = (I-kS) \tilde{p}(\underline{\psi}; \underline{x}, t_{c(m)}), \tag{3.19}$$

$$\tilde{p}(\underline{\psi}; \underline{x}, t_m) = (I+kE) \tilde{p}(\underline{\psi}; \underline{x}, t_r) . \tag{3.20}$$

The value of  $\tilde{p}$  after the mixing operation is an approximation to  $\tilde{p}(\underline{\psi}; \underline{x}, t+k)$ , and according to equation (3.16),

$$\tilde{p}(\underline{\psi}; \underline{x}, t+k) = \tilde{p}(\underline{\psi}; \underline{x}, t_m) + O(k^2) . \tag{3.21}$$



### 3.4 Monte Carlo Simulation

A method is devised to modify the ensembles  $\Phi(\underline{h}\underline{\ell}, t)$  so as to simulate each of the four processes -- diffusion, convection, reaction and mixing. The effect that each process has upon  $\tilde{q}$  can be determined by multiplying equations (3.17) - (3.20) by  $Q(\underline{\psi})$  and integrating. The simulations are constructed so that, to within truncation error, the effects upon  $\hat{q}$  are the same. To be more precise, let  $t'$  and  $t''$  be the notional times before and after a particular process, and let the ensemble and pdf be equivalent at  $t'$ :

$$\hat{q}(\underline{h}\underline{\ell}, t') \rightarrow \tilde{q}(\underline{h}\underline{\ell}, t') . \quad (3.22)$$

We seek a simulation of the process such that

$$\hat{q}(\underline{h}\underline{\ell}, t'') \rightarrow \tilde{q}(\underline{h}\underline{\ell}, t'') + k\mathcal{D}(h, k) . \quad (3.23)$$

This condition is sufficient to ensure that, as  $N$ ,  $h^{-1}$  and  $k^{-1}$  tend to infinity, the ensemble  $\Phi(\underline{h}\underline{\ell}, t)$  converges to the pdf  $\tilde{p}(\underline{\psi}; \underline{h}\underline{\ell}, t)$ . In other words, if this condition is satisfied for each simulated process, then the Monte Carlo method as a whole provides a true simulation of the pdf transport equation (2.8). In section 3.6 it is estimated that finite values of  $N$ ,  $h^{-1}$  and  $k^{-1}$  cause an error of order  $(h, k, N^{-\frac{1}{2}})$ .

#### Diffusion

The effect upon  $\tilde{q}$  of diffusion in the  $x_i$ -direction is determined by multiplying equation (3.17) by  $Q(\underline{\psi})$  and integrating:

$$\tilde{q}(\underline{x}, t_{d(i)}) = (I + k\mathcal{D}_{(i)})\tilde{q}(\underline{x}) . \quad (3.24)$$

Here, and below,  $\tilde{q}(\underline{x})$  refers to the value before the process, i.e. to

$\tilde{q}(\underline{x}, t_{d(i-1)})$ . As a first step to developing a simulation, the differential operator is replaced by the three-point centered difference operator. At  $(\underline{x}, t) = (h\underline{\ell}, k\lambda)$  this yields

$$\begin{aligned} \tilde{q}(h\underline{\ell}, t_{d(i)}) = & (1 - \gamma_{i+} - \gamma_{i-})\tilde{q}(h\underline{\ell}) + \gamma_{i+} \tilde{q}(h(\underline{\ell} + \underline{e}_{(i)})) \\ & + \gamma_{i-} \tilde{q}(h(\underline{\ell} - \underline{e}_{(i)})) + k\mathcal{O}(h^2) , \end{aligned} \quad (3.25)$$

where  $\underline{e}$  is the unit vector and the Fourier numbers  $\gamma$  are

$$\gamma_{i\pm} = \frac{k}{h^2} \frac{1}{\langle \rho \rangle} \Gamma_T (h(\underline{\ell} \pm \frac{1}{2}\underline{e}_i), k\lambda). \quad (3.26)$$

Thus,  $\tilde{q}(h\underline{\ell}, t_{d(i)})$  is a weighted average of  $\tilde{q}(h\underline{\ell})$  and the values at the two neighboring nodes  $\tilde{q}(h(\underline{\ell} \pm \underline{e}_i))$ .

This process is simulated by forming  $\Phi(h\underline{\ell}, t_{d(i)})$  from elements selected at random from  $\Phi(h\underline{\ell})$  and  $\Phi(h(\underline{\ell} \pm \underline{e}_i))$  in appropriate proportions. The numbers of elements selected from  $\Phi(h(\underline{\ell} \pm \underline{e}_i))$  are

$$n_{di\pm} = N \gamma_{i\pm} \quad (3.27)$$

and the remaining  $n_{di}$  ( $= N - n_{di+} - n_{di-}$ ) elements are selected from  $\Phi(h\underline{\ell})$ . Thus, with  $\underline{\phi}^*$  denoting an element selected at random without replacement, the ensemble average after diffusion is

$$\begin{aligned} \hat{q}(h\underline{\ell}, t_{d(i)}) = & \frac{1}{N} \sum_{n_{di+}} Q(\underline{\phi}^*(h(\underline{\ell} + \underline{e}_{(i)}))) \\ & + \frac{1}{N} \sum_{n_{di-}} Q(\underline{\phi}^*(h(\underline{\ell} - \underline{e}_{(i)}))) + \frac{1}{N} \sum_{n_{di}} Q(\underline{\phi}^*(h\underline{\ell})). \end{aligned} \quad (3.28)$$

The expected value of the last term is

$$\begin{aligned}
E \frac{1}{N} \sum_{n_{di}} Q(\underline{\phi}^*(h\underline{\ell})) &= \frac{n_{di}}{N} E \frac{1}{n_{di}} \sum_{n_{di}} Q(\underline{\phi}^*(h\underline{\ell})) \\
&= (1 - \gamma_{i+} - \gamma_{i-}) \hat{q}(h\underline{\ell})
\end{aligned} \tag{3.29}$$

Applying the same procedure to the other terms yields

$$\begin{aligned}
E \hat{q}(h\underline{\ell}, t_{d(i)}) &= (1 - \gamma_{i+} - \gamma_{i-}) \hat{q}(h\underline{\ell}) + \gamma_{i+} \hat{q}(h(\underline{\ell} + e_{(i)})) \\
&\quad + \gamma_{i-} \hat{q}(h(\underline{\ell} - e_{(i)})).
\end{aligned} \tag{3.30}$$

As  $N$  tends to infinity  $\hat{q}(h\underline{\ell}, t_{d(i)})$  converges to its expected value.

Thus, if  $\hat{q} \rightarrow \tilde{q}$  prior to diffusion, a comparison of equations (3.25) and (3.30) reveals that

$$\hat{q}(h\underline{\ell}, t_{d(i)}) \rightarrow \tilde{q}(h\underline{\ell}, t_{d(i)}) + k^0(h^2). \tag{3.31}$$

This result confirms that the simulation of diffusion is valid (c.f. equation (3.23)).

An efficient implementation of the simulation of diffusion is the following. Each line of nodes in the  $x_i$ -direction is taken in turn. At each node along the line, groups of  $n_{di+}$  and  $n_{di-}$  elements are selected at random without replacement from the ensemble. The group of  $n_{di+}$  elements at  $h\underline{\ell}$  is then commuted with the group of  $n_{di-}$  elements at  $h(\underline{\ell} + e_i)$ . (From the definition of  $n_{di\pm}$  it may be seen that the sizes of these groups are the same.) This process is performed for each node along the line and for each line of nodes. The resulting ensembles are  $\Phi(h\underline{\ell}, t_{d(i)})$ .

### Convection

The development of a simulation of convection is similar to that for diffusion. Multiplying equation (3.18) by  $Q(\underline{\psi})$  and integrating shows the effect of convection in the  $x_i$ -direction to be

$$\tilde{q}(\underline{x}, t_{c(i)}) = (I - k C_{(i)}) \tilde{q}(\underline{x}). \quad (3.32)$$

$\tilde{q}(\underline{x})$  refers to the value prior to the process,  $q(\underline{x}, t_{c(i-1)})$ .

Replacing the differential operator by the two-point upwind difference operator yields,

$$\tilde{q}(h\underline{\ell}, t_{c(i)}) = (1 - c_i) \tilde{q}(h\underline{\ell}) + c_i \tilde{q}(h\underline{\ell} - e'_{(i)}) + k O(h). \quad (3.33)$$

$e'_i$  is the unit vector in the same direction as  $\tilde{U}_i$ , i.e.

$$e'_i = e_i, \quad \tilde{U}_i \geq 0 \quad (3.34)$$

$$e'_i = -e_i, \quad \tilde{U}_i < 0,$$

and the Courant number  $c_i$  is

$$c_i = \frac{k}{h} | \tilde{U}_i(h\underline{\ell}, k\lambda) |. \quad (3.35)$$

Thus,  $\tilde{q}(h\underline{\ell}, t_{c(i)})$  is the weighted average of  $\tilde{q}(h\underline{\ell})$  and the value at the upwind node  $\tilde{q}(h(\underline{\ell} - e'_i))$ .

Convection is simulated along each line of nodes in the  $x_i$ -direction taken in turn. At each node,  $n_{ci} = N c_i$  elements selected at random are replaced by  $n_{ci}$  elements selected at random from the upstream node. The resulting ensembles are  $\Phi(h\underline{\ell}, t_{c(i)})$ .

By arguments similar to those employed for the diffusive process, it can readily be shown that, if  $\hat{q} \rightarrow \tilde{q}$ , then

$$\hat{q}(h\underline{\ell}, t_{c(i)}) \rightarrow \tilde{q}(h\underline{\ell}, t_{c(i)}) + k O(h). \quad (3.36)$$

This confirms the validity of the simulation of convection.

### Reaction

Both convection and diffusion transport  $\tilde{p}(\psi; \underline{x}, t)$  in  $\underline{x}$ -space. Con-

sequently they are both simulated by the transfer of representative values from one node to another. Reaction and mixing, on the other hand, transport  $\tilde{p}(\underline{\psi}; \underline{x}, t)$  in  $\underline{\psi}$ -space. This is simulated by changing the composition of elements at each node. Of the four processes, only reaction is simulated deterministically.

