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Scalar dissipation rate modelling in variable density turbulent axisymmetric jets and diffusion flames

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In recent years several transport equation models for the scalar dissipation rate have been proposed to replace the well known algebraic expression based on equality of mechanical and scalar turbulent time scales. In this study various transport equation models are compared with each other and the model equation of Yoshizawa [J. Fluid Mech. **195**, 541 (1988)] is given special attention. The latter is shown to allow an algebraic solution that is different from the classical “equal-scales” algebraic model. The constants that appear in this equation are assigned values based on similarity behavior in turbulent jets and based on studies of homogeneous isotropic turbulence. Both algebraic models and the transport equation models are compared and applied to isothermal variable density jets and jet diffusion flames. It is found that general features, such as the behavior of scalar fluctuation intensities of variable density turbulent jets are relatively well predicted by all the models. Differences between the models exist regarding the predicted time scale ratios. © 1998 American Institute of Physics. [S1070-6631(98)01304-X]

I. INTRODUCTION

The mean scalar dissipation rate is defined as $\varepsilon_f = 2\kappa(\partial \overline{f''}/\partial x_i)^2$, where f is the scalar, “ $''$ ” denotes its fluctuation, and the tilde denotes a density weighted (Favre) average. The scalar can be the mass fraction of a chemical species or the temperature. The scalar dissipation rate signifies the destruction of turbulent scalar fluctuations by the action of the molecular diffusivity or conductivity (κ) and is the scalar analogue of the turbulent kinetic energy dissipation rate ε . The destruction of scalar fluctuations is associated with mixing at the small scales of the turbulent flow and plays an important role in turbulent combustion models: either as a descriptor of mixing¹ or as a descriptor of the stretching of laminar flamelets.² $1/\varepsilon_f$ can therefore be interpreted as a characteristic turbulent diffusion or mixing time. The stretching of the laminar flamelets gives rise to non-equilibrium chemistry which is of particular importance for the formation of pollutants such as nitric oxides in turbulent combustion.^{3–5}

To approximate the scalar dissipation rate, integral time scales of scalar and mechanical (velocity) turbulence are often assumed proportional. The resulting simple algebraic scalar dissipation rate model implies a constant turbulent Prandtl or Schmidt number in the framework of first order turbulence models. However, measurements and predictions of turbulent jets and diffusion flames in the literature indicate that mechanical and scalar scales are not always proportional. The measured Prandtl number in a heated round jet, by Chevray and Tutu,⁶ was not constant, neither were the mechanical to scalar time scale ratio and the Prandtl number measured by Sarh⁷ in a heated rectangular jet, nor the time scale ratio in a helium–air jet measured by Panchapakesan and Lumley.⁸ Shabbir and George⁹ found a varying mechani-

cal to scalar time scale ratio R_τ in their experiment on a buoyant axisymmetric plume. Buoyancy can have a significant influence on this time scale ratio, as observed by Hanjalic¹⁰ in his review. Drake *et al.*¹¹ argued that a constant turbulent Schmidt number may not be a useful concept in turbulent flames. If the time scale ratio is not constant, a transport equation for ε_f is required to calculate it independently.

Several transport equation models for the scalar dissipation rate have been published in the literature. In the present study many of these models are compared and especially the transport equation model of Yoshizawa,¹² which is based on his “two-scale direct interaction approximation” (TSDIA), is investigated and it is shown that an algebraic solution exists to this equation (the “non-equal” scales model). The coefficients in this equation are determined by considering scaling behavior in axisymmetric turbulent jets and homogeneous isotropic turbulence. The quantities predicted with the various models are the axial evolution of the scalar dissipation rate and the scalar variance, the asymptotic (large x) value of the center line intensity of scalar fluctuations, and profiles of the scalar variance across the jet and flame. They are compared with available measurements.

II. ANALYSIS OF SCALAR DISSIPATION RATE MODELS

A. Classical algebraic “equal-scales” model

As mentioned above, the simplest model for ε_f is based on the assumption that the time and length scales of mechanical and scalar turbulence are equal. The time and length scales for mechanical turbulence are $\tau_u \sim k/\varepsilon$ and $\ell_u \sim k^{3/2}/\varepsilon$, respectively, where k is the turbulent kinetic energy. On dimensional grounds, the time and length scales for

scalar turbulence are $\tau_s \sim \widetilde{f}^{n/2}/\varepsilon_f$ and $\ell_s \sim \widetilde{f}^{n/2} \varepsilon^{1/2}/\varepsilon_f^{3/2}$, respectively, where $\widetilde{f}^{n/2}$ is the scalar variance. Setting $\tau_u = \tau_s$ or $\ell_u = \ell_s$ gives the “equal-scales” model, $\varepsilon_f = R_\tau \widetilde{f}^{n/2} \varepsilon/k$, which relates the scalar dissipation rate linearly to the scalar variance and to the large eddy turnover time. The mechanical to scalar time scale ratio $R_\tau = (k/\varepsilon)/(\widetilde{f}^{n/2}/\varepsilon_f)$ is usually taken to be 2 according to experiments of Beguier *et al.*¹³ This leads to the “equal-scales” model

$$\varepsilon_f = 2 \widetilde{f}^{n/2} \varepsilon/k. \quad (1)$$

In the framework of first order turbulence models, a constant value of R_τ also leads to a constant turbulent Schmidt number. The turbulent Schmidt number, Sc_t , is defined as the ratio of the eddy viscosity $\nu_t \sim k^2/\varepsilon$ and the eddy diffusivity $\nu_s \sim \widetilde{f}^{n/2} \varepsilon/\varepsilon_f^2$. These expressions lead to a relationship between Sc_t and R_τ : $Sc_t = \nu_t/\nu_s \sim (k^2/\varepsilon)/(\widetilde{f}^{n/2} \varepsilon/\varepsilon_f^2)$, so $Sc_t = R_\tau^2$.

B. Discussion of scalar dissipation rate models in the literature

Various transport equation models for ε_f given in the literature are listed in Table I in chronological order. These models are given to present a complete overview of existing models. The equation for ε_f , to which all coefficients in Table I are related, is

$$\begin{aligned} \rho \frac{D\varepsilon_f}{Dt} = & D_{\varepsilon_f} + C_{P1} \frac{\varepsilon_f}{\widetilde{f}^{n/2}} P_f + C_{P2} \frac{\varepsilon_f}{k} P_k - C_{D1} \rho \frac{\varepsilon_f^2}{\widetilde{f}^{n/2}} \\ & - C_{D2} \rho \frac{\varepsilon_f \varepsilon}{k}, \end{aligned} \quad (2)$$

where D_{ε_f} is a diffusion term, $P_k = -\widetilde{\rho u_i'' u_k''} (\partial U_i / \partial x_k)$ is the production of turbulent kinetic energy, and $P_f = -2\widetilde{\rho u_k'' f''} (\partial F / \partial x_k)$ is the production of scalar fluctuations. Capitals (U and F) denote density weighted (Favre) averaged values of the velocity and mixture fraction (scalar) of the jet gas.

The coefficients of all models are listed in Table I, see also Eq. (2). It is now well established that in a non-homogeneous flow, such as a turbulent jet, the transport equation for ε_f should contain production terms due to scalar and velocity gradients and dissipation terms due to scalar as well as mechanical destruction of fluctuations.¹⁴ Therefore the older models that do not include these terms will not be used in the present study. The constants and also the characteristic time scales that occur in some of these terms, are not the same in every model. Large differences between the coefficients in Table I appear. In some (older) models the production term due to mean velocity gradients is absent ($C_{P2}=0$) and large differences appear in the numerical values of C_{P2} used. Striking differences are seen in both production term coefficients in Table I. The frequency factor in the production terms with C_{P1} is not the same in all models.

