Nonlocal expression for scalar flux in turbulent shear flow

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An exact expression for the scalar flux was derived using the Green’s function for a scalar. The nonlocal eddy diffusivity involved in the expression represents a contribution to the scalar flux from the mean scalar gradient at remote points in space and time. The direct numerical simulation of channel flow was carried out to validate the nonlocal expression. The velocity and scalar fields as well as the Green’s function were calculated in the cases of one- and two-dimensional mean scalar fields and of oscillating mean scalar field. It was shown that the nonlocal expression is accurate in all cases. A local expression for the scalar flux was also examined to show that the local approximation is not accurate enough and that the nonlocal effect is important. Some attempts were made to model the nonlocal effect. The nonlocal diffusivity was expressed algebraically using an exponential function, the local expression was modified by adding higher-order terms, and a differential equation for the nonlocal diffusivity was proposed. It was demonstrated that the analysis with the nonlocal expression gains insight into modeling the scalar transport in turbulent shear flows. © 2004 American Institute of Physics. [DOI: 10.1063/1.1697396]

I. INTRODUCTION

Modeling the turbulent transport of a scalar such as mass, heat, and concentration is an important problem in many fields including engineering and geophysics. The scalar flux needs to be evaluated to solve the equation for the mean scalar. In the eddy diffusivity model the scalar flux is assumed to be proportional to the mean scalar gradient and to be directed down the gradient. Although this model is widely used, the limitation of this approximation was also pointed out; a gradient transport model requires that the characteristic scale of the transport mechanism be small compared with the distance over which the mean gradient of the transported property changes appreciably. In turbulent flows the length scale of turbulence is often as large as that of the mean field variation. One of typical examples is the scalar transport in the atmospheric boundary layer; convective eddies driven by buoyancy are as large as the boundary layer height and the eddy diffusivity model is not always accurate.

Wyngaard and Brost showed that the value of the eddy diffusivity depends on whether the turbulent mixing is driven by the entrainment through the top boundary or the flux from the bottom surface. This is called the top-down and bottom-up diffusion. They defined the top-down scalar and the bottom-up scalar whose vertical fluxes at the height of are given by and respectively, where is the boundary layer height. They showed that the eddy diffusivity for the top-down scalar, , is greater than that for the bottom-up scalar, . This difference cannot be explained by the simple eddy diffusivity model if the eddy diffusivity is determined only by the wind turbulence and is independent of the scalar field. By superposing the two scalars they derived a generalized eddy diffusivity that depends on both the top and bottom boundary conditions. Hamba modified the eddy diffusivity model by introducing the second derivative of the mean scalar to explain the difference between the top-down and bottom-up scalars without the boundary conditions.

It is known that the upward heat flux is accompanied by a positive temperature gradient near the top boundary of the convective boundary layer. This countergradient transport cannot be accounted for by the eddy diffusivity model. The breakdown of the eddy diffusivity model is caused by the memory and vertical inhomogeneity of the turbulence. Deardorff proposed a countergradient term in addition to the eddy diffusivity term to explain the countergradient transport. Holtslag and Moeng examined data of large eddy simulation (LES) to obtain an expression for the countergradient term. Hamba showed that the second-derivative term in the modified eddy diffusivity model also accounts for the countergradient transport.

In these studies the eddy diffusivity model is modified within the framework of the local approximation. Since the nonlocal effect is important in the atmospheric boundary layer several attempts have been done to develop nonlocal models. Stull proposed the transient turbulence theory that describes the nonlocal transport using a matrix of mixing coefficients. Ebert et al. used tracers in their LES to directly obtain the matrix. The transient matrix model was also applied to stratospheric mixing and stellar convection. Fiedler proposed an integral model similar to the transient theory; Fiedler and Moeng used scalar profiles obtained from LES to construct the matrix in the integral model. Pleim and Chang used a nonlocal model named the asymmetrical convective model to apply to regional or mesoscale atmospheric chemical models. In addition to the nonlocal properties these models are different from the eddy diffusivity model as well as the Green's function were calculated in the cases of one- and two-dimensional mean scalar fields and of oscillating mean scalar field. It was shown that the nonlocal expression is accurate in all the cases. A local expression for the scalar flux was also examined to show that the local approximation is not accurate enough and that the nonlocal effect is important. Some attempts were made to model the nonlocal effect. The nonlocal diffusivity was expressed algebraically using an exponential function, the local expression was modified by adding higher-order terms, and a differential equation for the nonlocal diffusivity was proposed. It was demonstrated that the analysis with the nonlocal expression gains insight into modeling the scalar transport in turbulent shear flows. © 2004 American Institute of Physics. [DOI: 10.1063/1.1697396]
diffusivity model in the following respect: in the eddy diffusivity model the scalar flux is expressed in terms of the scalar gradient whereas in these nonlocal models the time advancement of the scalar is modeled in terms of the scalar itself.

On the other hand, Berkowicz and Prahm proposed a generalization of the eddy diffusivity; that is, the scalar flux is expressed by a spatial integral of the scalar gradient. The model has a coefficient corresponding to the eddy diffusivity; we call it the nonlocal eddy diffusivity in this paper. Nakayama et al. applied this model to the calculation of the scalar field in the turbulent boundary layer for engineering problems. This straightforward extension of the local eddy diffusivity is attractive because this approach is expected to be applicable to other fluxes such as the momentum flux. In fact, Nakayama and Vengadesan proposed a nonlocal eddy viscosity model for the Reynolds stress.

In addition to the application of nonlocal models the nonlocal expression for the scalar flux was also investigated theoretically. Using the direct interaction approximation (DIA) Kraichnan showed that the nonlocal eddy diffusivity can be approximated using the averaged Green’s function and the velocity correlation. Moreover, using the detailed Green’s function for the scalar equation Kraichnan derived an exact expression for the scalar flux. Georgopoulos and Seinfeld also derived a similar exact expression. However, their expressions involve the scalar flux also on the right-hand side; the scalar flux needs to be solved implicitly. Hamba modified the Green’s function to obtain an explicit exact expression for the scalar flux; using LES the Green’s function was calculated to evaluate the nonlocal diffusivity. Larson investigated the relationship between the turbulent and the Green’s function for the advection–diffusion equation. In addition to the Green’s function for the fundamental equation, the Green’s function for a model equation is also useful. Lin and Hildemann obtained an analytical solution of the atmospheric diffusion equation using its Green’s function. Zilitinkevich et al. examined the Green’s function for the model equation for the third-order moments to derive the nonlocal expression for the scalar flux.

Using the LES of the atmospheric boundary layer Hamba evaluated the Green’s function to obtain profiles of the nonlocal diffusivity and to examine the nonlocal effect. It was shown that the top-down and bottom-up diffusion and the countergradient diffusion can be explained using the nonlocal properties of scalar transport. This result indicates that the nonlocal analysis with the Green’s function can be a useful tool for better understanding turbulence and can give a clue to turbulence modeling. In this LES the turbulent motion is produced by buoyancy because no mean shear is set. On the other hand, in various flows turbulence is often produced by the mean shear. Therefore, it is also interesting to examine nonlocal properties in shear turbulence. As mentioned before the nonlocal analysis is expected to be applied to the eddy viscosity although the analysis must be more complicated owing to the nonlinearity in the velocity. In this work, as a first step to nonlocal modeling of the eddy diffusivity and viscosity, we examine nonlocal properties of scalar transport; we treat a channel flow as a basic example of shear turbulence. In the LES by Hamba the subgrid-scale part was modeled using a local model. This part is dominant compared with the grid-scale part near the wall and an approximate boundary condition was used for the surface layer. Therefore, nonlocal properties near the wall was not examined in detail. In the present work we carry out direct numerical simulation (DNS) with the no-slip boundary conditions to examine nonlocal properties accurately even near the wall.