The effect of reaction upon  $\tilde{q}$  is determined by multiplying equation (3.19) by  $Q(\underline{\psi})$  and integrating. At  $x = h\underline{\ell}$  this gives:

$$\tilde{q}(h\underline{\ell}, t_r) = \tilde{q}(h\underline{\ell}, t_{c(m)}) + k \tilde{r}(h\underline{\ell}, t_{c(m)}) \quad (3.37)$$

where  $\tilde{r}$  is the expected value of  $R(\underline{\phi})$ ,

$$R(\underline{\phi}) = S_{\alpha}(\underline{\phi}) \frac{\partial Q(\underline{\phi})}{\partial \phi_{\alpha}} . \quad (3.38)$$

For each element  $\underline{\phi}^{(n)} = \underline{\phi}^{(n)}(h\underline{\ell}, t_{c(m)})$  reaction proceeds according to

$$\underline{\phi}^{(n)}(h\underline{\ell}, t_r) = \underline{\phi}^{(n)} + \Delta \underline{\phi}^{(n)} , \quad (3.39)$$

where the undetermined quantity  $\Delta \underline{\phi}^{(n)}$  is of order  $k$ . The effect of reaction upon  $\hat{q}$  is determined from equation (3.39) by use of a Taylor expansion:

$$\begin{aligned} \hat{q}(h\underline{\ell}, t_r) &= \frac{1}{N} \sum_{n=1}^N Q(\underline{\phi}^{(n)} + \Delta \underline{\phi}^{(n)}) \\ &= \frac{1}{N} \sum_{n=1}^N \left\{ Q(\underline{\phi}^{(n)}) + \Delta \phi_{\alpha}^{(n)} \frac{\partial Q(\underline{\phi}^{(n)})}{\partial \phi_{\alpha}^{(n)}} + O(k^2) \right\} . \end{aligned} \quad (3.40)$$

The appropriate choice for  $\Delta \underline{\phi}^{(n)}$  is

$$\Delta \phi_{\alpha}^{(n)} = k S_{\alpha}(\underline{\phi}^{(n)}) + O(k^2) , \quad (3.41)$$

since equation (3.40) then becomes

$$\hat{q}(\underline{h}\underline{l}, t_r) = \hat{q}(\underline{h}\underline{l}, t_{c(m)}) + k \hat{r}(\underline{h}\underline{l}, t_{c(m)}) + O(k^2), \quad (3.42)$$

where  $\hat{r}$  is the ensemble average of  $R$ . And a comparison of equations (3.37) and (3.42) shows that, if  $\hat{q} \rightarrow \tilde{q}$  prior to reaction, then the required result is obtained, namely:

$$\hat{q}(\underline{h}\underline{l}, t_r) \rightarrow \tilde{q}(\underline{h}\underline{l}, t_r) + O(k^2). \quad (3.43)$$

A physical interpretation of the reaction process is simply that each element reacts independently for an interval of time  $k$  according to the ordinary differential equations

$$\frac{d\phi_\alpha^{(n)}}{dt} = S_\alpha(\underline{\phi}^{(n)}), \quad \alpha=1,2,\dots,\sigma. \quad (3.44)$$

The resulting change in  $\underline{\phi}^{(n)}$  is in accord with equation (3.41). The implementation of reaction is discussed further in section 3.5.

### Mixing

The effect of mixing upon  $\tilde{q}$  is determined by multiplying equation (3.20) by  $Q(\underline{\psi})$  and integrating. At  $\underline{x} = \underline{h}\underline{l}$  the result is

$$\tilde{q}(\underline{h}\underline{l}, t_m) = (1 - \omega k) \tilde{q}(\underline{h}\underline{l}, t_r) + \omega k v(\underline{h}\underline{l}, t_r), \quad (3.45)$$

where,

$$v = \int \tilde{p}(\underline{\psi}') \int \tilde{p}(\underline{\psi}) Q(\frac{1}{2}(\underline{\psi} + \underline{\psi}')) d\underline{\psi} d\underline{\psi}'. \quad (3.46)$$

In the simulation,  $\Phi(\underline{h}\underline{l}, t_m)$  is composed of  $N(1 - \omega k)$  elements selected at random from  $\Phi(\underline{h}\underline{l}, t_r)$  with the remaining  $n_m = N\omega k$  elements being "mixed". The elements from  $\Phi(\underline{h}\underline{l}, t_r)$  simulate the first term on the right-hand side of equation (3.45): the composition of the "mixed" elements should be

such that they account for the second term. This composition is determined by simulating the double integral  $v$ . If  $\hat{q}(t_r) \rightarrow \tilde{q}(t_r)$ , then for the inner integral of equation (3.46),

$$\int \tilde{p}(\underline{\psi}) Q(\frac{1}{2}(\underline{\psi} + \underline{\psi}')) d\underline{\psi} \rightarrow \frac{1}{N} \sum_{n=1}^N Q(\frac{1}{2}(\underline{\phi}^{(n)} + \underline{\psi}')). \quad (3.47)$$

Thus, for the outer integral,

$$\begin{aligned} v &\rightarrow \int \frac{1}{N} \sum_{n=1}^N Q(\frac{1}{2}(\underline{\phi}^{(n)} + \underline{\psi}')) \tilde{p}(\underline{\psi}') d\underline{\psi}' \\ &\rightarrow \frac{1}{N} \sum_{n=1}^N \frac{1}{N} \sum_{n'=1}^N Q(\frac{1}{2}(\underline{\phi}^{(n)} + \underline{\phi}^{(n')})). \end{aligned} \quad (3.48)$$

In this equation,  $\frac{1}{2}(\underline{\phi}^{(n)} + \underline{\phi}^{(n')})$  is the average value of the composition of two elements, and the summation is over all  $N^2$  pairs of elements. The same result is obtained if a random sample of size  $n_m$  is used:

$$v \rightarrow \frac{1}{n_m} \sum_{n_m} Q(\underline{\phi}^{\text{mix}}), \quad (3.49)$$

where each value of  $\underline{\phi}^{\text{mix}}$  is the average composition of a pair of elements selected at random with replacement from  $\Phi(h\underline{l}, t_r)$ .

In summary,  $n_m \equiv N$  mixed elements are formed from  $\Phi(t_r)$ : these are then used to replace  $n_m$  elements selected at random from  $\Phi(t_r)$ . The resulting ensemble is  $\Phi(t_m)$ .

With  $\underline{\phi}^*$  denoting an element selected at random without replacement from  $\Phi(h\underline{l}, t_r)$ , the ensemble average  $\hat{q}(h\underline{l}, t_m)$  is

$$\hat{q}(h\underline{l}, t_m) = \frac{1}{N} \sum_{N-n_m} Q(\underline{\phi}^*) + \frac{1}{N} \sum_{n_m} Q(\underline{\phi}^{\text{mix}}). \quad (3.50)$$

If  $\hat{q}(t_r) \rightarrow \hat{q}(t_m)$  then from (3.45), (3.49), (3.50) and the definition of  $n_m$

$$\begin{aligned} \hat{q}(h\underline{\ell}, t_m) &\rightarrow (1 - \omega k) \tilde{q}(h\underline{\ell}, t_r) + \omega k v(h\underline{\ell}, t_r) \\ &\rightarrow \tilde{q}(h\underline{\ell}, t_m), \end{aligned} \quad (3.51)$$

which is the required result.

### Conservation

The Monte Carlo simulation has been obtained by requiring that ensembles be equivalent to pdf's in the limit of large  $N$ . Numerical experiments show that the sampling error due to finite  $N$  is reduced if the simulation is made approximately conservative. Conservation requires that certain qualitative properties of the pdf equation are retained for any  $N$ . For example, the pdf equation shows that mixing does not affect the value of the means  $\tilde{\phi}$ . In the simulation of mixing described above, the means  $\hat{\phi}$  are affected, although their expected values are not. A conservative simulation of mixing is to perform the following process  $\frac{1}{2} n_m$  times: two elements are selected at random,  $\phi^{(n)}$  and  $\phi^{(n')}$ , and their values are replaced by their mean  $\frac{1}{2} (\phi^{(n)} + \phi^{(n')})$ . This is a valid simulation of mixing and, clearly, it does not affect the means  $\hat{\phi}$ .

The effect of convection and diffusion on the volume integral of  $\langle \rho \rangle \tilde{p}(\underline{\psi})$  is solely due to the flux of  $\tilde{p}(\underline{\psi})$  through the surface of the volume. In the Monte Carlo simulation of these processes there is an additional effect caused by the random sampling errors (although the expected value of this effect is zero). These random errors can be minimized by making the simulation approximately conservative. Consider diffusion in the  $x_i$ -direction in a constant-density flow. For the node at  $h\underline{\ell}$ ,  $n_{di+}$  elements are replaced by  $n_{di+}$  elements selected from the ensemble at  $h(\underline{\ell} + e_i)$ . For the node at  $h(\underline{\ell} + e_i)$ , exactly



the same number of elements are replaced by elements selected from the node at  $h\ell$ . Thus a conservative simulation of diffusion is obtained by commuting elements between neighboring ensembles. For variable-density flows the numbers of elements passed each way are not exactly the same and so the simulation becomes approximately conservative. In a similar way an approximately conservative simulation for convection is obtained by passing elements from node to node in the direction of the flow.

The proof of convergence of the method is unaffected by the use of approximately conservative simulations because the processes performed at each node are unaffected. The difference is that the sampling error at one node is approximately compensated by the sampling error at a neighboring node.

#### Time-step Restrictions

The processes described above can be performed only for the time step  $k$  being less than some limit. For example, after the mixing process, the ensemble contains  $n_m$  "mixed elements". If  $k$  is too large,  $n_m$  can exceed  $N$  and hence the process cannot be performed. The restrictions imposed by diffusion, convection and mixing are

$$(n_{di+} + n_{di-}) \leq N, \quad (3.52)$$

$$n_{ci} \leq N, \quad (3.53)$$

and

$$n_m \leq N. \quad (3.54)$$

From the definitions of the  $n$ 's, the above inequalities are satisfied for

$$\Gamma_T k/h^2 < \frac{1}{2}, \quad (3.55)$$

$$|\tilde{U}| k/h < 1, \quad (3.56)$$

and

$$k\omega < 1, \quad (3.57)$$

where  $\Gamma_T$ ,  $|\tilde{U}|$  and  $\omega$  are to be taken as the maximum values of these quantities over the whole flow field.

These time-step restrictions are of no consequence since (it is shown in the next section) the computational effort required per step is proportional to  $k$ . Hence a small value of  $k$  can be chosen (with a consequent gain in accuracy) without any penalty in computational expense.

