On the Role of Quasi-one-dimensional Dissipation Layers in Turbulent Scalar Mixing

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1. Motivation and background

Ever since Carl Gibson (1968) analyzed the fine scale structure of scalar mixing in terms of zero gradient points there has remained the question how these findings can be related to mixing models. Existing turbulent mixing models ignore the existence of minimal points. They are intuitively based on the picture that turbulent mixing is controlled by two processes: Stirring of the scalar field by turbulence and subsequent molecular diffusion. The general idea is that at sufficiently intense turbulence, stirring is the rate determining process and that molecular diffusion just completes the sequence. This follows from the hypothesis of a cascade process for scalar mixing, which suggests the use of the flow time to model scalar dissipation. This hypothesis is supported by experimental and DNS data, but since it recurs essentially to dimensional scaling only, it leaves open the question about the precise mechanism by which the interaction between turbulent stirring and molecular diffusion takes place.

There are a number of unresolved questions in scalar mixing. In pdf methods based on one-point statistics, for instance, the modeling of molecular mixing represents a challenging problem. The challenge lies in the existence of an exact form for the pdf equation of the conserved scalar which, however, is not well posed. For the special case of homogeneous turbulence this pdf equation reads (cf. O'Brien, 1980)

$$\frac{\partial P_Z}{\partial t} = -\frac{1}{2} \frac{\partial^2}{\partial Z^2} (\chi_Z P_Z) .$$  (1.1)

Here $Z$ is the mixture fraction which stands for a conserved scalar that is normalized such that it varies between $0 \leq Z \leq 1$, $P_Z$ is its probability density function and $\chi_Z$ is the conditional scalar dissipation rate defined as

$$\chi_Z = 2D \langle (\nabla Z')^2 | Z \rangle ,$$  (1.2)

where $D$ is the diffusion coefficient and $Z'$ is the mixture fraction fluctuation. In most situations in turbulent mixing the definition (1.2) can be replaced by

$$\chi_Z = 2D \langle (\nabla Z)^2 | Z \rangle ,$$  (1.3)

because the square of the mean gradient $(\nabla \bar{Z})^2$ is small compared to that of the fluctuating mixture fraction $(\nabla Z')^2$. Since $\chi_Z$ represents the gradient and therefore requires two-point information, it must be modeled. As pointed out by Pope (2000), the assumption of a constant conditional scalar dissipation rate equal to its mean unconditional value in (1.1) leads to an anti-diffusion equation, which is not well-posed, because it is non-realizable for arbitrary initial conditions. In most pdf methods the anti-diffusion term is therefore replaced by intuitively derived mixing models that do not make use of

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the exact formulation. From a fundamental point of view this is certainly unsatisfactory. Hence, the following questions may be posed: Is there an exact formulation for the molecular mixing process in a mathematically realizable form? If there is such a form, would this allow to model the process of stirring by the turbulent flow field and the subsequent molecular mixing process in a straightforward way? We will answer the first question in the affirmative and will outline aspects of the modeling below.

In the following, we will first derive an equation for the functional form of the scalar dissipation rate valid in a local region between a minimum and a maximum point in mixture fraction space. This equation exhibits analytical unsteady and quasi-steady state solutions which correspond in physical space to local convective-diffusive structures in which unsteady diffusion is enhanced by compressive strain (cf. Ashurst et al., 1987). We will call these structures quasi-one-dimensional dissipation layers (Q1DL). The distribution function of the mixture fraction within these layers is analytically related to the local scalar dissipation rate. In search of these Q1DLs we will then analyze the scalar DNS data of a time-evolving turbulent mixing layer by Rogers and Moser (1994) by generating trajectories between minimum and maximum points. Choosing a particular quasi-steady solution (the one that corresponds to a sine function in physical space) we will then reconstruct the probability density function of the mixture fraction $P_Z$ and the conditional scalar dissipation rate $\chi_Z$ using the joint pdf of minimum and maximum mixture fraction values of trajectories. Finally, we will derive an exact form for the joint distribution function of minimum and maximum mixture fractions, expressed in terms of their algebraic mean and their difference.