TABLE I. Coefficients in the scalar dissipation rate equations by various authors. Coefficients refer to Eq. (2). *Dibble *et al.* (Ref. 18) give a value of 2.45, which is probably erroneous. In their model also variable density terms are included. In the model of Mantel and Borghi (Ref. 23) also a term $0.9Re_t^{1/2}$ is included.

Author	C_{P1}	C_{P2}	C_{D1}	C_{D2}
Newman <i>et al.</i> ^a	1.0	0	1.01	0.88
Elghobashi and Launder ^b	0.9	0	1.1	0.8
Elghobashi and LaRue ^c	0.9	0.72	1.1	0.8
Dibble <i>et al.</i> ^d	0.5	1.45*	1.0	0.9
Chen ^e	0.5	1.45	1.15	0.65
Shih <i>et al.</i> ^f	$\frac{1}{2}\psi_1^f$	0	$1.0 - \frac{3}{2}II/R_{\tau,e}$	$\frac{1}{2}\psi_0 - 1 + \frac{3}{2}II$
Nagano and Kim ^g	0.9	0.72	1.1	0.8
Jones and Musonge ^h	$1.7R_\tau^{-1}$	1.45	1.0	0.9
Borghi ⁱ	$0.5R_\tau^{-1}$	1.0	1.9	0.95
Mantel and Borghi ^j	R_τ^{-1}	1.0	$0.625 Re_t^{1/2}$	0
Ruffin <i>et al.</i> ^k	0.5	1.78	1.0	0.9
Yoshizawa ^l	1.2	0.52	1.2	0.52
Sanders and Lamers ^m	1.5	$0.25C_{\varepsilon 1}$ =0.363	1.5	$0.25 C_{\varepsilon 2}$ = 0.48
Sommer <i>et al.</i> ⁿ	0.9	0.72	1.1	0.8
Non-equal (Present study)	1.0	$0.5 C_{\varepsilon 1}$ =0.725	1.0	$0.5 C_{\varepsilon 2}$ =0.95

^aReference 15.

^bReference 16.

^cReference 17.

^dReference 18.

^eReference 19.

^fReference 20.

^gReference 21.

^hReference 14.

ⁱReference 22.

^jReference 23.

^kReference 24.

^lReference 12.

^mReference 26.

ⁿReference 27.

Sometimes the scalar frequency $\varepsilon_f/\widetilde{f}^{n/2}$ in C_{P1} is replaced by the mechanical one ε/k , giving $C_{P1} \sim R_\tau^{-1}$.

The model equation proposed by Newman *et al.*¹⁵ includes both dissipation terms and one production term due to mean scalar gradients. It is also used by Elghobashi and Launder¹⁶ with slightly modified coefficients. Dibble *et al.*¹⁷ use this equation for the calculation of a turbulent Ar/H₂ flame, and consequently, due to the inhomogeneity of the flow, had to add a production term due to mean velocity gradients. They also added terms due to density fluctuations, which they showed to be not of great significance. Chen¹⁹ uses the same model but with modified values of the coefficients for calculations of turbulent flames.

Shih *et al.*²⁰ derive an ε_f -equation by applying the invariance principles of Lumley.²⁸ The comparison of their model with the others is difficult due to the functional forms of the constants which are given here for completeness,

$$\rho \frac{D\varepsilon_f}{Dt} = D_{\varepsilon_f} - \frac{1}{2} \rho \frac{\varepsilon_f^2}{\widetilde{f}^{n/2}} \psi^f, \quad (3)$$

with

$$\psi^f = \psi_0^f + \psi_1^f \frac{P_f}{\rho \varepsilon_f} \quad (4)$$

in which

$$\psi_0 = 2 - \frac{2 - \psi_0}{R_\tau} - 3 \frac{\Pi}{R_\tau} \left(\frac{R_\tau}{R_{\tau,e}} - 1 \right), \quad (5)$$

$$\psi_1 = \begin{cases} \left(2 + \frac{\psi_1 - 2}{R_{\tau,e}} \right) \left(\frac{R_\tau}{R_{\tau,e}} \right)^{10} & \text{if } R_\tau < R_{\tau,e} \\ \left(2 + \frac{\psi_1 - 2}{R_{\tau,e}} \right) \left(1 - 0.1 \left(1 - \frac{R_\tau}{R_{\tau,e}} \right) \right) & \text{if } R_\tau > R_{\tau,e} \end{cases} \quad (6)$$

with $\psi_0 = \frac{14}{5} + 0.98 \exp(-2.83/\text{Re}_t)[1 - 0.33 \ln(1 - 55\Pi)]$. The turbulent Reynolds number is $\text{Re}_t = 4k^2/9\varepsilon\nu$ and $\Pi = -\frac{1}{2}b_{ij}b_{ij}$, where Π is the second invariant of the anisotropy tensor $b_{ij} = \widetilde{u_i''u_j''}/2k - \frac{1}{3}\delta_{ij}$. Finally, $\psi_1 = 2.4$ and $R_{\tau,e}$, the equilibrium value of R_τ in the limit of isotropic turbulence, is taken to be 1.6.

Nagano and Kim²¹ use a transport equation model that has some similarity with the model proposed in the present study, but they apply it to heat transfer in wall bounded turbulent flows. All other models have been applied to jet type flows.

Jones and Musonge¹⁴ base their model on the proposal of Lumley²⁸ and determine the constants by considering temperature variances in homogeneous flow behind a grid with and without mean temperature gradient.

Borghi²² modified the model for the ε_f -equation of Zeman and Lumley.²⁹ Mantel and Borghi²³ propose a model which is Reynolds number dependent and which is aimed at modelling turbulent combustion with flamelet concepts. The equation is close to the equation for the flame surface density of Marble and Broadwell.³⁰ The models of Borghi²² and Mantel and Borghi²³ are close to flame surface density models for turbulent combustion of Marble and Broadwell.³⁰ However, scalar production and viscous dissipation terms are lacking in the flame surface density equation.

Ruffin *et al.*²⁴ do not give a reference for their model equation, but it closely resembles the model of Dibble *et al.*,¹⁸ except for C_{p2} .

III. SCALAR DISSIPATION RATE MODEL BASED ON YOSHIZAWA'S WORK

The model discussed in this section is based on the two-scale direct interaction approximation model of Yoshizawa. This model splits the Navier–Stokes equations in mean slow and fast fluctuating variables. The fluctuating field is isotropic and it is written in a series expansion. This field is then solved using the direct interaction approximation.^{12,25} This is a different method for deriving transport equations for turbulence quantities. The resulting scalar dissipation rate equation is concentrated on in the present work. It is investigated to what extent this equation can be useful in predictions of turbulent jet type of flows, reacting and non-reacting. It is shown that an analytical solution exists and that the original coefficients in the model need modifications in turbulent jets.