In the following section we derived an exact explicit expression for the scalar flux using the modified Green’s function. In Sec. III the nonlocal expression is validated using the DNS of channel flow. A local eddy diffusivity model is also examined to show the limitation of the local approximation and the importance of the nonlocal effect. In Sec. IV some attempts are made to model the nonlocal effect. Concluding remarks are given in Sec. V.

II. FORMULATION

In order to solve the transport equation for the mean scalar it is necessary to model the scalar flux. In the local eddy diffusivity model widely used, the scalar flux is approximated by

$$\langle u_i \theta' \rangle = -\kappa_{Tij} \frac{\partial \Theta}{\partial x_j}.$$ (1)

Here, $\langle \cdot \rangle$ denotes ensemble averaging, $\Theta = \langle \theta \rangle$ is the mean scalar, $u_i$ and $\theta'$ are the velocity and scalar fluctuations, respectively, and $\kappa_{Tij}$ is the eddy diffusivity tensor; the summation convention is used for repeated indices. Isotropic eddy diffusivity is often assumed; it is written as $\kappa_{Tij} = \kappa_T \delta_{ij}$ where $\delta_{ij}$ is the Kronecker delta symbol. The eddy diffusivity model is local in space in the sense that the scalar flux at a point is expressed in terms of physical quantities at the same point. This local approximation is valid only if the turbulence length scale is much less than the length scale of the mean field variation. However, this condition does not always hold for actual turbulent flows. For example, several nonlocal models have been developed for the scalar transport in the atmospheric boundary layer. In the transient turbulence theory proposed by Stull the equation for the mean scalar at the height of $y$ is given by

$$\Theta(y,t+\Delta t) = \int dy' G(y,t+\Delta t;y',t)\Theta(y',t),$$ (2)

where $\Delta t$ is the time step and $G(y,t+\Delta t;y',t)$ is the nonlocal mixing coefficient. The mean scalar at the height of $y$ at the present time is affected by that at the height of $y'$ at the previous time. Berkowicz and Prahm proposed a generalization of the local eddy diffusivity model; the vertical scalar flux is given by

$$\langle u' \theta' \rangle(y) = -\int dy' \kappa_{NL}(y;y') \frac{\partial \Theta(y)}{\partial y'},$$ (3)

where $\kappa_{NL}$ is a coefficient representing a nonlocal contribution; hereafter we call it the nonlocal eddy diffusivity. This expression is different from (2) in that the scalar flux is modeled instead of the time advancement of the scalar.
Using the DIA Kraichnan\textsuperscript{19} theoretically investigated the scalar transport. He showed a nonlocal expression for the scalar flux as

\[ \langle u'_i \theta' \rangle(x,t) = - \int dx' \int_0^t dt' \kappa_{NLij}(x,t;x',t') \times \frac{\partial}{\partial x'_j} \Theta(x',t'), \]

(4)

where

\[ \kappa_{NLij}(x,t;x',t') = \langle g(x,t;x',t') \rangle \langle u'_i(x,t) u'_j(x',t') \rangle. \]

(5)

Here \( g(x,t;x',t') \) is the Green's function satisfying

\[ \frac{\partial g}{\partial t} + u_i \frac{\partial g}{\partial x_i} - \kappa \frac{\partial^2 g}{\partial x_i \partial x_i} = \delta(x-x') \delta(t-t'), \]

(6)

where \( \kappa \) is the molecular diffusivity for the scalar. In this theory the nonlocal eddy diffusivity \( \kappa_{NLij} \) is expressed in terms of the mean Green’s function and the binary velocity correlation. Whether this approximate expression is good or not depends on the validity of the DIA.

Moreover, Kraichnan\textsuperscript{20} derived an exact expression for the scalar flux as follows. The transport equation for the scalar flux is given by

\[ \frac{\partial \theta'}{\partial t} + u_i \frac{\partial \theta'}{\partial x_i} - \kappa \frac{\partial^2 \theta'}{\partial x_i \partial x_i} = -u'_i \frac{\partial \Theta}{\partial x_i} + \frac{\partial}{\partial x_i} \langle u'_i \theta' \rangle. \]

(7)

Using the Green’s function satisfying (6) the scalar fluctuation can be solved formally as

\[ \theta'(x,t) = \int dx' \int_0^t dt' g(x,t;x',t') \left[ -u'_i(x',t') \frac{\partial}{\partial x'_j} \Theta(x',t') \right. \\
\left. + \frac{\partial}{\partial x'_j} \langle u'_i \theta' \rangle(x',t') \right]. \]

(8)

Here terms involving initial values \( \Theta(x',0) \) and \( \langle u'_i \theta' \rangle(x',0) \) are omitted because they do not contribute to the scalar flux \( \langle u'_i \theta' \rangle(x,t) \) when \( t \) is sufficiently large. Therefore, the scalar flux is written as

\[ \langle u'_i \theta' \rangle(x,t) = - \int dx' \int_0^t dt' \mu_{ij}(x,t;x',t') \frac{\partial}{\partial x'_j} \Theta(x',t') \\
\int dx' \int_0^t dt' \lambda_{ij}(x,t;x',t') \times \frac{\partial}{\partial x'_j} \langle u'_i \theta' \rangle(x',t'). \]

(9)

where

\[ \mu_{ij}(x,t;x',t') = \langle u'_i(x,t) g(x,t;x',t') u'_j(x',t') \rangle, \]

(10)

\[ \lambda_{ij}(x,t;x',t') = \langle u'_i(x,t) g(x,t;x',t') \rangle. \]

(11)

The first term on the right-hand side of (9) is an expression involving the nonlocal eddy diffusivity. Expression (5) for \( \kappa_{NLij} \) of the DIA can be considered an approximation to \( \mu_{ij} \) given by (10). Although (9) is exact, the second term on the right-hand side involves the scalar flux itself; it must be solved implicitly. This difficulty is originated from the fact that the scalar flux is involved on the right-hand side of (7).

Hamba\textsuperscript{22} introduced the modified Green’s function to obtain an explicit exact expression for the scalar flux. The equation for the modified Green’s function \( g_M \) is given by

\[ \frac{\partial g_M}{\partial t} + u_i \frac{\partial g_M}{\partial x_i} - \kappa \frac{\partial^2 g_M}{\partial x_i \partial x_i} = \delta(x-x') \delta(t-t'). \]

(12)

This equation is different from (6) in that the correlation \( \langle u'_i g_M \rangle \) is involved on the left-hand side. Owing to this modification the effect of the scalar flux term in (7) is incorporated into the Green’s function. Using \( g_M \) the formal solution for the scalar fluctuation can be written as

\[ \theta'(x,t) = - \int dx' \int_0^t dt' g_M(x,t;x',t') \times u_i(x',t') \frac{\partial}{\partial x'_j} \Theta(x',t'). \]

(13)

Unlike (8) the scalar flux is not involved in (13). This solution leads to expression (4) for the scalar flux with the nonlocal eddy diffusivity

\[ \kappa_{NLij}(x,t;x',t') = \langle u'_i(x,t) g_M(x,t;x',t') u'_j(x',t') \rangle. \]

(14)

Therefore, (4) and (14) compose an explicit exact expression for the scalar flux. For later use we introduce an equivalent Green’s function defined as

\[ g_i(x,t;x',t') = g_M(x,t;x',t') u'_i(x',t'). \]

(15)