2. Theory

We consider a small local fluid element with initial size of the order of $\pi L_0$ centered around its midpoint $O(x_0, t)$ which is convected by the velocity $v(x_0, t)$ within a constant density turbulent flow field. We also introduce a local cartesian coordinate system, unit vectors $\mathbf{i}, \mathbf{j}, \mathbf{k}$, aligned with the principal axis of strain ($\partial u/\partial x, \partial v/\partial y, \partial w/\partial z$) and a relative coordinate at $O(x_0, t)$ to the fluid element as $(x, y, z) = x - x_0$. The velocity field within the small fluid element can be expanded as

$$v(x, t) = v(x_0, t) + i \frac{\partial u}{\partial x} x + j \frac{\partial v}{\partial y} y + k \frac{\partial w}{\partial z} z.$$

We denote the most compressive rate of strain as $a = -\partial v/\partial y$ and assume that the scalar gradient is locally aligned with the most compressive rate of strain. This assumption is based on the DNS analysis by Ashurst et al. (1987) who found that ”there is an increased probability for the scalar gradient to align with the most compressive strain direction and that the average gradient is larger when pointing into that direction”. Therefore we will conduct a one-dimensional analysis based on the scalar equation

$$\frac{\partial Z}{\partial t} - a y \frac{\partial Z}{\partial y} = D \frac{\partial^2 Z}{\partial y^2},$$

where $D$ is assumed constant.

By differentiating (2.2) with respect to $y$ and multiplying it with $2 \partial Z/\partial y$ an equation for the square of the mixture fraction gradient can be derived

$$\frac{\partial}{\partial t} \left( \frac{\partial Z}{\partial y} \right)^2 - a y \frac{\partial}{\partial y} \left( \frac{\partial Z}{\partial y} \right)^2 - 2 a \left( \frac{\partial Z}{\partial y} \right)^2 = 2 \frac{\partial Z}{\partial y} \frac{\partial}{\partial y} \left( D \frac{\partial^2 Z}{\partial y^2} \right).$$
Using the one-dimensional form of the scalar dissipation rate as
\[ \chi_L = 2D (\partial Z/\partial y)^2 , \] (2.4)
and multiplying (2.3) with \(2D\) we obtain an equation for \(\chi_L\)
\[ \frac{\partial \chi_L}{\partial t} - a y \frac{\partial \chi_L}{\partial y} - 2 a \chi_L = D \frac{\partial^2 \chi_L}{\partial y^2} - \frac{1}{4} \left( \frac{\partial \chi_L}{\partial Z} \right)^2 . \] (2.5)
Here the identity
\[ \frac{\partial^2 Z}{\partial y^2} = \frac{1}{2} \frac{\partial}{\partial Z} \left( \frac{\partial Z}{\partial y} \right)^2 \] (2.6)
has been used. We call \(\chi_L\) the local dissipation rate within the quasi-one-dimensional dissipation layer.

In general a Q1DL lies between minimum and maximum values of the mixture fraction that differs from 0 and 1, respectively
\[ 0 \leq Z_{\text{min}}(t) \leq Z \leq Z_{\text{max}}(t) \leq 1 . \] (2.7)
Therefore we introduce the normalized coordinate
\[ Z^* = \frac{Z - Z_{\text{min}}}{\Delta Z} , \] (2.8)
where
\[ \Delta Z = Z_{\text{max}} - Z_{\text{min}} . \] (2.9)

We now introduce a flamelet-type transformation (cf. Peters, 2000) by replacing \(y\) by \(Z^*\) as independent variable and by setting the new time variable \(\tau = t\). Using the transformation rules
\[ \frac{\partial}{\partial t} = \frac{\partial Z^*}{\partial \tau} + \frac{\partial}{\partial \tau} , \] (2.10)
\[ \frac{\partial}{\partial y} = \frac{\partial Z^*}{\partial \tau} \frac{\partial}{\partial Z^*} , \] (2.11)
on (2.5) we obtain
\[ (\Delta Z)^2 \frac{\partial \chi_L}{\partial \tau} = \chi_L \frac{\partial^2 \chi_L}{\partial Z^{*2}} + 2 a^* \chi_L - \frac{1}{4} \left( \frac{\partial \chi_L}{\partial Z^*} \right)^2 + \left[ b^* - Z^* (c^* + b^*) \right] \frac{\partial \chi_L}{\partial Z^*} . \] (2.12)
This equation has several interesting features: The first term on the r.h.s. is a transport term where \(\chi_L\) itself is the diffusivity in \(Z^*\)-space. For \(a > 0\) the second term may be interpreted as a productive term, while the third term resembles a dissipation term since it contains the square of derivatives. The last term, finally, results from the time dependence of \(Z_{\text{min}}\) and \(Z_{\text{max}}\) defined by the quantities \(b\) and \(c\)
\[ b = \frac{1}{\Delta Z} \frac{\partial Z_{\text{min}}}{\partial t} , \quad c = - \frac{1}{\Delta Z} \frac{\partial Z_{\text{max}}}{\partial t} , \] (2.13)
with the parameters
\[ b^* = b (\Delta Z)^2 , \quad c^* = c (\Delta Z)^2 . \] (2.14)
appearing in (2.12). Let us note here that the time evolution of \(\Delta Z\) can be calculated from (2.13) by
\[ \frac{d \Delta Z}{dt} = -(b + c) \Delta Z = -2 \hat{b} \Delta Z \] (2.15)
N. Peters & P. Trouillet

where \( \hat{b} = (b + c)/2 \). This shows that the parameter \( \hat{b} \) describes the rate at which minima and maxima mixture fraction points move closer towards each other. We will therefore call \( \hat{b} \) the mixing rate.