A. Analytical solution

Yoshizawa,¹² using TSDIA, derived a model equation for ε_f given by

$$\frac{D\varepsilon_f}{Dt} = \lambda_1 \frac{\varepsilon_f}{\widetilde{f''^2}} \frac{D\widetilde{f''^2}}{Dt} + \lambda_2 \frac{\varepsilon_f}{\varepsilon} \frac{D\varepsilon}{Dt}. \quad (7)$$

The right hand side is a combination of the equations for the scalar variance and the dissipation rate of turbulent kinetic energy. The equations for the scalar variance $\widetilde{f''^2}$, the turbulent kinetic energy k and the turbulent energy dissipation rate ε are given by

$$\frac{D\widetilde{f''^2}}{Dt} = D_f \widetilde{f''^2} + P_f - \bar{\rho} \varepsilon_f, \quad (8)$$

$$\frac{Dk}{Dt} = D_k + P_k + G_k - \bar{\rho} \varepsilon, \quad (9)$$

and

$$\frac{D\varepsilon}{Dt} = D_\varepsilon + C_{\varepsilon,1} \frac{\varepsilon}{k} P_k - C_{\varepsilon,2} \frac{\varepsilon}{k} \bar{\rho} \varepsilon + C_{\varepsilon,3} \frac{\varepsilon}{k} G_k, \quad (10)$$

respectively. The first term in each equation represents turbulent diffusion which is approximated by the standard expression $D_\phi = C_\phi (\partial/\partial x_k) [\bar{\rho}(k/\varepsilon) \widetilde{v''^2} (\partial\phi/\partial x_k)]$. In the k and ε equations, the term G_k represents buoyancy induced turbulence production: $G_k = -\rho\beta_e \widetilde{u_i''f''}$ where β_e is the volumetric expansion coefficient $\beta_e = -(1/\bar{\rho})(\partial\rho/\partial f)$.

Equation (7) contains all production and dissipation terms that should be present: production due to scalar and velocity gradients and dissipation due to the dissipation of scalar and velocity fluctuations. It can be observed that buoyancy related production terms would be automatically present in Eq. (7) when they are present in Eq. (10). The form of this term is the same as that proposed by Hanjalic.¹⁰ The diffusion term in Eq. (7) consists of diffusion due to gradients of scalar fluctuations and to gradients of the dissipation rate of turbulent kinetic energy. This mixture of diffusion terms is called cross diffusion. The only difference between Eq. (2) and Eq. (7), when otherwise the same coefficients are used, is due to cross diffusion because in Eq. (2) the diffusion term is approximated as $D_{\varepsilon_f} = C_s (\partial/\partial x_k) [\bar{\rho}(k/\varepsilon) \widetilde{v''^2} (\partial\varepsilon_f/\partial x_k)]$. In conclusion, the model Eq. (7) is complete in the sense that it includes all terms that appear in the models in Table I, while it also accounts for cross diffusion terms, and possibly buoyancy effects.

The particular form of Eq. (7) allows an analytical solution based on a separation of variables

$$\varepsilon_f = \phi \widetilde{f''^2}^{\lambda_1} \varepsilon^{\lambda_2} \quad (11)$$

with ϕ a dimensional reference value

$$\phi = \frac{\varepsilon_{f0}}{\widetilde{f''^2}^{\lambda_1}_0 \varepsilon_0^{\lambda_2}} \quad (12)$$

in which the subscript 0 indicates a reference point in the flow.²⁶ An important feature of Eq. (11) is the absence of the turbulent kinetic energy k , compared to the equal-scales version $\varepsilon_f = R_\pi \widetilde{f''^2} \varepsilon/k$.

TABLE II. Decay coefficients n for axisymmetric jets and in homogeneous isotropic turbulence.

Variable	Axisymmetric jet	Homogeneous turbulence
U	x^{-1}	x^0
k	x^{-2}	x^{-n}
ε	x^{-4}	$x^{-(n+1)}$
F	x^{-1}	x^0
\widetilde{f}^{n2}	x^{-2}	x^{-m}
ε_f	x^{-4}	$x^{-(m+1)}$

B. Determination of the constants λ_1, λ_2 , and ϕ

Yoshizawa^{12,25} approximated the dimensionless constants λ_1 and λ_2 by using inertial range forms of spectrum functions, to be 1.2 and 0.306, respectively. He indicated that these values were only approximative, and that they should be adjusted by comparing results with experimental data. This can be done by using asymptotic jet similarity characteristics. In a self preserving jet, the axial velocity decays with axial distance as $U \sim x^{-n}$, with $n=1$ for an axisymmetric jet and $n=\frac{1}{2}$ for a plane jet. These values are based on momentum conservation $\int_0^\infty U^2(y)y^a dy = \text{constant}$, where y is the radial distance. Here, $a=0$ for a plane jet and $a=1$ for an axisymmetric jet. Since the jets spread linearly, $y \sim x$ so $U^2 x x^a = \text{constant}$, and this gives the above scaling relations, see also Hinze.³¹ The turbulent kinetic energy decays as $k \sim U^2 \sim x^{-2n}$ and the dissipation rate decays as $\varepsilon \sim k^{3/2}/\ell \sim x^{-3n-1}$ because the integral length scale ℓ increases linearly with x . When the velocity decay is known, the scalar decay can be derived based on the conservation of nozzle mass flux through each axial cross section of the jet: $\int_0^\infty U(y)F(y)y^a dy = \text{constant}$. Since $y \sim x$, the scalar decays as $F \sim x^{n-a-1}$, the scalar variance decays as $\widetilde{f}^{n2} \sim F^2 \sim x^{2(n-a-1)}$ and the scalar dissipation rate as $\varepsilon_f \sim x^{n-2a-3}$. Equating exponents of x in $\varepsilon_f \sim \widetilde{f}^{n2 \lambda_1} \varepsilon^{\lambda_2}$ and $\varepsilon_f \sim x^{n-2a-3}$, and using the scaling laws for \widetilde{f}^{n2} and ε , this leads to

$$2(n-a-1)\lambda_1 - (3n+1)\lambda_2 = n-2a-3. \quad (13)$$

In axisymmetric jets $a=1$ (because $\int_0^\infty U F y dy = \text{constant}$) and $n=1$, so $\lambda_1 + 2\lambda_2 = 2$. See Table II for a summary of these scaling characteristics. Since the original values of Yoshizawa do not obey Eq. (13), they cannot be used in axisymmetric jet flows and they will have to be adjusted.

At this stage it can already be anticipated that $\lambda_1=1$ since the dissipation rate of scalar fluctuations is expected to be proportional to the scalar variance itself. One of the arguments is that, when temperature fluctuations are considered instead of dimensionless mass fraction fluctuations, the dimension of temperature does not appear in ϕ . According to Eq. (13) this would give $\lambda_2=\frac{1}{2}$.

In addition, the decay of isotropic turbulence will be investigated in order to derive relations between λ_1, λ_2 and the decay exponents in this type of flow, which can be measured or estimated theoretically/numerically. In the homo-

geneous isotropic turbulence behind a grid, the velocity fluctuations k and the temperature fluctuations \widetilde{T}^{n2} decay as a function of axial distance x according to

$$U \frac{dk}{dx} = -\varepsilon; \quad U \frac{d\widetilde{T}^{n2}}{dx} = -\varepsilon_f \quad (14)$$

in which $(dx/dt)=U$ is used, where U is the mean constant velocity in the homogeneous flow. Due to flow homogeneity, no diffusion or production of turbulence occurs in the flow; the fluctuations are only generated at the grid. It is common practice to describe the decay by power laws in x :

$$k \sim x^{-n}; \quad \widetilde{T}^{n2} \sim x^{-m}, \quad (15)$$

which gives $\varepsilon \sim x^{-(n+1)}$ and $\varepsilon_f \sim x^{-(m+1)}$. Therefore, the time scale ratio in these flows is $R_\tau = m/n$. Equating powers of x in the second equation in Eq. (14), using $\varepsilon_f \sim \widetilde{T}^{n2 \lambda_1} \varepsilon^{\lambda_2}$ in which $\widetilde{T}^{n2} \sim x^{-m}$ and $\varepsilon \sim x^{-(n+1)}$, respectively, gives

