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S. B. Pope^a

^a Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA

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An Improved Turbulent Mixing Model

S. B. POPE† *Massachusetts Institute of Technology, Department of Mechanical Engineering, Cambridge, MA 02139*

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Abstract—In application to turbulent reactive flows, both stochastic models and pdf methods require a model of turbulent mixing. Models currently in use are due to Curl (1963), Dopazo (1979), and Janicka, Kolbe, and Kollmann (1979). For the simple case of decaying fluctuations of a passive scalar in homogeneous turbulence, measurements suggest that the probability density function (pdf) tends to a Gaussian. All the moments of the standardized Gaussian pdf are finite and, in particular, the fourth moment (the flatness factor) is equal to 3. It is shown that the existing models produce pdf's that differ significantly from the Gaussian; in particular, the predicted flatness factors are infinite. An improved class of mixing models is presented that produces pdf's with finite standardized moments. The shape of the pdf produced depends upon the choice of two model parameters. These parameters can be chosen so that the flatness is as small as 3.12 (cf. 3 for a Gaussian), while the recommended model, which has a better overall performance, results in a flatness of 3.70. The shape of this pdf (shown on Figure 5) is close to Gaussian.

1 INTRODUCTION

Two parallel theoretical approaches have been developed for dealing with the effects of turbulent fluctuations on chemical reactions. First, stochastic mixing models have been used by Kattan and Adler (1967), Flagan and Appleton (1974), and Pratt (1976) to study combustion in statistically homogeneous turbulence. Second, evolution equations for the joint probability density function (pdf) of the reactant concentrations have been solved. This approach, which is not restricted to the homogeneous case, has been studied by Dopazo and O'Brien (1974), Pope (1976, 1981a) and Janicka, Kolbe, and Kollmann (1978). In fact, the two approaches are equivalent, Pope (1979): the stochastic models can be regarded as Monte Carlo methods for solving the joint pdf equation.

The simplest case to study is a one-step reaction in constant-density homogeneous turbulence. Let $\phi(\mathbf{x}, t)$ be the progress variable (normalized reaction product) and let $p(\psi; t)$ be the pdf of ϕ . The pdf evolves in time due to the effects of reaction and molecular mixing. The notable feature of the pdf formulation is that the effect of reaction appears in closed form. Thus, only the effect of molecular mixing has to be modelled. Models currently in use are due to Curl (1963), Dopazo (1979) and Janicka, Kolbe, and Kollmann (1979). All of these

models can be written in pdf form and can also be used as stochastic models.

A useful test case to examine the performance of mixing models is the decay of fluctuations of ϕ in the absence of reaction. The mean $\langle\phi\rangle$,

$$\langle\phi\rangle = \int_{-\infty}^{\infty} \psi p(\psi) d\psi, \quad (1.1)$$

remains constant while the standard deviation σ ,

$$\sigma^2 = \langle\phi'^2\rangle = \int_{-\infty}^{\infty} (\psi - \langle\phi\rangle)^2 p(\psi) d\psi, \quad (1.2)$$

decreases with time. With the standardized variable $\hat{\psi}$ being defined by

$$\hat{\psi} \equiv (\psi - \langle\phi\rangle)/\sigma(t), \quad (1.3)$$

the standardized pdf

$$\hat{p}(\hat{\psi}; t) = p(\psi; t) \sigma(t), \quad (1.4)$$

has zero mean and unit standard deviation. For large t , as σ tends to zero it can be expected that the standardized pdf $\hat{p}(\hat{\psi}; t)$ approaches an asymptotic form that is independent of the initial condition.

Intuitively, the asymptotic form of the standardized pdf is a Gaussian,

$$\hat{p}(\hat{\psi}) = (2\pi)^{-1/2} \exp(-\frac{1}{2}\hat{\psi}^2). \quad (1.5)$$

The Gaussian, or normal, distribution has the important property that all of its standardized

†Present address: Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, NY 14853.

moments are finite. The standardized moments $\hat{\mu}_m$ are defined by

$$\begin{aligned}\hat{\mu}_m &\equiv \int_{-\infty}^{\infty} \hat{\psi}^m \hat{p}(\hat{\psi}) d\hat{\psi} \\ &= \frac{1}{\sigma^m} \int_{-\infty}^{\infty} \psi^m p(\psi) d\psi.\end{aligned}\quad (1.6)$$

Due to symmetry, all the odd moments (m odd) are zero, and, due to the standardization, the zeroth and second standardized moments are equal to unity. For the Gaussian pdf, Eq. (1.5), the flatness $\hat{\mu}_4$ is equal to 3 and the super skewness $\hat{\mu}_6$ is equal to 15.

While there is no proof that the pdf tends to a Gaussian in homogeneous turbulence there is strong experimental evidence that it does. Travoularis and Corrsin (1981) measured pdf's (with flatness equal to 3.0) that could not be distinguished from Gaussians.

The existing mixing models produce an asymptotic pdf as the limit of decaying fluctuations, but the pdf is far from Gaussian. In fact, all the even standardized moments ($\hat{\mu}_m$, $m > 4$) are infinite. Measurements in inhomogeneous flows (e.g. LaRue and Libby (1981), Venkataramini, Tutu, and Chevray (1975)) show that pdf's can depart significantly from the Gaussian distribution. But, even in the inhomogeneous case, there is no suggestion that the flatness is infinite.

The qualitatively incorrect behavior of existing models is a serious problem for two reasons. First, because of the infinite standardized moments, the statistical error in the stochastic models is large. Consequently, the models can be computationally expensive, and convergence cannot be guaranteed in all cases. Second, a major advantage claimed by pdf methods is that the pdf provides a complete statistical description of the turbulent fluctuations and consequently a more accurate closure is possible. Clearly this claim is vacuous if the model leads to qualitatively incorrect pdf's.

In this paper a new class of mixing models is presented. Their behavior is qualitatively correct in that all the standardized moments of the asymptotic pdf are finite. While the asymptotic pdf's are close to Gaussian, they are not exactly so. The minimum possible flatness is $\hat{\mu}_4 = 3.12$ (cf. $\hat{\mu}_4 = 3$ for a Gaussian), while the recommended model (that has a better overall behavior) yields $\hat{\mu}_4 = 3.70$.

2 BACKGROUND

2.1 The Test Problem

For inhomogeneous turbulent reactive flows, Janicka, Kolbe, and Kollmann (1978) and Pope (1981b) have reported successful calculations based on the solution of the pdf transport equation. A major advantage of this equation is that the effects of reaction appear in closed form. Models of turbulent transport and mixing are required. In order to study the modelling of mixing, an inert, constant-property, statistically-homogeneous flow is considered. For this case, the pdf evolves in time solely as a result of molecular mixing.

In the idealized test case there is a statistically-homogeneous turbulent velocity field $\mathbf{U}(\mathbf{x}, t)$ that does not decay. This is achieved (in principle) by supplying energy to the velocity fluctuations at the same rate as energy is removed by viscous dissipation. A frequency characteristic of the energy-containing motions is ϵ/k , where k is the turbulent kinetic energy and ϵ is its rate of dissipation. The fluid contains a conserved passive contaminant of concentration $c(\mathbf{x}, t)$ that obeys the transport equation

$$\frac{\partial c}{\partial t} + \mathbf{U}_t \frac{\partial c}{\partial x_t} = \Gamma \frac{\partial^2 c}{\partial x_t \partial x_t}.\quad (2.1)$$

The molecular diffusivity Γ is small compared with the turbulent diffusivity k^2/ϵ . Initially, at time $t=0$, there are packets of fluid whose size is of order $k^{3/2}/\epsilon$. Within each packet the concentration c is uniform and equal to one of two values— c_1 or c_2 , ($c_1 > c_2$). The mean concentrations is $\frac{1}{2}(c_1 + c_2)$.

