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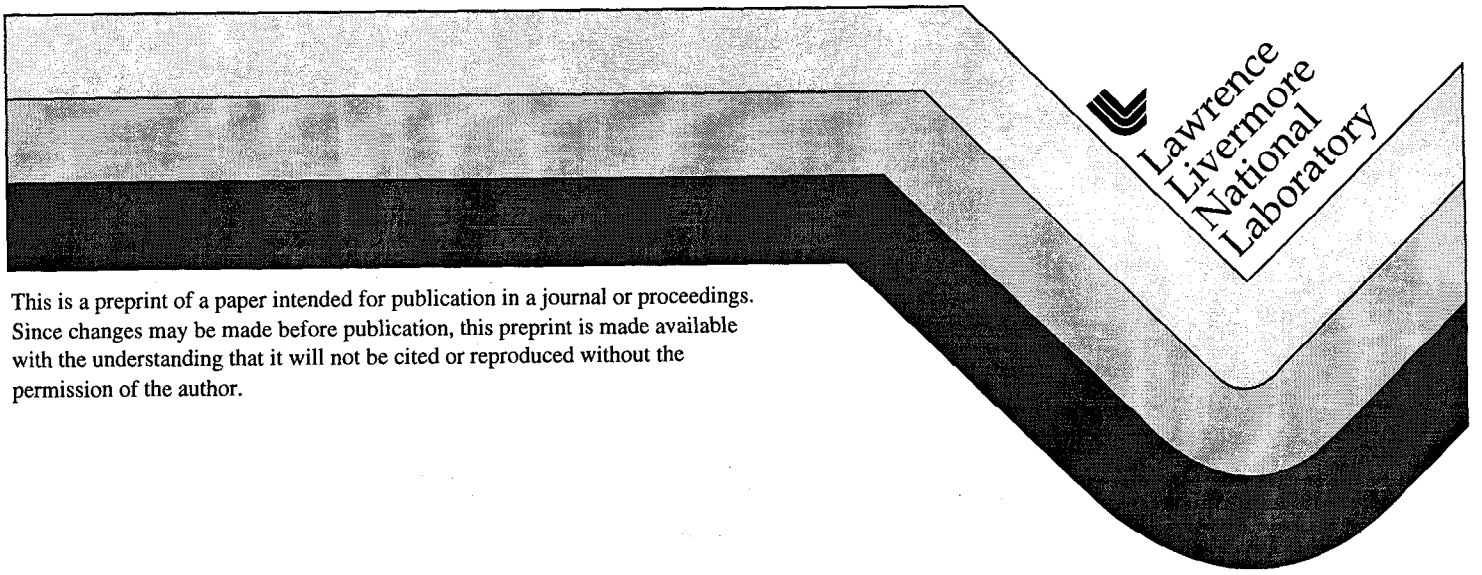

# A LAGRANGIAN STOCHASTIC DIFFUSION METHOD FOR INHOMOGENEOUS TURBULENCE

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**Abstract**—A Lagrangian stochastic method of solving the diffusion equation for inhomogeneous turbulence is presented in this paper. This numerical method uses (1) a first-order approximation for the spatial variation of the eddy diffusivity and (2) the corresponding first three particle position moments, to define a non-Gaussian particle position distribution. The method handles the case when the eddy diffusivity varies linearly to zero at a boundary. This is done by using the first few terms of the series representation of the analytic solution for this case to construct the non-Gaussian position distribution. Comparison of numerical simulation results to analytic solutions of the diffusion equation show that this method is accurate and significantly more efficient than a previously used methods that assume a Gaussian particle position distribution.

*Key word index:* Random walk dispersion model, diffusion equation, inhomogeneous turbulence

## 1. INTRODUCTION

In this paper, we present a Lagrangian stochastic, random walk method for solving the diffusion equation for inhomogeneous turbulence. This method is based on a stochastic

differential equation for particle displacement which describes the ensemble of possible fluid particle trajectories (Durbin, 1980 and 1983). The displacement equation describes the same process as the diffusion equation for the particle position probability density function. A basic assumption of the Lagrangian stochastic approach presented here is that the mean turbulent properties of the flow are known, and are described by an eddy diffusivity.

Models based on the diffusion equation have been shown to be useful tools for simulating the dispersion of material in the inhomogeneous turbulence found in the atmospheric boundary layer, and, in particular, in the surface layer. Nieuwstadt and van Ulden (1978) and Gryning *et al.* (1983) successfully simulated dispersion from a near-surface source in the surface layer under a wide range of stability conditions using an Eulerian diffusion equation model. Lagrangian stochastic models based on the diffusion equation have also been applied to the problem of dispersion in turbulent boundary layers (e.g., Durbin and Hunt, 1980; Boughton *et al.*, 1987; Näslund *et al.*; 1994; Luhar and Rao, 1994).

The diffusion equation approach assumes that the evolution of particle position is a Markov process, that is, a future particle position depends only on the current position, so that displacements are uncorrelated in time. Since displacements are correlated for times on the order of the Lagrangian velocity correlation time, $T_L$, the diffusion equation is valid for predictions at travel times, $t >> T_L$. Because both $T_L$ and wind speed approach zero near the surface (e.g., Hunt and Weber, 1979), the diffusion equation is valid even at very short times and downwind distance for near-surface sources. It is also valid for modeling vertical diffusion in stable boundary layers because $T_L$ becomes small compared to times typically of interest (Luhar and Rao, 1994). However, $T_L$ can become large above the surface layer, particularly in the convective boundary layer, and alternative Lagrangian stochastic models based on the Langevin equation (which

describes a Markov process for the particle velocity) must be used to simulate near-source dispersion (e.g., see review by Wilson and Sawford, 1996).

When valid, the diffusion equation approach can be significantly more efficient than the Langevin equation approach. In typical numerical simulation methods for integrating the Langevin equation the time step must be significantly smaller than $T_L$. As discussed by Durbin and Hunt (1980), this is very restrictive near the surface where parameterizations of $T_L$ approach zero, and, correspondingly, accurate numerical simulation of the Langevin equation using typical methods requires vanishingly small time steps. However, this is not a restriction on the diffusion equation approach.

In previous studies using Lagrangian stochastic models based on the diffusion equation, it has been typical to use lowest order (in time) numerical methods and Gaussian-distributed random displacements (e.g., Boughton *et al.*, 1987; Näslund *et al.*, 1994; Luhar and Rao, 1994). In this paper we present a more efficient and accurate higher order numerical simulation method for solving the diffusion equation when the eddy diffusivity, $K$, is a function of position. The method we present accounts for the fact that if $K$ is inhomogeneous, then the particle position probability distribution is non-Gaussian for finite time steps. In Section 2, we briefly review the Lagrangian stochastic approach based on the diffusion equation. In Section 3, we present a new method for solving the diffusion equation that uses the first three moments of particle position to determine accurate approximations to the non-Gaussian probability distribution of particle position. In Section 4, we demonstrate the accuracy of this method by comparing Monte Carlo numerical simulation results to analytic solutions of the diffusion equation. We also compare simulation results obtained using a lowest order numerical method, which uses a Gaussian particle position distribution, to the analytic solutions.

## 2. STOCHASTIC MODEL

Stochastic models determine the probability distribution of future particle positions, given the initial positions. This probability distribution can be used to calculate the ensemble-mean concentration of material at a desired time, given the concentration distribution at earlier times. Considering one dimension, the ensemble-mean air concentration (mass per unit length), $C(z,t)$, at position $z$ and time $t$ can be determined as follows:

$$C(z,t) = \int_{-\infty}^{t} dt_0 \int_{-\infty}^{\infty} dz_0 \, q(z_0,t_0) P(z,t \; ; \; z_0,t_0), \tag{1}$$

where $q(z_0,t_0)$ represents the source distribution term at position $z_0$ at time $t_0$ (trace material mass emitted per unit time per unit length), and $P(z,t \; ; \; z_0,t_0)$ is the probability density function for the particle position $z$ at time $t$ given it was at position $z_0$ at time $t_0$ (Tennekes and Lumley, 1972). If the source distribution term is constant with time and the turbulent flow is stationary, the ensemble-average concentration can be used as an estimate of the time-average concentration using the ergodic hypothesis (Lumley and Panofsky, 1964).