$$m+1 = m\lambda_1 + (n+1)\lambda_2. \quad (16)$$

The exponents n and m remain to be determined to obtain a relation between λ_1 and λ_2 . Theoretically, assuming complete self-preservation such that the Reynolds number is constant during decay, it can be shown that the value of n should be unity: $n=1$ (Hinze³¹). In the final stage of the decay, however, viscosity effects become important and the fluctuations decay faster so that $n>1$, but then the flow is no longer self-preserving. Experimental data of Gibson and Dakos³² and those in the review of Mohamed and LaRue³³ show values of $n>1$, namely $n \approx 1.3$. However, the experimental studies of Batchelor and Townsend,³⁴ Stewart and Townsend,^{35,36} Kistler and Vrebalovich,³⁷ Van Atta and Chen,³⁸ Portfors and Keller,³⁹ Dickey and Mellor,⁴⁰ Groth and Johansson,⁴¹ and Hanarp⁴² all report $n=1$. Groth and Johansson⁴¹ explain the larger value of other researchers ($n \approx 1.3$) by the fact that these included data close to the grid, where the turbulence is still strongly anisotropic. When Groth and Johansson⁴¹ included data of the anisotropic near field in their own evaluation of n , they also obtained a larger value: $n=1.32$. This is confirmed by the data of Brown and Bilger⁴³ using a very anisotropic near field close to the grid, who find $n \approx 1.3$. Dickey and Mellor⁴⁰ state that the same experimental data can sometimes be fitted equally well by two different sets of decay exponent and virtual origin. There seems to be as yet no experimental consensus regarding the universality of the decay exponent in homogeneous isotropic turbulence. However, since the turbulent jet considered is fully self-preserving, we tentatively put emphasis on the self similar solutions to the homogeneous isotropic turbulence, leading to $n=1$.

Theoretical considerations to estimate n involve several flow “invariants:” the invariant associated with complete self-preservation and those of Saffman and Loitsianskii. These invariants are written in terms of the longitudinal double velocity correlation coefficient $f(r)$ in homogeneous isotropic turbulence. The function $f(r)$ obeys the Karman-Howarth equation (Hinze³¹). To have complete self-preservation, all coefficients in this equation should be pro-

portional to one another. This leads to the invariant $\ell_u u' = \text{constant}$, where u' is the rms velocity fluctuation, and “linear” decay is obtained: $n=1$. The use of Saffman’s dynamic invariant leads to $u'^2 \ell_u^3 = \text{constant}$ and $n=6/5$; while Loitsianskii’s invariant leads to $u'^2 \ell_u^5 = \text{constant}$ and $n=10/7$. The latter two do not allow complete self-preservation. It has been shown that Loitsianskii’s invariant is not a dynamic invariant, and that it may be applicable to the final stage of decay rather than the initial stage.

For the scalar decay, described by the exponent m , the same theoretical considerations can be used. These give for complete self-preservation: $m=3/2$ and the invariants of Saffman and Loitsianskii give $m=6/5$ and $m=6/7$, respectively (Hinze³¹). The experimental value of m seems to vary with the intensity of the temperature fluctuations generated at the grid; it increases with increasing values of the initial length scale ratio ℓ_u/ℓ_s and reaches a constant value for $\ell_u/\ell_s > 2.5$, see Mell *et al.*⁴⁴ and references therein. They attribute the dependence of m on the initial length-scale ratio to the decay, or non-stationarity, of the turbulence behind the grid. Indeed, Eswaran and Pope⁴⁵ find a universal decay in stationary turbulence which is independent of the initial length-scale ratio. The numerical “Test Field Model” study of Newman and Herring⁴⁶ in isotropic turbulence showed that $n=1$ and $m=1$, independently of initial conditions. It is interesting to note that these values, together with Eq. (16) give exactly Eq. (13) for axisymmetric turbulent jets. In Table III all experimental and theoretical values of n and m are listed.

However, the exact value of m is of no importance to the determination of λ_2 if proportionality between ε_f and \widehat{f}''^2 is retained because in that case $\lambda_1=1$ and Eq. (16) leads to

$$\lambda_2 = \frac{1}{n+1} \quad (17)$$

so that λ_2 is directly related to the velocity decay exponent and not to the scalar decay exponent m . In this way, the large uncertainty about the value of m is no longer of significance for determining λ_2 . The invariant associated with complete self-preservation and Saffman’s and Loitsianskii’s invariant, using Eq. (17) lead to $\lambda_2 = \frac{1}{2}$; $\frac{5}{11}$ and $\frac{7}{17}$, respectively. Assuming complete self-preservation with $n=1$ gives $\lambda_2 = \frac{1}{2}$. In that way, the new model for the scalar dissipation rate is proportional to the square root of the kinetic energy dissipation rate, which was also observed by Ashurst *et al.*⁴⁷ using Direct Numerical Simulations (DNS).

In the classical model the scalar dissipation rate was proportional to the large eddy strain rate ε/k , and in the new model the scalar dissipation rate can be considered to be related in some way to the small eddy strain rate, which is proportional to $\varepsilon^{1/2}$. Since the scalar dissipation rate is often associated with small scale mixing, relating the scalar dissipation rate to the small eddy strain rate seems realistic. However, this analogy should not be carried too far because in the macroscopic type of expression for ε_f that is sought, the small scale (molecular) parameters may not appear. The amount of scalar fluctuations that is dissipated is determined

TABLE III. Decay coefficients n and m in homogeneous isotropic turbulence.

Reference	n in $k \sim x^{-n}$	m in $T'^2 \sim x^{-m}$
Theoretical/Numerical		
Complete self-preservation ^a	1	$\frac{3}{2}$
Saffman’s invariant ^a	$\frac{6}{5}$	$\frac{6}{5}$
Loitsianskii’s invariant ^a	$\frac{10}{7}$	$\frac{6}{7}$
Test Field Model ^b	1	1
Experimental		
Gibson and Dakos ^c	≈ 1.3	
Mohamed and LaRue ^d	≈ 1.3	
Batchelor and Townsend ^e	1	
Stewart and Townsend ^f	1	
Kistler and Vrebalovich ^g	1	
Van Atta and Chen ^h	1	
Portfors and Keller ⁱ	1	
Dickey and Meller ^j	1	
Groth and Johansson ^k	1	
Hanarp ^l	1	
Brown and Bilger ^m	1.3	

^aReference 31.

^bReference 46.

^cReference 32.

^dReference 33.

^eReference 34.

^fReference 35 and 36.

^gReference 37.

^hReference 38.

ⁱReference 39.

^jReference 40.

^kReference 41.

^lReference 42.

^mReference 43.

by the large scale production of the fluctuations, assuming equilibrium in the scalar spectrum.

The dimension of the coefficient ϕ is completely determined by the values of λ_1 and λ_2 . Using $\lambda_1=1$ and $\lambda_2=\frac{1}{2}$, the coefficient ϕ should have the dimension of $\nu^{-1/2}$, so $m^{-1} s^{1/2}$. Since linear decay has been used to estimate λ_1 and λ_2 , this coefficient should be related to a certain power of the invariant $(u' \ell_u)^a$, associated with linear decay ($n=1$). Dimensional arguments lead to $a=-1/2$. Now, in a jet the velocity fluctuation u' is related to the jet exit velocity U and the length scale ℓ_u is proportional to the jet exit diameter D . This gives for ϕ

$$\phi = \phi_0 (UD)^{-1/2}, \quad (18)$$

in which ϕ_0 is a dimensionless constant, independent of U and D . This constant could be determined by comparing predictions in a jet with experiments. The invariant ϕ can be interpreted as a power of the momentum flux: $\phi \sim \mathcal{M}^{-1/4}$. It is interesting to note that using Saffman’s or Loitsianskii’s invariant, no simple physical interpretation of the invariant, i.e. ϕ , seems to exist.