Analytical solutions of (2.12) can be readily derived. For \( Z_{\min} = 0 \) and \( Z_{\max} = 1 \), for instance, the steady-state solution is given by eq. (3.47) in Peters (2000). For the unsteady case with \( a = 0 \) a closed form solution is also derived. For \( Z_{\min} = 0 \) but \( Z_{\max}(t) \neq 1 \) some unsteady solutions have recently been presented by Villermaux (2002).

Since we are dealing with a one-dimensional structure the local distribution function of \( Z^* \) within the Q1DL, denoted by \( P_L \), is analytically related to that of \( \chi_L \). This follows directly from the relation (cf. Papoulis, p. 95)

\[
P_L(Z^*) = \frac{P(y)}{|\partial Z^*/\partial y|},
\]

where \( P(y) \) is uniform. With the definition (2.4) and \( D \) being constant this leads to

\[
\chi_L(Z^*)^{1/2} \cdot P_L(Z^*) = \text{const}.
\]

For the local structure this relation can be used to derive from (2.12) an equation for \( P_L(Z^*) \)

\[
(\Delta Z)^2 \frac{\partial P_L}{\partial t} = -\frac{1}{2} \frac{\partial^2 (\chi_L P_L)}{\partial Z^*^2} + \left[ b^* - Z^* (c^* + b^*) \right] \frac{\partial P_L}{\partial Z^*} - a^* P_L,
\]

where \( \tau \) has been set equal to \( t \) again. In (2.18) the first term on the r.h.s. is reminiscent of the anti-diffusion term in (1.1). This will be used in section 4 below.

We now ask the question if there is a particular solution of (2.12) which is most likely to occur in a turbulent mixing field. For that purpose we need to go back to the original scalar equation (2.2). It is well known that, starting from an arbitrary initial condition for \( Z(y, t) \) at \( t = 0 \), higher order harmonics in the solution of a parabolic equation will die out very rapidly and the first harmonic representing a sine function will remain (cf. Kervokian, 1990, p.35, for example). For the reconstruction in section 4 we will therefore choose for \( Z(y, t) \) the particular form of a sine function in the interval between \( Z_{\min} \) and \( Z_{\max} \). Because of symmetry \( b = c = \hat{b} \) and the origin are placed at the center of the one-dimensional layer at \( Z = Z_m \) where \( Z_m \) is defined by

\[
Z_m = \frac{Z_{\max} + Z_{\min}}{2}.
\]

The zero gradient points \( Z_{\min} \) and \( Z_{\max} \) are placed at \( y = -\pi L/2 \) and \( y = +\pi L/2 \), respectively, where \( \pi L \) is the width of the layer. Since the velocity \( v \) at any position \( y \) is \( -ay \) we obtain for the change of \( L \)

\[
v(L) = \frac{dL}{dt} = -a \cdot L,
\]

which may be integrated as

\[
L(t) = L_0 e^{\int_0^t a(t) \, dt}.
\]

A Lagrangian form of (2.2) may be obtained by introducing the new coordinates

\[
\eta = y/L(t), \quad \tau = t.
\]

This leads with the transformation rules

\[
\frac{\partial}{\partial y} = \frac{1}{L} \frac{\partial}{\partial \eta}, \quad \frac{\partial}{\partial \tau} = a\eta \frac{\partial}{\partial \eta} + \frac{\partial}{\partial \tau}
\]
to
\[
\frac{\partial Z}{\partial \tau} = \frac{D}{L^2(t)} \frac{\partial^2 Z}{\partial \eta^2} .
\] (2.24)

It is easily seen that the sine function solution
\[
Z = Z_m + \frac{\Delta Z}{2} \sin \eta ,
\] (2.25)
equivalent to
\[
Z^* = \frac{1}{2} (1 + \sin \eta) ,
\] (2.26)
satisfies (2.24). Inserting (2.25) into (2.24) and using (2.19) it is seen that there exists
the following relation between \( \hat{b} \), \( L \) and \( D \)
\[
2 \hat{b} = \frac{D}{L^2} .
\] (2.27)

This shows that the mixing rate \( \hat{b} \) increases as \( L(t) \) decreases. This will occur if the time
integral in the exponent of (2.21) is positive, i.e. if the strain is compressive on time
average. This is generally the case under turbulent conditions. Therefore compressive
strain increases the mixing rate \( \hat{b} \) and thereby enhances mixing.

