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Sanders, J.P.H.; Lamers, A.P.G.G.

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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

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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-ε 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 $\varepsilon_s$. 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 $\epsilon_g$ 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

$$\nabla \cdot (\rho \nabla f) = \nabla \cdot (\rho \nu_s \nabla f)$$

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

$$\nabla \cdot (\rho \nabla g) = \nabla \cdot (\rho \nu_s \nabla g) + 2\rho \nu_s (\nabla f)^2 - \rho \epsilon_g$$

Here $\rho$ is the density, $\nabla f$ is the velocity and $\nu_s$ is the eddy diffusivity. Use was made of the gradient transport relations:

$$-u_i \nabla f = \nu \frac{\partial f}{\partial x_i} \text{ and } -u_i \nabla g = \nu_s \frac{\partial g}{\partial x_i}$$

and the definition of the scalar dissipation rate

$$\epsilon_g = 2D_f \overline{(\nabla f)^2}$$

in which $D_f$ is the molecular diffusivity.

The equation for $\epsilon_g$ given by Yoshizawa [1] reads

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

in which $\epsilon$ is the dissipation of turbulent kinetic energy, and $\frac{D}{Dt}$ is the total material derivative. Equation (5) can be solved analytically to yield
\[ \epsilon_g = \epsilon_g \left( \frac{g}{g_0} \right)^{\frac{1}{14}(e/\epsilon_0)^{\frac{1}{12}}} \]  

(6)

in which \( g_0 \), \( \epsilon_g \), and \( \epsilon_0 \) are the values of \( g \), \( \epsilon \), and \( \epsilon \) at some reference point. The values of the coefficients \( \lambda_1 \) and \( \lambda_2 \) were determined by Yoshizawa [1] to be 0.306 and 1.2 respectively.

To model \( \nu_s \), a scalar integral length scale \( \ell_f \) and a characteristic scalar time scale \( g/\epsilon_g \) is needed. On dimensional grounds it can be shown that

\[ \ell_f \approx g^{3/2} \left( \frac{\epsilon_0}{\epsilon_g} \right)^{1/2} \]  

(7)

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

\[ \nu_s = C_f g^{2} \epsilon/\epsilon_g^2 \]  

(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 \( \ell_k \approx \ell \) and \( \ell_f \) is made. This equality would lead to the commonly used model for the scalar dissipation rate

\[ \epsilon_g = 2 \ell_k \frac{\epsilon_g}{\epsilon} \]  

(9)

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

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 \( \nu_{ij} \) 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 \( \epsilon_g \), \( \epsilon \), 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 \( \epsilon \), leading to the same type of equation normally used in the standard \( k-\epsilon \) 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 $\lambda_1$ and $\lambda_2$.

In the far field on the axis of a turbulent round jet the concentration $f$ and fluctuations $g$ behave as $f \propto x^{-1}, g \propto x^{-2}$ while the integral scales $\ell$ and $\ell_f$ are proportional to $x$: $\ell \propto x, \ell_f \propto x$. The mean velocity and turbulent kinetic energy behave as $U \propto x^{-1}, k \propto x^{-2}$.

Therefore $\epsilon$ goes like $\epsilon \propto x^{-4}$. From $\ell_f \propto g^{3/2} \epsilon^{1/2} e^{-3/2} x$ and $\epsilon \propto g^{\lambda_1 \lambda_2}$ and equating powers in $x$ we get:

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

Comparing this with the values of the constants given by Yoshizawa where $\lambda_1 = 1.2$, $\lambda_2$ should be 0.4, while TSDIA gives 0.306, which is a deviation of 30%.

Apart from the constants $\lambda_1$, $\lambda_2$, and $C_f$, the values of $g, \epsilon$ and $e_g$ at a reference point are required. The only point in which these values are known is at the nozzle inlet, i.e.: $g = 0, \epsilon = 0$ and $\epsilon = C_{3/4}^3 \propto k^{3/2} / (\lambda_\ell D)$ with $\lambda_\ell = 0.03$, and $D$ the nozzle diameter. Because of equation (6) a problem emerges in the determination of the limit $\phi_0 = \lim (\epsilon_g(x) / g^{\lambda_1}(x))$ for, both $\epsilon_g$ and $g$ are 0 at the inlet. This limit influences the values of $\epsilon_g$ and therefore determines the maximum value of the scalar fluctuations $g$ on, for instance, the symmetry axis. The value of $\phi_0$ is determined so as to adjust this maximum value to the value obtained from experiments. From calculations it was inferred that the value of $\phi_0$ predominantly influences this maximum value and not the rest of the profiles, if $\phi_0$ has the correct order of magnitude.

Results

Several calculations, with and without satisfying condition (9), showed that $\lambda_1$ exerted the largest influence on the results while the best results were obtained with
\( \lambda_1 = 1.5 \) and consequently \( \lambda_2 = 0.25 \) 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.

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 \( \lambda_1 = 1.5 \). 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.
Concentration fluctuations on the symmetry axis. For further information see caption of Fig. 1.

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 ($\lambda_1 = 1.5; \lambda_2 = 0.25$) 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].

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Nomenclature

\begin{tabular}{|l|l|}
\hline
C_{\mu} & model constant in standard k-\epsilon model \\
C_f & model constant in scalar transport model \\
D & nozzle inner diameter, m \\
D_f & molecular viscosity, m^{2}s^{-1} \\
f & mean concentration \\
g & mean of the concentration fluctuations (\overline{f^2}) \\
k & mean turbulent kinetic energy, m^{2}s^{-2} \\
\ell & integral length scale, m \\
\ell_f & scalar integral length scale, m \\
\overline{u} & mean velocity, ms^{-1} \\
x & axial distance, m \\
\epsilon & mean of the dissipation of turbulent kinetic energy, m^{2}s^{-3} \\
\epsilon_g & mean scalar dissipation rate, s^{-1} \\
\phi_0 & limit of \epsilon_g^{-1} at the nozzle inlet, s^{-1} \\
\rho & mean density, kgm^{-3} \\
\lambda_1 & model constant in scalar transport model \\
\lambda_2 & model constant in scalar transport model \\
\hline
\end{tabular}
\( \lambda_{\varepsilon} \)  
model constant in inlet value for \( \varepsilon \)

\( \nu_t \)  
eddy viscosity coefficient, \( m^2s^{-1} \)

\( \nu_s \)  
eddy diffusivity coefficient, \( m^2s^{-1} \)

**Superscripts**
- \( \overline{\cdot} \) average
- \( \cdot \) fluctuation

**Subscript**
- \( \circ \) value at a reference point

References


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