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INT. COMM. HEAT MASS TRANSFER
Vol. 19, pp. 851-858, 1992
Printed in the USA

0735-1933/92 $5.00 + .00

SCALAR TRANSPORT IN A TURBULENT JET

J.P.H. Sanders and A.P.G.G. Lamers
Faculty of Mechanical Engineering
Eindhoven University of Technology
P.O. Box 513 Eindhoven, The Netherlands

(Communicated by D.B. Spalding)

ABSTRACT

A model equation for the scalar dissipation rate, based on the Two Scale Direct Interaction Approximation (TSDIA) of Yoshizawa [1] was solved and applied to a turbulent round jet in conjunction with turbulence modelling based on the eddy viscosity and diffusivity. The model coefficients were adjusted by using a similarity analysis for the round jet. This led to an improvement in the prediction of concentration fluctuations on the axis of a jet with respect to results obtained with the equal length scales model. The turbulent Schmidt number, no longer assigned an ad–hoc constant value, displays experimentally observed behaviour in the jet.

Introduction

In the modelling of a turbulent diffusion flame the mean concentration and concentration fluctuation fields are of importance. These scalar variables are the first two moments of a probability density function which is needed to calculate the mean density and temperature [2].

In the equation for the mixture fraction, which is invariant during combustion and is equal to the mean concentration in the equivalent isothermal flow, the turbulent flux term must be modelled. On dimensional grounds an eddy diffusivity coefficient should contain the scalar dissipation, which stands for the destruction of scalar fluctuations.

Using eddy viscosity and diffusivity models, such as the $k-\epsilon$ model of Jones and Launder [3] mostly the equality of integral velocity and scalar length scales [4] is invoked to circumvent the explicit modelling of the scalar dissipation ϵ_g. This implies a constant Schmidt number which is at variance with experiments in the round jet [5]. Furthermore, with the equal length scales model, the concentration fluctuations are not well predicted in a turbulent round variable density jet while the concentration is accurately predicted [2].

If the assumption of equal length scales is relaxed a transport equation for the scalar dissipation is needed. In the context of first order closures Yoshizawa [1] recently presented a model equation for ϵ_g based on his Two Scale Direct Interaction Approximation (TSDIA). This statistical theory makes use of the Direct Interaction Approximation (DIA) of Kraichnan [6], which is valid for the smallest scales of turbulence, and provides the link to the larger scales (grid scales) by introducing an expansion parameter into the transport equations. A derivative expansion with respect to the mean field is performed through which the inhomogeneities in the mean field are retained [7].

The equation for the scalar dissipation given by Yoshizawa is solved. It will be shown that the original TSDIA model constants of Yoshizawa are inadequate for predicting the concentration profiles in the turbulent round jet of Birch et al. [8]. A similarity analysis in the round jet leads to a relation between the two constants which is used to optimally adjust these constants to the experimental data. With the optimized constants the concentration and concentration fluctuation profiles are predicted very accurately.

Analysis

The scalar transport model consists of a convection diffusion equation for the mean scalar f, in this case the concentration

$$\vec{\nabla}\cdot(\rho\vec{u}f) = \vec{\nabla}\cdot(\rho\nu_s\vec{\nabla}f) \tag{1}$$

and the equation for the scalar fluctuations $g = \overline{f'^2}$, in which the prime denotes a fluctuation with respect to the mean and the overbar an average, reads [4]

$$\vec{\nabla}\cdot(\rho\vec{u}g) = \vec{\nabla}\cdot(\rho\nu_s\vec{\nabla}g) + 2\rho\nu_s(\vec{\nabla}f)^2 - \rho\epsilon_g \tag{2}$$

Here ρ is the density, $\vec{u}$ is the velocity and ν_s is the eddy diffusivity. Use was made of the gradient transport relations:

$$-\overline{u_i'f'} = \nu_s\frac{\partial f}{\partial x_i} \text{ and } -\overline{u_i'g'} = \nu_s\frac{\partial g}{\partial x_i} \tag{3}$$

and the definition of the scalar dissipation rate

$$\epsilon_g = 2D_f\overline{(\vec{\nabla}f')^2} \tag{4}$$

in which D_f is the molecular diffusivity.