The scalar dissipation rate is calculated from (2.25) as
\[
\chi_L = 2D \left( \frac{\partial Z}{\partial \eta} \right)^2 = \frac{D(\Delta Z)^2}{2L^2} \cos^2 \eta = \hat{b}^* \cos^2 \eta ,
\] (2.28)

where \( \hat{b}^* = \hat{b}(\Delta Z)^2 \). By replacing the cosine function by the sine function it is seen with
(2.26) that \( \chi_L \) can be expressed in terms of \( Z^* \) as
\[
\chi_L = 4 \hat{b}^* Z^*(1 - Z^*) ,
\] (2.29)

This solution satisfies for \( b = c \) the balance of the last two terms in (2.12). Inserting it
into the remaining part of (2.12) leads with \( \tau = t \) to
\[
\frac{d \hat{b}^*}{dt} = \hat{b}^* (2a - 4 \hat{b}) .
\] (2.30)

Combining (2.27), (2.20) and (2.19) shows that (2.30) is satisfied for any prescribed
function \( a(t) \).
\( \chi_L \) can also be written as
\[
\chi_L = 4 \hat{b}^* (Z - Z_{\text{min}})(Z_{\text{max}} - Z) .
\] (2.31)

Since \( \hat{b} \), \( Z_{\text{min}} \) and \( Z_{\text{max}} \) depend on time we call this a quasi-steady-state solution. Also,
using (2.17) we can calculate the local distribution function of \( Z \) within the Q1DLs as
\[
P_L(Z; Z_{\text{min}}, Z_{\text{max}}) = \frac{\pi^{-1}}{(Z - Z_{\text{min}})^{1/2}(Z_{\text{max}} - Z)^{1/2}} ,
\] (2.32)
where normalization has led to the elimination of the parameter \( \hat{b}^* \). In the following
we will use (2.31) and (2.32) to reconstruct the pdf \( P_Z(Z) \) and the conditional scalar
dissipation rate \( \chi_Z \) in the DNS data.
Table 1. Location of the boxes used to extract the DNS fields. The global dimensions of the DNS domain are [0, 100], [−4, 4] and [0, 24.7] in the x, y and z directions respectively.

<table>
<thead>
<tr>
<th>Box</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>[78, 90]</td>
<td>[−1.3, 1.3]</td>
<td>[3.2, 7.7]</td>
</tr>
<tr>
<td>2</td>
<td>[29, 41]</td>
<td>[−1.3, 1.3]</td>
<td>[3.2, 7.7]</td>
</tr>
<tr>
<td>3</td>
<td>[49, 61]</td>
<td>[−1.3, 1.3]</td>
<td>[7.7, 12.2]</td>
</tr>
<tr>
<td>4</td>
<td>[15, 26]</td>
<td>[−1.3, 1.3]</td>
<td>[7.7, 12.2]</td>
</tr>
</tbody>
</table>

3. A-priori testing using DNS data

The testing will be based on instantaneous flow and scalar fields extracted from the DNS of a time-evolving mixing layer performed by Rogers and Moser (1994). This DNS was computed using a pseudo-spectral method to solve the 3D incompressible Navier-Stokes equations on a 512 × 210 × 192 Fourier/Jacobi modes domain. A transport equation for a scalar with Schmidt number 1.0 was carried along in the simulation. After an initial development, the mixing layer becomes self-similar from \( t = 87.5 \) to \( t = 150 \) in non-dimensional units. During the simulation, the Reynolds number based on the vorticity thickness \( Re_l = \frac{\Delta \tilde{\omega}}{\nu} \) grows from 1370 to 10800.

Data from several times during this interval were used to test the theory. For each time, both velocity and scalar fields were extracted from four boxes centered around the midpoint \( y = 0 \) of the mixing layer. Table 1 gives a description of these subdomains. A conversion from Fourier space to physical space was performed. In physical space, the velocity and scalar fields were discretized on a regular structured grid with a resolution \( \Delta x \) which is of the order of the Kolmogorov scale.

The ensemble of the four boxes was then used to demonstrate the existence and relevance of the Q1DL structures presented in the theory above and to reconstruct both the pdf \( P_Z \) and the conditional scalar dissipation rate \( \chi_Z \). For brevity, we will only report data and analysis for one particular time, namely \( t = 150 \).

3.1. Evidence of one-dimensional dissipation layers

In Fig. 1 we show a portion of the scalar field \( Z(x, t) \) extracted from one of the boxes and in Fig. 2 the corresponding field of the instantaneous scalar dissipation rate \( \chi(x, t) \) defined by

\[
\chi = 2 D(\nabla Z)^2.
\]

Fig. 1 shows fairly large structures in the scalar field. At their edges these structures generate steep gradients and therefore thin layers with high values of the scalar dissipation rate as shown in Fig. 2. These layers have been observed both experimentally and in many DNS simulations and are the subject of the present analysis.