In this paper, we use the diffusion equation as a model for the time evolution of the transition probability density function for particle position. For a stationary, inhomogeneous turbulent flow with no mean Eulerian velocity, the diffusion equation for an inert, trace material away from any sources can be written, in one dimension, as

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial z}\left( K \frac{\partial P}{\partial z} \right), \tag{2}$$

where $P \equiv P(z,t \; ; \; z_0,t_0)$ and the eddy diffusivity is a function of $z$, $K = K(z)$. Below, we will study the case in which $z$ is the height above a surface. From Eqs. (1) and (2), it can be seen that $C(z,t)$ is also a solution to the diffusion equation, that is,

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(K\frac{\partial C}{\partial z}\right). \tag{3}$$

This is the eddy-diffusivity conservation of species equation. Eq. (1) can therefore be considered a general solution to this conservation of species equation.

The process described by the diffusion equation can also be described by a stochastic differential equation for the displacement of a fluid particle, that may be written as

$$dz = \frac{\partial K}{\partial z}dt + (2K)^{1/2}dW \tag{4}$$

where $dW$ is a random variate with zero mean and variance $dt$, i.e.,

$$\overline{dW} = 0,$$
$$\overline{dW^2} = dt,$$

that is uncorrelated in time, i.e.,

$$\overline{dW_{t_1}dW_{t_2}} = 0, \quad \text{if } t_1 \neq t_2$$

(Durbin, 1983). An overbar, $\overline{\ }$, represents the ensemble average of a quantity. This equation describes the ensemble of possible particle trajectories. Each trajectory represents one realization. Time integration of Eq. (4) provides a means to calculate the $z(t)$ trajectory of a particle. This provides a basis for Lagrangian, Monte Carlo numerical simulations in which a sample of $N$ independent particle trajectories, $\{z_i(t),\ i = 1,2,\ldots N\}$, from a source are used to estimate $P$ and, given a source distribution term, to estimate $C(\bar{z},t)$ using Eq. (1).

## 3. NUMERICAL METHOD

In lowest order (in time) numerical integration of Eq. (4), new particle positions $z(t)$ are generated from a Gaussian distribution $P_G(z,t\ ;\ z_0,t_0)$ with mean

$$\bar{z} = z_0 + \frac{\partial K}{\partial z}\Delta t, \tag{5}$$

and variance

$$\sigma_z^2 = \overline{(z-\bar{z})^2} = 2K\Delta t, \tag{6}$$

where $\Delta t = t - t_0$ is the numerical integration time step and $z_0(t_0)$ is the position at the beginning of the time step. This is repeated with the updated position successively to simulate a particle trajectory. In the presence of an impermeable boundary at $z$=0, particles displaced below the boundary are reflected (if $z$<0, then $z$=–$z$), so that the $P(z,t\ ;\ z_0,t_0) = P_G(z,t\ ;\ z_0,t_0) + P_G(-z,t\ ;\ z_0,t_0)$ for $z \geq 0$, and $P(z,t\ ;\ z_0,t_0)$=0 for $z < 0$.

In this section, we use the first three moments of the non-Gaussian distribution $P(z,t\ ;\ z_0,t_0)$ to develop a higher order (in time) numerical method for simulating the time evolution of particle position.

*3.1 Position moments*

The moments of the distribution $P(z,t\ ;\ z_0,t_0)$ are defined as follows:

$$\overline{z^n} = \int_0^\infty dz\ z^n P(z,t\ ;\ z_0,t_0), \qquad n = 1,2,\ldots\ . \tag{7}$$

Equations for the time evolution of these moments can be determined by first differentiating Eq. (7) with respect to time, yielding

$$\frac{\partial \overline{z^n}}{\partial t} = \int_0^\infty dz\ z^n \frac{\partial P}{\partial t}, \tag{8}$$

where $P = P(z,t\ ;\ z_0,t_0)$. Combining Eqs. (2) and (8), the time derivative of the $n$th moment is

$$\frac{\partial \overline{z^n}}{\partial t} = \int_0^\infty dz\ \ z^n \frac{\partial}{\partial z}\left(K\frac{\partial P}{\partial z}\right) \tag{9}$$

Using a first-order Taylor series approximation for $K(z)$,

$$K(z) = K_0 + \nu_0(z - z_0), \tag{10}$$

where

$$K_0 \equiv K(z_0), \text{ and} \tag{11}$$

$$\nu_0 \equiv \left.\frac{\partial K}{\partial z}\right|_{z_0}, \tag{12}$$

an approximation to Eq. (9) that is accurate to first order in $z$ is

$$\frac{\partial \overline{z^n}}{\partial t} = \int_0^\infty dz\ \ z^n \frac{\partial}{\partial z}\left(\left[K_0 + \nu_0(z - z_0)\right]\frac{\partial P}{\partial z}\right). \tag{13}$$

Performing the integration in Eq. (13) for $n$ = 1, 2, and 3 using the assumption that $P \to 0$ and $\partial P/\partial z \to 0$ faster than $z^n \to \infty$, yields equations for the time derivatives of the first three moments,

$$\frac{\partial \bar{z}}{\partial t} = \left(K_0 - \nu_0 z_0\right)P(0) + \nu_0, \tag{14}$$

$$\frac{\partial \overline{z^2}}{\partial t} = 2\left(K_0 - \nu_0 z_0\right) + 4\,\nu_0 \bar{z}, \tag{15}$$

$$\frac{\partial \overline{z^3}}{\partial t} = 6\left(K_0 - \nu_0 z_0\right)\bar{z} + 9\,\nu_0 \overline{z^2} \tag{16}$$

where $P(0) = F(0,t;z_0,t_0)$. If we assume either (a) $z_0$ is much greater than zero so that the particle has negligible probability of being displaced to $z = 0$ in a finite time step and therefore $P(0) \rightarrow 0$, or (b) for small $z_0$, $K$ varies linearly and vanishes at the surface (i.e., $K_0 \approx v_0 z_0$) in accordance with surface-layer similarity theory (e.g., Businger, 1973), then Eq. (14) may be simplified to

$$\frac{\partial \bar{z}}{\partial t} = v_0 \tag{17}$$

Integrating Eqs. (15-17) from $(z_0,\ t_0)$ to $(z,\ t)$ yields the following time-dependent moment equations:

$$\bar{z} = z_0 + v_0 \Delta t \tag{18}$$

$$\overline{z^2} = z_0^2 + 2(K_0 + v_0 z_0)\Delta t + 2v_0^2 \Delta t^2 \tag{19}$$

$$\overline{z^3} = z_0^3 + \left(3v_0 z_0^2 + 6K_0 z_0\right)\Delta t + \left(6v_0^2 z_0 + 12K_0 v_0\right)\Delta t^2 + 6v_0^3 \Delta t^3 \tag{20}$$

where $\Delta t \equiv t - t_0$. The mean, variance and third central moment of $z$ may be written, using Eqs. (18-20), as

$$\bar{z} = z_0 + v_0 \Delta t, \tag{21}$$

$$\sigma_z^2 \equiv \overline{\left(z - \bar{z}\right)^2} = 2K_0 \Delta t + v_0^2 \Delta t^2, \text{ and} \tag{22}$$

$$\zeta_z^3 \equiv \overline{\left(z - \bar{z}\right)^3} = 6K_0 v_0 \Delta t^2 + 2v_0^3 \Delta t^3, \tag{23}$$

Comparison to Eqs. (5-6) shows that Eqs. (21-23) provide a higher order in time approximation to the moments of the particle position when $v_0 \neq 0$. The skewness of $z$ is defined as

$$S_z \equiv \zeta_z^3 / \sigma_z^3. \tag{24}$$

It can be seen that for $K_0 \neq 0$ and $\Delta t << 1$, the skewness vanishes ($S_z \rightarrow 0$), and the probability distribution of $z$ approaches a Gaussian distribution. However, since we have assumed that $K_0 \rightarrow 0$ as $z_0 \rightarrow 0$ in accordance with surface-layer similarity theory relationships for $K$, the higher order terms are needed even for $\Delta t << 1$ in order to prevent the second and third moments from vanishing when the initial particle position is near the surface. It can be seen that as $K_0 \rightarrow 0$, $S_z \rightarrow 2$ for any non-zero values of $\Delta t$ and $v_0$.

