

RELIABILITY OF LARGE-EDDY SIMULATION OF BUOYANCY-DRIVEN TURBULENT MIXING

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Abstract. *The effects of unstable stratification on the turbulent transport in a shear layer are quantified by monitoring global geometric properties of constant density surfaces, such as their area and wrinkling. The flow is simulated using direct and large-eddy simulation, in which regularization modeling for the sub-grid scales in the momentum and the scalar equations is adopted and compared to dynamic sub-grid modeling. We establish the accuracy of the Leray regularization approach for the fluid flow and the scalar mixing. The LANS- α model was found to lead to an overestimation of the small scales, particularly at coarse grids. Predictions based on dynamic models were found to be comparable to the Leray model, but require more computational effort and do not provide a systematic framework for deriving sub-filter closure for complex problems.*

1 INTRODUCTION

We study gravity-driven turbulent mixing in a shear layer using large-eddy simulation. The dynamics of the sub-filter scales is derived systematically from an underlying regularization principle. In particular, we consider mixing of initially unstably stratified fluid layers using Leray and NS- α regularization. This configuration derives its motivation from transport processes over urban areas, or may be related to underwater pollution release in rivers, and, to geo-thermal activity in seas.

Regularization principles can be applied systematically to both the momentum equation and the equations governing the transport of scalar quantities. These principles provide a framework for deriving closure of the filtered nonlinear terms in large-eddy simulation. The dynamic range of the flow and the scalar fields, such as temperature and density, is determined by the Reynolds number (Re) of the dispersing flow, the Froude number (Fr) coupling the scalar field to the momentum equation and the Schmidt number (Sc) of the scalar quantity. These dimensionless parameters have a considerable influence

on the dynamics - we will investigate the mixing progress using direct numerical simulation. This provides a basis for assessing the quality of large-eddy modeling. We focus in particular on the limit of high Schmidt numbers at which the scalar transport generates scales that are much smaller than those of the turbulent momentum transport.

The regularization principles allow to systematically derive closure models for both the Navier-Stokes equations and the species equations in a spatially filtered large-eddy simulation context. This systematic approach is confronted with dynamic eddy-viscosity and eddy-diffusivity modeling. To assess the quality of the different sub-filter closure strategies, we monitor the development of large and small scales as the mixing progresses. The simulations start from an initially fully separated configuration in which a heavy fluid layer is placed on top of a lighter one. We compare the mixing efficiency as obtained from direct numerical simulation with the large-eddy simulations. We monitor fluid properties, such as the thickness of the mixed layer and the kinetic energy, as well as scalar quantities that quantify the interface between the heavy and lighter fluid domains. Of the regularization principles, we find the Leray approach robust and providing accurate capturing of momentum and scalar transport. The LANS- α model is found to produce too many small scales, particularly when a coarse grid is used. Phenomenological models based on the dynamic eddy-viscosity and eddy-diffusivity model were found to agree well with Leray, albeit requiring higher computational effort.

The organization of this paper is as follows. In Section 2 we discuss mixing under the influence of unstable stratification and present results of direct numerical simulation. The large-eddy approach to this flow problem is presented in Section 3 and simulation results based on regularization and eddy-viscosity modeling are shown in Section 4. Finally, concluding remarks are provided in Section 5.

2 Mixing due to unstable stratification

In this section we will present the mathematical model for unstably stratified turbulence and illustrate the evolution of the scalar mixing with direct numerical simulation results.

We consider the flow of an incompressible fluid, subject to the effect of gravity acting on density differences in the fluid. In non-dimensional form the governing equations can be written as [1]:

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \frac{1}{Re} \nabla^2 \mathbf{u} = \frac{1}{Fr^2} (c \mathbf{e}_g) \quad (2)$$

where \mathbf{u} denotes the velocity field, p the pressure, ∂_t denotes partial differentiation with respect to time t , and $\nabla = [\partial_x, \partial_y, \partial_z]$ is the vector differentiation operator with respect to the Cartesian x , y and z directions. The direction of the external gravity field is denoted by \mathbf{e}_g - it will be taken in the negative z direction. The flow dynamics is controlled by the Reynolds number $Re = U\ell/\nu$ and the Froude number $Fr = U/\sqrt{g\ell}$ in terms of reference scales for velocity (U), length (ℓ), kinematic viscosity (ν) and gravity (g). The effect of