3.2. Trajectories

In order to analyze the local dependence of the local scalar dissipation rate on mixture fraction, thereby identifying Q1DL structures, we calculate, starting from at every grid point in the boxes listed in Table 1, the direction of the scalar gradient (\( \nabla Z \)). We follow
On the Role of Q1DL in Turbulent Scalar Mixing

Figure 1. Mixture fraction field in a box extracted from the center of the mixing layer

Figure 2. Instantaneous scalar dissipation rate field from the same box as Fig. 1

this direction using a large number of small spatial steps of the order of $1/10$ of the grid resolution $\Delta x$, recalculating the scalar gradient after each step. The scalar field between the grid points is computed by tri-linear interpolation. With this procedure we move in the direction of increasing as well as decreasing values of the mixture fraction until we find a maximum as well as a minimum point. These extremal points correspond to the location where a continuation of the trajectory in the direction calculated at the previous
step would lead to a change in sign of the mixture fraction gradient. A further criterion for having reached a zero gradient point is that the scalar dissipation rate $\chi$ should be less than 0.0005. Trajectories which leave the box without ending at a minimum as well as a maximum point are not counted. Thereby we obtain from 21 million grid points within the four boxes 5 million trajectories. As a consequence of not counting trajectories that leave the box without reaching the two extremal points we will not capture the spike in the mixture fraction pdf at $Z = 0$ in figure 19 b for $\xi = 0$ in Rogers and Moser (1994).

For the trajectories that were completed within the box we obtain one minimum and one maximum point associated with the original starting point of the trajectory. It is important to note that we are not considering physical zero gradient points as such, but end points of trajectories. They are weighted by the number of starting points and their joint pdf reflects the trajectories rather than that of the zero gradient points themselves.

We calculate the scalar dissipation rate $\chi$ along the trajectory using the definition (3.1). The rates $b$ and $c$ defined by (2.13) are calculated by using the balance of the last two terms of (2.12) in the limit $\chi_L \to 0$. This leads to

$$b = \frac{1}{4\Delta Z} \frac{\partial \chi}{\partial Z}, \quad c = \frac{1}{4\Delta Z} \frac{\partial \chi}{\partial Z}$$

for $Z^* \to 0$ and $Z^* \to 1$, respectively.
In Fig. 3 we show three calculated scalar dissipation rate profiles along trajectories between different minima and maxima points $Z_{\text{min}}$ and $Z_{\text{max}}$. With these values and the mixing rate $\hat{b}$ calculated as the algebraic average of $b$ and $c$ we reconstruct in Fig. 4 the local scalar dissipation rate $\chi_L$ using (2.31). Using (2.32) we can also calculate the local distribution function $P_L$ which we show in Fig. 5. It is seen that, with the exception of trajectory 2, the shapes of $\chi$ in Fig. 3 are close to the inverse parabolas $\chi_L$ in Fig. 4. We believe that trajectory 2 passes close to a saddle point in the 3-D mixture fraction field, with the intermediate minimum of $\chi$ occurring in the vicinity of that saddle point. Trajectories with intermediate minima of $\chi$ were found quite frequently in the numerical analysis of the DNS data. They could have been split into two or more trajectories to obtain a closer agreement with the theory, but we believe that this would have introduced some additional arbitrariness.

The shapes of the local pdf $P_L$ shown in Fig. 5 are symmetric with respect to $Z_m$ of that trajectory and show singularities at their corresponding values $Z_{\text{min}}$ and $Z_{\text{max}}$. These singularities follow directly from $\chi_L = 0$ in (2.17) and indicate that the trajectories have long tails in physical space where the scalar gradients are small.

We will now use (2.32) to reconstruct the pdf $P_z$ of the mixture fraction using values from those points only from which complete trajectories have been started. For that purpose we calculate the joint pdf $Q(Z_{\text{min}}, Z_{\text{max}}, \hat{b})$ from the trajectories in the four boxes at time $t = 150$. The reconstructed pdf $P_{z,r}$ is then obtained from

$$ P_{z,r} = \int_0^1 \int_0^1 P_L(Z; Z_{\text{min}}, Z_{\text{max}}) \int_0^\infty Q(Z_{\text{min}}, Z_{\text{max}}, \hat{b}) \, d\hat{b} \, dZ_{\text{min}} \, dZ_{\text{max}}. \quad (3.3) $$

The comparison is shown in Fig. 6. The agreement is remarkably good, indicating that the symmetric shape of $P_L$ in (2.31) is sufficiently accurate to reconstruct the scalar pdf. Other symmetric shapes have also been used but the resulting pdf seems to be quite insensitive to that choice. It is remarkable that the reconstruction is successful even though the shape of the local pdf $P_L$ is bimodal with singularities at $Z_{\text{min}}$ and $Z_{\text{max}}$ and $P_Z$ has a bell-shaped form. The ability to reconstruct $P_Z$ is a strong argument in favor of the predominance of Q1DLs in the mixing process.