In summary, the position moments given in Eqs. (21-23) are exact if $K(z)$ is linear and also vanishes at $z$=0 so that $K(z) = v_0 z$, which is assumed to be the case here, at least near the surface. Far from the surface, Eqs. (21-23) are essentially exact if $K(z)$ varies linearly with $z$, i.e., $K(z) = K_0 + v_0(z - z_0)$, over the practical domain of $z$ during $\Delta t$. Obviously, the accuracy of these moments for cases when $K(z)$ is nonlinear will depend on the accuracy of the linear approximation over this domain.

*3.2 Analytic solution for special case:* $K(z) = vz$

The exact analytic solution to the diffusion equation, Eq. (2), for the special case in which there is an impermeable boundary at $z$=0, and $K(z) = vz$ is

$$P(z;\ z_0, \Delta t) = \frac{1}{v\Delta t}\ \exp\left[\frac{-(z+z_0)}{v\Delta t}\right]\ I_0\left[\frac{2(zz_0)^{1/2}}{v\Delta t}\right] \tag{25}$$

(Huang, 1979), where $I_0$ is the modified Bessel function of the first kind of order zero. This solution, Eq. (25), can also be represented by an infinite series:

$$P(z\ ;\ z_0, \Delta t) = \frac{1}{v\Delta t}\exp\left[\frac{-(z+z_0)}{v\Delta t}\right]\sum_{j=0}^{\infty}\frac{(zz_0)^j}{(j!)^2(v\Delta t)^{2j}}. \tag{26}$$

For the special case of $z_0 = 0$, Eqs. (25) and (26) reduce to an exponential distribution, $P(z;\ 0, \Delta t) = \frac{1}{v\Delta t}\exp\left[\frac{-z}{v\Delta t}\right]$, which has a skewness of 2 (consistent with $z$ moment

equations above for this case). Higher order terms in Eq. (26) can be also be represented using gamma distributions.

*3.3 Approximate form for $P(z)$*

We explored several approximate forms for $P(z)=P(z,t\ ;\ z_0,t_0)$. As shown in Sections 3.1 and 3.2, if $z_0 > 0$, then $P(z)$ is generally non-Gaussian (with non-zero skewness) and approaches a Gaussian distribution (with zero skewness) only in the limit as $\Delta t \rightarrow 0$. For $z_0 = 0$ and the physically realistic case in which $K$ is linear and vanishes at $z$=0, $P(z)$ is exponential (with skewness value of 2) regardless of the size of the time step, $\Delta t$. Therefore, in order to use longer time steps in numerical simulations we need a skewed distribution function from which we can generate random numbers. This distribution must allow a large range of skewness, with absolute values from 0 to 2, and must accurately simulate the case in which $K$ is linear and vanishes at a boundary.

The general form for $P(z)$ that we use is

$$P(z) \cong f_0 P_0(z) + f_1 P_1(z). \tag{27}$$

$P_0(z)$ is a skewed probability density function constructed from the lower order terms in the series representation of the analytic solution given in Eq. (26). These lower order terms are important near the surface and allow for accurate approximation of the highly skewed form of $P(z)$ as $z_0 \rightarrow 0$. $P_1(z)$ is a probability density function which can have zero or non-zero skewness. For $z_0 >> 0$, $P_1(z)$ can be used alone as an accurate approximation for $P(z)$.

We define the two terms of $P(z)$ in Eq. (27) in the following way. First, the term $f_0 P_0(z)$ is set equal to the first $m$+1 terms from the series representation of the analytic solution

given in Eq. (26). $P_0(z)$ can, then, be represented as a combination of gamma distribution functions, and has the form

$$P_0(z) = \frac{1}{f_0} \sum_{j=0}^{m} f_{gj} P_{gj}(z), \tag{28}$$

where

$$P_{gj}(z) = \frac{z^j}{(v_0 \Delta t)^{j+1} j!} \exp\left[\frac{-z}{v_0 \Delta t}\right], \tag{29}$$

$$f_{gj} = \frac{z_0^j}{(v_0 \Delta t)^j j!} \exp\left[\frac{-z_0}{v_0 \Delta t}\right], \text{ and} \tag{30}$$

$$f_0 = \sum_{j=0}^{m} f_{gj}. \tag{31}$$

Each $P_{gj}$ is a gamma probability density function (for the special case when $j = 0$, it is the exponential distribution function). This form for $P_0(z)$ is used because if $m = \infty$, then $f_0 P_0(z)$ is the exact solution for $P(z)$ when $K(z) = v_0 z$, as given in Eq. (26).

We then determine $f_1$ and the parameters of $P_1(z)$ from the normalization condition, $\int_{-\infty}^{\infty} P(z)dz = 1$, and the desired first three moments of $z$ given in Eqs. (21-23). Using Eq. (27), the $n$th moment of $z$ can be written as

$$\overline{z^n} = \int_0^{\infty} z^n P(z)dz \cong f_0 \int_0^{\infty} z^n P_0(z)dz + f_1 \int_{-\infty}^{\infty} z^n P_1(z)dz, \tag{32}$$

or

$$\overline{z^n} \cong f_0 \overline{z_0^n} + f_1 \overline{z_1^n}, \tag{33}$$

where

$$\overline{z_0^n} \equiv \int_0^\infty z^n P_0(z)dz, \tag{34}$$

$$\overline{z_1^n} \equiv \int_{-\infty}^\infty z^n P_1(z)dz. \tag{35}$$

(Note that the notation $\overline{z_0^n}$ is used here to represent the moments of the distribution $P_0(z)$, and does not refer to $z_0=z(t_0)$ used above.) Since $P_0(z)$ and $f_0$ are known, the moments $\overline{z_0^n}$, defined by Eq. (34), can be calculated using Eqs. (28-31) and are

$$\overline{z_0^n} = \frac{1}{f_0}\sum_{j=0}^{m}\left[ f_{gj}\frac{(j+n)!}{j!}\left(v_0\Delta t\right)^n \right]. \tag{36}$$

We now have all the information we need to solve Eqs. (33) for $f_1$ and the three moments $\overline{z_1}$, $\overline{z_1^2}$, and $\overline{z_1^3}$ of $P_1(z)$. Consequently, we determine $f_1$ and the three moments $\overline{z_1}$, $\overline{z_1^2}$, and $\overline{z_1^3}$ of $P_1(z)$ (four unknowns) from the following four equations:

$$1 = f_0 + f_1, \tag{37}$$

$$\bar{z} = f_0\overline{z_0} + f_1\overline{z_1}, \tag{38}$$

$$\overline{z^2} = f_0\overline{z_0^2} + f_1\overline{z_1^2}, \tag{39}$$

$$\overline{z^3} = f_0\overline{z_0^3} + f_1\overline{z_1^3}. \tag{40}$$

We explored two general types of skewed $P_1(z)$ functions: (i) transformed Gaussian distributions, and (ii) linear combinations of two distributions (including two different Gaussian distributions). The first type proved to be more accurate. In specifying a transformed Gaussian distribution, we first define the desired random variable $z$ from distribution $P_1(z)$ as follows

$$z = \overline{z_1} + x \tag{41}$$

where the non-Gaussiar random variable $x$ has zero mean and is generated by transforming a Gaussian* random variable $r$ (with zero mean and variance of 1) using

$$x = \frac{a}{b}\left( e^{br} - e^{\frac{b^2}{2}} \right). \tag{42}$$

(A series expansion useful for evaluating $x$ is given in the Appendix.) The value of $\overline{z_1}$ is know from Eq. (38). The parameters $a$ and $b$, needed to calculate $x$, are determined so that z has the desired variance and skewness given by

$$\sigma_{z_1}^2 \equiv \overline{z_1^2} - \overline{z_1}^2 \tag{43}$$

$$S_{z_1} \equiv \frac{\overline{z_1^3} - 3\overline{z_1^2}\,\overline{z_1} + 2\overline{z_1}^3}{\sigma_{z_1}^3} \tag{44}$$

where $\overline{z_1}$, $\overline{z_1^2}$, and $\overline{z_1^3}$ are defined by Eqs. (38-40). Given that $P(r)$ is a Gaussian distribution, the analytic expression for $P(x)$ is then

$$P(x) = P(r)\frac{dr}{dx} = \frac{1}{a\sqrt{2\pi}} e^{-\frac{r(x)^2}{2}} e^{-br(x)} \tag{45}$$

where

$$-\frac{a}{b} e^{\frac{b^2}{2}} < x < \infty,$$

and

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* Alternate distributions may be used for $r$ which are sums of $k$ uniform random numbers, $r = \sum_{i=1}^{k} r_i$, where $r_i$ is a uniform random number on $(-l, +l)$ and $l = \sqrt{3/k}$ .The random variable $r$ , then, has zero mean, variance of one, and a symmetric probability distribution with a shape that varies with $k$. In the limit as $k \to \infty$, $r$ approaches a Gaussian random number according to the Central Limit Theorem.