It satisfies

\[ \frac{\partial g_i}{\partial t} + u_j \frac{\partial g_i}{\partial x_j} - \kappa \frac{\partial^2 g_i}{\partial x_j \partial x_j} = u'_i \delta(x-x') \delta(t-t'), \]

(16)

and the nonlocal eddy diffusivity given by (14) can be written as

\[ \kappa_{NLij}(x,t;x',t') = \langle u'_i(x,t) g_j(x,t;x',t') \rangle. \]

(17)

Using this nonlocal diffusivity the nonlocal expression for the scalar flux is given by

\[ \langle u'_i \theta' \rangle(x,t) = - \int dx' \int_0^t dt' \kappa_{NLij}(x,t;x',t') \times \frac{\partial}{\partial x'_j} \Theta(x',t') \langle u'_i \theta' \rangle_{NL}. \]

(18)

Here, let us mention the relation between the nonlocal expression (18) and the local approximation. The nonlocal
eddy diffusivity $\kappa_{NLij}$ has a nonzero value if the distance $|x-x'|$ and the time difference $t-t'$ are comparable with or less than the turbulence length and time scales, respectively. If in this region in space and time the scalar gradient $\partial \Theta / \partial x_i'$ is nearly constant, the scalar flux can be approximated by

$$\langle u'_i \theta' \rangle = -\kappa_{Li}(x,x,t) = \frac{\partial \Theta}{\partial x_i} = \left( \frac{\partial \langle u'_i \theta' \rangle}{\partial x} \right)_{TL},$$

(19)

where $\kappa_{Li}$ is the local eddy diffusivity defined as

$$\kappa_{Li}(x,t) = \int d\mathbf{x}' \int_0^T dt' \kappa_{NLi}(x,t',x,t').$$

(20)

Therefore, whether the local approximation is good or not depends on the relation in the length and time scales between profiles of $\kappa_{NL}$ and $\partial \Theta / \partial x_i'$.  

III. VALIDATION USING DNS RESULTS

In this section we show results from the DNS of channel flow. Using DNS data we examine the following two points: whether the nonlocal expression (18) is exact or not and how good the local approximation (19) is. In the DNS we numerically solve the equations for the velocity and the scalar given by

$$\frac{\partial u_i}{\partial t} = -u_j \frac{\partial u_i}{\partial x_j} - \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_i \partial x_j} + f_s \delta_{ij},$$

(21)

$$\frac{\partial u_i}{\partial x_i} = 0,$$

(22)

and

$$\frac{\partial \theta}{\partial t} = -u_i \frac{\partial \theta}{\partial x_i} + \kappa \frac{\partial^2 \theta}{\partial x_i \partial x_j} + f_\theta,$$

(23)

where $p$ is the pressure, $\nu$ is the molecular viscosity, $f_s$ is an external force, and $f_\theta$ is an external source. The equation for the Green’s function $g_i'$ given by (16) is also solved. The variables $x_i(=x,y)$ and $x_3(=z)$ denote the coordinate in the streamwise, wall-normal, and spanwise directions, respectively; corresponding velocity components are given by $u_i(=u)$, $u_3(=v)$, and $u_3(=w)$. Hereafter, all quantities except for $\theta$ are nondimensionalized by the wall-friction velocity $u_+$ and the channel half-width $L_x/2$ unless otherwise mentioned. Since the equations treated are linear in $\theta$, it can be normalized arbitrarily.

The Reynolds number based on $u_+$ and $L_x/2$ is set to $Re_x = 180$ and the Prandtl number is $Pr = 0.7$. The size of the computational domain is $L_x \times L_y \times L_z = 9.6 \times 2 \times 4.8$. A staggered grid is adopted; it is uniform in the $x$ and $z$ directions and is stretched in the $y$ direction using a hyperbolic tangent function. The number of the grid points is $N_x \times N_y \times N_z = 256 \times 128 \times 256$. The periodic boundary conditions for $u_i$, $\theta$, and $g_i'$ are used in the $x$ and $z$ directions. No-slip conditions $u_i = 0$ are imposed at the walls ($y = \pm 1$). The upper-wall boundary condition for the scalar is $\theta = 0$ whereas the lower-wall boundary condition is $\theta = \theta_0(x,t)$; the function will be described later. The wall boundary condition for the Green’s function is $g_i' = 0$ because the boundary condition for the scalar is of the Dirichlet type. We use the second-order finite-difference scheme in space and the Adams–Bashforth method for time marching. The computational time step is $\Delta t = 1.5 \times 10^{-3}$. The computation was run for a sufficiently long time to be statistically independent of the initial condition; then statistics such as the scalar flux were accumulated over a time period of 18 unless otherwise mentioned.

We calculated four cases as shown in Table I. In all the cases the same velocity field is used; it is a typical channel flow statistically steady in time and homogeneous in the $x$ and $z$ directions. In cases 1 and 2 the scalar at the lower wall is set to $\theta = 0$. Instead, the source term is nonzero; it is set to $f_\theta = 2$ in the whole region in case 1 whereas it is nonzero only near the center line at $y = 0$ in case 2. In cases 3 and 4 the source term is set to zero and the dependence of $\theta_0$ on $x$ or $t$ is introduced. In case 3, $\theta_0$ is periodic in $x$ with the period of $L_x/2$; two cycles are included in the computational domain at $0 < x < L_x$. In case 4, $\theta_0$ is periodic in time with the period of $T = 1.2$. This period is longer than a turbulence time scale defined by $k/\epsilon$ where $k$ is the turbulent kinetic energy and $\epsilon$ is its dissipation rate. For example, $k/\epsilon = 0.2$ at $y = -0.9$ and $k/\epsilon = 0.71$ at $y = 0$.

A. One-dimensional mean scalar field

Since the source term $f_\theta$ in cases 1 and 2 is a function of $y$ only, the scalar field is statistically homogeneous in the $x$ and $z$ directions like the velocity field. We take an average over the $x-z$ plane and in time; statistics depend only on $y$. In this case the scalar flux given by (18) and (17) can be expressed as

$$\langle u'_i \theta' \rangle_{NL}(y) = -\int dy' \kappa_{NLi}(y,y') \frac{\partial \Theta(y')}{\partial y'},$$

(24)

$$\kappa_{NLi}(y,y') = \int dx' \int dz' \int_0^T dt' \langle u'_i(x,t) \rangle$$

$$\times g_i'(x,t;x',t'),$$

(25)

because the scalar gradient $\partial \Theta / \partial y'$ does not depend on $x'$, $y'$, or $t'$. The local eddy diffusivity $\kappa_{NL}$ is a function of $y$ and $y'$ only. Here and hereafter, the space integral extends over the whole computational domain unless otherwise mentioned. To evaluate $\kappa_{NL}$ we need to obtain the value of $g_i'$ satisfying (16). It is difficult to solve (16) straightforwardly because of its computing cost. Making use of the homogeneity of the velocity field we decrease the computing cost as shown in the Appendix. The scalar flux given by (19) and (20) is also expressed as