In a similar way we reconstruct $\chi_Z$ by using (2.31) and the joint pdf $Q(Z_{\text{min}}, Z_{\text{max}}, \hat{b})$. The reconstructed conditional scalar dissipation rate $\chi_{z,r}$ follows from

$$ \chi_{z,r} = \int_0^1 \int_0^1 \int_0^\infty \chi_L(Z; Z_{\text{min}}, Z_{\text{max}}, \hat{b}) \, Q(Z_{\text{min}}, Z_{\text{max}}, \hat{b}) \, dZ_{\text{min}} \, dZ_{\text{max}} \, d\hat{b}. \quad (3.4) $$

and is denoted as “reconstruction 1” in Fig. 7. The comparison is not as favorable as that in Fig. 6, when we take the mixing rate $\hat{b}$ from the trajectories. It is seen that “reconstruction 1” does not reproduce the two humps of the DNS around $Z = 0.2$ and $Z = 0.8$. As an alternative we could use the maximum value of $\chi$ from each trajectory to parameterize (2.31). Rather than to take these values directly we will derive an approximate relation between the maximum of $\chi$ and $b^*$ and correct $b^*$ in (2.31) accordingly.

It is evident that the sine function solution and therefore $\chi_L$ in (2.29) does not capture the initial unsteady development of the Q1DLs. With the solution of (2.15) there exists a monotonic relation between the time and $\Delta Z$ of a Q1DL. Therefore one may parameterize the additional time dependence of $\chi_L$ by a correlation for $b^*$ in (2.29) that depends on $\Delta Z$ only. The analysis of the trajectories from the DNS shows in fact that the maximum values of $\chi$, which occur at $Z^* = 0.5$ and therefore according to (2.29) would be equal to
\( \hat{b}^* \), can reasonably well be approximated by
\[
\chi_{\text{max}}/\hat{b}^* = 1.0 + 2.0 \Delta Z/(\Delta Z)_{\text{max}} \tag{3.5}
\]
Here the maximum values of \( \Delta Z \) are:
\[
(\Delta Z)_{\text{max}} = \begin{cases} 
2 - 2Z_m & \text{for } Z_m \geq 0.5 \\
2Z_m & \text{for } Z_m < 0.5 
\end{cases} \tag{3.6}
\]
which follow from (4.5) below for \( Z = 0 \), \( Z^* = 0 \) and \( Z = 1 \), \( Z^* = 1 \), respectively. Dissipation layers that extend to \( Z = 0 \) and \( Z = 1 \) will therefore have dissipation rates which are significantly larger than predicted by (2.31).

In the second reconstruction, shown as "reconstruction 2" in Fig. 7, we have multiplied (2.31) by the approximation of the r.h.s. of (3.5). This curve shows higher values than the DNS curve, but also shows its characteristic humps. By comparison with "reconstruction 1" we conclude that the humps in the \( \chi_Z \) profile result from dissipation layers that extend either to \( Z = 0 \) or to \( Z = 1 \). Similar profiles of \( \chi_Z \) with two humps, for instance, are found in the constant density DNS data of Pantano et. al. (2002).

4. An equation for the joint distribution function of \( Z_m \) and \( \Delta Z \)

Rather than considering the joint pdf of minimum and maximum points we will derive an equation for the joint distribution function of \( Z_m \) and \( \Delta Z \) from first principles. The corresponding normalized pdf calculated from the \( Z_m \) and \( \Delta Z \) values of the 5 million trajectories is shown in Fig. 8.

Based on (2.9), (2.13) and (2.19) the substantial changes of \( Z_m \) and \( \Delta Z \) are
\[
\frac{dZ_m}{dt} = \frac{b - c}{2} \Delta Z, \quad \frac{d\Delta Z}{dt} = -(b + c) \Delta Z. \tag{4.1}
\]
We realize that depending on the sign of \( (b - c) \) the value of \( Z_m \) either increases or decreases with time, while \( \Delta Z \) always decreases. We also note that (cf. Gibson, 1968) minimum and maximum points are convected by the flow field but due to their nature, they do not diffuse. This is also valid for \( Z_m \) and \( \Delta Z \). In a flow field \( Z_m \) and \( \Delta Z \) are therefore governed by the following convective-reactive equations
\[
\frac{\partial Z_m}{\partial t} + v \cdot \nabla Z_m = \frac{b - c}{2} \Delta Z, \quad \frac{\partial \Delta Z}{\partial t} + v \cdot \nabla \Delta Z = -(b + c) \Delta Z. \tag{4.2}
\]
In deriving the joint distribution function of $Z_m$ and $\Delta Z$, we follow O’Brien (1980) who considered the pdf of a reactive-diffusive scalar. In such a derivation the formulation of the reaction term is exact while the diffusion term must be modelled. We are fortunate that $Z_m$ and $\Delta Z$ are non-diffusive such that, based on (4.2), the equation for the joint distribution function $P$ of $Z_m$ and $\Delta Z$ becomes