$$r(x) = \frac{1}{b}\ln\left(e^{\frac{b^2}{2}} + \frac{bx}{a}\right). \tag{46}$$

The mean of $x$ is zero, $\bar{x} = 0$. Using the expression for $P(x)$, the variance of $x$ is

$$\sigma_x^2 \equiv \overline{(x-\bar{x})^2} = \frac{a^2}{b^2} e^{b^2}\left(e^{b^2} - 1\right). \tag{47}$$

The skewness of $x$ is

$$S_x \equiv \frac{\overline{(x-\bar{x})^3}}{\sigma_x^3} = \left(e^{b^2} + 2\right)\left(e^{b^2} - 1\right)^{1/2}. \tag{48}$$

Therefore, $b$ can be determined using Eq. (48) with $S_x = S_{z_1}$, where $S_{z_1}$ is computed using Eq. (44). However, there is no explicit solution for $b(S_x)$. We use an accurate polynomial approximation (see Appendix) for $b(S_x)$ (Newton's method can also be used to obtain a solution for $b$ iteratively to any accuracy desired). After determining the value for $b$, the value of $a$ can be determined using Eq. (47) with the value of $\sigma_x^2 = \sigma_{z_1}^2$ calculated using Eq. (43). This can be done in an efficient and accurate manner by using a series expansion for $a/\sigma_x$ (see Appendix). Random values of $z$ (for use in Monte Carlo numerical simulations) can be calculated simply by obtaining a random value of $r$, transforming it to $x$ using Eq. (42), and generating a random value of $z$ with Eq. (41).

Examples of the exact $P(z)$ for the case of $K(z)=vz$ and the corresponding approximate $P(z)$ and its individual terms for $m$=3 are shown in Figs. 1 and 2. Fig. 1a shows the exact and approximate dimensionless distributions, $v\Delta tP(z)$, versus dimensionless height $z/v\Delta t$ for $z_0/v\Delta t$=2. Fig. 1b shows the corresponding terms of the approximate dimensionless distribution: $v\Delta tf_{g0}P_{g0}(z)$, $v\Delta tf_{g1}P_{g1}(z)$, $v\Delta tf_{g2}P_{g2}(z)$, $v\Delta tf_{g3}P_{g3}(z)$, and $v\Delta tf_1P_1(Z)$. Fig. 2 shows the same distributions for $z_0/v\Delta t$=4. These figures show that

for $z_0$ close to zero the terms from $P_0(z)$ dominate the approximate $P(z)$. For larger $z_0$, the $P_1(Z)$ term makes a larger contribution.

The numerical simulation method based on this approximate non-Gaussian $P(z)$ can be summarized as follows. Given position $z_0(t_0)$ at the beginning of a time step, a new particle position $z(t)$ is generated from the non-Gaussian distribution $P(z,t\ ;\ z_0,t_0)$, given by Eq. (27), which has the first three moments given by Eqs. (21-23). This is done by first calculating $f_{gj}$, $j=0,\ 1,\ldots m$, and $f_0$. Then, a uniform random number $U$ on (0,1) is generated. If $U \le \sum_{i=0}^{j} f_{gi}$ (the smallest value of $j$ that meets this criteria is used), then a value of $z$ from the gamma distribution $P_{gj}(z)$ is generated. Random values of $z$ can easily be generated from a gamma distribution $P_{gj}(z)$ using $j$+1 uniform random numbers as follows:

$$z = -v_0 \Delta t\ \ln\left(\prod_{i=1}^{j+1} U_i\right), \tag{49}$$

where the $U_i$, $i=1,\ 2,\ \ldots\ (j+1)$, are independent uniform random variables on (0,1) (Ross, 1993). If $U > f_0$, then (i) calculate $\sigma_{z_1}^2$ and $S_{z_1}$, (ii) use these to calculate $a$, $b$, and $x$, and (iii) obtain a value of $z$ from the $P_1$ distribution, as discussed above. When $S_{z_1}$ is negative (when $v_0 < 0$), $x$ can be calculated using $S_x = |S_{z_1}|$, and then changing the sign of $x$ (i.e., $x=-x$). For particle positions well above the surface (we use the criteria $z_0^2 > 10K_0\Delta t + 5v_0^2\Delta t^2$), it is assumed that $P(z)=P_1(z)$. Depending on the values of $z_0$, $\Delta t$, and $m$, and on the form of $K(z)$, there may be a small probability of $z < 0$. Simple reflection is used when this occurs (i.e., if $z < 0$, then $z=-z$).

## 4. EVALUATION OF METHOD

In this section, numerical simulations using the higher order, non-Gaussian method described in the previous section are evaluated using the analytic solution to the diffusion

equation for the case in which there is an impermeable boundary at $z = 0$ and $K = vz$. This is a physically realistic case since it is consistent with eddy diffusivity relationships for the neutral (adiabatic) atmospheric surface layer, and with relationships for the diabatic surface layer for heights much less than the absolute value of the Monin-Obukhov length ($z << |L|$).

For this case, the numerical method is exact as $z_0 \rightarrow 0$ (except for statistical error due to the finite number of trajectories computed) because the first few terms in the analytic solution for this case were used to construct the $f_0 P_0(z)$ term in the *P(z)* distribution. As $z_0 \rightarrow 0$, the first few terms of $f_0 P_0(z)$ dominate the exact solution for this case. We used a value of $m$ =3 for $P_0(z)$, given by Eq. (28), for the simulations in this paper. For $z_0$>>0, the accuracy of the method depends on the accuracy of $P_1(z)$, which dominates.

Numerical simulations were performed in which particle positions were all initialized to a value of $z_0$ at the beginning of the simulation. A total of $5 \times 10^5$ particle trajectories were computed in each simulation. Particle position distributions, $P(z)$, were calculated by sampling particles in 40 evenly spaced bins between $z$=0 and $4\bar{z}$.

Figure 3 shows examples of the dimensionless probability density, $P(Z)$, where $Z = z/vt$, simulated using the non-Gaussian method, as well as the analytic solution, given in Eq. (25), for initial particle positions at the surface, $Z_0$=0. This method is exact after a single time step for this case ( $P(z) = P_{g0}(z)$, an exponential distribution). This is reflected in the excellent agreement between the analytic solution and numerical solution using a single step, i.e., a dimensionless time step of $\Delta t/t$=1 (Fig. 3a). The results of simulations with the non-Gaussian method are also excellent using a smaller time step, $\Delta t/t$=0.1 (Fig. 3b), with very small error introduced because the method is approximate for particle positions greater than zero at intermediate times in this simulation.

For comparison, numerical simulations were also performed using the lower order, Gaussian numerical method. This method was described at the beginning of Section 3, and uses a Gaussian position distribution with moments defined by Eqs. (5) and (6). Figure 4 shows the results for $Z_0$=0 obtained using the Gaussian method and time steps of $\Delta t/t$=1, 0.1, and 0.01. These results show that, compared to the non-Gaussian method, the Gaussian method requires considerably smaller time steps (by a factor of more than 100) to approach the analytic solution for this case. Consequently, the computer CPU time required to achieve accurate solutions for this case with the Gaussian method is considerably greater (by a factor of more than 50).

