# LEVEL-SET DYNAMICS AND MIXING EFFICIENCY OF PASSIVE AND ACTIVE SCALARS IN DNS AND LES OF TURBULENT MIXING LAYERS

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## ABSTRACT

The mixing efficiency in a turbulent mixing layer is quantified by monitoring the surface-area of level-sets of scalar fields. The Laplace transform is applied to numerically calculate integrals over arbitrary level-sets. The analysis includes both direct and large-eddy simulation and is used to assess the suitability of specific subgrid parameterizations in relation to predicting mixing efficiency. We incorporate several subgrid models in the comparison, e.g. the scale similarity model of Bardina, the dynamic eddy-viscosity model and the dynamic mixed model. For accurate predictions, dynamic models are favored. It is observed that the ratio between LES-filterwidth $\Delta$ and grid-spacing $h$ has a considerable influence; a ratio of four appears suitable. Gravity driven flows can be modeled by 'active' scalar fields which couple to the momentum and energy equations. The significant increase in mixing efficiency due to buoyancy effects is directly quantified.

## INTRODUCTION

In recent years, advances in computational power and numerical methods have brought about the possibility to simulate turbulent fluid motion in all its detail by means of so-called direct numerical simulation (DNS). This approach gives rise to extensive data-bases, e.g. containing large numbers of snapshots of the instantaneous solution which form the raw material for further analysis. In this paper we concentrate on dynamical features of global properties of evolving level-sets in turbulent flow. This information can be used to quantify the changes in complexity of a flow as a function of time and spatial coordinate and can also characterize dominant behavior e.g. in mixing or in dispersive processes. In addition, properties of an evolving interface are of central importance e.g. in combustion and chemistry and in relation to multi-phase flows.

This paper contains three main elements. First, a new method for calculating iso-surface integrals is presented. This method involves Laplace transform (Vervisch et al. 1994), and a new, locally exact, quadrature approach to treat the rapidly oscillating integrals that arise. The surface area of level-sets of scalar fields can be calculated accurately, including contributions arising from very intense and localized turbulent events.

The second main point is related to the use of Large-Eddy Simulation (LES) for the prediction of mixing efficiency. In LES one attempts to predict generic flow features and to obtain

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a smoothed representation of the solution at a fraction of the computational costs associated with DNS. This can only be achieved at the expense of introducing a subgrid-model for the turbulent stresses. Problems which involve details of turbulent mixing, possibly in combination with chemical reactions such as combustion, or turbulent dispersion of polluting agents, may require a more detailed representation of the smallest structures in the flow. This could require extensions of 'traditional' subgrid modeling or numerical treatment. The suitability of present-day subgrid modeling and the appropriate ratio between LES-filterwidth $\Delta$ and grid-spacing $h$ will be considered.

The third main point in this paper involves quantifying the influence of buoyancy effects on mixing efficiency. Gravity currents of heavy fluid which propagate in an environment of lighter fluid are encountered in numerous geophysical applications. Likewise this type of flows arises in many problems related to industrial safety and environmental protection (Härtel et al., 2000). The buoyancy effects on mixing will be quantified by evaluating the surface area of the interface between the 'heavy' and the 'light' fluid, as a function of time. It is shown that buoyancy can lead to significantly enhanced mixing. Depending on the Froude number, a variation in the mixing rate of a factor of about three can readily be obtained.

The organization of this paper is as follows. First we introduce the method to evaluate surface integrals over arbitrary iso-surfaces. Then we formulate the evolution of active and passive scalars and illustrate the global scenario of the flow. Results of DNS and LES predictions of the mixing efficiency of passive scalars will be discussed afterwards. Moreover, we apply the approach to mixing in gravity driven mixing layers. Finally, we will summarize our findings.