The equation for ϵ_g given by Yoshizawa [1] reads

$$\frac{D\epsilon_g}{Dt} = \lambda_1\frac{\epsilon_g}{g}\frac{Dg}{Dt} + \lambda_2\frac{\epsilon_g}{\epsilon}\frac{D\epsilon}{Dt} \tag{5}$$

in which ϵ is the dissipation of turbulent kinetic energy, and $\frac{D}{Dt}$ is the total material derivative. Equation (5) can be solved analytically to yield

$$\epsilon_g = \epsilon_{g_0} (g/g_0)^{\lambda_1} (\epsilon/\epsilon_0)^{\lambda_2} \tag{6}$$

in which g_0, ϵ_{g_0} and ϵ_0 are the values of g, ϵ_g and ϵ at some reference point. The values of the coefficients λ_1 and λ_2 were determined by Yoshizawa [1] to be 0.306 and 1.2 respectively.

To model ν_s a scalar integral length scale ℓ_f and a characteristic scalar time scale g/ϵ_g is needed. On dimensional grounds it can be shown that

$$\ell_f \simeq g^{3/2} \epsilon^{1/2} \epsilon_g^{-3/2} \tag{7}$$

Now the eddy diffusivity coefficient ν_s (in $m^2 s^{-1}$) can be formed as

$$\nu_s = C_f g^2 \epsilon / \epsilon_g^2 \tag{8}$$

in which C_f is a constant determined by Yoshizawa [1], $C_f = 0.446$.

In the described scalar transport model no assumption about equality of the velocity fluctuation length scale $\ell \simeq k^{3/2} \epsilon^{-1}$ and ℓ_f is made. This equality would lead to the commonly used model for the scalar dissipation rate

$$\epsilon_g = 2 \frac{\epsilon}{k} g \tag{9}$$

in which the number 2 is empirical [9]. Inserting equation (9) into equation (8) gives $\nu_s \simeq k^2 \epsilon^{-1}$ which implies a constant Schmidt number, which is the ratio of the eddy viscosity and diffusivity, because the eddy viscosity itself is modelled as $\nu_t = C_\mu k^2 \epsilon^{-1}$ with $C_\mu = 0.09$.

It should be mentioned that Yoshizawa in fact used non–isotropic relations instead of equation (3) in which the anisotropy was included via a tensor coefficient ν_{ij} combined with the scalar gradient. This term has been dropped to be able to compare the TSDIA model results with results from the equal length scales isotropic model. In the expression for the turbulent transport of scalar fluctuations, equation (3), cross diffusion terms, including gradients of ϵ_g, ϵ, and other variables were included. Also here, only the standard term was retained, taking the same constant C_f.

An important question concerns the reliability of the constants. Yoshizawa [1] points out that the values determined using inertial range concepts should be viewed as approximate only. For instance, the TSDIA has been used by Yoshizawa [10] to derive an equation for the dissipation of turbulent kinetic energy ϵ, leading to the same type of equation normally used in the standard k–ϵ model, apart from cross diffusion effects. The commonly used constants in the standard model for the modelling of the production and dissipation terms are 1.45 and 1.92 respectively, while TSDIA gives the value 1.7 for both of them. This gives an indication of the "accurateness" of the constants.

It was found that the standard TSDIA constants are inadequate for the prediction of concentration and concentration fluctuation profiles in the variable density turbulent round methane jet into air of Birch et al. [8]. Therefore a way has to be found for adjusting these constants. A similarity analysis of the round jet leads to a relation between λ_1 and λ_2.

In the far field on the axis of a turbulent round jet the concentration f and fluctuations g behave as $f \simeq x^{-1}$, $g \simeq x^{-2}$ while the integral scales ℓ and ℓ_f are proportional to x: $\ell \simeq x$, $\ell_f \simeq x$. The mean velocity and turbulent kinetic energy behave as $U \simeq x^{-1}$, $k \simeq x^{-2}$. Therefore ϵ goes like $\epsilon \simeq x^{-4}$. From $\ell_f \simeq g^{3/2} \epsilon^{1/2} \epsilon_g^{-3/2} \simeq x$ and $\epsilon_g \simeq g^{\lambda_1} \epsilon^{\lambda_2}$ and equating powers in x we get:

$$\lambda_1 + 2\lambda_2 = 2 \qquad (9)$$

Comparing this with the values of the constants given by Yoshizawa where λ_1=1.2, λ_2 should be 0.4, while TSDIA gives 0.306, which is a deviation of 30%.