Figure 5 shows an example of $P(Z)$ simulated using the non-Gaussian method and the analytic solution for a initial position above the surface, $Z_0$=4. This numerical method is not exact in a single step for this $Z_0$, but the numerically simulated distribution is a very good approximation to the analytic distribution when using a time step equal to the total simulation time, $\Delta t/t$=1 (Fig. 5a). The small numerical error quickly vanishes as the time step is decreased, as shown by the results of a simulation using $\Delta t/t$=0.1 in Fig. 5b. Figure 6 shows the results for $Z_0$=4 obtained using the Gaussian method and time steps of $\Delta t/t$=1, 0.1, and 0.01. These results again show that considerably smaller time steps are required for this lower order, Gaussian method to approach the analytic solution.

When $K$ is a non-linear function of $z$, the time step must be restricted so that the first-order approximation to $K$ does not introduce unacceptable numerical error. Simulations were performed using the higher order, non-Gaussian method with the quadratic function $K = vz\left(1-\frac{z}{h}\right)$ and an initially uniform distribution of particles in order to determine the size time step needed to maintain the correct steady-state uniform distribution. The results of these simulations (not shown) indicate that restricting the time step so that $\sigma_z(\Delta t)/h$ is

less than or equal to 0.1 results in fractional error of less than approximately 4% in the calculated probability density.

## 5. SUMMARY

We presented the development and testing of a higher order Lagrangian stochastic method for solving the diffusion equation that uses a non-Gaussian particle position distribution. This method uses a first-order approximation for the spatial variation of the eddy diffusivity. An approximation to the non-Gaussian particle position distribution is defined using the first three position moments. The case when the eddy diffusivity varies linearly to zero at a boundary is handled by using the first few terms of the series representation of the analytic solution for this case in constructing the approximate non-Gaussian distribution. This approach accounts for the effect that the first-order spatial variation of the eddy diffusivity has on the mean, variance, and third moment of the particle position distribution. In contrast, the previously used method that employs a Gaussian particle position distribution only accounts for this effect on the mean of the distribution. The new non-Gaussian method is of higher order in time than this previously used Gaussian method. Comparison of numerical simulation results to analytic solutions for a linear eddy diffusivity show that this new higher order, non-Gaussian method is accurate and significantly more efficient than the lower order, Gaussian method.

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## REFERENCES

Boughton, B.A., J.M. Delaurentis, and W.E. Dunn (1987) A stochastic model of particle dispersion in the atmosphere, *Boundary-Layer Meteor.*, **40**, 147-163.

Businger, J.A. (1973) Turbulent transfer in the atmospheric surface layer, In: *Workshop on Micrometeorology* (D.A. Haugen, ed.), American Meteorological Society, Boston, MA, pp. 67-100.

Durbin, P.A. (1980) A random flight model of inhomogeneous turbulent dispersion, *Phys. Fluids*, **23**, 2151-2153.

Durbin, P.A. and J.C.R. Hunt (1980) Dispersion from elevated sources in turbulent boundary layers, *J. de Mécanique*, **19**, 679-695.

Durbin, P.A. (1983) *Stochastic differential equations and turbulent dispersion.* NASA Reference Publication 1103, 69 pp. (Available from NTIS as N8322546)

Gryning, S.-E., A.P. van Ulden, and S.E. Larsen (1983) Dispersion from a continuous ground-level source investigated by a *K* model, *Quart. J. R. Met. Soc.*, **109**, 355-364.

Huang, C.H. (1979) A theory of dispersion in turbulent shear flow, *Atmos. Environ.*, **13**, 453-463.

Hunt, J.C.R. and A.H. Weber (1979) A Lagrangian statistical analysis of diffusion from a ground-level source in a turbulent boundary layer, *Quart. J. R. Met. Soc.*, **105**, 423–443.

Luhar, A.K. and K.S. Rao (1994) Lagrangian stochastic dispersion model simulations of tracer data in nocturnal flows over complex terrain. *Atmos. Environ.*, **28**, 3417-3431.

Lumley, J.L. and H.A. Panofsky (1964) *The Structure of Atmospheric Turbulence.* John Wiley and Sons, Inc., New York.

Näslund E., H.C. Rodean, and J.S. Nasstrom, 1994: A comparison between two stochastic diffusion models in a complex three-dimensional flow. *Boundary-Layer Meteorol.*, **67**, 369-384.

Nieuwstadt, F.T.M. and A.P. van Ulden (1978) A numerical study on the vertical dispersion of passive contaminants from a continuous source in the atmospheric surface layer, *Atmos. Environ.*, **12**, 2119-2124

Ross, S.M. (1993) *Introduction to Probability Models*, Academic Press, Inc., San Diego, 556 pp.

Tennekes H., and J.L. Lumley (1972) *A First Course in Turbulence.* The MIT Press, Cambridge, MA.

Wilson, J.D. and B.L. Sawford: 1996, 'Review of Lagrangian stochastic models for trajectories in the turbulent atmosphere', *Boundary-Layer Meteorol.*, **78**, 191-210.

## APPENDIX

A truncated series expansion may be used to accurately evaluate $x$ as follows:

$$x = a\left(x_{br} - x_{bb}\right)$$

where

$$x_{bb} = \left(\frac{b}{2}\right)\left[1 + \left(\frac{b}{2}\right)^2 + \frac{2}{3}\left(\frac{b}{2}\right)^4 + \frac{1}{3}\left(\frac{b}{2}\right)^6\right],$$

and, in general,

$$x_{br} = \frac{1}{b}\left(e^{br} - 1\right).$$

However, for small absolute values of $br$, $|br| < 0.1$, we use the approximation

$$x_{br} = r\left[1 + \left(\frac{br}{2}\right) + \frac{2}{3}\left(\frac{br}{2}\right)^2 + \frac{1}{3}\left(\frac{br}{2}\right)^3 + \frac{2}{15}\left(\frac{br}{2}\right)^4\right].$$

An accurate polynomial approximation for $b$ is

$$b(S_x) \cong c_1 S_x + c_3 S_x^3 + c_5 S_x^5 + c_7 S_x^7$$

where $c_1 = \frac{1}{3}$, $c_3 = -0.02124555359$, $c_5 = 0.002368933581$, $c_7 = -0.000165946201$. The form of this approximation was taken from the reversion of the series expansion for $S_x$. The first term is identical to the first term of the reversion series expansion. The coefficients for the third, sixth and seventh order terms, however, were determined using a least squares procedure to achieve the best overall fit to the exact values in the range $0 \le S_x \le 2$. This approximation results in $b$ values which produce $S_x$ values with fractional errors less than 0.0003, compared to the desired $S_x$ value in the range $0 \le S_x \le 2$. A series expansion approximation for $a/\sigma_x$, truncated after sixth order in $b$, is

$$\frac{a}{\sigma_x} \cong 1 - \tfrac{3}{4}b^2 + \tfrac{25}{96}b^4 - \tfrac{7}{128}b^6.$$

## FIGURE CAPTIONS

Fig. 1. Example of dimensionless probability density, $v\Delta tP(z)$, versus dimensionless height, $z/v\Delta t$, for $z_0/v\Delta t$=2: (a) exact analytic distribution (solid line) and approximate distribution used with the higher order non-Gaussian numerical method (dashed line), and (b) terms in the approximate distribution, $v\Delta tf_{g0}P_{g0}(z)$, $v\Delta tf_{g1}P_{g1}(z)$, $v\Delta tf_{g2}P_{g2}(z)$, $v\Delta tf_{g3}P_{g3}(z)$ (solid lines), and $v\Delta tf_1P_1(z)$ (dashed line).