$$\frac{\partial P}{\partial t} + \langle v \cdot \nabla P \rangle + \frac{1}{2} \left( \frac{\partial ((b-c) \frac{\partial P}{\partial Z_m})}{\partial \Delta Z} - \frac{\partial ((b+c) \frac{\partial P}{\partial \Delta Z})}{\partial Z_m} \right) = \Sigma(Z_m, \Delta Z).$$  \hspace{1cm} (4.3)

Here a yet unknown source term $\Sigma(Z_m, \Delta Z)$ has been added on the r.h.s. The convective term containing the fine-grained joint density $P$ must be modelled. The rates $(b-c)$ and $(b+c)$ in (4.3) are assumed to be fixed quantities that are known.

Gibson (1968) discussed the initial production of zero gradient points by vortices that are strong enough to overturn the imposed scalar gradient. He also argued that secondary splitting would continuously generate new zero gradient points. Based on these considerations we expect that the production term $\Sigma(Z_m, \Delta Z)$ in the equation for $P$ must depend on properties of the turbulent flow field. Since the only quantity representing the flow field in the theory developed above is the strain rate $\alpha$, we expect that $\Sigma(Z_m, \Delta Z)$ will depend on this quantity.
We want to show that, knowing the joint distribution function \( P(Z_m, \Delta Z) \), we would be able to reconstruct \( P_Z \). One way to do this is to reproduce in the homogeneous limit the exact equation (1.1) which governs \( P_Z \). For that purpose we make use of our knowledge about the local distribution function \( P_L \) following from (2.18). We first multiply (4.3) by \( P_L \) to obtain

\[
P_L \frac{\partial \mathcal{P}}{\partial t} + \langle \mathbf{v} \cdot \mathbf{\nabla} (P_L \mathcal{P}) \rangle + \frac{1}{2} \frac{\partial ((b - c) \Delta Z P_L)}{\partial Z_m} - \frac{\partial ((b + c) \Delta Z P_L)}{\partial \Delta Z}
\]

\[
= \mathcal{P} \left[ \frac{1}{2} (b - c) \Delta Z \frac{\partial P_L}{\partial Z_m} - (b + c) \Delta Z \frac{\partial P_L}{\partial \Delta Z} \right] + P_L \Sigma(Z_m, \Delta Z) . \tag{4.4}
\]

With the definition

\[
Z^* = \frac{1}{2} + \frac{Z - Z_m}{\Delta Z}
\]

(4.5)

the grouping in square brackets in the third term on the r.h.s. of (4.4) becomes

\[
\frac{1}{2} (b - c) \Delta Z \frac{\partial P_L}{\partial Z_m} - (b + c) \Delta Z \frac{\partial P_L}{\partial \Delta Z} = -[b - Z^*(b + c)] \frac{\partial P_L}{\partial Z^*} . \tag{4.6}
\]

Combining (2.18) and (4.4) with (4.6) then leads to

\[
\frac{\partial P_L \mathcal{P}}{\partial t} + \langle \mathbf{v} \cdot \mathbf{\nabla} (P_L \mathcal{P}) \rangle = -\frac{1}{2} \frac{\partial^2 (\chi_L P_L \mathcal{P})}{\partial Z^2} + \frac{1}{2} \frac{\partial ((b - c) \Delta Z P_L \mathcal{P})}{\partial Z_m} + \frac{\partial ((b + c) \Delta Z P_L \mathcal{P})}{\partial \Delta Z} - a P_L \mathcal{P} + P_L \Sigma(Z_m, \Delta Z) . \tag{4.7}
\]

Integration over \( Z_m \) and \( \Delta Z \) shows that the third and the fourth term on the r.h.s. cancel after integration because \( \mathcal{P} \) must be zero at the boundaries. Furthermore, the last two terms cancel if the source in (4.3) satisfies the condition

\[
\int_0^1 \int_0^{(\Delta Z)_{\text{max}}} (\Sigma(Z_m, \Delta Z) - a \mathcal{P}) P_L \Delta Z dZ_m = 0 . \tag{4.8}
\]

If (4.8) is to be valid for any form of \( P_L \) it follows immediately that

\[
\Sigma(Z_m, \Delta Z) = a \mathcal{P} . \tag{4.9}
\]