## MIXING EFFICIENCY AND ISO-SURFACE INTEGRALS

We concentrate on dynamical features of so-called 'global' variables. The global variable corresponding to a density function $f$ and the level-set $S(a,t)$ is denoted by $I_f(a,t)$. Here $S(a,t)$ is defined by the set where $F(\mathbf{x},t)=a$ for a 'level-function' $F$. The global variable $I_f(a,t)$ is defined as

$$I_f(a,t) = \int_{S(a,t)} dA\ f(\mathbf{x},t)$$

$$= \int_V d\mathbf{x}\ \delta(F(\mathbf{x},t)-a)|\nabla F(\mathbf{x},t)|f(\mathbf{x},t) \quad (1)$$

where $V$ is a fixed and arbitrary volume which encloses the level-set $S(a,t)$. The evolution of $I_f(a,t)$ is governed by

$$\frac{\partial I_f(a,t)}{\partial t} + \frac{\partial}{\partial a}\Big(\int_V d\mathbf{x}\ \delta(F-a) f|\nabla F|\frac{\partial F}{\partial t}\Big) = \int_V d\mathbf{x}\ \delta(F-a)\frac{\partial}{\partial t}(f|\nabla F|) \quad (2)$$

Here we can identify different transport terms. In specific applications, such as the mixing of scalar fields, the present quadrature method allows for an accurate assessment of the magnitude of the various transport mechanisms.

If one wants to evaluate $I_f(a,t)$ as defined in (1) or any of the fluxes in (2) one can use the Laplace transform in order to efficiently deal with the delta-function that arises in the integrand. After some calculation one then arrives at

$$I_f(a,t) = \frac{1}{\pi}\int_0^\infty d\tau\Big(\int_V d\mathbf{x}\, f|\nabla F|e^{-(F-a)} \times \cos(\tau(F-a))\Big) \quad (3)$$

The global variable $I_f(a,t)$ is written as a double integral; one over the volume $V$ and one over the variable $\tau$. If we divide the volume $V$ into a large number of grid-cells $\Omega_{ijk}$ we can split the integral in (3) into integrals over grid-cells which can each be treated with the new, locally exact, quadrature method. Details of this approach will be published elsewhere (Geurts, 2001).

This method to evaluate iso-surface integrals can be adopted to determine the area of the surface separating regions with high values of a scalar field from regions with low values. By monitoring this surface during transitional and turbulent flow in a mixing layer the mixing efficiency $\eta$ can be quantified. We may introduce

$$\eta(a,t) = I(a,t)/I(a,0) \quad (4)$$

to define the amount of 'stretching' of the iso-surface corresponding to $F(\mathbf{x},t)=a$. Here we consider the mixing of two fluids. The region occupied by fluid 'A' or fluid 'B' can be characterized effectively by introducing a scalar field $c$ with values ranging between 0 and 1. We adopt the convention that fluid 'A' corresponds to a value of $c=0$ and fluid 'B' is identified by $c=1$. In the sequel we refer to 'A' as the carrier fluid with density $\rho$ and 'B' the carried fluid with density $\rho_h$ where the subscript '$h$'

denotes 'heavy', which is relevant in case buoyancy effects are included. As a definition of the interface between the two fluids we adopt the value $c = 1/2$ in the rest of this paper. The determination of the surface area of the interface between 'A' and 'B' can be used to quantify the increased complexity of the flow-field during mixing.

## ACTIVE AND PASSIVE SCALARS IN A MIXING LAYER

In many applications, gravity driven currents may arise in which a heavy fluid can propagate in a surrounding lighter fluid under the influence of gravity. The effects of gravity on the flow can be represented through the introduction of source terms in the momentum and energy equations. In particular, using the Boussinesq approximation we have (Gebhart et al., 1979):

$$\partial_t \rho + \partial_j(\rho u_j) = 0$$
$$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) + \partial_i p - \partial_j \sigma_{ij} = -\frac{\alpha \rho c \delta_{i2}}{Fr^2}$$
$$\partial_t e + \partial_j((e+p)u_j) - \partial_j(\sigma_{ij} u_i) + \partial_j q_j = -\frac{\alpha \rho c u_2}{Fr^2}$$