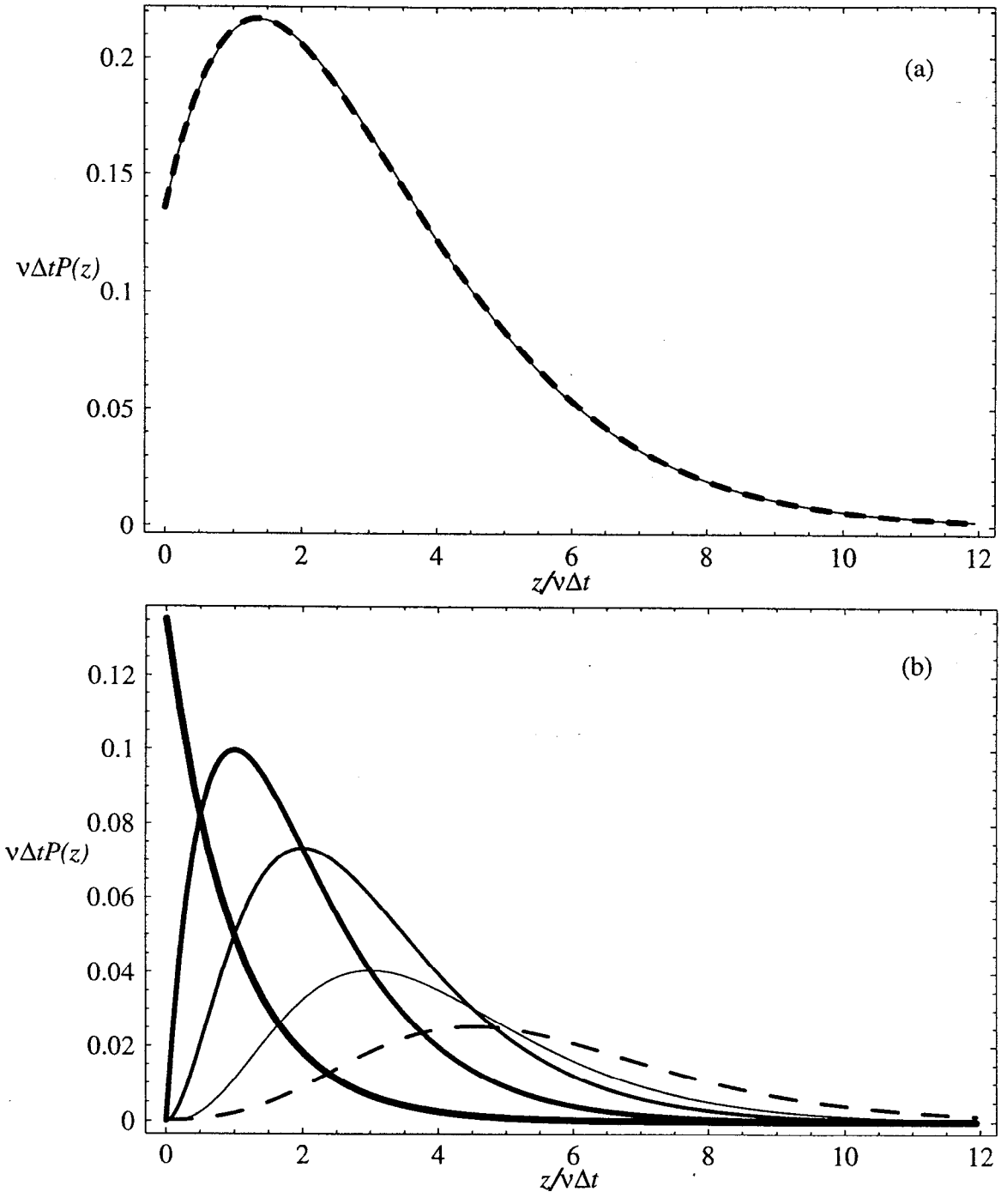
Fig. 2. Same as Fig. 1, except for $z_0/v\Delta t$=4.

Fig. 3. Dimensionless probability density scaled by the mean height, $\overline{Z}\,P(Z)$, versus height, $Z/\overline{Z}$ (where $Z=z/vt$) for initial height $Z_0$=0 calculated from simulations using the higher order, non-Gaussian method and time steps of (a) $\Delta t/t$=1 and (b) $\Delta t/t$=0.1.

Fig. 4. Dimensionless probability density scaled by the mean height, $\overline{Z}\,P(Z)$, versus height, $Z/\overline{Z}$, for initial height $Z_0$=0 calculated from simulations using the lower order, Gaussian method and time steps of (a) $\Delta t/t$=1, (b) $\Delta t/t$=0.1, and (c) $\Delta t/t$=0.01.

Fig. 5. Same as Fig. 3 except for initial height $Z_0$=4.

Fig. 6. Same as Fig. 4 except for initial height $Z_0$=4.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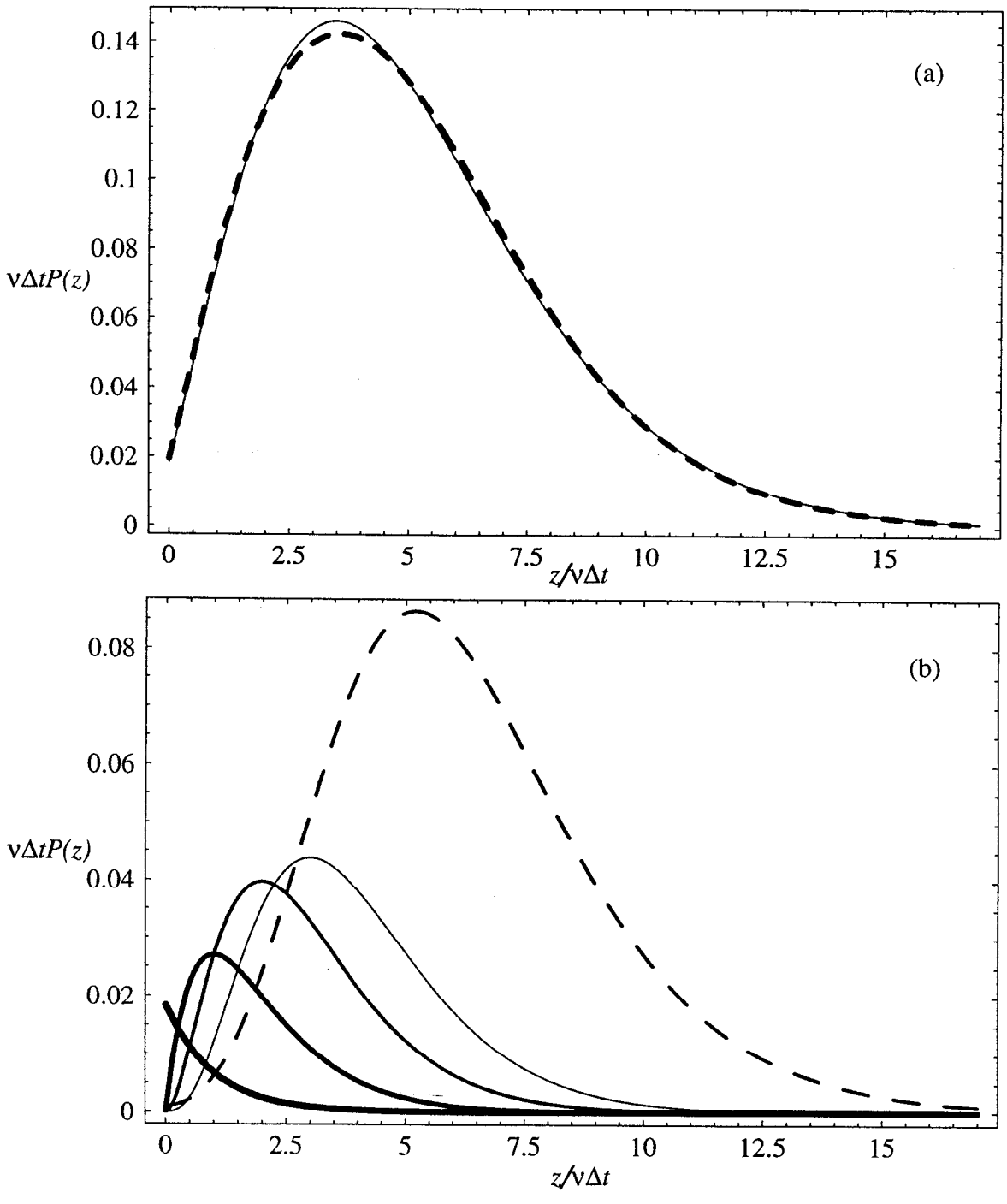
0.1
0.05
0
νΔtP(z)
0
2
4
6
8
10
12
z/νΔt
(b)
0.12
0.1
0.08
0.06
0.04
0.02
0
νΔtP(z)
0
2
4
6
8
10
12
z/νΔt

Fig. 1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5
7.5
10
12.5
15
z/νΔt
(b)
0.08
0.06
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12.5
15
z/νΔt