<table>
<thead>
<tr>
<th>Case</th>
<th>$\theta_0$</th>
<th>$f_\theta$</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>2</td>
<td>$x$, $z$, $t$</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>$\exp(-y^2/0.09)$</td>
<td>$x$, $z$, $t$</td>
</tr>
<tr>
<td>3</td>
<td>$\sin(4\pi x/L_x)$</td>
<td>0</td>
<td>$z$, $t$</td>
</tr>
<tr>
<td>4</td>
<td>$\sin(2\pi z/L_z)$</td>
<td>0</td>
<td>$x$, $z$</td>
</tr>
</tbody>
</table>
The components $\kappa_{NL22}$ and $\kappa_{NL12}$ are involved in $(u' \theta')_{NL}$ and $(u' \theta'')_{NL}$, respectively. The profiles represent a contribution of the scalar gradient at $y'$ to the scalar flux at a given point of $y$. In Fig. 2(a) the profile of $\kappa_{NL22}$ becomes wider as $y$ increases. Let us evaluate the width of the profile as the distance between the two points where the value of $\kappa_{NL22}$ is $e^{-1}$ times its peak value; the width is 0.05 for $y = -0.942$ and 0.12 for $y = 0$. The peak of each curve is located at $y' = y$. This means that the contribution of the scalar gradient at the same point is the largest. In Fig. 2(b) the value of $\kappa_{NL12}$ is negative except for the case of $y = -0.017$ since the values of $(u' \theta')$ and $\partial \Theta / \partial y$ are positive at $-1 < y < 0$. The profile of $\kappa_{NL12}$ is somewhat wider than that of $\kappa_{NL22}$ at the corresponding location of $y$. For example, the width of $\kappa_{NL12}$ is 0.12 for $y = -0.945$; it is about twice the width of $\kappa_{NL22}$ for $y = -0.942$. The profile of $\kappa_{NL12}$ for $y = -0.017$ is different from the other three profiles; it is negative at the lower half ($-1 < y < 0$) and positive at the upper half ($0 < y < 1$). Although the absolute value is small the profile shows fairly nonlocal contribution. Here, we should note that the value of $\kappa_{NL12}$ defined by (25) is common for cases 1 and 2. This is because $g_2$ involved in (25) is determined solely by the velocity field. The value of $\kappa_{NL12}$ does not depend on the specific mean scalar field.

Here, let us compare the present result with the LES of the atmospheric boundary layer. The profile of $\kappa_{NL22}$ was obtained in the LES; its width is 0.49$y_b$ for $y = 0.6y_b$ near

![Figure 1](Image 1)

**FIG. 1.** Profiles of mean scalar and its gradient as functions of $y$ for cases 1 and 2: (a) mean scalar and (b) scalar gradient. Solid line for the mean scalar denotes the result of DNS by Horiuti (Ref. 26).

![Figure 2](Image 2)

**FIG. 2.** Profiles of nonlocal eddy diffusivity as a function of $y$ in the case of one-dimensional mean scalar field: (a) $\kappa_{NL22}(y, y')$ and (b) $\kappa_{NL12}(y, y')$. The components $\kappa_{NL22}$ and $\kappa_{NL12}$ are involved in $(u' \theta')_{NL}$ and $(u' \theta'')_{NL}$, respectively. The profiles represent a contribution of the scalar gradient at $y'$ to the scalar flux at a given point of $y$. In Fig. 2(a) the profile of $\kappa_{NL22}$ becomes wider as $y$ increases. Let us evaluate the width of the profile as the distance between the two points where the value of $\kappa_{NL22}$ is $e^{-1}$ times its peak value; the width is 0.05 for $y = -0.942$ and 0.12 for $y = 0$. The peak of each curve is located at $y' = y$. This means that the contribution of the scalar gradient at the same point is the largest. In Fig. 2(b) the value of $\kappa_{NL12}$ is negative except for the case of $y = -0.017$ since the values of $(u' \theta')$ and $\partial \Theta / \partial y$ are positive at $-1 < y < 0$. The profile of $\kappa_{NL12}$ is somewhat wider than that of $\kappa_{NL22}$ at the corresponding location of $y$. For example, the width of $\kappa_{NL12}$ is 0.12 for $y = -0.945$; it is about twice the width of $\kappa_{NL22}$ for $y = -0.942$. The profile of $\kappa_{NL12}$ for $y = -0.017$ is different from the other three profiles; it is negative at the lower half ($-1 < y < 0$) and positive at the upper half ($0 < y < 1$). Although the absolute value is small the profile shows fairly nonlocal contribution. Here, we should note that the value of $\kappa_{NL12}$ defined by (25) is common for cases 1 and 2. This is because $g_2$ involved in (25) is determined solely by the velocity field. The value of $\kappa_{NL12}$ does not depend on the specific mean scalar field.
the center of the layer where $y_b$ is the boundary layer height. Considering the channel width is 2 in the present simulation we can see that the width of 0.49$y_b$ is about eight times larger than that of 0.12 for $y=0$ in the channel. The profile of $\kappa_{NL,2}$ for the atmospheric boundary layer is wider than that for the present channel. This is due to the difference in the mechanism of turbulence production. In the atmospheric boundary layer plumes produced near the bottom surface rise to the upper boundary; the resulting turbulent field can be nonlocal in the vertical direction. On the other hand, in the channel flow vortices produced by the mean shear are stretched in the streamwise direction; the nonlocal effect in the wall-normal direction is not very strong. Nevertheless, the profiles of the nonlocal diffusivity in the channel flow cannot be approximated by $\partial(y'-y)$; some nonlocal effect may remain and its strength is determined by the relation between the width of the nonlocal diffusivity and the length scale of the mean field variation.

Next, we examine the profiles of the scalar flux for case 1. Figure 3(a) shows the profiles of the vertical component $\langle v'\theta' \rangle$. In Fig. 3(a) the DNS by Horiuti, the present DNS, and the nonlocal expression $\langle v'\theta' \rangle_{NL}$ agree well with each other at $-1<y'<0$. This agreement means that the nonlocal expression (24) is valid and the nonlocal diffusivity (25) is appropriately evaluated from the DNS data. Compared with the DNS result the absolute value of $\langle v'\theta' \rangle_L$ is somewhat greater at $y=-0.9$ and is slightly smaller away from the wall. To compare with the local diffusivity we define the effective diffusivity as

$$\kappa_{E,2} = -\langle u'_i\theta' \rangle L \frac{\partial \theta}{\partial y}. \tag{28}$$

This value depends on the mean scalar profile unlike $\kappa_{L,2}$; if the local approximation is good, $\kappa_{E,2}$ should be equal to $\kappa_{L,2}$. In Fig. 3(b) the effective diffusivity $\kappa_{E,2}$ is greater than the local diffusivity $\kappa_{L,2}$ in the center region; the former is slightly smaller than the latter at $y=-0.9$. The value of $\kappa_{E,2}$ at $y=0$ is inaccurate because both the numerator and denominator in (28) are very small. Figure 3(c) shows the profiles of the streamwise component $\langle u'\theta' \rangle$ for case 1. The value of $\langle u'\theta' \rangle$ by the present DNS is slightly less than that of the DNS by Horiuti. The nonlocal expression $\langle u'\theta' \rangle_{NL}$ agrees well with the result of the present DNS. On the other hand, $\langle u'\theta' \rangle_L$ is much greater than the DNS result near the wall. The overestimate of $\langle u'\theta' \rangle_L$ is larger than that of $\langle u'\theta' \rangle_{NL}$. This is because the profile of $\kappa_{NL,2}$ is wider than that of $\kappa_{NL,2}$ near the wall in Fig. 2 and the nonlocal effect is more important. At the center line the scalar gradient $\partial \theta/\partial y$ vanishes. Since the scalar flux in the local model is proportional to the scalar gradient, the value of $\langle u'\theta' \rangle_L$ also vanishes at $y=0$. Reflecting the small value of the scalar gradi-

![Figure 3](image-url)
ent near the center line the DNS value of $\langle u' \theta' \rangle$ shows a small value at $y = 0$. However, it does not vanish but has a positive value. As shown in Fig. 2(b) the nonlocal diffusivity has a broad profile for $y = 0$. Since the scalar gradient changes its sign at $y = 0$ the contributions of the upper and lower halves in (24) are both positive; they induce a positive scalar flux at $y = 0$. This difference between the nonlocal and local expressions is clearly seen in the effective diffusivity $\kappa_{E12}$ in Fig. 3(d). It diverges at $y = 0$ because $\langle u' \theta' \rangle \neq 0$ and $\partial \theta / \partial y = 0$. Therefore, the local diffusivity model cannot describe a positive value of the scalar flux at $y = 0$.