(It can be noted that, as  $N$  tends to infinity, the Monte Carlo simulation converges to the finite-difference scheme given by equation (3.16) with the differential operators  $\mathcal{C}$  and  $\mathcal{D}$  replaced by finite-difference operators. This is an explicit scheme which is stable, conditional on (3.55) and (3.56).)

### Boundary Conditions

In most applications either the boundary values of  $\tilde{p}(\underline{\psi})$  are specified, or the normal gradient of  $\tilde{p}(\underline{\psi})$  is zero (corresponding to a plane of symmetry or an outflow boundary). The first condition can be implemented by choosing the boundary ensembles in the same way as the initial ensembles are chosen. The zero-normal-gradient condition is implemented by equating the boundary ensemble (after each operation) to its inward neighbouring ensemble.

### 3.5 Computational Efficiency

In this section it is shown that the computational effort required for each cycle of the simulation is linearly proportional to  $Nk\sigma$ . This result is important for two reasons. That the work rises only linearly with  $\sigma$  (the dimensionality of  $\underline{\psi}$ -space) shows that the method is practicable for large  $\sigma$ . (This is in marked contrast to a finite-difference scheme for which the work is estimated to rise as  $e^{a\sigma}$ ,  $a \approx 6$ .) The second significance of the result is that the work per step is proportional to  $k$ . If the simulation

is performed for a time  $T$ , then  $T/k$  steps are required. The total work is then proportional to  $(Nk\sigma)(T/k) = NT\sigma$ . Consequently, since the total work is independent of  $k$ , there is no penalty in choosing a small time step and hence virtually eliminating the associated truncation error.

The dependence of the work upon  $\sigma$ ,  $N$  and  $k$  is now determined assuming  $h$  and  $m$  to be fixed.

Interestingly, both the diffusion and convection processes involve no arithmetic, only data manipulation. Of order  $n_{di}$  or  $n_{ci}$  elements are involved and the number of operations per element is proportional to  $\sigma$ . Since  $n_{di}$  and  $n_{ci}$  are of order  $kN$ , the number of operations per node per time step is of order  $kN\sigma$ . A similar argument leads to the same result for the mixing operation.

The implementation of reaction as described in section 3.4 is not computationally efficient. An efficient algorithm exploits the fact that, between mixing operations, only reaction affects the composition of an element. If a given element has not been involved in mixing for  $\lambda_r$  steps, then its composition can be obtained by integrating the equations

$$\frac{d\phi_\alpha}{dt} = S_\alpha(\underline{\phi}) \quad \alpha=1,2,\dots,\sigma, \quad (3.58)$$

for a time  $\tau = k\lambda_r$ , taking the composition after the last mixing as the initial condition. Thus, rather than integrating equations (3.58) for all  $N$  elements for an interval  $k$ , the efficient algorithm integrates the equations for the  $2n_m$  elements involved in mixing for the longer intervals  $\tau$ . (The average value of  $\tau$  is  $\omega^{-1}$ .)

The amount of work required by this algorithm depends upon the complexity of the reaction scheme. We assume that the work required to evaluate one reaction rate  $S_{\alpha}(\underline{\phi})$  is independent of  $\sigma$ , and that equations (3.58) are integrated using a scheme such as that of Young and Boris (1977). Then the total work requirement at one node for one cycle is proportional to  $kN\sigma$ .

For each of the four processes, and hence for the scheme as a whole, the number of computations per time step is of order  $kN\sigma$ . Hence to perform the simulation for a time  $T$  (i.e. for  $T/k$  steps) requires of order  $NT\sigma$  operations. This confirms that the computer requirements are independent of  $k$  and rise only linearly with  $\sigma$ .

By comparison, the number of computer operations required by a straightforward finite-difference scheme increases exponentially with  $\sigma$ . If  $\underline{\psi}$ -space is discretized into, say, 20 divisions in each direction, then the number of nodes in the space is  $(20)^{\sigma}$ . The double integral in equation (2.9) requires the evaluation of a volume integral in  $\underline{\psi}$ -space for each  $\underline{\psi}$ -node: this requires of order  $(20)^{2\sigma}$  operations. Thus, at each node in  $\underline{\psi}$ -space, for each time step, of order  $(20)^{2\sigma} \approx e^{6\sigma}$  operations are required. The values shown on Table 1 may be compared with current computation rates of order  $10^6 \text{ s}^{-1}$ .

Table 1: Computer operations required by a finite-difference scheme.	dimensionality of the joint pdf $\sigma$	approximate number of operations required by finite-difference scheme $e^{6\sigma}$
	1	$4.0 \times 10^2$
	2	$1.6 \times 10^5$
	3	$6.6 \times 10^7$
	4	$2.6 \times 10^{10}$
	5	$1.1 \times 10^{13}$

If not impracticable, solutions for  $\sigma=3$  would be very expensive. For  $\sigma=4$ , finite-difference solutions are definitely impracticable. The main point to note, however, is that the operation requirement increases exponentially with  $\sigma$ . As long as this is so, no conceivable refinement to the finite-difference scheme or improvement in computing speed can facilitate solutions for large  $\sigma$ .

### 3.6 Estimation of Error

The error in the simulation is due to both truncation and sampling error. As  $N$  tends to infinity, the sampling error tends to zero, thus isolating the truncation error. This--according to equation (3.23)--is of order  $k$  and  $h$ , and hence the scheme is first-order accurate in space and time. The sampling error caused by a finite value of  $N$  is more difficult to determine. Here we estimate that the standard sampling error is of order  $N^{-1/2}$  and independent of  $k$  and  $\sigma$ . These error estimates are supported by test calculations in section 4.

For each process, the sampling error is defined as the difference between  $\hat{q}$  and its expected value based on a knowledge of the ensemble prior to the process. Thus, for the mixing process at  $(x,t) = (h\underline{\lambda}, k\lambda)$  the sampling error is

$$\varepsilon_m(h\underline{\lambda}, k\lambda) = \hat{q}(h\underline{\lambda}, t_m) - E\hat{q}(h\underline{\lambda}, t_m) . \quad (3.59)$$

And for diffusion and convection in the  $x_i$ -direction, the sampling errors  $\varepsilon_{di}$  and  $\varepsilon_{ci}$  are similarly defined. It follows trivially from equation (3.59) that the expected value of  $\varepsilon_m$  is zero; so also are the expected values of  $\varepsilon_{di}$  and  $\varepsilon_{ci}$ .

Consider the performance of the Monte Carlo simulation for a time interval  $0 < t \leq T$ . If  $\Lambda$  steps are taken then the time increment  $k$  is

$$k = T/\Lambda \quad . \quad (3.60)$$

In order to estimate the total sampling error at the end of the simulation  $\epsilon_T(\underline{h}\underline{\lambda})$ , we make three assumptions: that the individual errors ( $\epsilon_m$  etc.) are small, that they are independent, and that they are neither amplified nor attenuated in successive time steps. Subject to these assumptions, the total sampling error is just the sum of the individual errors:

$$\epsilon_T(\underline{h}\underline{\lambda}) = \sum_{\lambda=1}^{\Lambda} (\epsilon_m(\underline{h}\underline{\lambda}, k\lambda) + \sum_{i=1}^m \epsilon_{di}(\underline{h}\underline{\lambda}, k\lambda) + \sum_{i=1}^m \epsilon_{ci}(\underline{h}\underline{\lambda}, k\lambda)) \quad . \quad (3.61)$$

The assumption that the errors are small and independent is valid for large  $N$ . Although it is necessary to the present analysis, the remaining assumption is unlikely to hold. The consequences of this are discussed at the end of this section.

Since the expected values of  $\epsilon_m$  etc. are zero, the expected value of  $\epsilon_T$  given by equation (3.61) is also zero. Thus, the method provides an unbiased estimate of  $\hat{q}$  for any  $N$ .

The standard error  $\epsilon_{st}(\underline{h}\underline{\lambda})$  -- which is the standard deviation of  $\epsilon_T(\underline{h}\underline{\lambda})$  -- is a measure of the probable sampling error. With the argument  $\underline{h}\underline{\lambda}$  being implied (here and below)  $\epsilon_{st}$  is given by

$$\epsilon_{st}^2 = \mathbb{D} \epsilon_T \quad . \quad (3.62)$$

( $\mathbb{D}$  is the variance operator)

Substituting for  $\epsilon_T$  from equation (3.61) and making use of the independence property, we obtain

$$\epsilon_{st}^2 = \sum_{\lambda=1}^{\Lambda} ( \mathbb{D} \epsilon_m(k\lambda) + \sum_{i=1}^m \mathbb{D} \epsilon_{di}(k\lambda) + \sum_{i=1}^m \mathbb{D} \epsilon_{ci}(k\lambda) ) \quad . \quad (3.63)$$

Since the right-hand side is the sum of  $\Lambda(2m+1)$  variances, it is clear that

$\varepsilon_{st}$  satisfies the inequality

$$\varepsilon_{st}^2 \leq \Lambda(2m+1) \sup_{\lambda, i} \{ D \varepsilon_m(k\lambda), D \varepsilon_{di}(k\lambda), D \varepsilon_{ci}(k\lambda) \} . \quad (3.64)$$

We show below that for fixed  $h$  each of the three variances is of order  $k/N$ . Hence,

$$\varepsilon_{st}^2 \leq O(\Lambda k/N) \quad (3.65)$$

or, recalling that  $\Lambda = T/k$ ,

$$\varepsilon_{st}^2 \leq O(1/N) \quad (3.66)$$

Thus, the standard error is of order  $N^{-1/2}$  and independent of  $k$  and  $\sigma$ .