The normalized concentration $\phi(\mathbf{x}, t)$ is defined by

$$\phi = 2\{c - \frac{1}{2}(c_1 + c_2)\}/(c_1 - c_2),\quad (2.2)$$

so that the mean value $\langle \phi \rangle$ is zero and, initially, the variance $\langle \phi'^2 \rangle$ is unity. The present study of turbulent mixing centers on the evolution of the pdf of ϕ , $p(\psi; t)$. Its initial value is

$$p(\psi; 0) = \frac{1}{2} \delta(1 - \psi) + \frac{1}{2} \delta(1 + \psi),\quad (2.3)$$

where the first delta function corresponds to fluid with $\phi = 1$ ($c = c_1$), and the second to fluid with $\phi = -1$ ($c = c_2$). As mixing proceeds, the standard deviation $\sigma(t)$

$$\sigma^2 = \int_{-\infty}^{\infty} \psi^2 p(\psi) d\psi,\quad (2.4)$$

decreases from its initial value of unity. Values of ϕ in the range $-1 \leq \phi \leq 1$ occur, while absolute values of ϕ greater than unity are impossible. The pdf remains symmetrical about $\psi=0$, and consequently all the odd moments of $p(\psi)$ are zero.

The initial distribution Eq. (2.3) is discontinuous, but in the early stages of mixing a continuous distribution forms in the range $-1 \leq \psi \leq 1$, and the magnitude of the two delta functions decreases. After some time the delta functions disappear and the continuous distribution contracts, as the standard deviation σ decreases. As σ tends to zero, the pdf tends to a Gaussian.

The various mixing models presented here are judged according to the pdf shapes that they predict. Specifically, a good model should produce a continuous distribution that tends asymptotically to a Gaussian. We are not concerned here with determining the rate at which the pdf evolves. Rather, we specify that the standard deviation decreases at a constant rate ω :

$$\frac{d\sigma}{dt} = -\omega\sigma. \quad (2.5)$$

With the initial condition $\sigma(0)=1$, the solution to this equation is,

$$\sigma(t) = e^{-\omega t}. \quad (2.6)$$

According to conventional modelling, the decay frequency is

$$\omega = C_\phi \epsilon/k, \quad (2.7)$$

where Spalding (1971) suggests the value 1.0 for the constant C_ϕ . However, the works of Béguier, Dekeyser, and Launder (1978) and Warhaft and Lumley (1978) show clearly that C_ϕ is not a universal constant.

2.2 Curl's Model

The first and simplest mixing model is due to Curl (1963). Curl expressed the model in pdf form while Spielman and Levenspiel (1965) devised the equivalent stochastic model.

In stochastic models, the pdf $p(\psi;t)$ is represented indirectly by an ensemble of N sample values $\phi^{(1)}, \phi^{(2)} \dots \phi^{(n)} \dots \phi^{(N)}$.

The mean $\langle Q(\phi) \rangle$ of any function of ϕ , $Q(\phi)$, can be obtained from the pdf by

$$\langle Q(\phi) \rangle = \int_{-\infty}^{\infty} Q(\psi) p(\psi) d\psi, \quad (2.8)$$

while, in stochastic models, $\langle Q(\phi) \rangle$ can be estimated by

$$\langle Q(\phi) \rangle \approx \frac{1}{N} \sum_{n=1}^N Q(\phi^{(n)}). \quad (2.9)$$

The error involved in this approximation is proportional to $N^{-1/2}$ and so a large ensemble should be used. In the analysis, the limit of N tending to infinity is used.

To apply Curl's stochastic model to the test problem, the initial ensemble is specified to correspond to the initial double-delta-function pdf, Eq. (2.3). Half of the elements ($n=1,2 \dots N/2$, say) are ascribed the value $\phi^{(n)}=1$, and the remaining $N/2$ elements are ascribed the value $\phi^{(n)}=-1$. The initial time is $t=0$, and the model advances time through a sequence of small steps Δt ($\Delta t \omega \ll 1$) by performing the following stochastic process. Pairs of elements are selected at random from the ensemble. The number of pairs selected N_p is the nearest integer to $N_p' = \beta \Delta t \omega N$, where β is a constant that is determined by the condition that σ decays at the rate ω . (For Curl's model $\beta=2$.) Let the two elements in a pair be denoted by n and m , and their values when selected are

$$\phi^{(n)}(t) = \phi_a, \quad \phi^{(m)}(t) = \phi_b. \quad (2.10)$$

Mixing is performed by changing the values of ϕ to

$$\phi^{(n)}(t+\Delta t) = \phi_a^*, \quad \phi^{(m)}(t+\Delta t) = \phi_b^*, \quad (2.11)$$

where

$$\phi_a^* = \phi_b^* = \frac{1}{2}(\phi_a + \phi_b). \quad (2.12)$$

This mixing process is performed for each pair of elements selected to produce the ensemble at time $t+\Delta t$. For elements not selected, their value of ϕ is unaltered.

It is clear that this simulation of mixing leaves the mean value unchanged, since,

$$\frac{1}{2}(\phi_a^* + \phi_b^*) = \frac{1}{2}(\phi_a + \phi_b), \quad (2.13)$$

while the variance decreases, since,

$$\begin{aligned} \phi_a^{*2} + \phi_b^{*2} &= \phi_a^2 + \phi_b^2 \\ -\frac{1}{2}(\phi_a - \phi_b)^2 &\leq \phi_a^2 + \phi_b^2. \end{aligned} \quad (2.14)$$

The equivalent pdf model can be obtained from

$$p(\psi; t + \Delta t) \approx p(\psi; t) + (N_p/N) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p(\psi_a) p(\psi_b) \\ \times \{ -\delta(\psi - \psi_a) - \delta(\psi - \psi_b) \\ + \delta(\psi - \psi_a^*) + \delta(\psi - \psi_b^*) \} d\psi_a d\psi_b. \quad (2.15)$$

The integral $p(\psi_a) d\psi_a$ represents the selection of the element n ($\phi^{(n)} = \psi_a$), and similarly $p(\psi_b) d\psi_b$ represents the selection of the element m ($\phi^{(m)} = \psi_b$). The four delta functions represent, respectively, the removal of elements with values $\phi^{(n)} = \psi_a$ and $\phi^{(m)} = \psi_b$, and the addition of elements with values $\phi^{(n)} = \psi_a^*$ and $\phi^{(m)} = \psi_b^*$, where

$$\psi_a^* = \psi_b^* = \frac{1}{2}(\psi_a + \psi_b). \quad (2.16)$$

The double integral divided by N represents the change in the pdf caused by the mixing of one pair of elements. Since N_p pairs of elements mix in the time interval Δt , the double integral is multiplied by N_p/N .

The pdf evolution equation is obtained by dividing Eq. (2.15) by Δt and taking the limits $\omega \Delta t \rightarrow 0$ and $N \omega \Delta t \rightarrow \infty$. The result is

$$\frac{\partial p}{\partial t} = -2\beta\omega p + 2\beta\omega \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \\ \times p(\psi_a) p(\psi_b) K(\psi, \psi_a, \psi_b) d\psi_a d\psi_b, \quad (2.17)$$

where the kernel K is

$$K(\psi, \psi_a, \psi_b) = \delta(\psi - \frac{1}{2}(\psi_a + \psi_b)). \quad (2.18)$$

The corresponding evolution equation for the standard deviation $\sigma(t)$ is obtained by multiplying Eq. (2.17) by ψ^2 and integrating. The result is

$$\frac{d\sigma}{dt} = -\frac{1}{2}\beta\omega\sigma, \quad (2.19)$$

and hence, for compatibility with Eq. (2.5), β takes the value 2.

This completes the description of Curl's model in both pdf and stochastic form. The application of the stochastic model to the test problem immediately reveals a flaw in the model. Initially, ϕ takes the value -1 or 1 . After the first time step, the possible values are $-1, 0$ and 1 ; after the second step they are $-1, -\frac{1}{2}, 0, \frac{1}{2}$ and 1 ; after the k th step they are integer multiples of 2^{1-k} . Thus, the pdf is composed of delta functions and, although the

number of delta functions becomes infinite, a continuous distribution never evolves.