To demonstrate that the nonlocal diffusivity is independent of the mean scalar field, in case 2 we adopt another type of $f_\theta$ that has a peak at $y = 0$. In Fig. 4(a) $\langle u' \theta' \rangle_{NL}$ agrees well with the DNS result. On the other hand, the absolute value of $\langle u' \theta' \rangle_L$ is much greater than the DNS result near the center line. This overestimate is due to the short length scale of the mean field variation in case 2 as shown in Fig. 1(b). The effective diffusivity $\kappa_{E22}$ near the center line in case 2 is much smaller than the local diffusivity $\kappa_{L22}$ in Fig. 4(b). The effective diffusivities in cases 1 and 2 are quite different near the center line. This difference means that the effective diffusivity depends on the mean scalar profile. To obtain better profiles of the scalar flux with the local eddy diffusivity model, we need to incorporate the mean-field effect into the eddy diffusivity. A typical example is the top-down and bottom-up diffusion in the atmospheric boundary layer. However, it is not clear whether such a modeling can be used for general cases other than the atmospheric boundary layer. On the other hand, the present analysis suggests that the nonlocal expression is a straightforward extension of the local eddy diffusivity and it is exact for arbitrary mean scalar field. The agreement between $\langle u' \theta' \rangle_{NL}$ and the DNS result in cases 1 and 2 demonstrates that the nonlocal expression (18) is exact in the case of one-dimensional mean scalar field.

B. Two-dimensional mean scalar field

In Sec. III A we examined the nonlocal effect in the wall-normal direction. Here, we investigate the nonlocal contribution not only in the wall-normal direction but also in the streamwise direction. In case 3 the value of the scalar at the lower wall, $\theta_b$, is set to be periodic in $x$; the period length is $L_x = 2a$, the resulting scalar field is homogeneous only in the $z$ direction. We take an average in the $z$ direction and in time; statistics depend on $x$ and $y$. In this case the scalar flux given by (18) and (17) can be expressed as

$$
\langle u' \theta' \rangle_{NL}(x,y) = -\int dx' \int dy' \left[ \kappa_{NL1}(x,y;x',y') \frac{\partial \Theta(x',y')}{\partial x'} + \kappa_{NL2}(x,y;x',y') \frac{\partial \Theta(x',y')}{\partial y'} \right],
$$

(29)

$$
\kappa_{NLij}(x,y;x',y') = \int dz' \int dt' (u'_j(x,t)g_j(x,t;x',t')).
$$

(30)

Since the velocity field is homogeneous in the $x$ direction and inhomogeneous in the $y$ direction, $\kappa_{NLij}(x,y;x',y')$ is a function of $x' - x$, $y$, and $y'$. Similarly, the scalar flux given by (19) and (20) is expressed as

$$
\langle u' \theta' \rangle_L(x,y) = -\kappa_{L11}(x,y) \frac{\partial \Theta}{\partial x} - \kappa_{L12}(x,y) \frac{\partial \Theta}{\partial y},
$$

(31)

$$
\kappa_{Lij}(x,y) = \int dx' \int dy' \kappa_{NLij}(x,y;x',y').
$$

(32)

Figure 5 shows the two-dimensional contour plot of the mean scalar for case 3. Half of the computational domain is shown in the $x$ direction. At the lower wall $\Theta$ is positive at $0 < x < 2.4$ and negative at $2.4 < x < 4.8$. The absolute value of the mean scalar near the wall decreases rapidly as $y$ increases because the source term $f_\theta$ is zero in this case. The scalar gradient in the $y$ direction is greater than that in the $x$ direction. Away from the wall the phase of the variation of $\Theta$ in the $x$ direction is shifted downstream owing to the effect of convection by the mean flow.

Figure 6 shows the contour plots of $\kappa_{NL22}$ as functions of $x' - x$ and $y'$ for $y = -0.901$ and $y = -0.605$. The diffusivity $\kappa_{NL22}$ represents a contribution of the scalar gradient $\partial \theta / \partial y$ at $(x' - x, y')$ to the scalar flux $\langle u' \theta' \rangle$ at $(0, y)$. The profiles
are elongated in the upstream direction due mainly to the mean flow convection. The elongated profiles imply that the scalar gradient at remote points in the upstream direction affects the scalar flux at (0, y). The size of the contour in this direction is longer for y = −0.605 than for y = −0.901. This difference is because the mean flow is faster and the time scale k/ε is greater for y = −0.605. Some wiggle is seen just downstream the point at (0, y). Its amplitude is as large as half the maximum of κNL22. The reason for the wiggle is not clear; it may be due to the error of the finite-difference scheme. If the viscous effect is negligible and the contribution from upstream is dominant, the profile of κNL22 should behave like the step function in the x direction. Such a profile cannot be precisely expressed by the finite-difference scheme.

Figures 7(a), 7(b), and 7(c) show the contour plots of ⟨u′θ′⟩ evaluated from the DNS, ⟨u′θ′⟩NL, and ⟨u′θ′⟩L, respectively. The value of ⟨u′θ′⟩NL agrees well with the DNS result whereas the absolute value of ⟨u′θ′⟩L is fairly greater than the DNS result near the wall. The overestimate of ⟨u′θ′⟩L is clearly seen in Fig. 7(d) in which the scalar flux is plotted as a function of y for x = 2.01. Moreover, the location of the peak of ⟨u′θ′⟩L in Fig. 7(c) is shifted upstream compared with the DNS result in Fig. 7(a); the positive peak of ⟨u′θ′⟩L is located at (1.7, −0.93) whereas that of the DNS result is at (2.0, −0.92). The nonlocal expression is required to predict the peak location accurately.

An overestimate of the peak value and a shift of the peak location are also seen for the streamwise scalar flux ⟨u′θ′⟩. Figure 8 shows the scalar flux ⟨u′θ′⟩ as a function of y for x = 4.2 for case 3. The value of ⟨u′θ′⟩NL agrees well with the DNS result whereas ⟨u′θ′⟩NL is clearly overestimated near the wall. The overestimate of ⟨u′θ′⟩L is greater than that of ⟨u′θ′⟩L in Fig. 7(d). This difference is because the width of κNL12 in the y direction is wider than that of κNL22 as was discussed in the preceding section; the nonlocal effect is greater for ⟨u′θ′⟩L. The peak location is also poorly predicted by the local expression; the positive peak of ⟨u′θ′⟩L is located at (3.7, −0.95) whereas that of the DNS result is at (4.2, −0.94) (figures are not shown here).