For variable density jets, in which the jet density ρ_j is different from the ambient density ρ_a , the density ratio $\omega = \rho_a/\rho_j$ influences the flow field as well. In non-buoyant flows this can be taken into account by replacing the nozzle diameter D by an effective diameter $D^* = D(\rho_j/\rho_a)^{1/2} = D\omega^{-1/2}$ (Thring and Newby⁴⁸). This effective diameter is the diameter of a jet having the same momentum flux and jet exit velocity as the real jet considered, but with

$\rho_j = \rho_a$, so $\omega = 1$. In fact, this concept will work only in the far field of the jet, where the actual density will be very close to the air density ρ_a . All velocity and scalar profiles in the far field of jets with different ω can be collapsed onto the same curve when the distances are scaled with D^* instead of D .⁴⁹ When turbulent flames are considered, the far field density will not approach the ambient air density very quickly and it is more useful to relate the diameter D^* to a jet with the same momentum flux and velocity as the original flame, but having a density equal to the *local* density in the physical position considered. This concept will also work for isothermal jets because it is somewhat more general. However, the effective diameter in this case, $D^* = D(\rho_j/\rho)^{1/2}$, is not a constant anymore, but it depends on the position in the flow. In all predictions to be presented, ϕ is determined as

$$\phi = \phi_0 (UD^*)^{-1/2} \quad (19)$$

in which $D^* = D(\rho_j/\rho)^{1/2}$. In the present study the value of ϕ_0 has been determined to be $\phi_0 \approx 5$ by comparison of model predictions in the far field with experimental data.^{50,51}

C. Comparison with other models

Following the previous discussion, the scalar dissipation rate in the non-equal scales algebraic model is given by

$$\varepsilon_f = \widetilde{\phi f^{n_2}} \varepsilon^{1/2}. \quad (20)$$

This algebraic model for the scalar dissipation rate will be called the “non-equal scales” model, in contrast with the classical “equal-scales” model. The values for C_{P1}, C_{P2}, C_{D1} and C_{D2} associated with the values $\lambda_1 = 1$ and $\lambda_2 = \frac{1}{2}$ are shown in the last line of Table I. They are very close to those of Nagano and Kim²¹ while the dissipation coefficients C_{D1}, C_{D2} are close to all other models. The largest differences are observed for the coefficient C_{P1} . Notwithstanding the fact that the coefficients associated with the present non-equal scales model resemble those in the model of Nagano and Kim,²¹ their transport equation can not be solved analytically because their coefficients do not allow their model to be cast into the form of Eq. (7).

The non-equal scales expression can also be compared to an algebraic expression given by Libby and Bray⁵² for the scalar dissipation rate in turbulent premixed flames: $\varepsilon_f \sim u_l \widetilde{f^{n_2}} \varepsilon/k^{3/2}$, where u_l is the laminar burning velocity. Their analysis shows that the influence of chemical reactions on the scalar dissipation rate may be very large. In premixed flames, the scalar dissipation rate is directly related to the presence of the reaction zone. In the fresh unburned gases no concentration fluctuations occur, because they are perfectly mixed. In the burned gases, the same holds if no unburned gases pass through the reaction zone. Therefore, the scalar dissipation rate shows a peak close to the reaction zone and it is negligible elsewhere. The additional terms due to density variations in the model of Dibble *et al.*¹⁸ are designed for non-premixed (diffusion) flames, but they were shown not to be very influential.

IV. TURBULENCE AND COMBUSTION MODELS

The second order turbulence model used in the present study is based on the work of Launder *et al.*⁵³ It is described in Sanders *et al.*⁴⁹ where the return to isotropy constant has been changed to have a correct round jet spreading rate. The scalar flux turbulence model is also described in Ref. 49. Turbulent combustion is modelled with the laminar flamelet model, the theory of which is given by Peters.² For applications see also Sanders and Lamers⁵⁴ and Sanders *et al.*¹² In this model, the turbulent flame is considered as an ensemble of laminar one dimensional stretched flames, called flamelets. These laminar flamelets are embedded in the turbulent flow and undergo strain or stretch due to the turbulent flow field which can lead to chemical non-equilibrium effects such as temperature decrease or even local extinction. The flame structure of laminar flamelets is computed using detailed chemistry and it is used as a database for turbulent flame computations. The flamelet computations are performed with a numerical code that is a precursor of the laminar flame code RUNIDL (Rogg⁵⁵). The flamelet structure is given as a function of the mixture fraction and a parameter that describes the non-equilibrium state of the flamelet. According to theory (Peters²), and also according to the latest numerical studies on *NO* formation by Sanders *et al.*,¹² this parameter is the scalar dissipation rate.

For the calculation of the turbulent flow field, the mean density is the only variable that directly translates the influence of combustion on the flowfield. The density varies significantly from the cold outer flowfield towards the hot regions in the flame. A parabolic marching algorithm is used to compute the jets and jet diffusion flames. It is described in Sanders *et al.*⁴⁹ In the same reference, the mechanical turbulence model used in the present study was validated by comparing it with experimental data.

V. RESULTS AND DISCUSSION

Computations for reacting and non-reacting jets are presented using several of the models listed in Table I. Both algebraic models are used since it is interesting to compare these models which are easily implemented. Further, transport equation models are chosen which are based on different techniques. Those of Chen¹⁹ and Jones and Musonge¹⁴ are of the same type but they are often used in reacting flows. The model of Shih *et al.*²⁰ is based on Lumley's technique and the one of Mantel and Borghi²³ was developed to predict turbulent premixed flames.

A. Isothermal jets

The isothermal jets considered are mainly methane-air jets with a corresponding density ratio of $\omega = \rho_a/\rho_j \approx 1.6$. In Ref. 49 it was found that normalised quantities in the jet do not depend on the initial density ratio (spreading rates, centreline scalar fluctuation intensities) while even center line mixture fraction and velocity decay do not depend on ω when the axial distance is scaled by an effective diameter that takes the initial density ratio into account.

Regarding the production of the scalar dissipation rate, it should be noted that the boundary conditions for $\widetilde{f^{n_2}}$ and ε_f

are zero at all boundaries of the jet. Hence, if all production terms in the ε_f transport equation are proportional to ε_f itself, which is the case in most models in Table I, then ε_f will remain zero in the complete flow field. In some models in Table I, the frequency (ε/k) is used in one of the production terms, which alleviates this problem. However, a very small, non-zero, value of $\widetilde{f''^2}$ and ε_f at the nozzle, also solves this problem. The solution should not, and does not depend on the particular value of these variables at the nozzle. In the present study, typically $\widetilde{f''^2}_0 = 10^{-20}$ and $\varepsilon_{g0} = 2\widetilde{f''^2}_0 \varepsilon_0 / k_0$ has been used.