The pdf can be written

$$p(\psi; t) = \sum_l P_l(t) \delta(\psi - \psi_l), \quad (2.20)$$

where ψ_l is the location of the l th delta function, P_l is its magnitude, and the summation is over the infinite number of delta functions. Note that the normalization condition is

$$\int_{-\infty}^{\infty} p(\psi) d\psi = \sum_l P_l = 1. \quad (2.21)$$

Figure 1 shows the delta function magnitudes for the test problem at the nondimensional time $t^* = \omega t = 0.5$. Only the 65 delta functions that are located at integer multiples of 2^{-6} are shown, but these contain more than 96 percent of the total probability. (These results were obtained by numerical integration of the equations for the first 2^{10} delta function magnitudes.)

Although Curl's model exhibits this unacceptable behavior, it provides a basis for better models.

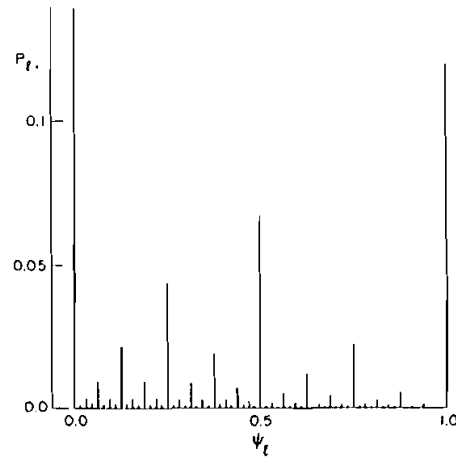


FIGURE 1 Delta function magnitudes P_l against their locations ψ_l , according to Curl's model for the test problem at time $t^* = 0.5$.

2.3 Modified Curl Model

Dopazo (1979) and Janicka, Kolbe, and Kollmann (1979) independently suggested a modification to

Curl's model that results in continuous pdf's. In the stochastic model, the modification is to the mixing process. Consider replacing Eq. (2.12) with the equations

$$\phi_a^* = (1 - \alpha)\phi_a + \frac{1}{2}\alpha(\phi_a + \phi_b), \quad (2.22)$$

and

$$\phi_b^* = (1 - \alpha)\phi_b + \frac{1}{2}\alpha(\phi_a + \phi_b). \quad (2.23)$$

The role of the new parameter α is to control the extent of the mixing: with $\alpha=0$ no mixing occurs, with $\alpha=1$ Curl's model is recovered. The pdf equation appropriate to the modified stochastic model is, as before, Eq. (2.17), but the kernel K is

$$K(\psi, \psi_a, \psi_b) = \delta(\psi - (1 - \alpha)\psi_a - \frac{1}{2}\alpha(\psi_a + \psi_b)). \quad (2.24)$$

This model with any given value of α ($0 < \alpha < 1$) does not overcome the problem of discontinuous pdf's: it merely changes the location of the delta functions. But if α is chosen to be a random variable with a continuous pdf $A(\alpha)$, then the model itself produces continuous pdf's. Again, Eq. (2.17) governs the evolution of the pdf and the kernel is

$$K(\psi, \psi_a, \psi_b) = \int_0^1 A(\alpha)\delta(\psi - (1 - \alpha)\psi_a - \frac{1}{2}\alpha(\psi_a + \psi_b))d\alpha. \quad (2.25)$$

This is the idea behind the models of Dopazo (1979) and Janicka, Kolbe, and Kollmann (1979). The delta-function kernel of Curl's model, Eq. (2.18), is replaced by a smooth kernel, Eq. (2.25). (Note that Curl's model can be recovered by the choice $A(\alpha) = \delta(1 - \alpha)$.) A suitable choice of the pdf $A(\alpha)$ is discussed by Dopazo and Janicka *et al.*, and it is also discussed below. For the moment we follow Janicka *et al.* in the simplest choice,

$$A(\alpha) = 1. \quad (2.26)$$

The constant β depends upon the choice of $A(\alpha)$ and can be determined from the rate of decay of the standard deviation. The evolution equation for $\sigma(t)$ can, again, be obtained by multiplying the pdf equation by ψ^2 and integrating. The result is

$$\frac{d\sigma}{dt} = -\omega\sigma\beta(a_1 - \frac{1}{2}a_2), \quad (2.27)$$

where a_m is the m th moment of $A(\alpha)$,

$$a_m = \int_0^1 \alpha^m A(\alpha)d\alpha. \quad (2.28)$$

Thus, for compatibility with Eq. (2.5), β is given by

$$\beta = (a_1 - \frac{1}{2}a_2)^{-1}, \quad (2.29)$$

and, for the choice of $A(\alpha) = 1$, this yields $\beta = 3$.

The evolution of the pdf for the test problem was calculated using the stochastic model with $A(\alpha) = 1$. The pdf comprises delta functions of magnitude $P_1(t)$ at $\psi = \pm 1$, and a continuous distribution in between:

$$p(\psi; t) = p_c(\psi; t) + P_1(t)\{\delta(1 - \psi) + \delta(1 + \psi)\}. \quad (2.30)$$

Initially, $P_1(0)$ is equal to one half, and $p_c(\psi; 0)$ is zero. Figure 2 shows $p_c(\psi, t)$ for different values of t^* , and the decay of $P_1(t)$. At $t^* = 0.5$ the delta functions have nearly disappeared and the continuous pdf p_c is almost flat. With increasing time the maximum value $p_c(0; t)$ increases and the pdf becomes narrower. The modification to Curl's model is seen to be successful in producing a continuous pdf.

As expected, as t^* tends to infinity, the standardized pdf $\hat{p}(\hat{\psi})$ adopts an asymptotic shape. The standardized pdf is

$$\hat{p}(\hat{\psi}) = \sigma p(\psi), \quad (2.31)$$

where

$$\hat{\psi} = \psi/\sigma. \quad (2.32)$$

Figure 3 shows $\hat{p}(\hat{\psi})$ compared with a Gaussian, and significant differences are evident. Because of the standardization, the standard deviation of each distribution is unity. But at first sight it appears that $\hat{p}(\hat{\psi})$ is narrower than the Gaussian. Closer examination reveals that the tails of $\hat{p}(\hat{\psi})$ approach zero very slowly, and consequently they contribute significantly to the variance.

The observed long tails of the asymptotic pdf suggest that the fourth and higher even standardized moments are large. Figure 4 shows the evolution of the flatness and superskewness for the test problem. At $t^* \approx 1$, both of these quantities have attained their Gaussian values, $\hat{\mu}_4 = 3$ and $\hat{\mu}_6 = 15$. But as t^* increases both $\hat{\mu}_4$ and $\hat{\mu}_6$ continue to grow (more rapidly than linearly) and they are infinite for the asymptotic distribution.

It can be concluded that the modified Curl model produces continuous pdf's, but that the asymptotic pdf is far from Gaussian. The maximum value of the pdf, $\hat{p}(0)$, is over 50 percent greater than the Gaussian value, and the fourth and higher even moments of the standardized asymptotic pdf are

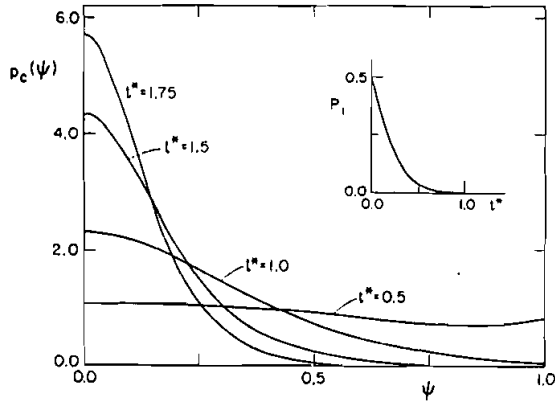


FIGURE 2 Evolution of pdf for the test problem according to the modified Curl model.