It remains to be shown that the variances of the individual sampling errors ( $\varepsilon_m$  etc.) are of order  $k/N$ . The value of  $\hat{q}$  after the mixing process is given by equation (3.50):

$$\hat{q}(h\underline{x}, t_m) = \frac{1}{N} \sum_{N-n_m} Q(\underline{\phi}^*) + \frac{1}{N} \sum_{n_m} Q(\underline{\phi}^{mix}) . \quad (3.67)$$

Taking the variance of both sides of this equation we obtain

$$\begin{aligned} D \varepsilon_m(h\underline{x}, t_m) &= \frac{1}{N^2} \{ n_m(1 - n_m/N) D Q(\underline{\phi}^*) + n_m D Q(\underline{\phi}^{mix}) \} \\ &= (k/N)\omega \{ (1-\omega k) D Q(\underline{\phi}) + D Q(\frac{1}{2}(\underline{\phi}+\underline{\phi}')) \} \\ &= O(k/N) . \end{aligned} \quad (3.68)$$

Similarly for diffusion and convection the sampling error variances are

$$\begin{aligned} D \varepsilon_{di}(h\underline{x}, k\lambda) &\approx (k/N)(4\Gamma D Q(\underline{\phi})/h^2) \\ &= O(k/N) \end{aligned} \quad (3.69)$$

and

$$\begin{aligned} \mathbb{D} \varepsilon_{ci}(h\underline{\ell}, k\lambda) &\approx (k/N) (2|\tilde{U}| \mathbb{D} Q(\underline{\phi})/h) \\ &= O(k/N) \end{aligned} \tag{3.70}$$

Equations (3.68) - (3.70) contain the required result that, for fixed  $h$ , all the variances are of order  $k/N$ . In the expressions for the sampling error variance, the only functions of the composition space that appear are variances such as  $\mathbb{D} Q(\underline{\phi})$ . These are not functions of  $\sigma$  per se, and so neither is  $\varepsilon_{st}$ .

The last two equations show that  $\mathbb{D} \varepsilon_{di}$  and  $\mathbb{D} \varepsilon_{ci}$  are proportional to  $h^{-2}$  and  $h^{-1}$  respectively. Consequently the analysis predicts that the standard error varies as  $1/(hN^{\frac{1}{2}})$ . The calculations reported in the next section show that, fortunately, this does not happen and in fact the standard error is independent of  $h$ . The likely reason is that the conservative simulations of convection and diffusion ensure that the sampling error is confined to the highest wave numbers that the grid can resolve. Since diffusion damps out fluctuations at a rate proportional to the square of the wave number, it is to be expected that these errors rapidly disappear. In other words, contrary to the earlier assumption, the sampling error is rapidly attenuated. (In support of this explanation is the finding that with a non-conservative scheme the sampling error does increase with decreasing  $h$ . In this case the sampling error is uniformly distributed over all wave numbers.)

### 3.7 Accuracy

The Monte Carlo method has been shown to be first-order accurate in both space and time. In spite of this low order of accuracy, accurate results can be obtained without excessive computation.

It has already been shown that the work required to perform the



simulation for a given time interval is independent of the time step  $k$ . Consequently there is no penalty in taking small time steps to reduce the associated truncation error to any desired level.

The Monte Carlo method can only be applied to difference operators with positive weights. It is for this reason that the first-order accurate upwind difference is used for the convective terms instead of the second-order accurate central difference. However the method can be made pseudo-second-order accurate by using a hybrid difference scheme (see Gosman et al. 1969). In this scheme the upwind difference is replaced by a central difference wherever the convective and diffusive operators combined result in positive weights: the two processes would then be simulated together. With this modification the Monte Carlo method has the same spatial truncation error as most current turbulent flow calculation procedures (see for example, Gosman & Pun 1973).

The third source of error is the sampling error due to finite  $N$ . It has been shown that as  $N$  tends to infinity the standard error  $\epsilon_{st}$  in  $\hat{q}$  is of order  $q'N^{-1/2}$  and independent of the dimensionality  $\sigma$ . As well as the obvious dependence upon  $N$ , the error depends upon the function being sampled  $Q(\phi)$  through its standard deviation  $q'$ . Consider, for example,  $Q(\phi)$  being a spike function centered in a region of low probability - the tail of the distribution, say. Then since  $q'$  is large the sampling error is large. This situation is encountered in the construction of histograms and then indeed many samples are required to determine the tails accurately. More often, however, simpler functions such as means are of more interest: then the results of the next section indicate that with one hundred elements the sampling error is less than 5%.

#### 4. TEST CALCULATIONS

In order to test its performance, the Monte Carlo method was used to simulate the pdf transport equation for a model problem. The calculations reported here demonstrate the use of the method and consolidate the error estimates of the previous section. The results show the following:

- i) the Monte Carlo simulation converges to the solution of the differential equation,
  - ii) the expected value of the error is independent of  $N$  (i.e. the method is unbiased),
  - iii) the standard error is proportional to  $N^{-1/2}$ ,
- and
- iv) the standard error is independent of  $h$ .

##### 4.1 The Model Problem

The model problem corresponds to a plug-flow reactor with imperfect mixing. The flow is one-dimensional with the uniform velocity  $U$  being in the  $\bar{x}$ -direction. The density  $\rho$ , the turbulent diffusion coefficient  $\Gamma_T$  and the turbulent frequency  $\omega$  are also uniform. A single scalar  $\phi$  represents the concentration of reaction products which is zero at the start of the reactor ( $\phi=0$  at  $\bar{x}=0$ ) and is everywhere bound by zero and unity ( $0 \leq \phi \leq 1$ ). Two cases are considered: in the first--the linear case--the reaction rate of  $\phi$  is a linear function of  $\phi$ ; in the second--the non-linear case--there is an Arrhenius reaction rate.

The velocity  $U$  and the length of the reactor  $L$  are used to define the following dimensionless quantities:

$$\begin{aligned}
t^* &\equiv t U/L & , & & x &\equiv \bar{x}/L & , \\
\Gamma^* &\equiv \Gamma_T/(\rho UL) & , & & \omega^* &\equiv \omega L/U & ,
\end{aligned}
\tag{4.1}$$

$$S^*(\psi) \equiv S(\psi)L/U \quad \text{and} \quad E^*(\psi; x, t) \equiv E(\psi; x, t)/\omega .$$

The pdf of  $\phi(x, t^*)$  is  $p(\psi; x, t^*)$ . The pdf transport equation for the model problem is obtained from equation (2.8) and the above definitions:

$$\frac{\partial p}{\partial t^*} + \frac{\partial p}{\partial x} + \frac{\partial}{\partial \psi} (p S^*(\psi)) = \Gamma^* \frac{\partial^2 p}{\partial x^2} + \omega^* E^* . \tag{4.2}$$

The boundary conditions are

$$p(\psi; 0, t^*) = \delta(\psi) , \tag{4.3}$$

and

$$\frac{\partial^2}{\partial x^2} p(\psi; 1, t^*) = 0 , \tag{4.4}$$

and the initial condition--corresponding to complete reaction--is

$$p(\psi; x, 0) = \delta(1-\psi) . \tag{4.5}$$

The normalized reaction rate for the linear case is

$$S^*(\psi) = a_1(1-\psi) \tag{4.6}$$

where  $a_1$  is a constant. The main reason for considering this case is that there is an exact solution for the mean value  $\langle \phi \rangle$  in the steady state:

$$\langle \phi \rangle = 1 - \exp(-bx) \tag{4.7}$$

where

$$b = \frac{1}{2} \{ (1 + 4a_1\Gamma^*)^{\frac{1}{2}} - 1 \} / \Gamma^* . \quad (4.8)$$

(In fact this solution satisfies the downstream boundary condition only approximately, but the effect of the discrepancy is unimportant.)

The Arrhenius expression used in the non-linear case is

$$S^*(\psi) = a_2 \times 2183. \psi(1-\psi) \exp(-20/(1+3\psi)) . \quad (4.9)$$

$a_2$  is a constant and the multiplier 2183 is chosen so that the maximum value of  $S^*(\psi)$  is  $a_2$ .

The values of the constants are selected so that each of the four processes--convection, diffusion, reaction and mixing--are of approximately equal importance. The values are

$$a_1 = 3., \quad a_2 = 10., \quad \omega^* = 20., \quad \Gamma^* = 0.1. \quad (4.10)$$

In general, the Monte Carlo calculations reported below were performed with  $N=40$  and  $h=0.1$ . The smallest possible time step was used which, for the given  $N$  and  $h$ , is  $k=0.0025$ .

#### 4.2 The Linear Case

All the results for the linear case are at  $t^*=2$ , by which time the steady state has been reached. The mean  $\langle \phi \rangle$  and standard deviation  $\phi'$  are plotted against  $x$  on figure 1. The dashed line is the exact solution equation (4.7) and the full circles are the ensemble average values  $\hat{\phi}$ . The expected value of  $\hat{\phi}$  was estimated by taking the arithmetic mean of  $\hat{\phi}$  over 25 similar calculations (the sole difference between each calculation being the random numbers used). The expected value  $E \hat{\phi}$  is shown as

the solid line on the figure. Sampling error is evident from the differences between  $\hat{\phi}$  and  $E \hat{\phi}$ .

According to the theory of the previous section, as  $N$  tends to infinity, the Monte Carlo simulation converges to the finite-difference scheme given by equations (3.17) - (3.20) with the differential operators  $C$  and  $D$  replaced by finite-difference operators. Because the pdf equation is linear, the value of the mean given by the finite-difference equations  $\langle \phi \rangle_{fd}$  can readily be computed. It is found that  $\langle \phi \rangle_{fd}$  is equal to the expected value  $E \hat{\phi}$ . This observation provides strong evidence for the convergence and lack of bias in the method. As  $N$  tends to infinity,  $\hat{\phi}$  tends to  $E \hat{\phi}$  which is equal to  $\langle \phi \rangle_{fd}$ : as  $h$  tends to zero  $\langle \phi \rangle_{fd}$  converges to the exact solution. Thus, as  $N$  and  $h^{-1}$  tend to infinity,  $\hat{\phi}$  tends to the exact solution. The difference between the values of  $\hat{\phi}$  and  $E \hat{\phi}$  is sampling error due to finite  $N$ : the difference between  $E \hat{\phi}$  and the exact solution is truncation error due to finite  $h^{-1}$ . The fact that  $E \hat{\phi}$  is equal to  $\langle \phi \rangle_{fd}$  for finite  $N$  ( $N=40$ ) strongly suggests that the method is unbiased.

The standard deviation  $\phi'$  and its expected value are also shown on figure 1.  $\phi'$  reaches a maximum of almost 0.2 at  $x=0.2$  and then decays monotonically.

In order to study the dependence of the solution upon  $N$ , calculations were performed with values of  $N$  ranging from 10 to 400. Plotted against  $N^{-1/2}$  on figure 2 is the expected value  $E \hat{\phi}$  at  $x=0.5$  with error bars showing (twice) the standard error  $\epsilon_{st}$ ,

$$\epsilon_{st}^2 = D \hat{\phi} \quad . \quad (4.11)$$

The exact value of  $E \hat{\phi}$  cannot be determined from a finite number of calculations: the dashed lines correspond to plus and minus one standard deviation uncertainty centered on the finite-difference solution  $\langle \phi \rangle_{fd}$ . The plot shows (to within the uncertainty of the test) that the expected value  $E \hat{\phi}$  is equal to the finite-difference solution  $\langle \phi \rangle_{fd}$  for all  $N$ . In other words,  $\hat{\phi}$  is an unbiased estimate of  $\langle \phi \rangle$ . It may also be seen from the error bars that the standard error rises linearly with  $N^{-1/2}$ .