At this point it can be noted that due to the fact that the coefficient ϕ in the algebraic non-equal scales model depends on the boundary conditions of the jet, also the direct solution of the corresponding transport equation would depend on these conditions. The transport equation also contains cross diffusion terms that may lead to numerical instability. Even if cross diffusion is negligible, the equality of the constants C_{P1} and C_{D1} , which is a necessary condition for the equation to be solvable analytically, will lead to instability. For instance, if in a certain region of the jet diffusion and convection balance each other, and if also equilibrium prevails such that $P_f \approx \bar{\rho} \varepsilon_f$ and $P_k \approx \bar{\rho} \varepsilon$, then ε_f can be approximated in that region by $\varepsilon_f \approx -[(C_{P2} - C_{D2}) / (C_{P1} - C_{D1})](\varepsilon/k) \widetilde{f''^2}$. This expression becomes singular when $C_{P1} = C_{D1}$. In test calculations in which the transport equation corresponding to the analytical solution was solved but without cross diffusion, not shown here, it was indeed observed that there exists an asymptotic state for $(\widetilde{f''^2})^{1/2}/F$ if $C_{P1} \neq C_{D1}$ while it does not exist for $C_{P1} = C_{D1}$. This may explain why the model of Ref. 21, having coefficients very close to those in the non-equal scales model, although with $C_{P1} \neq C_{D1}$, does yield an asymptotic constant value of $(\widetilde{f''^2})^{1/2}/F$.

One of the characteristic parameters of the scalar field in a turbulent jet is the asymptotic (large x) center line value of the scalar fluctuation intensity $(\widetilde{f''^2})^{1/2}/F$. Experimentally, this value is independent of x if buoyancy effects are absent. In Table IV the values of the scalar fluctuation intensity and the time scale ratio, predicted with various transport equation and algebraic models, are shown. The center line mechanical to scalar time scale ratio R_τ becomes constant for large x with all models, the experimental value of Beguier *et al.*¹³ being close to 2.

All models show an asymptotic behavior, although the predicted values are somewhat higher than the experimental value of Richards and Pitts.⁵⁰ They also show no dependence of the far field results on the initial value of the scalar dissipation rate. It can be observed that in general a higher time scale ratio implies a lower value of the scalar fluctuation intensity.

In Fig. 1 the far field axial variation of the rms of the scalar fluctuations is shown to be predicted quite well with all models, when compared to the experiments of Birch *et al.*⁵¹ of a methane–air jet. The axial variation of the scalar dissipation rate in Fig. 2 also shows that all models behave similarly.

TABLE IV. Asymptotic values of the scalar fluctuation intensity $(\widetilde{f''^2})^{1/2}/F$ and time scale ratio R_τ : experiments and predictions using the models in Table I.

Author	$(\widetilde{f''^2})^{1/2}/F$	R_τ
Richards and Pitts ^a (expt.)	0.23	...
Beguier <i>et al.</i> ^b (expt.)	...	2.00
Dibble <i>et al.</i> ^c	0.28	1.70
Chen ^d	0.28	1.70
Shih <i>et al.</i> ^e	0.30	1.55
Nagano and Kim ^f	0.32	1.42
Jones and Musonge ^g	0.20	2.48
Mantel and Borghi ^h	0.31	1.48
Ruffin <i>et al.</i> ⁱ	0.22	2.15
Equal scales	0.24	2.00
Non-equal scales	0.22	2.30

^aReference 50.

^bReference 13.

^cReference 18.

^dReference 19.

^eReference 20.

^fReference 21.

^gReference 14.

^hReference 23.

ⁱReference 24.

The radial profiles of the rms of the scalar fluctuations are shown in Fig. 3. Away from the axis, the calculations agree very well with the experiments of Richards and Pitts.⁵⁰ The agreement at larger axial distances would be better because there the center line values between models and experiment are closer. The radial profiles of the scalar dissipation rate are shown in Fig. 4, where again all models behave approximately in the same way. The experimental data of Antonia and Mi,⁵⁶ when normalized to the equal-scales center line value, do not show a local maximum, although it is present in all model calculations. The time scale ratio R_τ in Fig. 5 shows significant differences between all models. A decreasing behavior, such as predicted with the non-equal scales model was also predicted by Dibble *et al.*¹⁸ This agrees with the (plane jet) experiments of Sarh.⁵ However, all other models predict the inverse behavior.

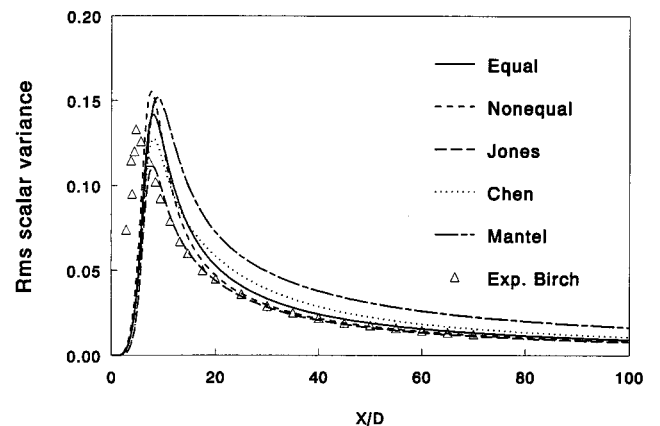


FIG. 1. Center line rms of scalar fluctuations $(\widetilde{f''^2})^{1/2}$ predicted with several models and compared to the experiments of Birch *et al.* (Ref. 51).

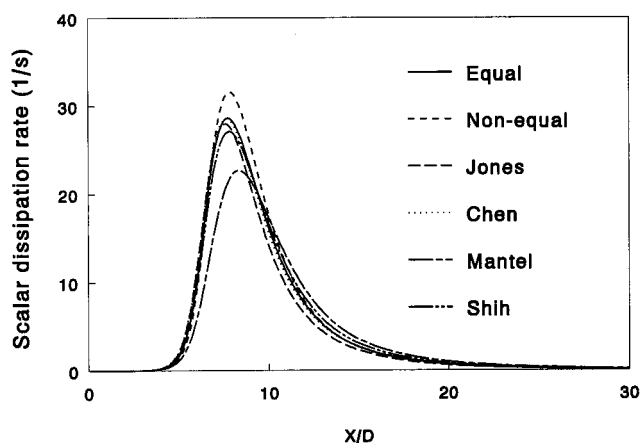


FIG. 2. Center line values of ε_f predicted with several models for the same jets as in Fig. 1.

Regarding variable density effects, it is important to verify whether a model predicts a value for the scalar fluctuation intensity $(\tilde{f}^{n2})^{1/2}/F$ that is independent of the initial density ratio, as shown experimentally by Richards and Pitts.⁵⁰ All models predict this behavior. However, it is stressed that ϕ in the non-equal scales model must be determined using the effective diameter D^* in Eq. (18). Otherwise the model predicts a value of the asymptotic scalar fluctuation intensity which increases with ω , which does not agree with the experiments.

B. Turbulent diffusion flames

The vertical diluted hydrogen flames (75% H_2 and 25% N_2), measured at the DLR in Stuttgart by Meier *et al.*,⁵⁷ are considered. The nozzle diameter is $D=0.008$ m and exit velocities are $U_j=56.4; 42.3; 28.2$ m/s, with a coflow of $U_{\text{coflow}}=0.3$ m/s. The Reynolds and Froude numbers of these flames are approximately $(Re; Fr) = (14200; 40530); (10650; 22800)$ and $(7100; 10130)$, respectively.