C. Oscillating mean scalar field

In Sec. III B we showed profiles of the nonlocal diffusivity elongated owing to the convection effect. This effect is closely related to the temporally nonlocal effect, that is, a contribution of the scalar gradient at a previous time to the scalar flux at the present time. To examine this contribution we set the value of θ0 in case 4 to be periodic in time with the period of T = 1.2. The resulting scalar field is not statistically steady while it is homogeneous in the x–z direction. We take an average over the x–z direction and a phase average over 16 cycles; statistics depend on y and t. The scalar flux given by (18) and (17) can be expressed as

\[
\langle u'_i \theta' \rangle_{NL}(y,t) = \int dy' \int dt' \kappa_{NL22}(y,t;y',t') \frac{\partial}{\partial y} \Theta(y',t') \left( u'_i(x,t) g^*_L(x,t;x',t') \right).
\]  

(33)

\[
\kappa_{NL22}(y,t;y',t') = \int dx' \int dz' \int u'_i(x,t) g^*_L(x,t;x',t').
\]

(34)

Since the velocity field is statistically steady, κNL22(y,t;y',t') is a function of y, y', and t'−t. The scalar flux given by (19) and (20) is expressed as
Expression (35) is different from (26) in that $\kappa_{L_2}(y,t)$ varies with time.

$$
\langle u' \theta' \rangle_L(y,t) = - \kappa_{L_2}(y,t) \frac{\partial \Theta}{\partial y}, \tag{35}
$$

$$
\kappa_{L_2}(y,t) = \int dy' \int_{0}^{t} dt' \kappa_{NL_2}(y,t;y',t'). \tag{36}
$$

Figure 9 shows the contour plot of the mean scalar for case 4 as a function of $y$ and $t$. One period in time is shown; at the lower wall $\Theta$ is positive at $0 < t < 0.6$ and negative at $0.6 < t < 1.2$. The absolute value of the mean scalar near the wall rapidly decreases as $y$ increases; compared with the near-wall region the phase of the temporal variation of $\Theta$ is delayed in the region away from the wall. This figure is similar to the mean scalar profile for case 3 as a function of $x$ and $y$ shown in Fig. 5.
IV. TOWARDS MODELING NONLOCAL EFFECTS

In Sec. III using the DNS results we showed that the nonlocal expression for the scalar flux given by (18) is accurate. This means that if the profile of the nonlocal eddy diffusivity is known in advance the scalar flux can be exactly estimated for arbitrary mean scalar field. However, we were able to evaluate the nonlocal diffusivities because detailed values of \( u'_i(x,t) \) and \( g_j(x,t';x',t') \) were calculated in the DNS. In general such detailed values are not available; instead the nonlocal diffusivity needs to be modeled. In the previous work\(^{22} \) we made no attempt to model the nonlocal diffusivity. At present it is very difficult to derive an accurate general model for the nonlocal diffusivity. In this section we examine the DNS results in an attempt to model the nonlocal effect in the following three ways. The first approach is the most straightforward: the profile of \( \kappa_{NLij} \) is expressed in terms of some local quantities. The second one is to improve the local approximation by adding higher-order terms suggested by the nonlocal expression. The third one is to solve a differential equation for \( \kappa_{NLij} \) because algebraic expressions in the first approach may be too simple.

First, we examine the profiles of the nonlocal diffusivity in more detail. Figure 12(a) shows semilog plots of \( \kappa_{NL22} \) in the case of one-dimensional mean scalar field as a function of \( y' \). Since the region near the peak at \( y'=y \) mainly contributes to the integral in (24), we do not attempt to model the profiles of tails which vary for different values of \( y \). Then, the profile can be roughly approximated by

\[
\kappa_{NL22}(y;y') \approx \exp[-|y-y'|/\ell(y,y')],
\]

where \( \ell(y,y') \) is a length scale. The length scale \( \ell \) becomes longer as \( y \) increases. As shown in the dashed line for \( y = -0.796 \), the profile is not always symmetric with respect to \( y' = y \). Therefore, the length scale \( \ell \) may depend not only on \( y \) but also on \( y' \). Here, we do not attempt to express the length scale in terms of model variables such as \( k \) and \( \epsilon \). This is because the choice of model variables depends on what kind of turbulence model is used such as the \( k-\epsilon \) model, the \( k-e \cdot v^2 \) model\(^{27} \) and the Reynolds stress model. We concentrate on examining expressions that can be commonly used in turbulence models.

In addition to the dependence on \( y' \) the nonlocal diffusivity depends on \( x' \) and \( t' \) in cases 3 and 4, respectively. Since it is too complicated to model the two-dimensional profile, we integrate the nonlocal diffusivity over \( y' \) and examine the dependence on \( x' \) or \( t' \) only. Figure 12(b) shows semilog plots of the integral of the nonlocal diffusivity \( \kappa_{NL22} \) as a function of \( (x'-x)/U(y) \) or \( t'-t \). In both cases the gradient of the profile is less steep for \( y = -0.605 \) compared with that for \( y = -0.901 \) because the time scale is longer for the former as mentioned previously. The profile of \( \kappa_{NL22}(x,y;x') \) in case 3 is similar to that of \( \kappa_{NL22}(y,t;t') \) in case 4. These similar figures suggest that the effect of the convection term \( \mathbf{U} \cdot \nabla \theta' \) in case 3 is nearly equivalent to the effect of the time derivative \( \partial \theta'/\partial t \) in case 4. Then, the profile of the nonlocal diffusivity can be approximated by

![Figure 10: Contour plot of nonlocal eddy diffusivity \( \kappa_{NL22}(y,y',t') \) as a function of \( y \) and \( t' - t \) for case 4.](./image.png)
In the present case, if the mean velocity is small compared with the convection effect in the region at $x > x'$, there should be some contribution from the downstream region at $x' > x$. This diffusion effect is not examined here because it is small compared with the convection effect in the present case. If the mean velocity $U(y)$ is negligibly small and the diffusion effect is dominant, then the profile should be similar to (37) in which $y$ and $y'$ are replaced by $x$ and $x'$, respectively. In (38) not the velocity gradient but the velocity itself is involved; this expression is not Galilean invariant. This is not unphysical because the two-time Eulerian correlation is treated in (30). In the preceding section it was shown that the nonlocal expression with the Eulerian correlation can be a good tool for analyzing the scalar transport. However, there may be some problems with modeling the scalar flux because an expression like (38) is not Galilean invariant and depends on the coordinate. Modeling based on the Lagrangian correlation is more appropriate. It is much more complicated and difficult to evaluate the Lagrangian correlation in this type of simulation; it remains as future work.

Although it is straightforward to algebraically express the nonlocal diffusivity, it is not clear whether good expressions can be found for general cases. Another way to model the scalar flux is to improve the local approximation by adding higher-order terms. For example, in addition to the local eddy diffusivity term Hamba introduced a term involving the second derivative of the mean scalar to examine the scalar transport in the atmospheric boundary layer. Using the statistical theory Yoshizawa pointed out that a term involving the Lagrange derivative of the scalar gradient, $D(\nabla \theta)/Dt$, can be included in the expression for the scalar flux. Such extensions can be investigated using the nonlocal expression as follows.

In the case of one-dimensional mean scalar field, the scalar flux is given by (24). Using the Taylor expansion of the scalar gradient $\partial \theta / \partial y'$ at $y' = y$ and truncating it up to the second order we have

$$\langle u' \theta' \rangle_{\text{LE}}(y) = -\kappa_{\text{LE}2}(y) \frac{\partial \theta}{\partial y} - \kappa_{\text{LE}2}(y) \frac{\partial^2 \theta}{\partial y^2} - \kappa_{\text{LE}2}(y) \frac{\partial^3 \theta}{\partial y^3},$$

(40)
finally the whole region from $y$ to the result is almost the same as that of the local expression.

On the other hand, little improvement is shown near the center line. The dotted line agrees well with that of the nonlocal expression. This is why we chose the value of $h=0.1$. The range of integral in (41) and (42) is originally the whole region from $y=-1$ to $y=1$. However, we found that the integral over the whole region did not give better results compared with the local expression $\langle u' \theta' \rangle_L$. Figure 13(a) shows the profiles of $\langle u' \theta' \rangle_{LE}$ in case 2 in which the nonlocal effect is important near $y=0$. The dashed line denotes the expression involving only the first term on the right-hand side of (40); this expression is the same as $\langle u' \theta' \rangle_L$ given by (26) and was shown in Fig. 4(a). The dotted line denotes the expression involving the first and second terms on the right-hand side of (40). Near the wall the result agrees well with that of the nonlocal expression $\langle u' \theta' \rangle_{NL}$ plotted by the solid line. This is why we chose the value of $h=0.1$; if a higher value such as $h=0.2$ is used then the absolute value of $\langle u' \theta' \rangle_{LE}$ near the wall becomes too small.