Fig. 2

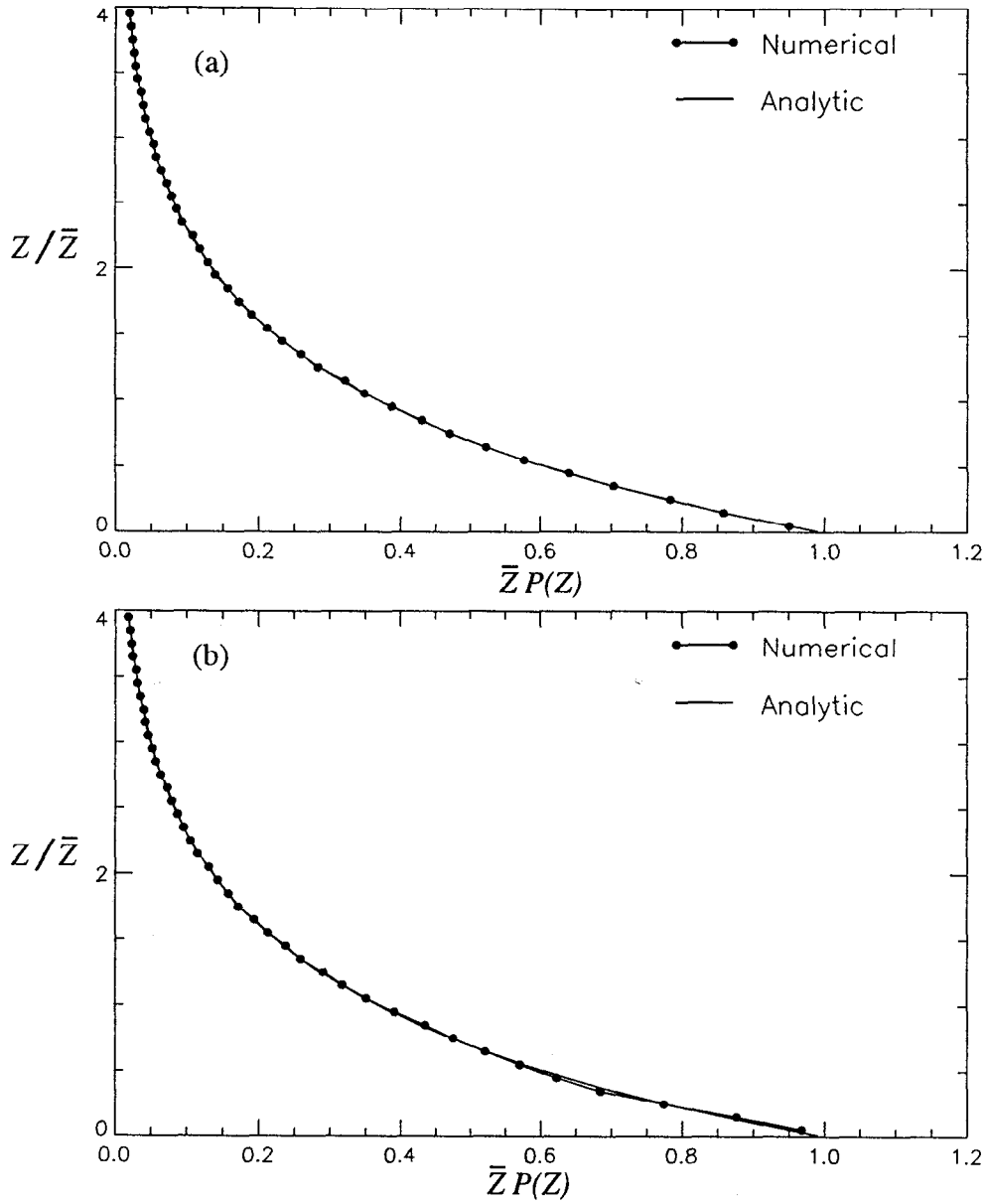

(a)
Numerical
Analytic
$Z/\bar{Z}$
$\bar{Z}\,P(Z)$
(b)
Numerical
Analytic
$Z/\bar{Z}$
$\bar{Z}\,P(Z)$

Fig. 3

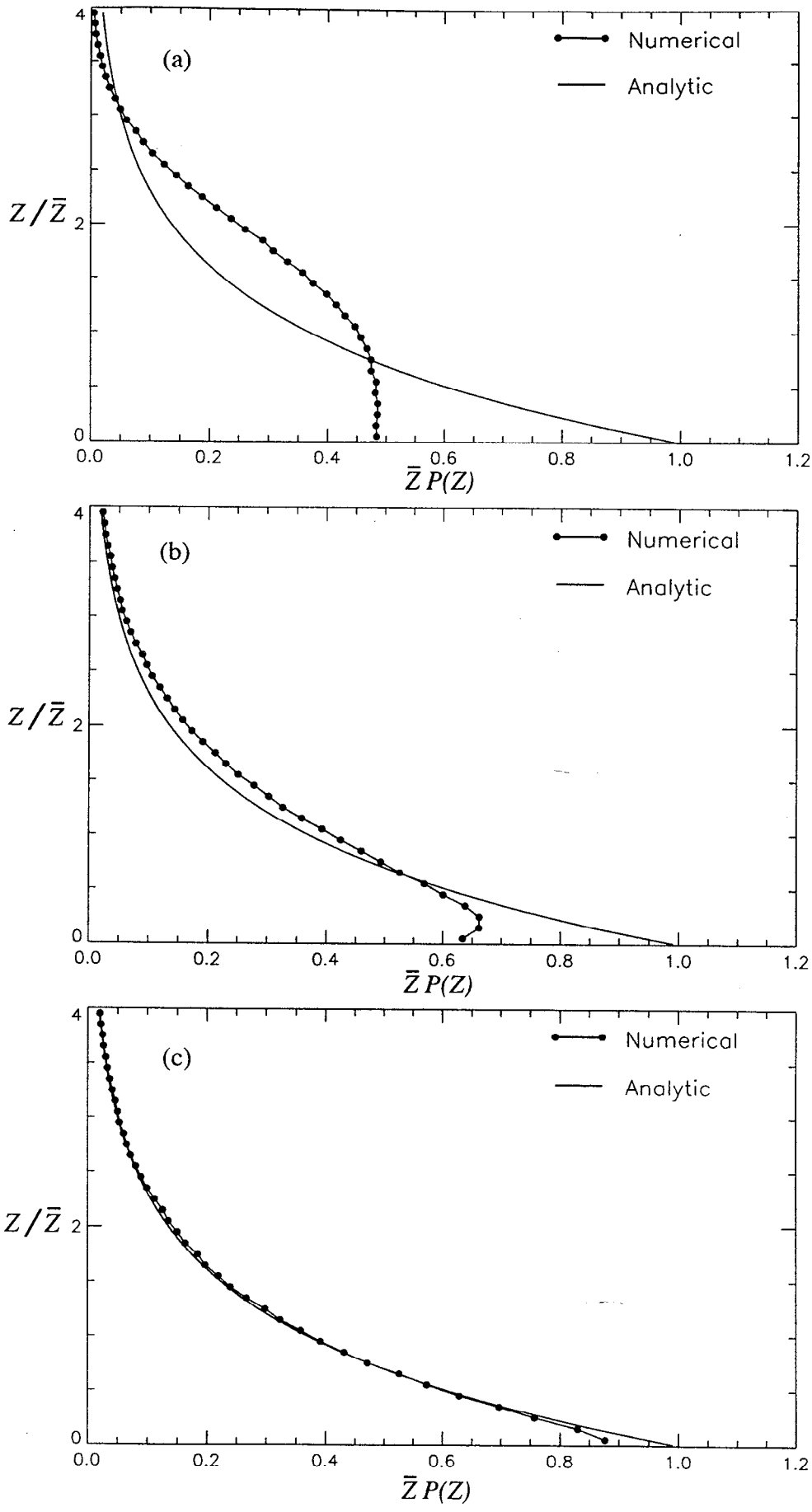
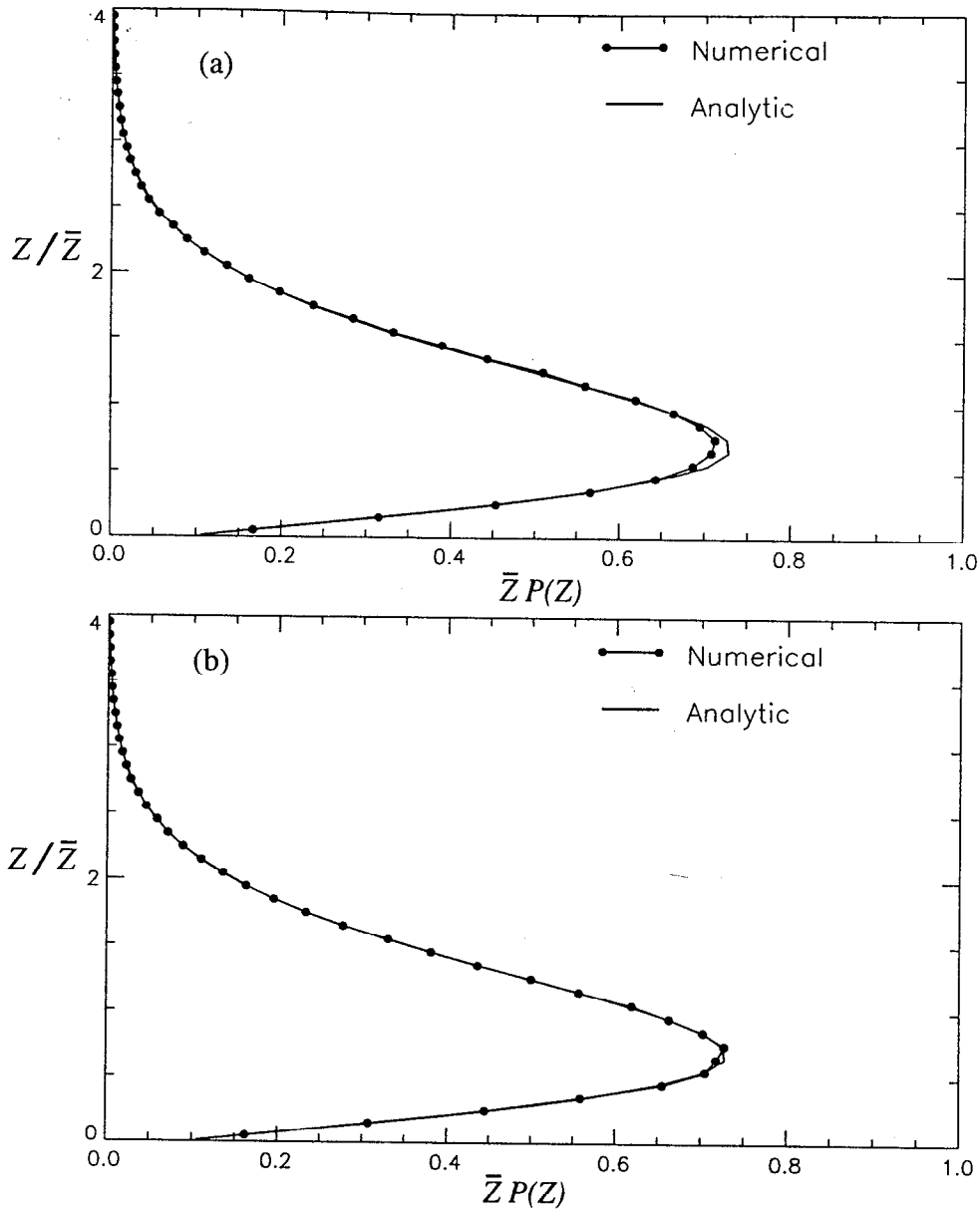