where we introduced the relative density variation parameter $\alpha = (\rho_h - \rho)/\rho$ and the Froude number $Fr = U^*/\sqrt{g^* L^*}$ with $g^*$ the gravitational constant and $U^*$, $L^*$ a reference velocity and length scale respectively. Here, we consider the gravitational force to act in the negative $x_2$ direction and use $\alpha = 1$. Moreover, $\partial_t$ and $\partial_j$ denote partial derivatives with respect to time $t$ and Cartesian coordinate $x_j$ respectively. Also, $\rho$ denotes the density of the 'lighter' fluid, $u_j$ the velocity component in the $x_j$ direction and $\sigma_{ij}$ is the viscous stress tensor defined by $\sigma_{ij} = S_{ij}/Re$ with $Re$ the Reynolds number and $S_{ij}$ the strain rate tensor. Moreover, $p$ is the pressure, $e$ the total energy density and $q_j$ the heat flux vector. For further details see Vreman et al. (1997). Finally, $c$ denotes a scalar field which varies between 0 and 1 and which relates to the local density $\tilde{\rho}$ as $\tilde{\rho} = (1-c)\rho + c\rho_h$. The scalar field $c$ is assumed to evolve according to

$$\partial_t(\rho c) + \partial_j(u_j \rho c) - \frac{1}{Sc}\partial_{jj} c = 0 \qquad (5)$$

where $Sc$ denotes the Schmidt number which characterizes molecular diffusion transport. The scalar field $c$ is convected by the flow field $u_j$ and the finer features of $c$ such as regions of large gradients are smoothed by the action of diffusion effects.

In this paper we identify two types of scalar fields. If the Froude number $Fr$ tends to infinity, we observe that the source terms in the momentum and energy equation reduce to zero. In that case there is only a one-way coupling and the scalar field will be referred to as 'passive'. At finite Froude number the scalar field is seen as 'active' and determines part of the flux of the momentum and energy equation, i.e. there is a two-way coupling.

For illustration purposes, we simulate the compressible three-dimensional temporal mixing layer and use a convective Mach number $M = 0.2$ and a Reynolds number based on upper stream velocity and half the initial vorticity thickness of 50. This is sufficiently high to allow a mixing transition to small scales. The governing equations are solved in a cubic geometry of side $L$. Periodic boundary conditions are imposed in the streamwise ($x_1$) and spanwise ($x_3$) direction, while in the normal ($x_2$) direction the boundaries are free-slip walls. These settings correspond to the simulation as reported in Vreman et al. (1997).

Visualization of the DNS data corresponding to infinite Froude number demonstrates the roll-up of the fundamental instability and successive pairings (figure 1). As can be observed, a highly three-dimensional flow field arises around $t = 80$, yielding a single roller in which the flow exhibits a complex structure, with many regions of positive spanwise vorticity. The dispersion of passive scalar corresponding to this field is considered next.

The initial condition for the scalar field is chosen such that all 'heavy' fluid is located in the upper half of the domain and the 'light' fluid is in the lower half. An example of the evolution of a passive scalar field is shown in figure 2 at a Schmidt number of $Sc = 10$. It is clear that during transition the interface between the two regions rolls up and becomes quite distorted. We also considered a higher Schmidt number of $Sc = 100$; the global features of that simulation correspond to those of figure 2 but many more small scale features remain within the rollers, due to the smaller influence of diffusion. This qualitative impression of increased complexity during transition, will be further quantified in the next sections.

## DNS AND LES OF MIXING OF PASSIVE SCALARS

In this section we first turn to evaluating the mixing efficiency $\eta$ using DNS data. In particular we consider the dependence of $\eta$ on Schmidt