An unfavourable prediction of the error estimates obtained in the last section is that the standard error varies inversely with  $h$ . Figure 3 shows the difference between  $E \hat{\phi}$  and  $\langle \phi \rangle_{fd}$  at  $x=0.5$  (with error bars showing the standard error) this time plotted against  $h^{-1}$ . It appears that the standard error is independent of  $h$ --a fortunate result. (The likely reason for the erroneous prediction is given in section 3.6.)

In order to estimate the magnitude of the sampling error, the quantity

$$\varepsilon^* = N^{1/2} \varepsilon_{st} / \phi' \quad (4.12)$$

is plotted against  $x$  on figure 4 for  $N=10$ , 40 and 400. Although there is considerable scatter, it is clear that  $\varepsilon^*$  is of order unity: the maximum value is 1.4. Consequently, inverting equation (4.12), the standard error can be estimated from

$$\varepsilon_{st} = \varepsilon^* \phi' N^{-1/2} \quad , \quad (4.13)$$

where (at least for this case)  $\varepsilon^*$  is of order unity.

### 4.3 The Non-linear Case

A transient non-linear case was investigated to confirm the generality of the conclusions drawn from the steady-state linear case. In this series of tests the Arrhenius reaction rate was employed and the solution examined at times before the steady state had been reached.

The expected values  $E\hat{\phi}$  are plotted against  $x$  on figure 5 for the times  $t^* = 0.5, 1.0$  and  $1.5$ : the dashed line is the expected value of  $\phi'$  and the circles are values of  $\hat{\phi}$  at  $t^* = 1.0$ . It may be seen that the maximum value of  $\phi'$  is about twice that of the linear case which accounts for the larger sampling error.

For  $x = 0.5$  and  $t^* = 1.0$ , the expected value  $E\hat{\phi}$  is plotted against  $N^{-1/2}$  on figure 6. The error bars show (twice) the standard error and, as in figure 2, the dashed lines correspond to plus and minus one standard deviation uncertainty. Again, it appears that (to within the uncertainty of the test)  $E\hat{\phi}$  is independent of  $N$  and the standard error  $\epsilon_{st}$  is proportional to  $N^{-1/2}$ . That  $E\hat{\phi}$  is independent of  $N$  confirms the lack of bias in the method.

Figure 7 shows a plot of  $\epsilon^*$  (see equation 4.12) against  $x$  for  $N=10, 40$  and  $400$ . As in the linear case, there is a good deal of scatter but the mean value of  $\epsilon^*$  is close to unity: the greatest value is 1.65.

In summary: test calculations for both a steady-state linear case and a transient non-linear case show that the Monte Carlo method is unbiased, and that the standard sampling error (of  $\hat{\phi}$ ) is

$$\epsilon_{st} = \epsilon^* \phi' N^{-1/2}$$

where  $\epsilon^*$  is of order unity and independent of  $h$ .

## 5. MIXING LAYER CALCULATIONS

The Monte Carlo method in conjunction with the  $k - \epsilon$  turbulence model was used to calculate pdf's of temperature in a turbulent mixing layer. The results reported here show good agreement with the experimental data of Batt (1977). These data were obtained in a two-dimensional mixing layer in which the velocities of the two streams were 23 ft/s and 1.6 ft/s. The temperature difference between the streams was 5° C.

In the calculations the slight density variation was ignored and, because of the nature of the flow, the boundary layer assumptions were invoked. The single scalar  $\phi$  represents the normalized temperature ( $\phi = 0$  in the high speed stream,  $\phi = 1$  in the low speed stream). For this flow there is no heat source and hence  $S(\phi)$  is zero. Thus, with  $U$  and  $V$  being the velocities in the  $x$  and  $y$  (flow and normal) directions, the transport equation for  $p(\psi; x, y)$  is

$$U \frac{\partial p(\psi)}{\partial x} + V \frac{\partial p(\psi)}{\partial y} = \frac{\partial}{\partial y} \frac{\Gamma_T}{\rho} \frac{\partial p(\psi)}{\partial y} + E(\psi; x, y) \quad (5.1)$$

Equations are also solved for the velocity  $U$ , the turbulent kinetic energy  $k$  and its rate of dissipation  $\epsilon$ . These equations are:

$$\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0, \quad (5.2)$$

$$U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} = \frac{\partial}{\partial y} \nu_T \frac{\partial U}{\partial y}, \quad (5.3)$$



$$U \frac{\partial k}{\partial x} + V \frac{\partial k}{\partial y} = \frac{\partial}{\partial y} \frac{\nu_T}{\sigma_k} \frac{\partial k}{\partial y} + \nu_T \left( \frac{\partial U}{\partial y} \right)^2 - \epsilon, \quad (5.4)$$

and

$$U \frac{\partial \epsilon}{\partial x} + V \frac{\partial \epsilon}{\partial y} = \frac{\partial}{\partial y} \frac{\nu_T}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial y} + C_{\epsilon 1} \frac{\nu_T \epsilon}{k} \left( \frac{\partial U}{\partial y} \right)^2 - C_{\epsilon 2} \epsilon^2/k, \quad (5.5)$$

where the turbulent viscosity  $\nu_T$  is given by

$$\nu_T = C_\mu k^2/\epsilon. \quad (5.6)$$

The constants  $C_\mu$ ,  $C_{\epsilon 1}$ ,  $C_{\epsilon 2}$ ,  $\sigma_k$  and  $\sigma_\epsilon$  are ascribed the standard values 0.09, 1.45, 1.9, 1.0, and 1.3.

It remains to specify  $\Gamma_T$  and  $\omega$  in terms of  $k$  and  $\epsilon$ . This is achieved by requiring that the pdf equation (5.1) be consistent with the standard model equation for  $\langle \phi'^2 \rangle$  (Spalding 1971). This yields,

$$\Gamma_T = \rho \nu_T / \sigma_\phi, \quad (5.7)$$

and

$$\omega = 2 C_\phi \epsilon / k, \quad (5.8)$$

where the constants  $\sigma_\phi$  and  $C_\phi$  take the values 0.7 and 2.0.

Equations (5.2) - (5.6) were solved by a finite-difference procedure (Pope 1977) with boundary and initial conditions appropriate to the mixing layer. The pdf equation was solved by a variant of the Monte Carlo method

which exploits the fact that equation (5.1) is parabolic. Rather than marching in time (as described in section 3) the method marches in the downstream direction  $x$ . Thus initial ensembles are specified at  $x = 0$  and each step of the simulation advances the ensembles a distance  $\Delta x$  downstream. In the cross-stream direction there were 24 nodes at each of which there was an ensemble of 100 elements. The step length  $\Delta x$  was very small - typically one tenth of the mixing-layer thickness.

In order to make comparisons with measured pdf's, histograms (with 20 intervals) were constructed from the calculated ensembles. Figure 8 shows a comparison of these histograms with measured pdf's at seven cross-stream locations at  $x = 15.5$  inches. It may be seen that in general the agreement is good: for the five central pdf's, the locations of the peaks and the shapes and spreads of the distributions are closely matched. (The measurements at the extreme locations are suspicious: in neither case does the pdf integrate to unity and, from similar data [e.g. Birch et al. 1978], a spike resembling an exponential decay can be expected at the bounds  $\psi = 0$  and  $\psi = 1$ .)

These calculations demonstrate the use of the Monte Carlo method and the good agreement with experimental data is encouraging considering the known shortcomings of some of the modelling assumptions.

## 6. DISCUSSION

### Summary

A Monte Carlo method has been developed to solve the pdf equations of turbulent flow. At each node of a finite-difference grid covering the solution domain, the joint pdf is represented by an ensemble of  $N$  elements. Each element is ascribed a complete set of values of the relevant fluid properties. In a simulation of the scalar pdf equation (2.8), elements are commuted between neighboring nodes (simulating diffusion) and they are transferred from node to node in the flow direction (simulating convection). Two elements mix by adopting the average values of their properties and, between mixing operations, the properties change according to the instantaneous reaction rates. The precise manner in which these operations are performed is determined in section 3.

The performance of the method has been determined by analysis and by computational experiments. For large  $N$ , the truncation error is proportional to the grid spacing  $h$  and the time step  $k^\dagger$ . A finite value of  $N$  results in a random sampling error. The expected value of this error is zero (i.e. the method is unbiased) and the standard error is of order  $N^{-1/2}$ . From computational tests it appears that the standard sampling error (in determining the mean  $\langle\phi\rangle$ ) is

$$\epsilon_{st} = \epsilon^* \phi' N^{-1/2} \quad (6.1)$$

where  $\epsilon^*$  is of order unity and independent of  $h$ .

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<sup>†</sup> The scheme can be made pseudo-second-order accurate in  $h$  by using the hybrid scheme instead of straight forward upwind differencing (see Gosman et al 1969). Also, it has been shown that there is no penalty in choosing a very small value of  $k$  and hence eliminating that source of error.

The usefulness of the method stems from the fact that the computational work required increases only linearly with  $\sigma$ , the dimensionality of the joint pdf. Consequently, calculations of turbulent flows with many reactive species are possible.

The Monte Carlo method in conjunction with the  $k - \epsilon$  turbulence model has been used to calculate pdf's of temperature in a mixing layer. The results agree well with the measurements of Batt (1977).

#### Computer Requirements

It has been shown in section 3.5 that the computer time required is proportional to  $N\sigma$ : it is also approximately proportional to the number of nodes  $n$ . For the non-linear test case ( $N = 40$ ,  $n = 11$ ,  $\sigma = 1$ ) the computer time on a VAX 11 was 4s. Using this information, the cost of a two-dimensional calculation can be estimated. With a  $20 \times 20$  grid ( $n = 400$ ) and  $N = 100$  (which, according to equation (6.1) gives a standard error of less than 5%) the estimated time is  $360 \sigma$  s -- that is, six minutes per species. On the VAX installation used, the cost of such a calculation would be \$10. per species.