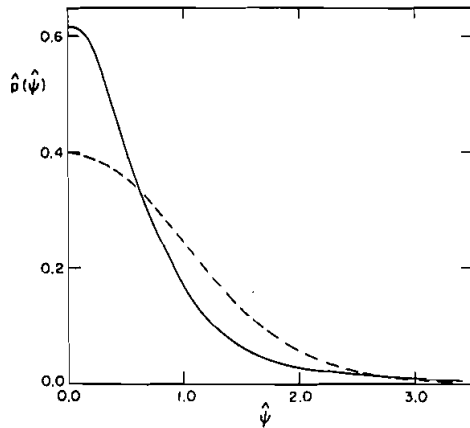


FIGURE 3 Standardized asymptotic pdf for the modified Curl model —; Gaussian - - -.

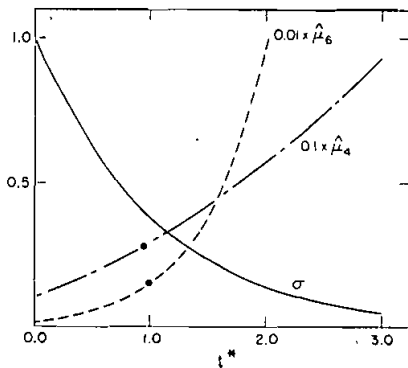


FIGURE 4 Evolution of moments for the test problem according to the modified Curl model: — standard deviation σ ; - - - flatness $\hat{\mu}_4$; - - - super skewness $\hat{\mu}_6$; ● Gaussian values $\hat{\mu}_4=3, \hat{\mu}_6=15$.

infinite. This latter conclusion holds for any choice of the mixing pdf $A(\alpha)$.

3 IMPROVED MIXING MODEL

A new class of mixing models is presented that produces continuous pdf's with finite standardized moments. The models are similar to the modified Curl model, except that the selection of elements for mixing is biased. The bias depends upon the age of the element, which is defined in Section 3.1. A derivation and analysis of the model equations is provided in Appendix A, and the performance of the models is discussed in Section 3.2. An efficient implementation of the stochastic version of the model is presented in Section 3.3.

3.1 Age Distributions

In the stochastic model, the age of an element is defined as the normalized time since it mixed with another element. Let $t^{(n)}$ be the last time that the element n was selected for mixing. Then, with t being the current time, the age of the n th element is

$$\tau^{(n)} = \omega(t - t^{(n)}). \quad (3.1)$$

Thus, for every element there is a value of ϕ , $\phi^{(n)}$, and an age $\tau^{(n)}$.

The age distribution $r(s)$, where s is the independent age variable, is defined to be the pdf of τ . In Appendix A, it is shown that for the modified Curl model the age distribution is

$$r(s) = 2\beta \exp(-2\beta s). \quad (3.2)$$

It is further shown that, with this age distribution, any choice of $A(\alpha)$ leads to a standardized asymptotic pdf with infinite higher moments. But if the age distribution is modified to decay more rapidly with s , then pdf's with finite moments are possible.

In the stochastic model, the age distribution can be changed by biasing the sampling according to the age of the elements. Specifically, let $z(s)$ be the relative probability of sampling the element n of age $\tau^{(n)} = s$. The sample bias $z(s)$ is normalized so that

$$\int_0^\infty r(s) z(s) ds = 1. \quad (3.3)$$

This biased sampling procedure results in the age

distribution (see Appendix A),

$$r(s) = 2\beta \exp\left(-2\beta \int_0^s z(s')ds'\right), \quad (3.4)$$

or, alternatively, the age distribution $r(s)$ results from the bias

$$z(s) = \frac{-1}{2\beta} \frac{d}{ds} \ln r(s). \quad (3.5)$$

In the modified Curl model there is no sample bias, and so $z(s)$ is a constant (unity). Then Eq. (3.4) yields the age distribution Eq. (3.2). If the bias is linearly proportional to the age, *i.e.*

$$z(s) = \pi\beta s,$$

then the corresponding age distribution is

$$r(s) = 2\beta \exp(-\pi\beta^2 s^2). \quad (3.6)$$

The age distributions encountered so far, Eq. (3.2) and Eq. (3.6), extend from $s=0$ to $s=\infty$. Distributions of finite extent can be obtained by letting $z(s)$ become infinite at a finite value of s . For example, the age distribution of the recommended model is

$$\begin{aligned} r(s) &= 2\beta(1-y^2)^2, \quad 0 \leq y \leq 1, \\ &= 0, \quad y < 0 \text{ and } y > 1, \end{aligned} \quad (3.7)$$

where

$$y = \frac{16}{15}\beta s. \quad (3.8)$$

This corresponds to the bias

$$z(s) = \frac{32y}{15(1-y^2)}, \quad (3.9)$$

which clearly becomes infinite as y tends to unity.

3.2 Model Performance

The improved mixing model is defined by the two pdf's $A(a)$ and $r(s)$. The implementation of the stochastic version of the model is the same as the modified Curl model (Section 2.3), except that the sampling of the elements is biased according to $z(s)$. An efficient algorithm to achieve this biased sampling is described in Section 3.3.

The pdf form of the model is expressed as an evolution equation for the joint pdf of ϕ and τ , $q(\psi, s; t)$. The individual pdf's can be recovered from

the joint pdf by

$$p(\psi; t) = \int_0^\infty q(\psi, s; t) ds, \quad (3.10)$$

and

$$r(s; t) = \int_{-\infty}^\infty q(\psi, s; t) d\psi. \quad (3.11)$$

The evolution equation for $q(\psi, s; t)$ is (see Appendix A),

$$\begin{aligned} \frac{\partial q}{\partial t} + \omega \frac{\partial q}{\partial s} &= -2\beta\omega qz + 2\beta\omega\delta(s) \\ &\times \int_{-\infty}^\infty \int_{-\infty}^\infty h(\psi_a)h(\psi_b)K(\psi, \psi_a, \psi_b) d\psi_a d\psi_b, \end{aligned} \quad (3.12)$$

where $h(\psi)$ is the pdf of the sampled elements,

$$h(\psi) = \int_0^\infty z(s)q(\psi, s) ds. \quad (3.13)$$

An evolution equation for $p(\psi; t)$ is obtained by integrating Eq. (3.12) over all s :

$$\begin{aligned} \frac{\partial p}{\partial t} &= -2\beta\omega h + 2\beta\omega \\ &\times \int_{-\infty}^\infty \int_{-\infty}^\infty h(\psi_a)h(\psi_b)K(\psi, \psi_a, \psi_b) d\psi_a d\psi_b \end{aligned} \quad (3.14)$$

It may be noted that this equation is the same as the modified Curl model equation, Eq. (2.17), except that, on the right-hand side, the pdf $p(\psi)$ is replaced by the sampled pdf $h(\psi)$.

It is shown in Appendix A that Eq. (3.14) admits self-similar solutions which correspond to the pdf for the test problem in the limit as t tends to infinity. These solutions are examined for the thirty-six models obtained from six choices of $A(a)$ (*a-f*) and six choices of $r(s)$ (I-VI). From the analysis, the values of flatness $\hat{\mu}_4$, the super skewness $\hat{\psi}_6$, and the constant β are obtained. These are given in Tables I, II and III in Appendix A.

The model that produces moments closest to a Gaussian is model Ia defined by

$$A(\alpha) = \delta(1 - \alpha) \quad (3.15)$$

and

$$r(s) = 2\beta, \quad 0 \leq s \leq \frac{1}{2\beta},$$

$$= 0, \quad s < 0 \text{ and } s > \frac{1}{2\beta}. \quad (3.16)$$

For this model the flatness is $\hat{\mu}_4 = 3.12$ and the superskewness is $\hat{\mu}_6 = 16.8$, which may be compared with the Gaussian values $\hat{\mu}_4 = 3$ and $\hat{\mu}_6 = 15$. All other models produce larger values of $\hat{\mu}_4$ and $\hat{\mu}_6$.