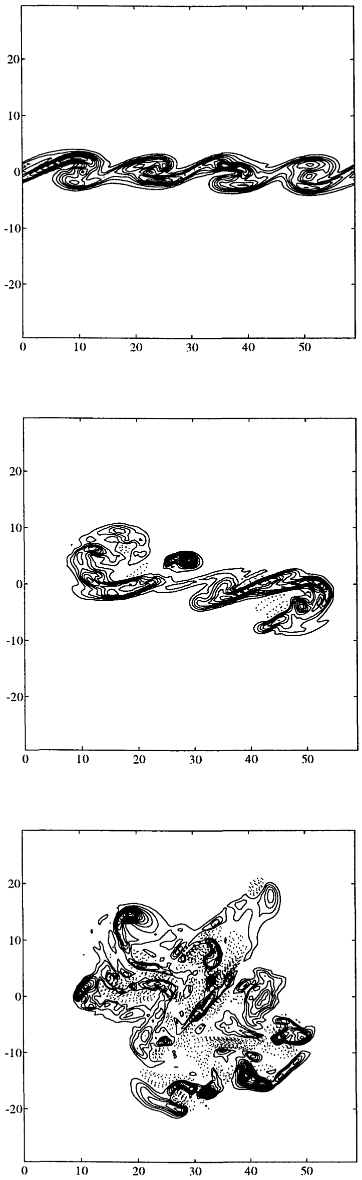


Figure 1: Development of spanwise vorticity in DNS of a temporal mixing layer; from top to bottom $t = 20$, $t = 40$ and $t = 80$.

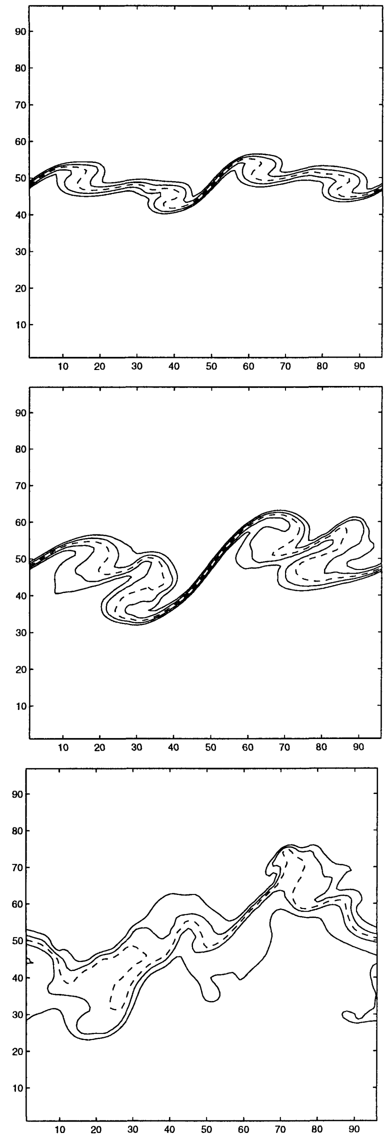


Figure 2: Evolution of passive scalar at Schmidt number $Sc = 10$; from top to bottom; $t = 20$, $t = 40$ and $t = 80$. The initial condition consisted of a layer of level 1 on top of a layer of level 0. The dashed line corresponds to $c = 0.5$, solid contours with $c = 0.3$, 0.4 (generally below) and $c = 0.6$, 0.7 (generally above).

number and investigate the role of the spatial resolution. Subsequently we turn to LES predictions of the mixing efficiency and compare predictions from different subgrid models at different ratios of LES-filterwidth $\Delta$ and grid-spacing $h$.

In figure 3 we have plotted the DNS-prediction of the mixing efficiency for two Schmidt numbers, at various resolutions. We observe that an increase in the Schmidt number corresponds to a strong increase in mixing, as was to be expected. Moreover, although not quite fully resolved, a resolution in the range of $96^3$–$128^3$ appears to capture most of the flow-features quantitatively correctly. Clearly, the larger amount of small scale features that remain at $Sc = 100$ require a higher resolution than needed for $Sc = 10$. Changing the Schmidt number from 10 to 100 results in about a factor of 3 increase in $\eta$. Since the global features of the scalar field are not changed significantly, this increase arises from small scale contributions only.

The sensitive dependence of the mixing efficiency $\eta$ on Schmidt number, i.e. on the amount of small scales that emerge in the passive scalar field, will now be considered in the LES context. For this purpose we follow a traditional LES modeling of the Navier-Stokes equations. The turbulent stress tensor $\tau_{ij} =$

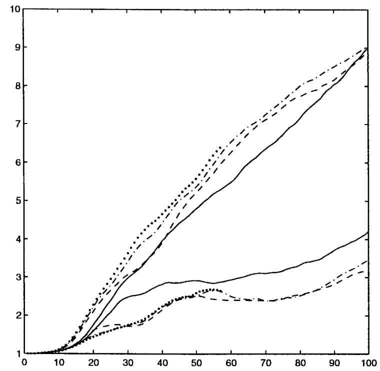

Figure 3: Evolution of surface of $c = 0.5$ level set in DNS at resolution $32^3$ (solid), $64^3$ (dashed), $96^3$ (dash-dotted) and $128^3$ (dotted) at $Sc = 10$ (bottom set) and $Sc = 100$ (upper set of curves).