In case 4 the scalar flux is given by (33). Using the Taylor expansion of the scalar gradient $\partial \theta / \partial y'$ at $(y',t')=(y,t)$ and truncating it up to the first order of $y'$ or $t'$ we have

$$\langle u' \theta' \rangle_{LE}(y,t) = - \kappa_{L2}(y,t) \frac{\partial \theta}{\partial y} - \kappa_{L2}^{(1)}(y,t) \frac{\partial^2 \theta}{\partial y^2}$$

and

$$\langle u' \theta' \rangle_{NL}(y,t) = \int_{y-h}^{y+h} dy' \frac{1}{2} \left( \langle \theta' \rangle^2_{NL} - \langle \theta \rangle^2 \right),$$

where

$$\kappa_{L2}^{(1)}(y) = \int_{y-h}^{y+h} dy' \langle u' \theta' \rangle_{NL}(y',y),$$

and

$$\kappa_{L2}^{(2)}(y) = \int_{y-h}^{y+h} dy' \langle u' \theta' \rangle^2_{NL}(y',y').$$

FIG. 12. Profiles of nonlocal eddy diffusivity: (a) $\kappa_{NL2}(y,y')$ as a function of $y'$ in the case of one-dimensional mean scalar field, and (b) $f dy' \kappa_{NL2}(x,y',x',y')$ as a function of $(x'-x)/U$ for case 3 and $f dy' \kappa_{NL2}(y,y',t')$ as a function of $t'-t$ for case 4.

FIG. 13. Profiles of scalar flux: (a) $\langle u' \theta' \rangle$ as a function of $y$ for case 2 and (b) $\langle u' \theta' \rangle_{LE}$ as a function of $y$ for $t=0.498$ for case 4. Three local expressions $\langle u' \theta' \rangle_{LE}$ are given by (40) or (43); local 1 contains only the first term, local 2 the first and second terms, and local 3 all three terms.
\[
\kappa_{L2}^{(0,1)}(y,t) = \int dy' \int_{t-s}^{t} dt' (t-t') \kappa_{NL2}(y,t';y',t'),
\]
and \(h = 0.1\) and \(s = 0.1\). These values are chosen so that the profile of \((u' \theta')_{LE}\) approximately agrees with the DNS result as follows. Figure 13(b) shows the profiles of \((u' \theta')_{LE}\) in case 4. The dashed line denotes the expression involving only the first term on the right-hand side of (43); this expression is the same as \((u' \theta')_{L}\) given by (35) and shown in Fig. 11(d). The dotted line denotes the expression involving the first and second terms on the right-hand side of (43). Owing to the second term the peak value decreases whereas the profile at \(y' > -0.75\) is not improved. The dotted–dashed line denotes the expression involving all three terms on the right-hand side of (43). Adding the third term makes the value at \(y' > -0.75\) closer to the nonlocal expression plotted by the solid line. This improvement for \(y' > -0.75\) can be explained as follows. The turbulence time scale \(k/e\) away from the wall is greater than that near the wall. This means that away from the wall the nondimensional period \(T e/k\) is smaller and the effect of the oscillating mean field on the scalar flux is larger. Therefore, compensating for the effect using the time derivative term improves the profile for \(y' > -0.75\). These results show that adding higher-order terms we can improve the local approximation although the range of integral needs to be selected for a better agreement.

Next, we try to construct a differential equation for the nonlocal diffusivity in the case of one-dimensional mean scalar field. In general, nonlocal effects are often expressed in terms of an elliptic equation. For example, an elliptic relaxation equation is proposed to model the nonlocal pressure effect near the wall. Here, we assume that \(\kappa_{NL2}(y;\gamma)\) satisfies the following equation:

\[
\frac{\partial^2 f}{\partial y^2} + a \frac{\partial f}{\partial y} - cf = -\langle u'^2 \rangle \delta(y - \gamma)
\]

where coefficients \(a\), \(b\), and \(c\) are functions of \(y\). Profiles of the coefficients are not known at this stage; they are evaluated from the DNS data in this work and should be modeled using local quantities in future work. If \(a = b = 0\) the nonlocal diffusivity is locally determined as \(\kappa_{NL2}(y;\gamma) = \langle u'^2 \rangle / c \delta(y - \gamma)\); this is equivalent to the local diffusivity \(\kappa_{L2}(y) = \langle u'^2 \rangle / c\). Since actual profile of \(\kappa_{NL2}\) is broad, \(a\) and \(b\) should have nonzero values. To obtain the value of the coefficients from the DNS we evaluated the value of \(\kappa_{NL2}(y;\gamma)\) as well as its first and second derivatives using five points at \(y = \gamma\), \(y' = \pm 4 \Delta y\), and \(y' = \pm 5 \Delta y\) where \(\Delta y\) is the grid interval. The profiles of the coefficients are shown in Fig. 14(a). Here, to better understand the meaning of the differential equation we further assume that \(a = a_0\), \(b = 0\), and \(c = c_0\) where \(a_0\) and \(c_0\) are constants. Under this condition the solution of (47) is given by

\[
f(y;\gamma') = \frac{\langle u'^2 \rangle}{2 \sqrt{a_0 c_0}} \exp\left(-\frac{|y-y'|}{\sqrt{a_0 c_0}}\right).
\]

Therefore, we can see that the algebraic expression (37) is the solution of the differential equation in this simplified case. This form is different from the Gaussian profile \(\exp[-(y-y')^2]\) usually seen in the diffusion problem. This difference is because (48) is a steady-state solution. Adding the time derivative term to the left-hand side of (47) and multiplying the delta function \(\delta(t-t')\) to the right-hand side we have

\[
-\frac{\partial f}{\partial t} + a \frac{\partial^2 f}{\partial y^2} + b \frac{\partial f}{\partial y} - cf = -\langle u'^2 \rangle \delta(y - \gamma) \delta(t - t').
\]
If we assume that \( a = a_0, \ b = 0, \) and \( c = c_0 \) the solution of this equation is given by

\[
f(y, t; y', t') = \frac{\langle v'^2 \rangle}{2\sqrt{\pi a_0(t-t')}} \exp \left[ -\frac{(y-y')^2}{4a_0(t-t')} \right] - c_0(t-t').\tag{50}\]

If we integrate the above solution with respect to \( t' \) from \(-\infty\) to \( t \) then we have (48).