While this model has the best performance for this test case, its overall performance is unacceptable. The choice of $A(\alpha)$ is the same as for Curl's model, and hence discontinuous pdf's can arise. The choice of $r(s)$ is also objectionable, because it implies complete age segregation. The bias $z(s)$ corresponding to Eq. (3.16) is

$$z(s) = \delta(2s\beta - 1), \quad (3.17)$$

which shows that an element selected for mixing at time $t = t_1$ will also be selected at the times $t = t_1 + (m/2\beta\omega)$ (where m is any positive integer). Thus, an element selected at t_1 and another element selected at $t_1 + (\xi/2\beta\omega)$ ($0 < \xi < 1$) can never mix with each other.

The recommended compromise between good overall behavior and low values of $\hat{\mu}_4$ and $\hat{\mu}_6$ is model IIIb, which is defined by

$$A(\alpha) = 10\alpha^3(1 - \frac{3}{2}\alpha), \quad (3.18)$$

and $r(s)$ given by Eq. (3.7). For this model the flatness is $\hat{\mu}_4 = 3.70$ and the superskewness is $\hat{\mu}_6 = 29.5$. The standardized asymptotic pdf $\hat{p}(\hat{\psi})$ was calculated using the stochastic form of the model and is shown on Figure 5. It may be seen that the shape of the pdf is close to Gaussian, in marked contrast to the modified Curl model pdf, Figure 3.

The decay of $p(\psi; t)$ for the test problem is shown on Figure 6. As before, the pdf comprises delta functions of magnitude $P_1(t)$ at $\psi = \pm 1$ and a continuous pdf $p_c(\psi; t)$ in the range $-1 < \psi < 1$, see Eq. (2.30). It may be seen from the figure that the delta functions have disappeared by $t^* = 1.0$, and that by $t^* = 1.5$ the pdf is a bell-shaped curve. Eventually as t^* tends to infinity, the pdf adopts the

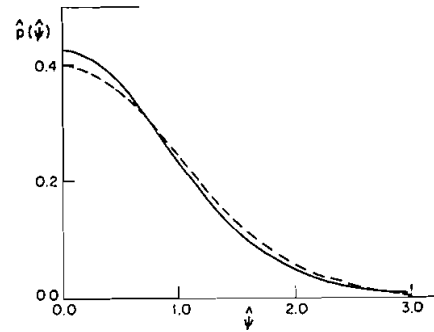


FIGURE 5 Standardized asymptotic pdf for the improved model IIIb ———; Gaussian - - - -.

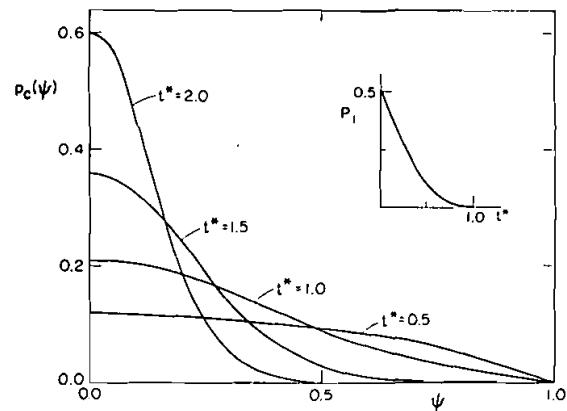


FIGURE 6 Evolution of the pdf for the test problem according to the improved model IIIb.

asymptotic (approximately Gaussian) form shown on Figure 5.

These results confirm the satisfactory performance of the improved model.

3.3 Stochastic Model Algorithm

In the improved model, the elements are selected randomly (though with the bias $z(s)$) so that the resulting age distribution is $r(s)$. An efficient, though indirect, algorithm to achieve the same result can be based on the pdf of element life expectancies. Let τ^* (a random variable) be the life expectancy of an element (*i.e.* its age when it mixes); and let $g(s)$ be the pdf of τ^* . It is shown in Appendix A that $g(s)$ and $r(s)$ are related by

$$g(s) = - \frac{1}{2\beta} \frac{dr(s)}{ds}. \quad (3.19)$$

Let τ be a random variable with pdf $g(s)$ given by Eq. (3.19). Then, if for each element the time

interval between mixing operations is specified to be τ , then the resulting age distribution is $r(s)$.

It should be noted that $g(s)$ is the pdf of life expectancy at birth, that is, when the age is zero. If the age $\tau=s$ has already been attained, the conditional pdf of the age $\tau^*=s^*$ at mixing is

$$g_c(s^*|s) = H(s^*-s)g(s^*) / \int_s^\infty g(s')ds', \quad (3.20)$$

where H is the Heaviside function.

These observations lead to the following efficient algorithm for the test problem. Each of the N elements has a value of ϕ , $\phi^{(n)}$, an age, $\tau^{(n)}$, and a life expectancy $\tau^{*(n)} > \tau^{(n)}$. Initially, half the elements are ascribed the value $\phi^{(n)}=1$ and the remainder $\phi^{(n)}=-1$. Each element is randomly prescribed an age $\tau^{(n)}=s$ (with pdf $r(s)$) and a life expectancy $\tau^{*(n)}=s^*$ (with pdf $g_c(s^*|s)$). The initial time is $t=0$. In the step that advances time from t to $t+\Delta t$, all the elements age by an amount $\omega\Delta t$,

$$\tau^{(n)}(t+\Delta t) = \tau^{(n)}(t) + \omega\Delta t. \quad (3.21)$$

An element is selected for mixing if its age exceeds its life expectancy, that is, if

$$\tau^{(n)}(t+\Delta t) > \tau^{*(n)}. \quad (3.22)$$

If an element is selected for mixing, its age is set to zero and its life expectancy is randomly reset according to the pdf $g(s)$.

The elements selected for mixing randomly choose partners and mix as in the modified Curl model. Let the two elements in a pair be denoted by n and m , with initial values $\phi^{(n)}(t)=\phi_a$ and $\phi^{(m)}(t)=\phi_b$. Then mixing occurs by

$$\phi^{(n)}(t+\Delta t) = \phi_a^*, \quad \phi^{(m)}(t+\Delta t) = \phi_b^*, \quad (3.23)$$

where

$$\phi_a^* = (1-\alpha)\phi_a + \frac{\alpha}{2}(\phi_a + \phi_b), \quad (3.24)$$

$$\phi_b^* = (1-\alpha)\phi_b + \frac{\alpha}{2}(\phi_a + \phi_b), \quad (3.25)$$

and α is a random variable with pdf $A(\alpha)$.

This stochastic model was used to obtain the results shown on Figures 5 and 6.

4 CONCLUSION

It has been shown that Curl's model and the modified Curl model lead to standardized asymptotic pdf's with infinite fourth and higher (even) moments. The improved models, presented in the previous section, produce finite moments by changing the age distribution. Model Ia produces a pdf with flatness $\hat{\mu}_4=3.12$ and superskewness $\hat{\mu}_6=16.8$, but the model's overall performance is unacceptable. The recommended model is IIIb, for which the asymptotic values of $\hat{\mu}_4$ and $\hat{\mu}_6$ are 3.70 and 29.5. The asymptotic pdf for this model is shown on Figure 5, and it may be seen that it is close to Gaussian.

The model has been presented for the simple case of a single scalar in homogeneous turbulence. Extension to the general case is straight forward. The age of an element was defined by, Eq. (3.1),

$$\tau^{(n)} = \omega(t - t^{(n)}). \quad (4.1)$$

For the inhomogeneous case, the turbulent frequency ω can vary, and so in general the definition of age is

$$\tau^{(n)} = \int_{t^{(n)}}^t \omega(t')dt'. \quad (4.2)$$

If, instead of the single scalar ϕ , there is a set of σ scalars,

$$\phi = \phi_1, \quad \phi_2 \dots \phi_\sigma, \quad (4.3)$$

then, in the stochastic model, each element has a set of values $\phi^{(n)}$, and an age $\tau^{(n)}$. Mixing occurs as before, with Eqs. (3.24) and (3.25) applying to each scalar.