Apart from the constants λ_1, λ_2 and C_f, the values of g,ϵ and ϵ_g at a reference point are required. The only point in which these values are known is at the nozzle inlet, i.e.: g=0; ϵ_g=0 and $\epsilon = C_\mu^{3/4} k^{3/2} / (\lambda_\epsilon D)$ with λ_ϵ=0.03, and D the nozzle diameter. Because of equation (6) a problem emerges in the determination of the limit $\phi_0 = \lim_{x \downarrow 0} (\epsilon_g(x) / g^{\lambda_1}(x))$ for, both ϵ_g and g are 0 at the inlet. This limit influences the values of ϵ_g and therefore determines the maximum value of the scalar fluctuations g on, for instance, the symmetry axis. The value of ϕ_0 is determined so as to adjust this maximum value to the value obtained from experiments. From calculations it was inferred that the value of ϕ_0 predominantly influences this maximum value and not the rest of the profiles, if ϕ_0 has the correct order of magnitude.

Results

Several calculations, with and without satisfying condition (9), showed that λ_1 exerted the largest influence on the results while the best results were obtained with

λ_1=1.5 and consequently λ_2=0.25 and C_f=0.5 instead of 0.446. In Fig.1 and Fig.2 the axial concentration and fluctuation profiles obtained with the original and the adjusted coefficients are shown. The improvement over the original coefficients is very significant.

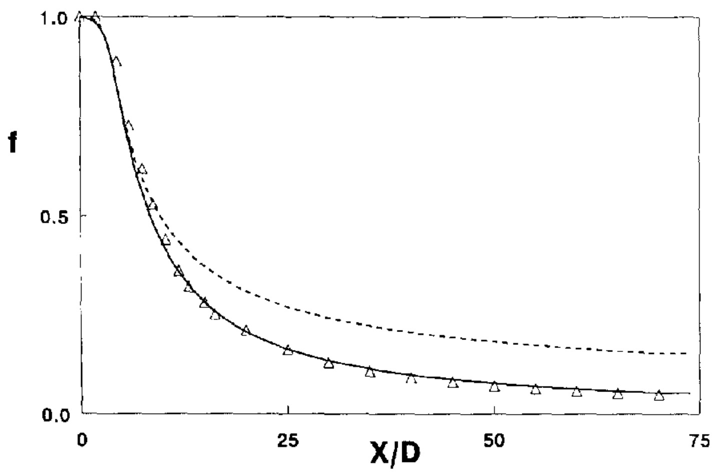

FIG.1
Concentration of nozzle fluid on the symmetry axis as a function of axial distance normalized by the inner nozzle diameter D. Calculations with original TSDIA constants (dashed line) and adjusted constants (λ_1=1.5;λ_2=0.25 and C_f=0.5) (drawn line). Experiments (triangles) are of Birch et al. [8].

The influence of the change of C_f from 0.446 to 0.5 on the radial concentration profiles is shown in Fig.3, both calculations being done with λ_1=1.5. The choice of C_f=0.5 was made so as to match the calculated spreading rate for the concentration halfwidth with the experimental value, namely 0.097. The concentration halfwidth is defined as the radial distance at which the concentration is half its centre line value.
The Gaussian fit to the radial profiles gives slightly underestimated values at the edge of the shear layer [11], but still this fit is best to use due to possible experimental error. Taking this into account the profile with C_f=0.5 is very satisfactory while the change in the axial profiles due to the increase of C_f from 0.446 to 0.5 is negligible.

The turbulent Schmidt number is also shown in Fig.3. The predicted trend is correct as can be concluded from experiments [5,12]. The measurements of Chevray and Tutu [12], where a turbulent Prandtl number was calculated from experimental data of a turbulent heated round jet, indeed showed a maximum in the Prandtl number. These data can be used for a rough comparison if the Lewis number is constant.

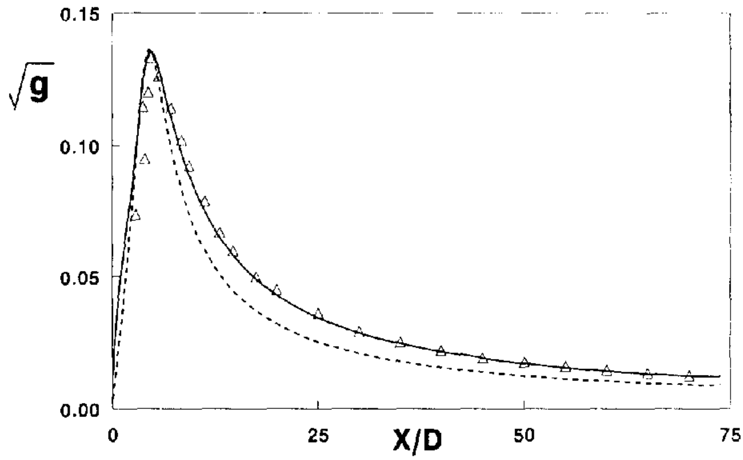

FIG.2
Concentration fluctuations on the symmetry axis. For further information see caption of Fig.1.