In (48) the length scale \( \ell \) can be evaluated as \( \sqrt{a/c} \). However, near the wall this estimate is not valid because \( c \) becomes negative as shown in Fig. 14(a). Here, using the value of \( \sqrt{a/c} \) at \( y = y_0 \) we assume a linear positive profile near the wall as

\[
L(y) = \begin{cases} 
\sqrt{a(y_0)/c(1+y)/(1-y_0)} & \text{for } -1 < y < -y_0, \\
\sqrt{a(y)/c(y)} & \text{for } -y_0 < y < y_0, \\
\sqrt{a(y_0)/c(y_0)(1-y)/(1-y_0)} & \text{for } y < y_0 < 1,
\end{cases}
\tag{51}\]

where \( y_0 = 0.885 \). The profile of the length scale is also plotted in Fig. 14(a). Using this length scale we can express the scalar flux as

\[
\kappa_{NL22}(y; y') = \left\{ \frac{\langle v'^2 \rangle}{2\sqrt{\pi a_0(t-t')}} \exp \left[ -\frac{(y-y')^2}{4a_0(t-t')} \right] - c_0(t-t') \right\} L(y),
\tag{52}\]

where

\[
\kappa_0 = \langle v'^2 \rangle L/(2a).
\tag{53}\]

Figure 14(b) shows the profiles of \( \kappa_{NL22}(y; y') \) as functions of \( y' \) for case 1. The solid line denotes the nonlocal diffusivity evaluated using its definition (25), the dashed line is the solution of (47), and the dotted line is the exponential form (52). The three profiles fairly agree well with each other; not only the differential equation (47) but also the algebraic expression (52) can reproduce the nonlocal diffusivity. This result suggests that in the case of one-dimensional mean scalar field the algebraic expression (52) can be used to predict the scalar flux accurately if profiles of \( \kappa_0(y) \) and \( L(y) \) are modeled appropriately. However, in the case of two-dimensional or oscillating mean scalar field the algebraic expression may be as complex as (50); it can be simpler to solve a differential equation like (49). This differential equation is closely related to the second-order model for the scalar flux. Multiplying \( \partial \Theta/\partial y' \) and integrating with respect to \( y' \) on the both sides of (49) we obtain

\[
-\frac{\partial}{\partial t} \langle \nu'^2 \rangle + a \frac{\partial^2}{\partial y^2} \langle \nu'^2 \rangle + b \frac{\partial}{\partial y} \langle \nu'^2 \rangle + c \langle \nu'^2 \rangle = \langle v'^2 \rangle \frac{\partial \Theta}{\partial y}.
\tag{54}\]

This suggests that the nonlocal expression can also be used to evaluate the coefficients for the second-order model for the scalar flux and that a simple second-order model can work as well as a complicated nonlocal first-order model.

In Fig. 14(a) the profile of coefficient \( c \) has a peak at \( y = -0.916 (y^+ = 15) \) and its value decreases to negative values as \( y \) decreases to \(-1\). As mentioned above the length scale \( \ell \) cannot be evaluated near the wall; the negative value means that the approximation by the simple exponential form is not valid near the wall. Figure 15(a) shows the profile of \( \kappa_{NL22}(y; y') \) as a function of \( y' \) for four locations of \( y \) in the close vicinity of the wall. Each profile is normalized by its maximum value. Although the location of \( y \) is different, the peak location is nearly the same; it is at \( y^+ = 4.7 \). This is in contrast to Fig. 2(a) in which \( y \) is set away from the wall and the peak is located at \( y' = y \). The profiles of the nonlocal diffusivity in Fig. 15(a) mean that the contribution of the scalar gradient at \( y^+ = 5 \) is the largest for the scalar flux at \( y^+ < 5 \). In this region the turbulence production is very small and the molecular diffusion is a dominant gain term in the kinetic energy balance.32 Turbulent fluctuations driven at \( y^+ > 5 \) is transported by the molecular diffusion into the viscous sublayer; in this sublayer the velocity fluctuation is rather passive. This situation agrees well with the numerical examination of the vorticity in channel flow by Miyake.33 His result showed that the convection velocity of streamwise vortices near the wall is nearly constant at \( y^+ < 10 \). Figure 15(b) shows the two-dimensional plot of
\( \kappa_{NL22}(x,y;x',y') \) as a function of \( x' - x \) and \( y' \) for \( y' = 0.4 \) in case 3. The scalar gradient in the region away from the wall contributes to the scalar flux at \( y' = 0.4 \). Therefore, the profile of \( \kappa_{NL22} \) near the wall cannot be approximated by an exponential form. Instead, some self-similar profiles may exist as suggested by Fig. 15(a). This result suggests that nonlocal contribution should be included in near-wall modeling. Damping functions are often used in the eddy viscosity and the eddy diffusivity. Some functions adopted in the \( k-e \) models involve local values of \( k \) and \( \epsilon \). If nonlocal properties of the eddy viscosity are similar to those of the eddy diffusivity shown in Fig. 15, damping function at \( y' < 5 \) should involve not only local values but also values at \( y' = 5 \) where the contribution is the largest.

V. CONCLUSIONS

A nonlocal expression for the scalar flux was derived using the Green’s function for a scalar. The nonlocal diffusivity involved in the expression represents a contribution to the scalar flux from the scalar gradient at remote points in space and time. To validate the nonlocal expression the DNS of channel flow was carried out; the velocity and scalar fields as well as the Green’s function were calculated in the cases of one- and two-dimensional mean scalar fields and of oscillating mean scalar field. It was shown that the nonlocal expression is accurate in all the cases. At the same time a local expression for the scalar flux was examined; the scalar flux near the wall is overestimated and the peak location is shifted in the streamwise direction or in time compared with the DNS results. This shows that the local approximation is not accurate enough and the nonlocal effect is important.

In general the value of the nonlocal diffusivity is not known in advance; it needs to be modeled. Three attempts were made: the nonlocal diffusivity was expressed algebraically using an exponential function, the local approximation was improved by adding higher-order derivative terms, and a differential equation for the nonlocal diffusivity was proposed. Although much more work needs to be done to construct a general nonlocal model, it was demonstrated that the analysis with the nonlocal expression gains insight into modeling the scalar flux.

As future work, this approach should be applied to more complex flows than channel flow. It is interesting to examine two-dimensional or unsteady mean velocity field and its effect on the scalar flux. We expect that this approach can also be applied to the Reynolds stress. The nonlocal viscosity then represents the nonlocal contribution of the velocity gradient to the Reynolds stress.

APPENDIX: CALCULATION OF GREEN’S FUNCTION

To obtain the value of the Green’s function \( g_i(x,t;x',t') \) we need to solve (16). Since the right-hand side of (16) depends on \( x' \) and \( t' \) it is necessary to solve the equation \( N_x \times N_x \times N_t \times N_t \) times where \( N_t \) is the number of time step in \( t' \). Therefore, it is difficult to solve (16) straightforwardly because of its computing cost. In this work, making use of the homogeneity of the velocity field we decrease the computing cost as follows. In the case of one-dimensional mean scalar field the nonlocal diffusivity \( \kappa_{NLij}(y;y') \) given by (25) can be written as

\[
\kappa_{NLij}(y;y') = \langle u'_i(x,t) g_j^*(x,t;y') \rangle,
\]

where

\[
g_j^*(x,t;y') = \int dx' \int dz' \int_0^t dt' g_i'(x,t;x',t').
\]

The equation for \( g_j^* \) can be derived by integrating the both sides of (16) with respect to \( x' \), \( z' \), and \( t' \) as follows:

\[
\frac{\partial g_j^*}{\partial t} + u_j \frac{\partial g_j^*}{\partial x_j} - \frac{\partial}{\partial x_j}(u'_j g_j^*) = -\kappa \frac{\partial^2 g_j^*}{\partial x_j^2} + u'_j \delta(y-y').
\]

As a result, the location of the source term depends only on \( y' \); we need to solve the equation only \( N_y \) times.

Here, we should mention the averaged term involved on the left-hand sides of (16) and (A3). Since we take an average over the \( x-z \) plane and in time, the term \( \langle u'_j g_j^* \rangle \) cannot be evaluated until the time marching is finished. Instead, in this work the average on the left-hand side is approximated by that over the \( x-z \) plane only. The error involved in dropping the time average was not estimated. It seems negligible because the results obtained from the nonlocal model agree very well with the DNS results as already shown.

17A. Nakayama, H. D. Nguyen, and M. B. Daif, “Nonlocal diffusion model