The method does not make great demands upon computer storage. At first sight, the two-dimensional calculation mentioned above requires 40,000 storage locations per species which, on some computers, would be prohibitive. However, the storage requirement can be reduced at will by splitting the calculation into several smaller calculations. Because the method is unbiased, the average of ten calculations with  $N = 10$  has the same statistical error as one calculation with  $N = 100$ : the smaller calculations require the same computer time (altogether) but require only one tenth of the storage.

### Relationship to other approaches

For homogeneous turbulence, where  $p(\psi;t)$  is independent of  $\underline{x}$ , the Monte Carlo method reduces to a simulation of reaction and mixing. Then the method differs only in detail from that of Spielman and Levenspiel (1965), which has subsequently been used by Flagan and Appleton (1974), Pratt (1976) and others. Indeed, the idea of the ensemble representation was taken from these works.

It has been known for some time that the Monte Carlo method in the form of random walks can be used to solve elliptic differential equations; Courant, Friedrichs and Lewy (1928). In these random walks, a "walker" passes from node to node of a finite-difference grid according to prescribed probabilities. At each node the value ascribed to the walker can be modified according to another prescription. Eventually the walker reaches the boundary of the solution domain where, we assume, the boundary value is specified. An estimate of the solution of the differential equation at the walker's point of origin can then be obtained from the boundary value and the final value of the walker. The accuracy of the result is improved by taking the average of the estimates obtained from many random walks.

Similarities between random walks and the present method are obvious. Minor differences are that, in the present method, an estimate of the solution is obtained over the whole field and that the walker's (element's) values originate from the boundary conditions. The major difference is that in the present method the walkers (elements) interact in the mixing process. For this reason ensembles of many elements are required rather than requiring a single walker to take many walks. Because of these differences the present analysis is completely different from that used for random walks.

### Physical interpretation

A physical interpretation of the Monte Carlo method is unnecessary and, in the author's opinion, should be avoided. It may be tempting to interpret a representative value  $\phi^{(n)}$  as referring to the properties of a "particle" or "element of fluid." Since these "particles" conserve neither mass nor volume and since they can simply disappear, such an interpretation is likely to be misleading. Neither should the randomness of turbulence be seen reflected in the randomness of the Monte Carlo method. The method simulates a deterministic equation: random fluctuations in  $\hat{\phi}$  are not due to turbulence but to sampling error (caused by finite N). Nor should the method be thought of as a physical model.

The physics is embodied in the pdf transport equation. The joint pdf is a well-defined, measurable quantity for which an exact transport equation can be derived. Modelling is applied to the exact equation in order to obtain equation (2.8), and the Monte Carlo method is no more than a numerical method for solving this equation.

### Applications

The direct application of the method is to turbulent reactive flows. In

spite of modelling uncertainties, the pdf equation most likely provides the best theoretical description (available at present) of such flows. Consequently, the Monte Carlo method is of direct practical value in enabling the solution of the equation, even when many species and complex kinetics are involved.

In recent years, many measurements have been made of pdf's and joint pdf's of velocity and a passive scalar in turbulent shear flows. Riberio and Whitelaw (1975) measured the joint pdf of velocity  $p(v_1, v_2; \underline{x}, t)$  in a fully developed turbulent jet, and Wallace and Brodkey (1977) obtained similar measurements in a turbulent channel flow. For a heated turbulent jet, Venkataramini, Tutu and Chevray (1975) measured the joint pdf of velocity  $p(v_1, v_2; \underline{x}, t)$  and also the joint pdf of velocity and temperature  $p(\psi_1, v_1; \underline{x}, t)$ . None of these data has been compared with theoretical calculations. Application of Monte Carlo method to the transport equations for  $p(\underline{v}; \underline{x}, t)$  and  $p(\underline{v}, \underline{\psi}; \underline{x}, t)$  would make such a comparison possible.

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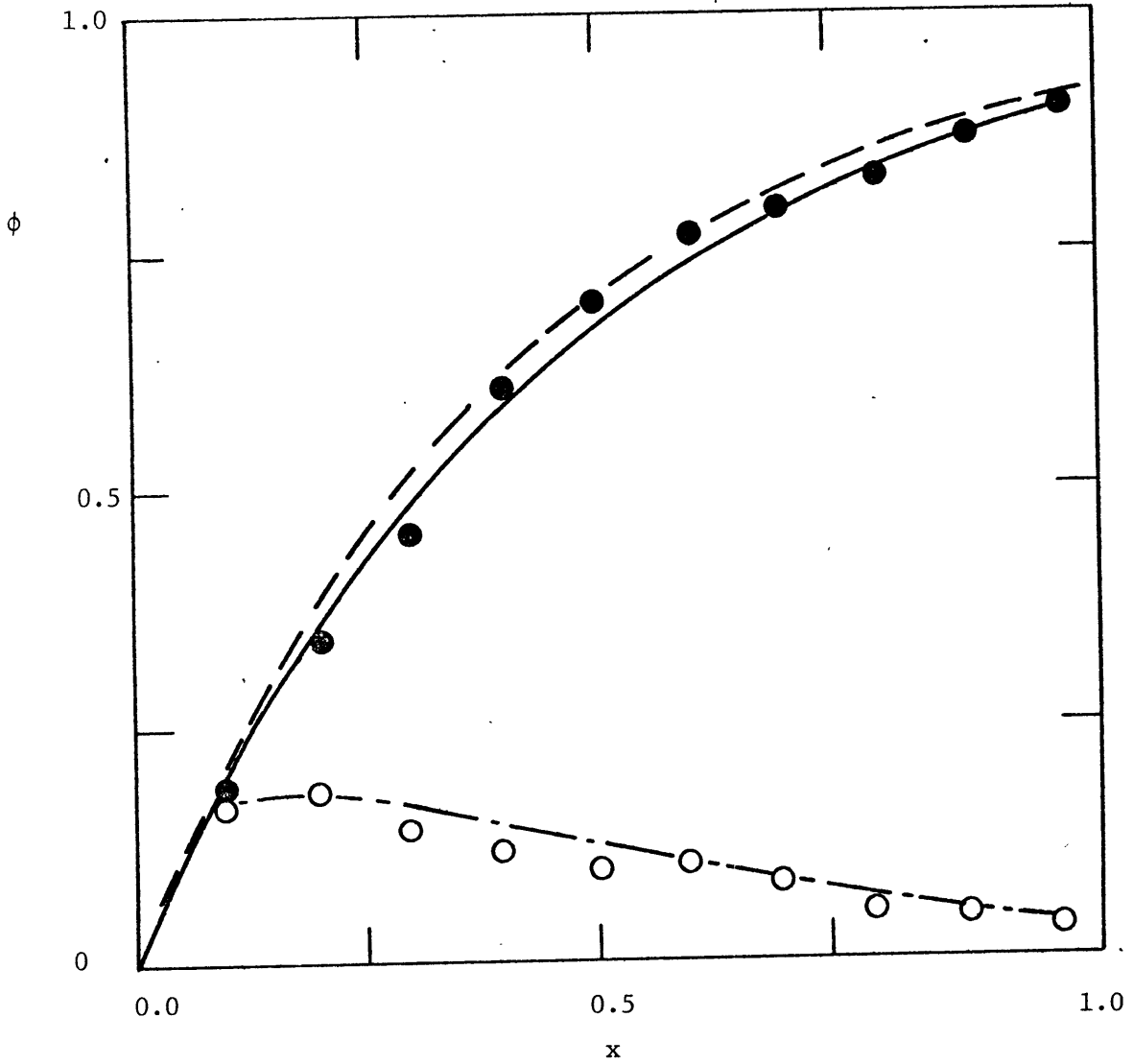
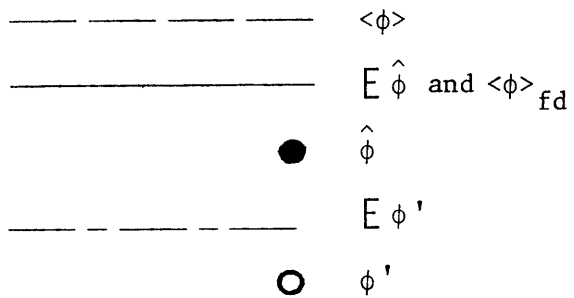


Fig. 1:  $\langle \phi \rangle$  and  $\phi'$  against  $x$ : linear case,  $N = 40$ ,  $h = 0.1$ .



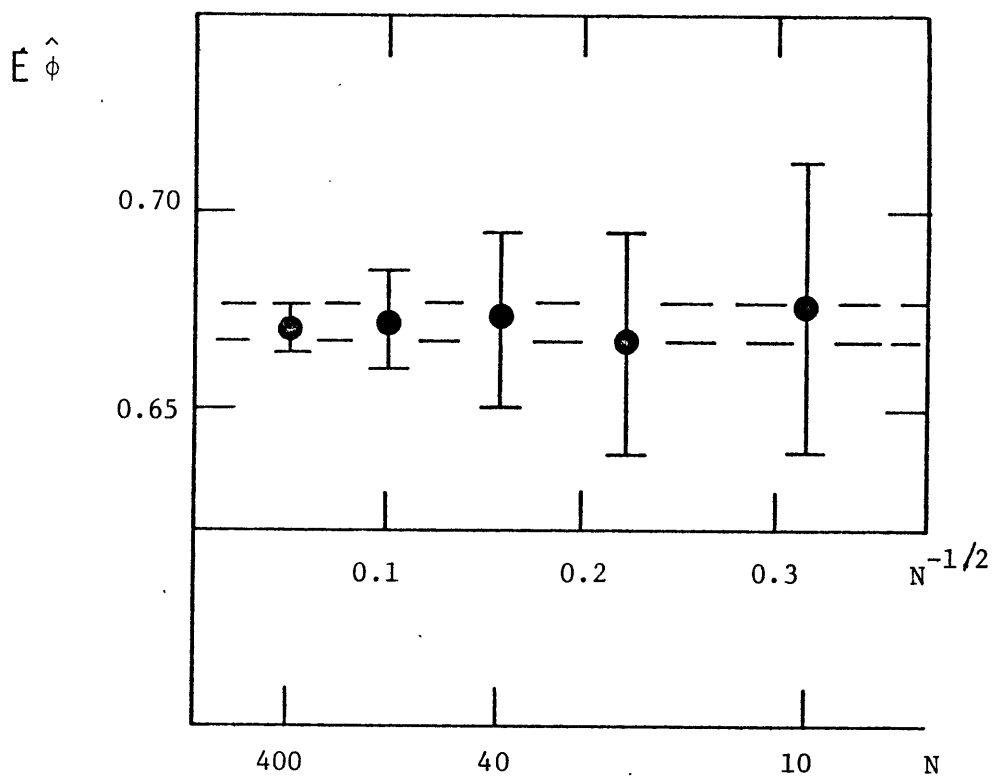


Fig 2:  $E \hat{\phi} \pm \epsilon_{st}$  against  $N^{-1/2}$ : linear case,  $x = 0.5$ ,  $h = 0.1$ .