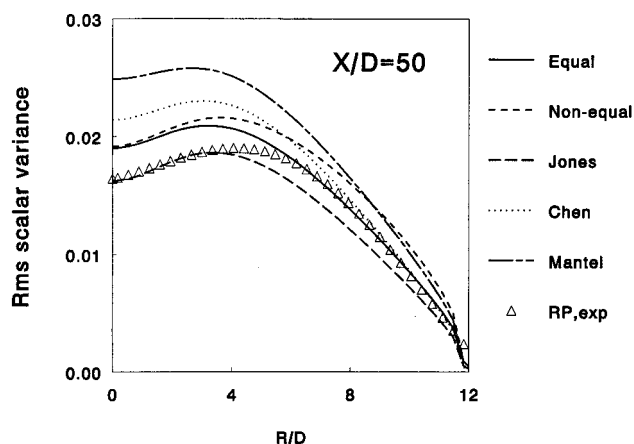


FIG. 3. Rms of scalar fluctuations $(\tilde{f}^{n2})^{1/2}$ across a methane-air jet at $x/D=50$. Measurements are from Richards and Pitts (Ref. 50).

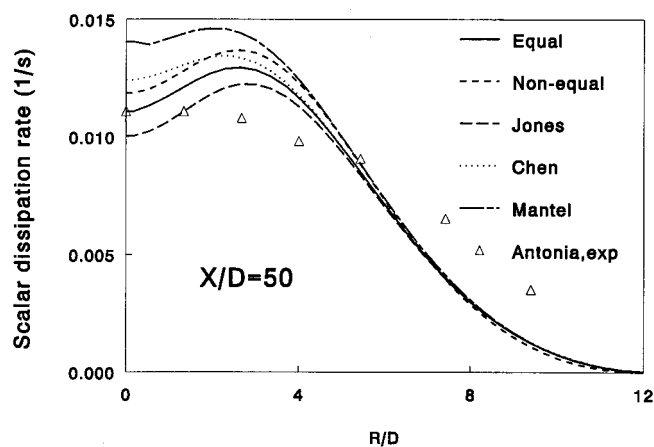


FIG. 4. Scalar dissipation rate ε_f across the jet predicted with several models compared to the experimental data of Antonia and Mi (Ref. 56).

The mean center line mixture fraction, based on the hydrogen element mass fractions, is shown in Fig. 6. The computations compare well with the measurements. The center line scalar fluctuation intensity predicted with the equal-scales model is shown in Fig. 7. Both predictions and measurements show an increase of the fluctuation level with decreasing exit velocity. This is due to gravity effects, that are taken into account in the equations and those become more important at lower velocities. The more important the gravity effects are, the faster the mean center line mixture fraction decays (Fig. 6). Since the mixture fraction fluctuations themselves are not so much influenced by gravity effects, the overall behavior is an increase of the intensity with increasing gravity effects.

In Fig. 8 the differences between the results of computations with the non-equal scales model at the several jet exit velocities are smaller. However, the far field values are underpredicted when compared to the measurements. The scalar fluctuation intensity predicted with the transport equation model of Chen¹⁹ is too high in the far field while it is underpredicted in the near field (Fig. 9). The predictions with the

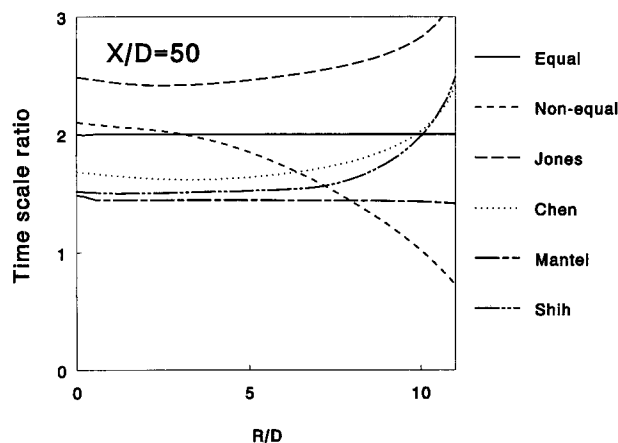


FIG. 5. Time scale ratio R_τ across the jet predicted with several models.

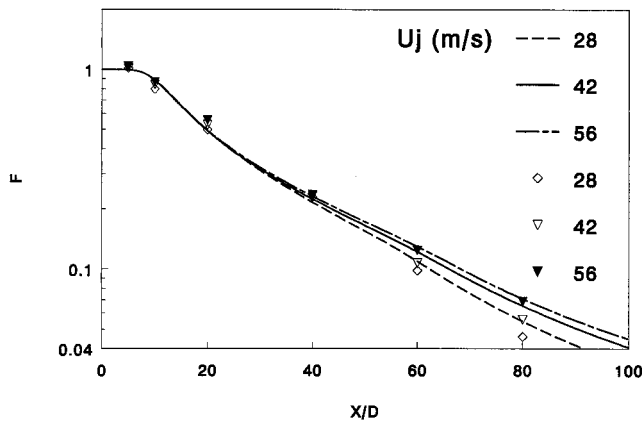


FIG. 6. Center line variation of the mixture fraction for the 3 flames measured at DLR Stuttgart by Meier *et al.* (Ref. 57). Lines are predictions and symbols represent measurements.

model of Jones and Musonge,¹⁴ Fig. 10, show the same behavior in the near field, but they correspond rather well with the experimental data in the far field. Both transport equation models and the non-equal scales model tend to show intensities for different exit velocities that approach each other in the far field.

Center line mean temperatures predicted with equilibrium chemistry are shown in Fig. 11. The far field temperature levels are lower for the flames at lower exit velocities due to the higher scalar fluctuation intensities at lower exit velocities. This is caused by the effect of “unmixedness,” which prevents the coexistence of fuel and oxydizer at the same time at the same location.

VI. SUMMARY AND CONCLUSIONS

Several existing scalar dissipation rate models have been reviewed and in particular the model equation of Yoshizawa,¹² based on TSDIA, is investigated because it constitutes a different method to derive turbulence equations.

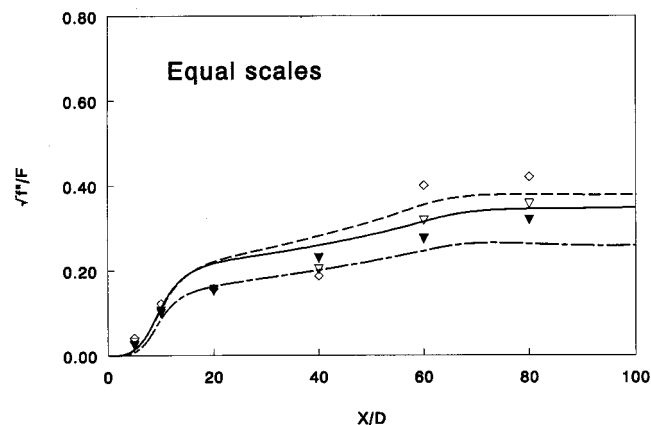


FIG. 7. Center line variation of the mixture fraction fluctuation intensity $(\overline{f''^2})^{1/2}/F$ for the 3 flames measured at DLR Stuttgart by Meier *et al.* (Ref. 57). Predictions with the equal scales model. See Fig. 6 for details.