With the definitions

\[
P_Z = \int_0^1 \int_0^{(\Delta Z)_{\text{max}}} P_L \mathcal{P} \Delta Z dZ_m
\]

(4.10)

\[
\mathcal{P}_Z = \int_0^1 \int_0^{(\Delta Z)_{\text{max}}} P_L \mathcal{P} \Delta Z dZ_m
\]

(4.11)

integration of (4.7) over \( Z_m \) and \( \Delta Z \) leads to a pdf equation for \( Z \) in the form

\[
\frac{\partial P_Z}{\partial t} + \langle \mathbf{v} \cdot \mathbf{\nabla} P_Z \rangle = -\frac{1}{2} \frac{\partial^2 \chi_Z P_Z}{\partial Z^2} , \tag{4.12}
\]

which reduces to (1.1) in the limit of homogeneous turbulence as anticipated. In (4.12)

\[
\chi_Z P_Z = \int_0^1 \int_0^{(\Delta Z)_{\text{max}}} \chi_L P_L \mathcal{P} \Delta Z dZ_m , \tag{4.13}
\]

which is consistent with the use of Bayes’ theorem by O’Brien (1980) in the definition of
\( \chi_Z \) as a conditional mean scalar dissipation rate. O’Brien also introduced a gradient flux approximation for the convective term which reads for the convective term in (4.3)

\[
< v \cdot \nabla P > = < v > \cdot \nabla D_t \cdot \nabla P,
\]

(4.14)

where \( D_t \) is the turbulent diffusivity. Equation (4.3) then becomes with (4.9) and (4.14)

\[
\frac{\partial P}{\partial t} + < v > \cdot \nabla P - \nabla D_t \cdot \nabla P + \frac{1}{2} \frac{\partial ((b - c) \Delta Z P)}{\partial Z_m} - \frac{\partial ((b + c) \Delta Z P)}{\partial \Delta Z} = a P.
\]

(4.15)

Apart from the modeling of the convective term this equation is exact if the rates \( a, b \) and \( c \) are assumed to be fixed known quantities.

5. Modeling aspects

In the present analysis we have replaced the direct formulation for the scalar pdf equation for \( Z \) by an indirect formulation for the joint distribution function of \( Z_m \) and \( \Delta Z \). Both are exact as far as the scalar field is concerned. The former is not well-posed and therefore requires ad-hoc modeling of the molecular mixing term. In transported pdf models this modeling is usually based on the assumption of a constant scalar-to-flow time scale ratio. (cf. Pope, 2000). On the contrary, in the present formulation molecular mixing occurs exclusively within the Q1DLs. The independent variables in the present formulation are \( Z_m \) and \( \Delta Z \), where \( Z_m \) represents \( Z \) in a certain way while \( \Delta Z \) captures non-local effects since the Q1DLs may span over a large distance within the turbulent flow. Modeling is required for the mixing rate \( \bar{b} = (b + c)/2 \), the asymmetry coefficient \( (b - c) \) and the strain rate \( a \). In the case of constant density turbulence the statistics of \( a \) are determined entirely by the velocity field, with the mean of \( a \) being proportional to \( \varepsilon/k \) where \( \varepsilon \) is the viscous dissipation and \( k \) is the kinetic energy of turbulence. The influence of the statistics of \( a \) on \( \bar{b} \) and \( (b - c) \) can in principle be determined by solving (2.2) with the use of (2.13) for various initial conditions. Such an approach will, to a certain extend, be problem-dependent. Since the mean of the mixing rate \( \bar{b} \) represents the inverse of the scalar time and \( k/\varepsilon \) represents the flow time, the approach offered here appears somewhat less empirical than the assumption of a constant scalar-to-flow time scale ratio used in current modeling approaches for the scalar pdf \( P_Z \).

Details of the modeling will be addressed in a more complete paper on the subject.

6. Conclusions

By identifying quasi-one-dimensional dissipation layers as key elements we have outlined a non-local theory of turbulent mixing. In this theory molecular mixing and its enhancement by compressive strain occurs exclusively within the local Q1DLs, while their transport by turbulence and their formation and disappearance is described by a pdf transport equation. That equation remains to be modeled. The main assumption of the theory is that the layers are one-dimensional and that they can be parametrized by four parameters, the minimum and the maximum mixture fraction and the mixing rates \( b \) and \( c \).

This has been tested by generating trajectories and by reconstructing the mixture fraction pdf and the conditional scalar dissipation rate from DNS data of Rogers and Moser. The reconstructed scalar pdf \( P_{Z,X} \) shows good agreement with the scalar pdf \( P_Z \) of the starting points of the trajectories. The reconstruction of the scalar dissipation
rate turns out to be quite sensitive to the mixing rate $\hat{b}$ and its dependence on other parameters of the problem.

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