In the velocity pdf equation and the velocity-scalar joint pdf equation the effect of viscous dissipation has to be modelled. Previously Curl's model was used (Pope, 1981c,d), but clearly the improved model can be applied, with an expected gain in accuracy.

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Appendix A

AGE DISTRIBUTION EQUATION

An evolution equation for the age distribution $r(s)$ is obtained from

$$r(s+\omega\Delta t; t+\Delta t) \approx r(s; t) + 2\beta\omega\Delta t\{\delta(s) - r(s)z(s)\}. \quad (\text{A.1})$$

The argument $s+\omega\Delta t$ on the left-hand side reflects the fact that an element (not selected for mixing) ages an amount $\omega\Delta t$ in the time interval Δt . The fraction of elements selected is $2\beta\omega\Delta t$, and the effect is to remove an amount $r(s)z(s)$ from $r(s)$ and to add it to $r(0)$: that is, the mixed elements have zero age. In the limit as $\Delta t \rightarrow 0$, Eq. (A.1) becomes,

$$\frac{1}{\omega} \frac{\partial r}{\partial t} + \frac{\partial r}{\partial s} = 2\beta\delta(s) - 2\beta r(s)z(s). \quad (\text{A.2})$$

In the steady state, $\partial r/\partial t$ is zero, and an analytic solution for $r(s)$ can be obtained. Since negative ages are impossible, $r(s)$ is zero for negative s . Thus, by integrating Eq. (A.2) from 0_- to 0_+ (i.e. over the delta function) we obtain

$$r(0) = 2\beta. \quad (\text{A.3})$$

For s greater than zero, the first term on the right-hand side of Eq. (A.2) is zero and hence,

$$\frac{d}{ds} \ln r(s) = -2\beta z(s), \quad s > 0. \quad (\text{A.4})$$

Integrating this equation and using Eq. (A.3) to eliminate the constant of integration we obtain the

steady-state age distribution

$$r(s) = 2\beta \exp\left(-2\beta \int_0^s z(s') ds'\right). \quad (\text{A.5})$$

It may be noted that $z(s)$ can be determined from $r(s)$ by

$$z(s) = \frac{-1}{2\beta} \frac{d}{ds} \ln r(s). \quad (\text{A.6})$$

It is convenient to introduce the variable $x = \beta s$ and the pdf $\hat{r}(x)$

$$\hat{r}(x) = r(s)/\beta. \quad (\text{A.7})$$

Then Eqs. (A.5) and (A.6) can be rewritten,

$$\hat{r}(x) = 2 \exp\left(-2 \int_0^x z(x') dx'\right) \quad (\text{A.8})$$

and

$$z(x) = -\frac{1}{2} \frac{d}{dx} \ln \hat{r}(x). \quad (\text{A.9})$$

Joint pdf Equation

The evolution equation for the joint pdf of ϕ and τ , $q(\psi, s; t)$, can be derived in the same way as Eq. (2.15)

and Eq. (A.2):

$$\begin{aligned}
 q(\psi, s + \omega \Delta t; t + \Delta t) &\approx q(\psi, s; t) + \\
 &+ \beta \omega \Delta t \int_{-\infty}^{\infty} \int_0^{\infty} \int_{-\infty}^{\infty} \int_0^{\infty} q(\psi_a, s_a) \\
 &\times q(\psi_b, s_b) z(s_a) z(s_b) \\
 &\times \int_0^1 A(\alpha) \left\{ -\delta(\psi - \psi_a) \delta(s - s_a) \right. \\
 &- \delta(\psi - \psi_b) \delta(s - s_b) + \delta \left(\psi - \left[1 - \frac{\alpha}{2} \right] \psi_a - \frac{\alpha}{2} \psi_b \right) \\
 &\times \delta(s) + \delta \left(\psi - \left[1 - \frac{\alpha}{2} \right] \psi_b - \frac{\alpha}{2} \psi_a \right) \delta(s) \left. \right\} \\
 &\times d\alpha ds_b d\psi_b ds_a d\psi_a. \tag{A.10}
 \end{aligned}$$

The argument $s + \omega \Delta t$ in the first term reflects the aging of elements not selected for mixing. The integral

$$q(\psi_a, s_a) z(s_a) ds_a d\psi_a,$$

represents the selection of an element with $\phi = \psi_a$ and $\tau = s_a$; and similarly the integral

$$q(\psi_b, s_b) z(s_b) ds_b d\psi_b,$$

represents the selection of an element with $\phi = \psi_b$ and $\tau = s_b$. The first two delta-function products account for the removal of the elements with the values (ψ_a, s_a) and (ψ_b, s_b) while the second two account for the addition of the mixed elements. The mixed elements have zero age, and the values of ϕ given by Eqs. (2.22) and (2.23). Since α is a random variable, the expression is multiplied by the pdf $A(\alpha)$, and integrated over all α .

Dividing Eq. (A.10) by $\Delta t \rightarrow 0$, we obtain the evolution equation for $q(\psi, s; t)$:

$$\begin{aligned}
 \frac{\partial q}{\partial t} + \omega \frac{\partial q}{\partial s} &= -2\beta\omega qz + 2\beta\omega \delta(s) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \\
 &\times h(\psi_a) h(\psi_b) K(\psi, \psi_a, \psi_b) d\psi_a d\psi_b, \tag{A.11}
 \end{aligned}$$

where the kernel K is given by Eq. (2.25), and the pdf of sampled elements is

$$h(\psi) = \int_0^{\infty} z(s) q(\psi, s) ds. \tag{A.12}$$

Self-Similar Solution

The joint pdf evolution equation, Eq. (A.11) admits a self-similar solution of the form

$$q(\psi, s; t) = r(s) f(\psi/\sigma_c) / \sigma_c, \tag{A.13}$$

where f is a standardized pdf and

$$\sigma_c(s, t) = \sigma_0 \exp(s - \omega t) - \sigma_* e^s. \tag{A.14}$$

Here σ_0 is a constant and σ_* is written for $\sigma_0 \exp(-\omega t)$.

By differentiating Eq. (A.13) we obtain an expression for the left-hand side of the evolution equation, Eq. (A.11):

$$\begin{aligned}
 \frac{\partial q}{\partial t} + \omega \frac{\partial q}{\partial s} &= \frac{\omega f}{\sigma_c} \frac{dr}{ds} \\
 &= 2\beta\omega f \delta(s) / \sigma_* - 2\beta\omega qz. \tag{A.15}
 \end{aligned}$$

And comparing this equation with the right-hand side of Eq. (A.11) we obtain

$$\begin{aligned}
 f(\psi/\sigma_*) / \sigma_* &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} h(\psi_a) h(\psi_b) \\
 &\times K(\psi, \psi_a, \psi_b) d\psi_a d\psi_b. \tag{A.16}
 \end{aligned}$$

Since $h(\psi)$ is known in terms of $r(s)$ and f , this equation could, in principle, be solved for f .