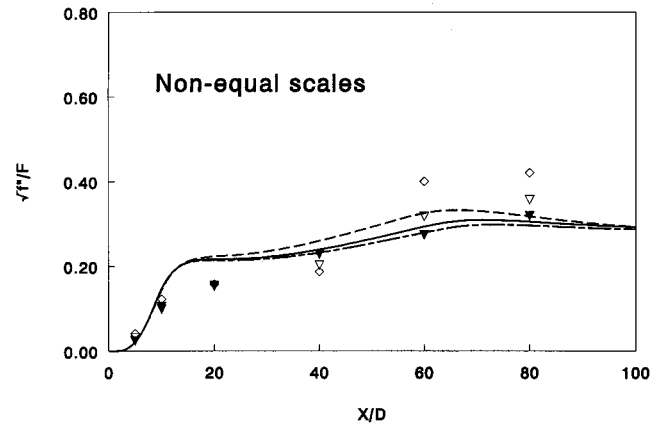


FIG. 8. Center line variation of the mixture fraction fluctuation intensity $(\overline{f''^2})^{1/2}/F$ for the 3 flames measured at DLR Stuttgart by Meier *et al.* (Ref. 57). Predictions with the non-equal scales model. See Fig. 6 for details.

An analytical solution to this equation is given, which does not rely on assumptions made about scalar time scales being related to mechanical time scales, such as in the classical equal scales algebraic model. The model is extensively discussed and applied to isothermal variable density turbulent jets and turbulent jet diffusion flames. The coefficients in the equation were originally determined by Yoshizawa but it was shown that they cannot be universal. New coefficients have been estimated using the decay scaling laws in turbulent jets and decay of homogeneous and isotropic turbulence. Experimental and theoretical/numerical results on homogeneous turbulence have been extensively reviewed and this showed that there is no consensus yet on universality of the decay exponents in homogeneous turbulence. Many experiments indicate however a linear decay for velocity fluctuations while temperature fluctuations seem to decay with exponents that vary with initial conditions.

In the new algebraic model, the dimensional parameter ϕ , the dimension of which depends on the values of the coefficients λ_1 and λ_2 , is associated with a certain power of

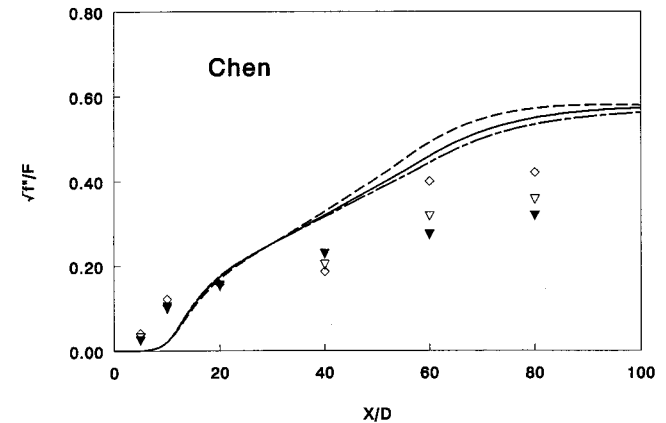


FIG. 9. Center line variation of the mixture fraction fluctuation intensity $(\overline{f''^2})^{1/2}/F$ for the 3 flames measured at DLR Stuttgart by Meier *et al.* (Ref. 57). Predictions with the model of Chen (Ref. 19). See Fig. 6 for details.

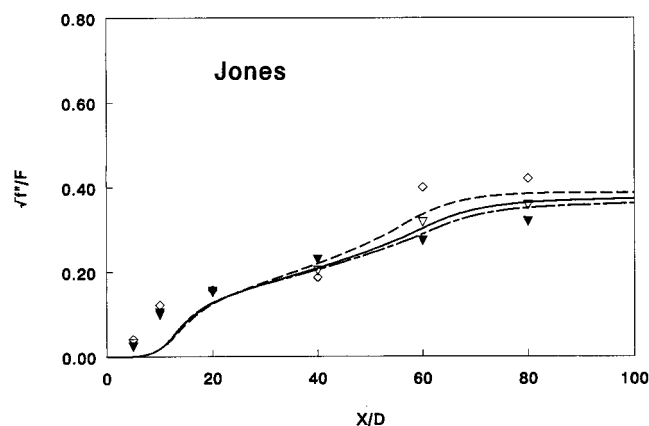


FIG. 10. Center line variation of the mixture fraction fluctuation intensity $(\overline{f''^2})^{1/2}/F$ for the 3 flames measured at DLR Stuttgart by Meier *et al.* (Ref. 57). Predictions with the model of Jones and Musonge (Ref. 14). See Fig. 6 for details.

an invariant of the flow. With the chosen values of $\lambda_1 = 1$ and $\lambda_2 = \frac{1}{2}$, this invariant is the momentum flux in a jet, which depends on the jet exit velocity and the nozzle diameter. In variable density jets, the ratio of the local density and the jet density should enter in the determination of ϕ in the form of an effective diameter. Due to the appearance of the coefficients λ_1 and λ_2 and ϕ , the model is not free from empiricism. However, most scalar dissipation rate models do contain empirical input. The final equation is similar in form to other models in the literature, but the coefficients and derivation are different.

The scalar variance, the scalar dissipation rate itself and the mechanical to scalar time scale ratio are most prone to be influenced by the scalar dissipation rate model. All scalar dissipation rate models investigated show approximately the same behavior for the predicted scalar variance and the scalar dissipation rate in turbulent axisymmetric jets. This means that a simple algebraic model is sufficient for this type of flows. The only variable that shows different behavior

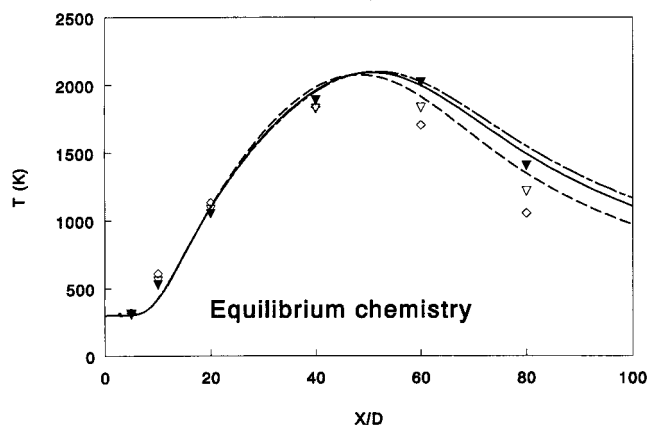


FIG. 11. Center line temperature variation predicted with equilibrium chemistry for the 3 flames measured at DLR Stuttgart by Meier *et al.* (Ref. 57). See Fig. 6 for details.

between the models is the mechanical to scalar time scale ratio. The non-equal scales model results decrease with radial distance and this agrees with the (plane jet) experiments of Sarh⁷ and with the predictions of Dibble *et al.*¹⁸ However, all other models predict the inverse behavior.

The center line asymptotic scalar fluctuation intensity in isothermal variable density jets predicted with the non-equal scales model and all other models is independent of the air to jet density ratio, which agrees with experimental findings in the literature.

In turbulent flames, density differences are more persistent and buoyancy effects can play a role. The far field scalar fluctuation intensities for different jet exit velocities predicted by the algebraic equal scales model show more scatter than do the predictions based on the transport equations of Chen¹⁹ and Jones and Musonge¹⁴ or the non-equal scales algebraic model. In the near field however, the algebraic models show better agreement with the experimental data.

It can be concluded that in jet type of flows, reacting and non-reacting, an algebraic model for the scalar dissipation rate is sufficient to predict the major characteristics of the flow. The time scale ratio between mechanical and scalar turbulence can only be predicted by transport equation models, or the algebraic non-equal scales model that is based on a transport equation. The applicability of the non-equal scales model may be limited to jet type of flows because typical characteristics of jet flows have been used to determine the coefficients in the model.

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