(a)
Numerical
Analytic
$Z/\bar{Z}_2$
$\bar{Z}\,P(Z)$
(b)
Numerical
Analytic
$Z/\bar{Z}_2$
$\bar{Z}\,P(Z)$
(c)
Numerical
Analytic
$Z/\bar{Z}_2$
$\bar{Z}\,P(Z)$

Fig. 4


(a)
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$Z/\bar{Z}$
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(b)
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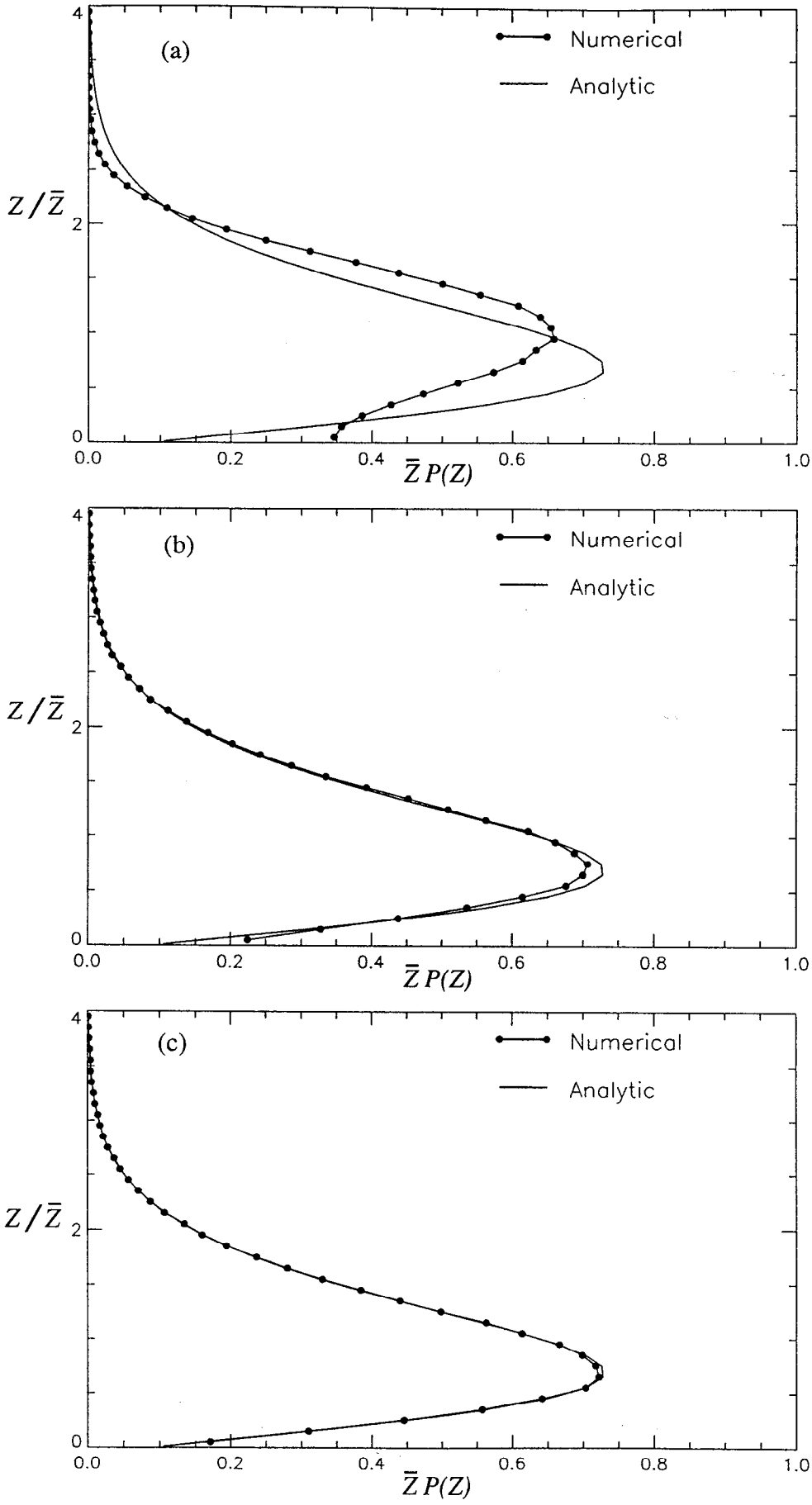
Fig. 5


(a)
Numerical
Analytic
$Z/\bar{Z}$
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(b)
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Analytic
$Z/\bar{Z}$
$\bar{Z}\,P(Z)$
(c)
Numerical
Analytic
$Z/\bar{Z}$
$\bar{Z}\,P(Z)$

Fig. 6