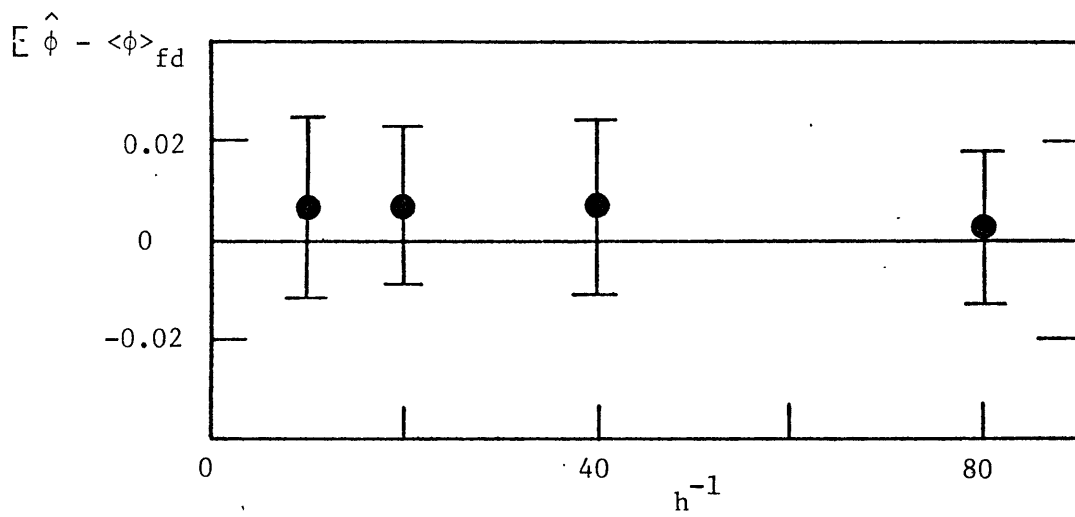


Fig. 3:  $E \hat{\phi} \pm \epsilon_{st} - \langle \phi \rangle_{fd}$  against  $h^{-1}$ : linear case,  $x = 0.5$ ,  $N = 40$ .

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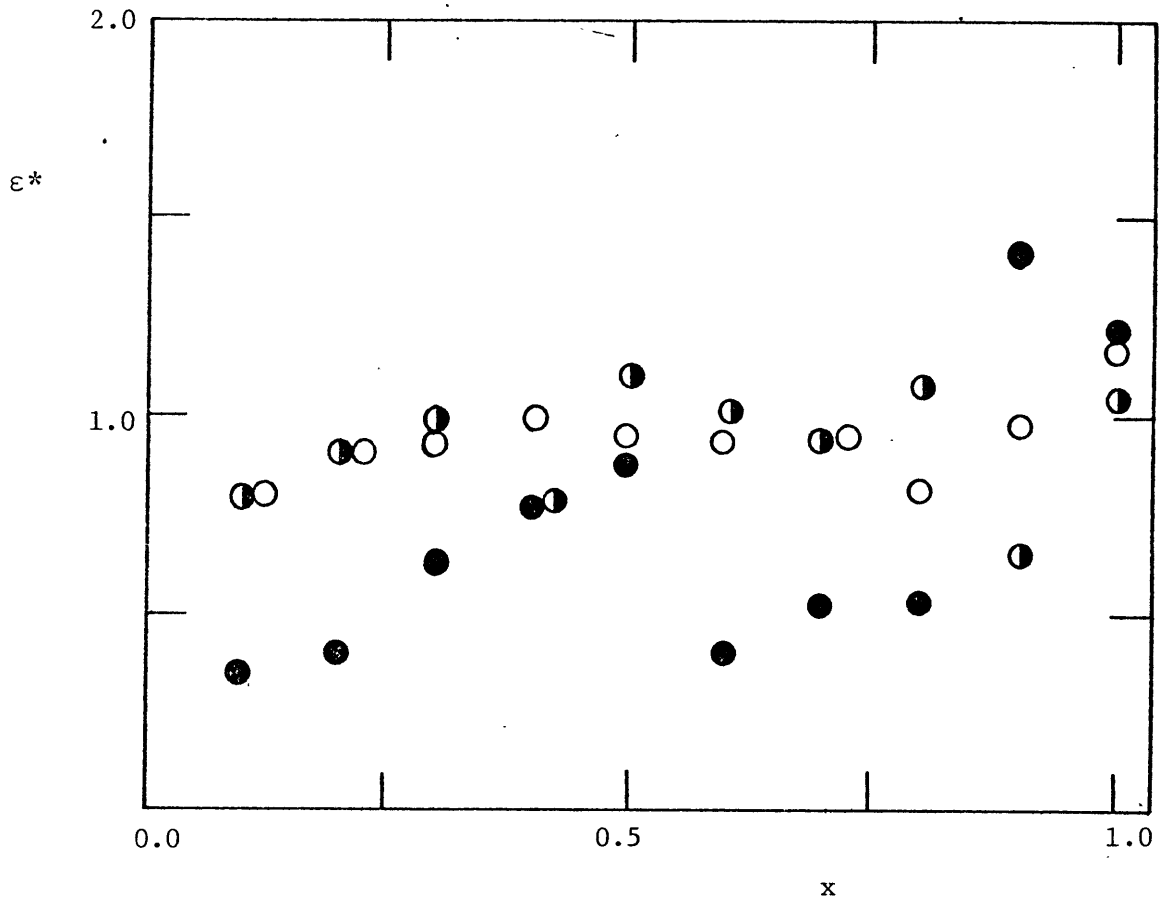


Fig 4:  $\epsilon^*$  against  $x$ : linear case,  $h = 0.1$ .

○  $N = 10$ ,   ●  $N = 40$ ,   ●  $N = 400$

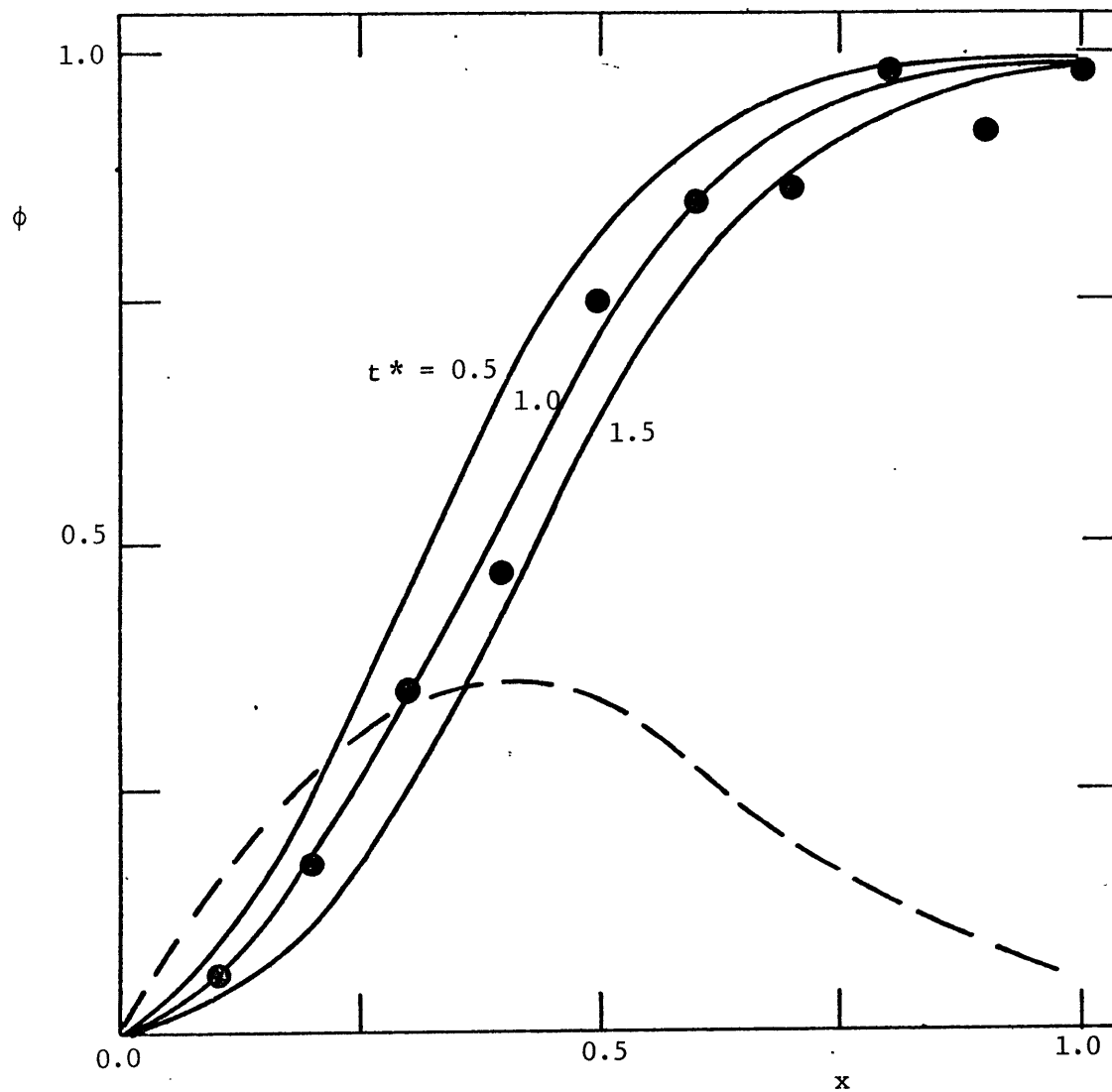
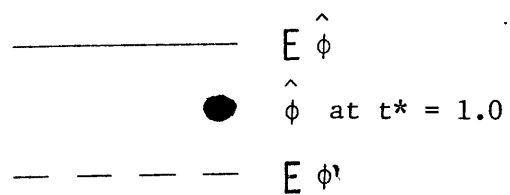


Fig 5:  $\hat{\phi}$  and  $\phi'$  against  $x$ : non-linear case,  $N = 40$ ,  $h = 0.1$ .