In the absence of such an explicit solution, we seek a solution in terms of the moments of f . Accordingly, the following moments and integrals are defined:

$$\mu_m = \int_0^{\infty} \int_{-\infty}^{\infty} \psi^m q(\psi, s) d\psi ds, \tag{A.17}$$

$$\gamma_m = \int_{-\infty}^{\infty} \eta^m f(\eta) d\eta, \tag{A.18}$$

$$\lambda_m = \int_{-\infty}^{\infty} \psi^m h(\psi) d\psi, \tag{A.19}$$

$$R_m = \int_0^{\infty} e^{ms} r(s) ds, \tag{A.20}$$

and

$$\begin{aligned} \kappa_m = & \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi^m h(\psi_a) h(\psi_b) \\ & \times K(\psi, \psi_a, \psi_b) d\psi_a d\psi_b d\psi. \end{aligned} \quad (\text{A.21})$$

Making use of the self-similar solution, Eq. (A.13), μ_m can be expressed as,

$$\begin{aligned} \mu_m = & \int_0^{\infty} \int_{-\infty}^{\infty} \psi^m r(s) f(\psi/\sigma_c) / \sigma_c d\psi ds \\ = & \int_0^{\infty} \sigma_c^m r(s) \int_{-\infty}^{\infty} (\psi/\sigma_c)^m f(\psi/\sigma_c) d\psi / \sigma_c ds \\ = & \sigma_*^m R_m \gamma_m. \end{aligned} \quad (\text{A.22})$$

Similarly, λ_m can be reexpressed as,

$$\begin{aligned} \lambda_m = & \int_0^{\infty} \int_{-\infty}^{\infty} \psi^m z(s) r(s) f(\psi/\sigma_c) / \sigma_c d\psi ds \\ = & \sigma_*^m \gamma_m \int_0^{\infty} e^{ms} z(s) r(s) ds \\ = & \sigma_*^m \gamma_m \{1 + (m/2\beta) R_m\}. \end{aligned} \quad (\text{A.23})$$

The last step is achieved by integrating by parts after $z(s)r(s)$ has been replaced by,

$$z(s)r(s) = -\frac{1}{2\beta} \frac{dr(s)}{ds}. \quad (\text{A.24})$$

The self-similar equation, Eq. (A.16) can be used to relate κ_m and γ_m . Multiplying both sides by ψ^m and integration yields,

$$\sigma_*^m \gamma_m = \kappa_m. \quad (\text{A.25})$$

In Appendix B it is shown that κ_m can be written in terms of λ_m ; specifically,

$$\begin{aligned} \kappa_2 = & c_{2,2} \lambda_2, \\ \kappa_4 = & c_{4,4} \lambda_4 + c_{4,2} \lambda_2^2, \end{aligned} \quad (\text{A.26})$$

and

$$\kappa_6 = c_{6,6} \lambda_6 + c_{4,2} \lambda_4 \lambda_2,$$

where the constants c depend upon the moments of $A(\alpha)$.

Sufficient relationships have now been obtained to determine β and the normalized moments $\hat{\mu}_4$ and $\hat{\mu}_6$:

$$\hat{\mu}_m = \mu_m / \mu_2^{m/2}, \quad (m \text{ even}). \quad (\text{A.27})$$

With $m=2$, Eqs. (A.25) and (A.26) give

$$\kappa_2 = \sigma_*^2 \gamma_2 = c_{2,2} \lambda_2. \quad (\text{A.28})$$

Because of the standardization, γ_2 is equal to unity. Hence, using Eq. (A.23) to eliminate λ_2 , we obtain

$$1 = c_{2,2} \{1 + R_2/\beta\}, \quad (\text{A.29})$$

or,

$$\begin{aligned} R_2/\beta = & \frac{1}{\beta} \int_0^{\infty} \exp(2x/\beta) \\ & \times \hat{r}(x) dx = 1/c_{2,2} - 1. \end{aligned} \quad (\text{A.30})$$

For a given model, $c_{2,2}$ and $\hat{r}(x)$ are known and so this implicit equation can be solved for β . It is clear from the integral expression that R_2/β goes monotonically from infinity to zero as β goes from zero to infinity. Consequently, Eq. (A.30) has a unique solution.

Once β has been determined, Eqs. (A.23), (A.25) and (A.26) can be combined to produce explicit expressions for γ_4 and γ_6 . These are,

$$\gamma_4 = \frac{c_{4,2}}{c_{2,2}^2} \left/ (1 - c_{4,4} \{1 + 2R_4/\beta\}) \right., \quad (\text{A.31})$$

and

$$\begin{aligned} \gamma_6 = & \frac{c_{6,4}(\gamma_4 - c_{4,2}/c_{2,2}^2)}{c_{4,4} c_{2,2}} \left/ \right. \\ & \times (1 - c_{6,6} \{1 + 3R_6/\beta\}). \end{aligned} \quad (\text{A.32})$$

And, finally, from Eqs. (A.22) and (A.27), the normalized moments are obtained,

$$\hat{\mu}_m = \gamma_m R_m / R_2^{m/2}. \quad (\text{A.33})$$

To summarize the determination of β , $\hat{\mu}_4$ and $\hat{\mu}_6$: for a given model (given $A(\alpha)$ and $\hat{r}(x)$), the constants c can be determined (Appendix B). The implicit equation Eq. (A.30) can then be solved for β and hence R_m can be determined. The moments $\hat{\mu}_4$ and $\hat{\mu}_6$ can then be obtained from Eqs. (A.31)–(A.33).

Modified Curl Model

For the modified Curl model there is no sample bias and so $z(s)$ is a constant (unity). Equation (A.5) then gives the age distribution,

$$r(s) = 2\beta \exp(-2\beta s). \quad (\text{A.34})$$

The integral R_m , Eq. (A.20), is

$$R_m = 2\beta \int_0^\infty \exp(-s[2\beta - m]) ds. \quad (\text{A.35})$$

It is immediately apparent that, unless 2β exceeds m , R_m is infinite; and hence, from Eq. (A.33), $\hat{\mu}_m$ is infinite. Thus, for any choice of $A(\alpha)$ (which determines β), all the even moments for which $m \geq 2\beta$ are infinite.

For Curl's model β is equal to 2 and hence the fourth and higher even moments are infinite. For the modified Curl model ($A(\alpha)=1$, $\beta=3$), this analysis shows that the sixth and higher even moments are infinite. In fact, the numerical results of section 2.3 show that the fourth moment is also infinite. This, presumably, indicates that for this model γ_4 is infinite.

A necessary, though not sufficient, condition for a model to produce a pdf with finite moments is that $r(s)$ decays more rapidly than exponentially with s . This condition ensures that R_m is finite for all m .

Improved Models

The behavior of the model was investigated for six choices of $r(s)$ (denoted by I–VI) and six choices of $A(\alpha)$ (denoted by a–f). All of the age distributions produce finite values of R_m . They are,

- I *Uniform* $\hat{r} = 2$, $0 \leq x \leq \frac{1}{2}$,
- II *Parabolic* $\hat{r} = 2(1 - y^2)$, $0 \leq y = 4/3x \leq 1$,
- III *Quartic* $\hat{r} = 2(1 - y^2)^2$, $0 \leq y = 16/15x \leq 1$,
- IV *Cosine* $\hat{r} = 1 + \cos \pi x$, $0 \leq x \leq 1$,
- V *Linear* $\hat{r} = 2(1 - x)$, $0 \leq x \leq 1$,
- VI *Gaussian* $\hat{r} = 2 \exp(-\pi x^2)$, $0 \leq x$. (A.36)

Note that, except for VI, the age distributions are zero for s greater than some finite value: this implies that $z(s)$ becomes infinite.

TABLE I
Values of β for improved models

| | a | b | c | d | e | f |
|-----|-------|-------|-------|-------|-------|-------|
| I | 1.443 | 1.661 | 1.753 | 1.855 | 1.958 | 2.466 |
| II | 1.500 | 1.719 | 1.812 | 1.914 | 2.016 | 2.526 |
| III | 1.523 | 1.741 | 1.834 | 1.937 | 2.039 | 2.549 |
| IV | 1.531 | 1.750 | 1.843 | 1.945 | 2.048 | 2.557 |
| V | 1.592 | 1.812 | 1.905 | 2.008 | 2.111 | 2.622 |
| VI | 1.577 | 1.795 | 1.888 | 1.990 | 2.092 | 2.601 |

TABLE II
Flatness $\hat{\mu}_4$ for improved models

| | a | b | c | d | e | f |
|-----|------|------|------|------|------|------|
| I | 3.12 | 3.20 | 3.28 | 3.44 | 3.54 | 4.56 |
| II | 3.36 | 3.53 | 3.65 | 3.86 | 4.01 | 5.49 |
| III | 3.49 | 3.70 | 3.84 | 4.09 | 4.27 | 6.03 |
| IV | 3.54 | 3.77 | 3.93 | 4.19 | 4.38 | 6.26 |
| V | 3.80 | 4.18 | 4.41 | 4.80 | 5.10 | 8.21 |
| VI | 3.97 | 4.33 | 4.55 | 4.92 | 5.21 | 8.10 |