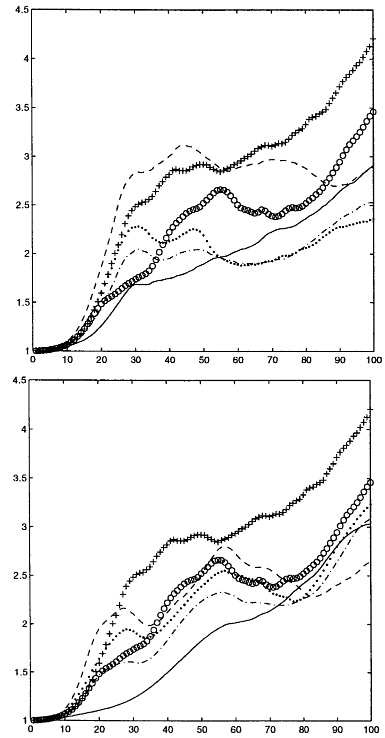

Figure 4: Evolution of surface of $c = 0.5$ level set in LES at resolution $32^3$ (top) and $64^3$ (bottom) using initial condition $A$ and $\Delta = L/16$; Smagorinsky model (solid), Bardina model (dashed), Dynamic model (dash-dotted) and Dynamic mixed model (dotted) at $Sc = 10$. The results without a subgrid model on $32^3$ are shown by $\times$ and the results at $96^3$ by $\circ$.

$\overline{u_i u_j} - \overline{u_i}\ \overline{u_j}$ which arises after spatial filtering of the nonlinear convective fluxes requires modeling. Here we compare four well-known subgrid models: (a) Smagorinsky's model with coefficient equal to 0.1, (b) Bardina's self-similarity model, (c) the dynamic model and (d) the dynamic mixed model combining Bardina's model with a dynamic eddy-viscosity contribution (see Vreman et al., 1997 for further details). We do not consider subgrid modeling of the passive scalar equation. Instead, we focus here on the dispersion of the passive scalar field due to convection in a smoothed velocity field. Specifically, this implies that $u_j$ in (5) is replaced by the Favre averaged velocity field $\tilde{u}_j = \overline{\rho u_j}/\overline{\rho}$. The incorporation of subgrid terms in the scalar equation will be considered elsewhere.

In figure 4 we have plotted the LES-predictions for the mixing efficiency. In all these simulations we kept the LES-filterwidth constant; $\Delta = L/16$. Next to the specific subgrid model, the numerical treatment can play a large role in LES. To investigate this in relation to $\eta$, we consider two different numerical settings. In the first, we use a grid with $32^3$ grid cells, which implies that the LES-filterwidth $\Delta$ is covered by two grid-cells, i.e. $\Delta/h = 2$. In the second case, we use $64^3$ grid-cells and consequently $\Delta/h = 4$. The second case corresponds to reduced numerical discretization errors, while the amount of detail that is retained in the velocity field is the same for the two settings. There is a considerable difference in the predictions of $\eta$ as can readily be inferred by comparing the top and bottom plots in figure 4. We notice that the use of Bardina's scale similarity model gives rise to an over prediction of $\eta$, in particular in combination with insufficient subgrid resolution. Moreover, the use of Smagorinsky's model, even at a reduced value of the coefficient of 0.1, is seen to lead to too low values of $\eta$ for small times, corresponding to too much dissipation arising from this subgrid model. The dynamic models perform roughly comparable, with a striking improvement in the long-term prediction of both models in case sufficient subgrid resolution is used. The dynamic mixed model appears to give predictions for $\eta$ which are closest to the unfiltered DNS results.