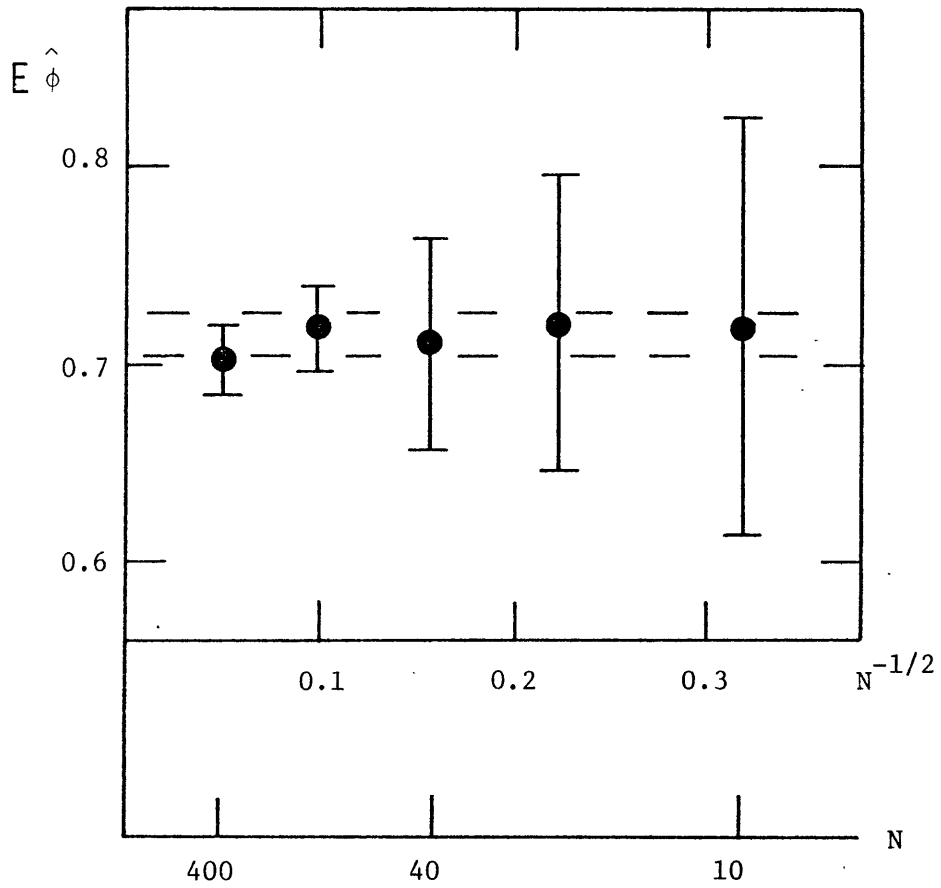


Fig 6:  $E \hat{\phi} \pm \epsilon_{st}$  against  $N^{-1/2}$ : non-linear case,  $x = 0.5$ ,  $t^* = 1.0$ ,  $h = 0.1$ .

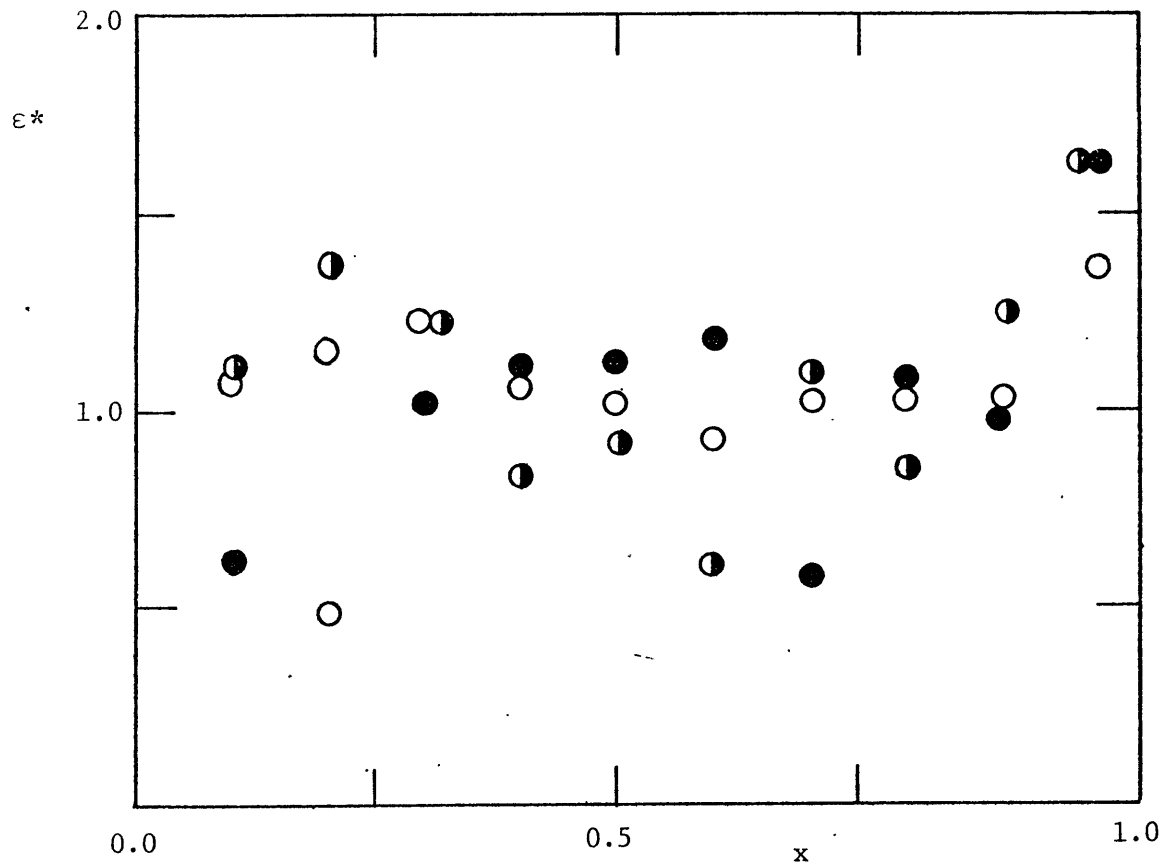


Fig 7:  $\epsilon^*$  against  $x$ : non-linear case,  $h = 0.1$ .

○  $N = 10$ , ◐  $N = 40$ , ●  $N = 400$



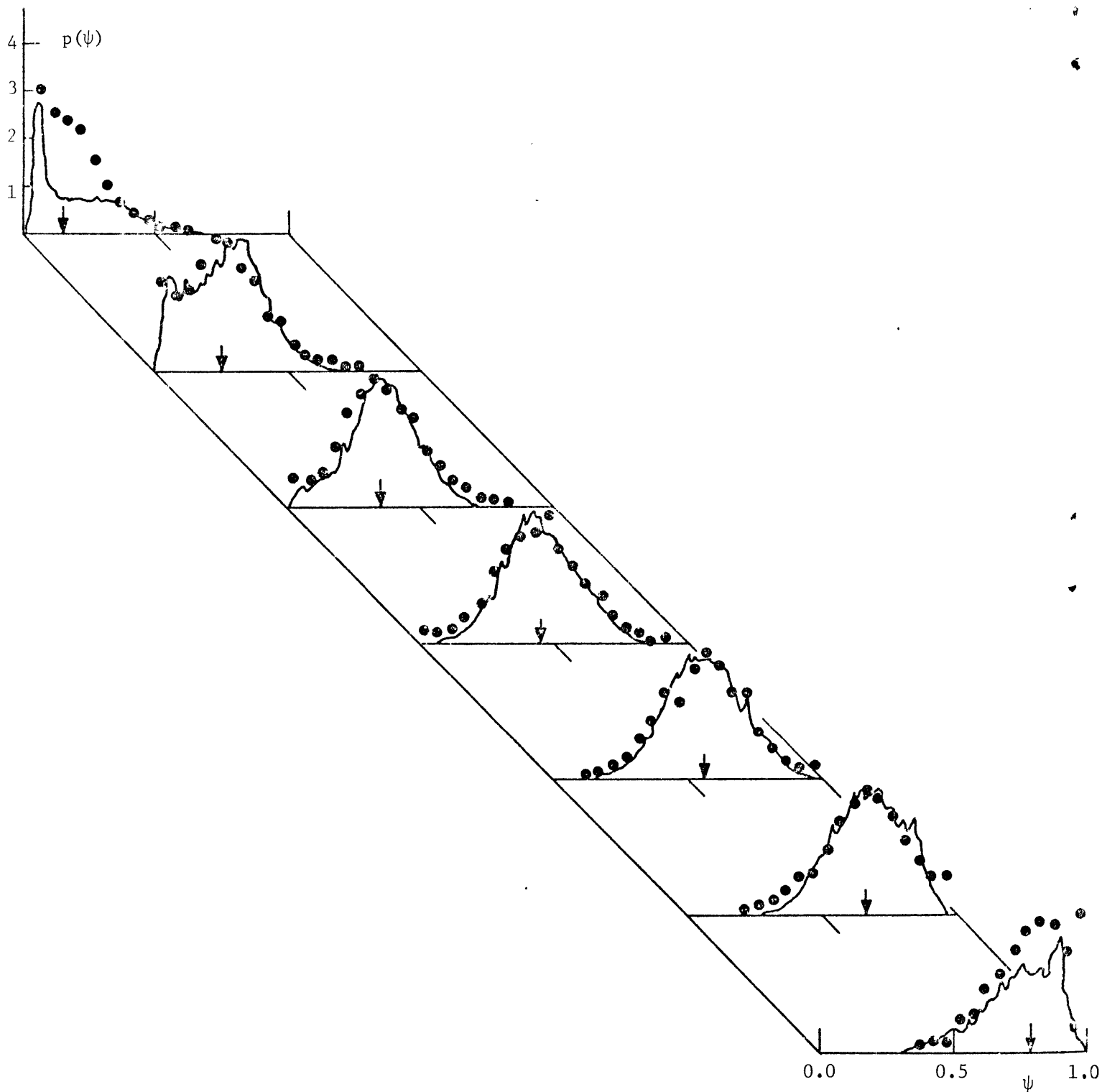


Fig. 3: pdf's of temperature in a mixing layer:  
 $p(\psi)$  against  $\psi$ . (Arrows show positions of means)

● Monte Carlo Calculations

~~~~~ Measurements of Batt (1977)