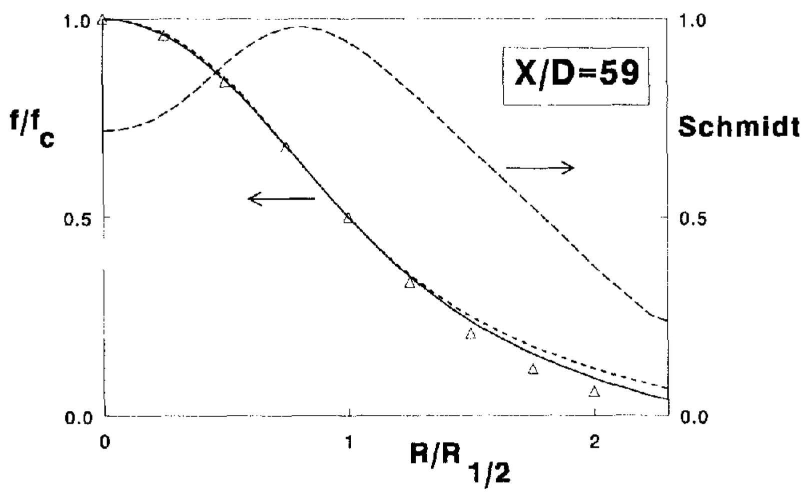

FIG.3
Radial profiles of the concentration of nozzle fluid, normalized by its centreline value f_c and the turbulent Schmidt number as a function of radial distance normalized by the concentration halfwidth $R_{1/2}$. Calculations are done with adjusted constants (λ_1=1.5;λ_2=0.25) and C_f=0.446 (dashed line) and 0.5 (drawn line) for the concentration and with C_f=0.5 for the Schmidt number. Experiments (triangles) are a Gaussian fit, according to Birch et al. [8].

Conclusions

It can be concluded that the TSDIA model, which has a stronger basis than the equal length scales model using an ad–hoc Schmidt number, gives improved results for the scalar fluctuations, while maintaining the good correspondence between concentration profiles from the equal length scales model and experiment. Furthermore, the turbulent Schmidt number, calculated using the new model, exhibits the experimentally observed behaviour in radial direction.

As this model has a firmer basis than the equal length scales model the scalar dissipation rate itself possibly could be calculated more accurately, although there are no measurements available. The scalar dissipation rate plays an important role in the description of non–equilibrium effects in turbulent flames [13].

Acknowledgement

We are grateful to dr. Krishna Prasad (Eindhoven University of Technology) for fruitful discussions.

Nomenclature

C_μ	model constant in standard k–ϵ model
C_f	model constant in scalar transport model
D	nozzle inner diameter, m
D_f	molecular viscosity, m^2s^{-1}
f	mean concentration
g	mean of the concentration fluctuations ($\overline{f'^2}$)
k	mean turbulent kinetic energy, m^2s^{-2}
ℓ	integral length scale, m
ℓ_f	scalar integral length scale, m
$\vec{u}$	mean velocity, ms^{-1}
x	axial distance, m
ϵ	mean of the dissipation of turbulent kinetic energy, m^2s^{-3}
ϵ_g	mean scalar dissipation rate, s^{-1}
ϕ_0	limit of $\epsilon_g g^{-\lambda_1}$ at the nozzle inlet, s^{-1}
ρ	mean density, kgm^{-3}
λ_1	model constant in scalar transport model
λ_2	model constant in scalar transport model

λ_ϵ	model constant in inlet value for ϵ
ν_t	eddy viscosity coefficient, m^2s^{-1}
ν_s	eddy diffusivity coefficient, m^2s^{-1}

Superscripts

$\overline{}$	average
'	fluctuation

Subscript

$_0$	value at a reference point

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Received August 3, 1992