## MIXING ENHANCEMENT DUE TO BUOYANCY

In the previous section we showed that the determination of the surface area of the interface which separates two regions of fluid, can be used to quantify the increased complexity of the flow-field, as a function of time or physical parameters. This concerned passive scalar fields. In case gravity acts on the two fluids, the specific spatial distribution determines the buoyancy contributions to the evolution of the momentum and energy. In this section we consider the effects of unstable stratification on the mixing efficiency $\eta$.

The evolution of the active scalar field at

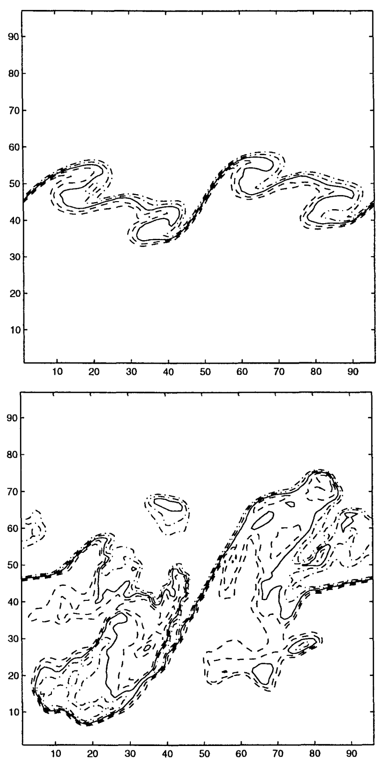


Figure 5: Evolution of active scalar at Schmidt number $Sc = 10$; from top to bottom; $t = 20$ and $t = 40$ and Froude-number equal to 2. The solid line corresponds to $c = 0.5$, dashed contours with $c = 0.3,\ 0.4$ and dash-dotted contours with $c = 0.6,\ 0.7$.

$Fr = 2$ is shown in figure 5. We use the same Schmidt number as in figure 2. The global features of the scalar field at $t = 20$ can still be compared well with the corresponding result for passive scalars. However, in the further development, we notice that the active scalar develops a larger interface much more rapidly. This difference is further illustrated in figure 6 where we compare the mixing efficiencies at three different Froude numbers. We observe that $Fr = 5$ provides mixing efficiencies which differ about 30 percent from the passive scalar case. Decreasing the Froude number to two gives a large increase in the mixing-rate of about a factor of three.

## CONCLUDING REMARKS

We developed a new method for calculating the surface of arbitrary iso-surfaces. This method was used to quantify the mixing that arises during transitional and turbulent flow in a temporal mixing layer. Accurate predictions of the mixing efficiency can be obtained. Moreover, the dependence of mixing efficiency on physical parameters can readily be quantified.

The amount of small-scale features in the passive scalar field obviously plays a considerable role in the mixing. Despite this, the

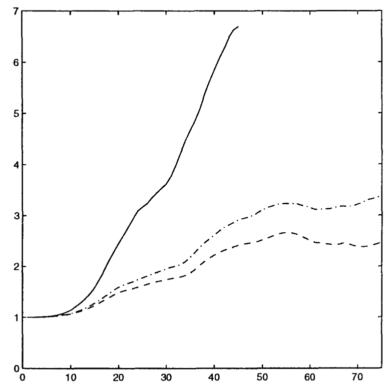


Figure 6: Evolution of surface of $c = 0.5$ level set at resolution $96^3$: $Fr = 2$ (solid), $Fr = 5$ (dash-dotted) and $Fr = \infty$ (dashed).

evolution of passive scalar fields due to convection in a smoothed LES-velocity field, gives rise to mixing efficiencies which compare well with those arising from DNS. The use of traditional subgrid models for the turbulent stress tensor appears sufficient. It was observed, however, that the role of the numerical scheme is quite pronounced and a ratio between LES-filterwidth and grid-spacing of about four was seen to considerably improve the predictions. This will be further investigated in the future.

Finally, we applied the surface integration method to determine the effect of buoyancy on mixing efficiency. At sufficiently low Froude numbers a strong increase in mixing efficiency arises from an initially unstably stratified configuration.

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