TABLE III
Superskewness $\hat{\mu}_6$ for improved models

| | a | b | c | d | e | f |
|-----|------|------|------|-------|-------|----------|
| I | 16.8 | 18.4 | 20.1 | 23.9 | 26.7 | 126.5 |
| II | 21.0 | 25.0 | 28.6 | 36.8 | 44.3 | ∞ |
| III | 23.6 | 29.5 | 34.7 | 47.2 | 59.9 | ∞ |
| IV | 24.8 | 31.6 | 37.7 | 52.7 | 68.7 | ∞ |
| V | 30.2 | 44.9 | 59.5 | 105.0 | 192.2 | ∞ |
| VI | 36.8 | 56.2 | 76.9 | 153.1 | 358.9 | ∞ |

The six distributions $A(\alpha)$ are,

- a *Delta function* $A(\alpha) = \delta(1 - \alpha)$,
- b *Quartic* $A(\alpha) = 10\alpha^3(1 - \frac{3}{4}\alpha)$,
- c *Cosine* $A(\alpha) = 1 - \cos \pi\alpha$,
- d *Linear* $A(\alpha) = 2\alpha$,
- e *Quadratic* $A(\alpha) = 3\alpha(1 - \frac{1}{2}\alpha)$,
- f *Uniform* $A(\alpha) = 1$.

For the thirty-six models comprising all combinations of $\hat{r}(x)$ and $A(\alpha)$, the values of β , $\hat{\mu}_4$ and $\hat{\mu}_6$ were calculated from Eqs. (A.30)–(A.33). The results are shown in Tables I, II and III. It may be seen that all the moments are finite except for $\hat{\mu}_6$ for models IIIf–VI f. In these cases, the denominator in Eq. (A.32) is negative, indicating that no finite values of γ_m can satisfy Eqs. (A.25) and (A.26).

The models are ordered so that $\hat{\mu}_4$ and $\hat{\mu}_6$ (and in general β) increase to the right and downward. Thus, the first model Ia has the smallest moments, $\hat{\mu}_4=3.12$ and $\hat{\mu}_6=16.8$, which may be compared with the Gaussian values of 3 and 15.

Life Expectancy

Closely related to the age distribution $r(s)$ is the pdf of life expectancy $g(s)$. Let the age of an element when it mixes be τ^* . Then $g(s)$ is the pdf of τ^* . The pdf's $r(s)$ and $g(s)$ are related by

$$g(s) = r(s)z(s) = -\frac{1}{2\beta} \frac{dr(s)}{ds}, \quad (\text{A.38})$$

or

$$\hat{g}(x) = -\frac{1}{\beta} \frac{d\hat{r}(x)}{dx}, \quad (\text{A.39})$$

where

$$\hat{g}(x) = g(s)/\beta. \quad (\text{A.40})$$

By differentiating Eq. (A.36), we find the life expectancy pdf's corresponding to the six age

distributions to be

- I $\hat{g} = \delta(x - \frac{1}{2})$,
- II $\hat{g} = 32/9x, 0 \leq x \leq \frac{3}{4}$,
- III $\hat{g} = 64/15y(1-y^2), 0 \leq y = 16/15x \leq 1$,
- IV $\hat{g} = \frac{1}{2}\pi \sin \pi x, 0 \leq x \leq 1$,
- V $\hat{g} = 1, 0 \leq x \leq 1$,
- VI $g = 2\pi x \exp(-\pi x^2), 0 \leq x$.

(Outside the indicated ranges, \hat{g} is zero.)

It may be seen that for I, the life expectancy τ^* is not a random variable but is fixed at $\tau^* = \frac{1}{2}\beta$. This implies that two elements that initially have different ages always have different ages and hence cannot mix with each other. This phase-locked behavior is unacceptable in a general model. Models II and V have \hat{g} 's that are discontinuous at the end of the age distribution, which could cause undesirable behavior. Thus, the age distribution III is to be recommended since (of the acceptable models) it has the smallest moments.

The delta-function distribution (a) for $A(\alpha)$ is the same as in Curl's model. It is unacceptable, therefore, since it can produce discontinuous pdf's.

The recommended model is, then, IIIb for which the moments are $\hat{\mu}_4 = 3.70$ and $\hat{\mu}_6 = 29.5$.

Appendix B

Starting from Eq. (A.21) an expression for κ_m in terms of λ_m is obtained. The procedure is demonstrated for $m=2$ and the results for $m=4$ and $m=6$ are given.

Substituting Eq. (2.25) for K in Eq. (A.21) yields

$$\begin{aligned} \kappa_m &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} h(\psi_a)h(\psi_b) \int_0^1 A(\alpha) \int_{-\infty}^{\infty} \\ &\times \psi^m \delta\{\psi - [1 - (\alpha/2)]\psi_a - (\alpha/2)\psi_b\} d\psi d\alpha d\psi_a d\psi_b \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} h(\psi_a)h(\psi_b) \int_0^1 A(\alpha) \{ [1 - (\alpha/2)]\psi_a \\ &+ \alpha/2 \psi_b \}^m d\alpha d\psi_a d\psi_b. \end{aligned} \quad (\text{B.1})$$

For the case $m=2$, the inner integral is

$$\begin{aligned} &\int_0^1 A(\alpha) \{ \psi_a^2(1 - \alpha + \alpha^2/4) + \psi_a \psi_b(\alpha - \alpha^2/2) \\ &+ \psi_b^2 \alpha^2/4 \} d\alpha = \psi_a^2(1 - a_1 + a_2/4) \\ &+ \psi_a \psi_b(a_1 - a_2/2) + \psi_b^2 a_2/4, \end{aligned} \quad (\text{B.2})$$

where a_n is the n th moment of $A(\alpha)$, Eq. (2.28). Substituting this result into Eq. (B.1) yields

$$\begin{aligned} \kappa_2 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} h(\psi_a)h(\psi_b) \{ \psi_a^2(1 - a_1 + a_2/4) \\ &+ \psi_a \psi_b(a_1 - a_2/2) + \psi_b^2 a_2/4 \} d\psi_a d\psi_b \end{aligned}$$

$$\begin{aligned}
&= \int_{-\infty}^{\infty} h(\psi_a) \{ \psi_a^2 (1 - a_1 + a_2/4) + \lambda_2 a_2/4 \} d\psi_a \\
&= \lambda_2 \{ 1 - a_1 + a_2/2 \}. \tag{B.3}
\end{aligned}$$

Here, λ_n is the n th moment of $h(\psi)$, Eq. (A.19), and use is made of the fact that odd moments of h are zero ($\lambda_n = 0$, n odd). Thus,

$$\kappa_2 = c_{2,2} \lambda_2, \tag{B.4}$$

where

$$c_{2,2} = (1 - a_1 + a_2/2). \tag{B.5}$$

For $m=4$, the same procedure yields,

$$\kappa_4 = c_{4,4} \lambda_4 + c_{4,2} \lambda_2^2, \tag{B.6}$$

where

$$c_{4,4} = 1 - 2a_1 + 3a_2/2 - a_3/2 + a_4/8, \tag{B.7}$$

and

$$c_{4,2} = 3a_2/2 - 3a_3/2 + 3a_4/8. \tag{B.8}$$

And for $m=6$, the result is

$$\kappa_6 = c_{6,6} \lambda_6 + c_{6,4} \lambda_4 \lambda_2, \tag{B.9}$$

where

$$\begin{aligned}
c_{6,6} &= 1 - 3a_1 + 15/4 a_2 - 5/2 a_3 \\
&\quad + (15a_4 - 3a_5 + a_6/2)/16, \tag{B.10}
\end{aligned}$$

and

$$c_{6,4} = 15/16(4a_2 - 8a_3 + 7a_4 - 3a_5 + a_6/2). \tag{B.11}$$