stratification is represented by the coupling of the scalar quantity c to the momentum equation. The evolution of the scalar is governed by an advection-diffusion equation:

$$\partial_t c + \mathbf{u} \cdot \nabla c - \frac{1}{ReSc} \nabla^2 c = 0 \quad (3)$$

in which the Schmidt number Sc represents the strength of the diffusive transport. If $Sc > 1$ small scale structures in the scalar field will be considerably smaller than the smallest eddies in the fluid flow. The flow in an unstably stratified temporal mixing layer [2] is simulated in a cubic volume of size L^3 with $L = 59$, starting from an initial condition with a heavy fluid layer ($c = 1$) on top of a lighter layer ($c = 0$). We adopt periodic conditions in the horizontal x and y directions and free slip conditions in the far-field of the vertical z direction. As a result of the mixing layer configuration, the fluid layers shear over each other, during which time the effects of gravity express themselves by transporting the heavier fluid down and, because of incompressibility, pushing the lighter fluid up. In total, these basic interactions give rise to a strongly anisotropic turbulent flow that we will discuss in more detail next.

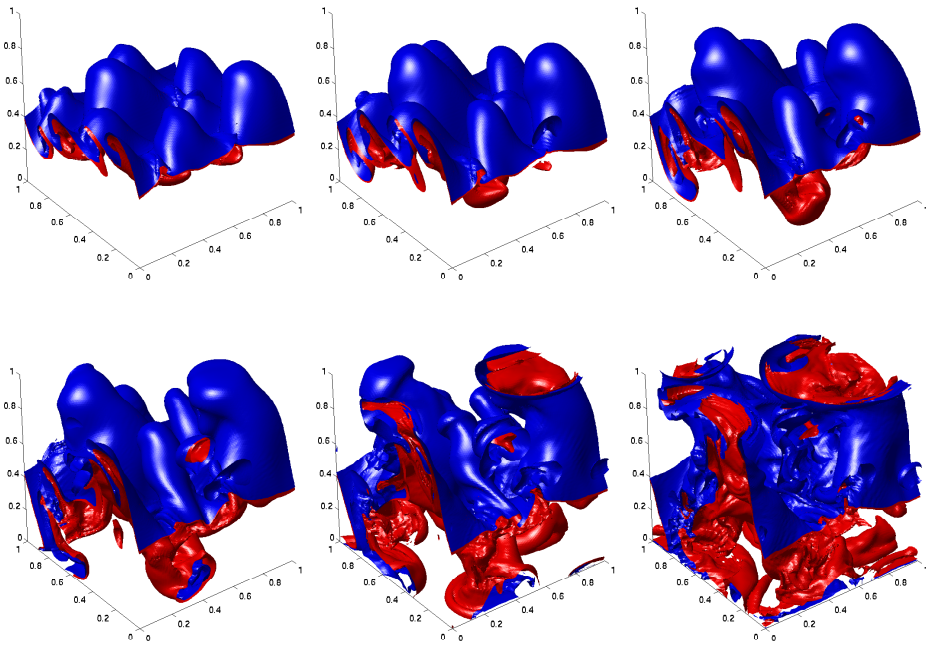


Figure 1: Development of iso-surfaces of the scalar c at $c = 0.55$ (blue) and $c = 0.45$ (red) at $t = 30, \dots, 55$ with steps of 5, counting from upper-left to lower-right. We adopted $Fr = 2$, $Re = 50$ and $Sc = 10$ at a resolution of 192^3 .

The development of turbulent mixing in an unstably stratified configuration is simulated using an energy-conserving, skew-symmetric discretization of the convective fluxes

and a positive definite discretization of the viscous terms [3]. This method is stable on any resolution and does not rely on the addition of artificial dissipation to stabilize a simulation. In Fig. 1 we display the development of iso-surfaces of the scalar at a characteristic setting of the parameters $Fr = 2$, $Re = 50$ and $Sc = 10$, corresponding to strong effects of gravity, emphasizing the development of small scales in the scalar, at flow conditions where the standard mixing layer shows a rapid transition to turbulence. During the initial stages the flow instabilities develop a pattern of interlocking fluid ‘fingers’ that penetrate from the heavy to the light layer, and vice versa. Further into the development of the flow, the gravitational effects show strong vertical structuring and the emergence of many small scale structures. This is visualized with slices through the scalar field as shown in Fig. 2 in which the emergence of plume structures is clearly visible.

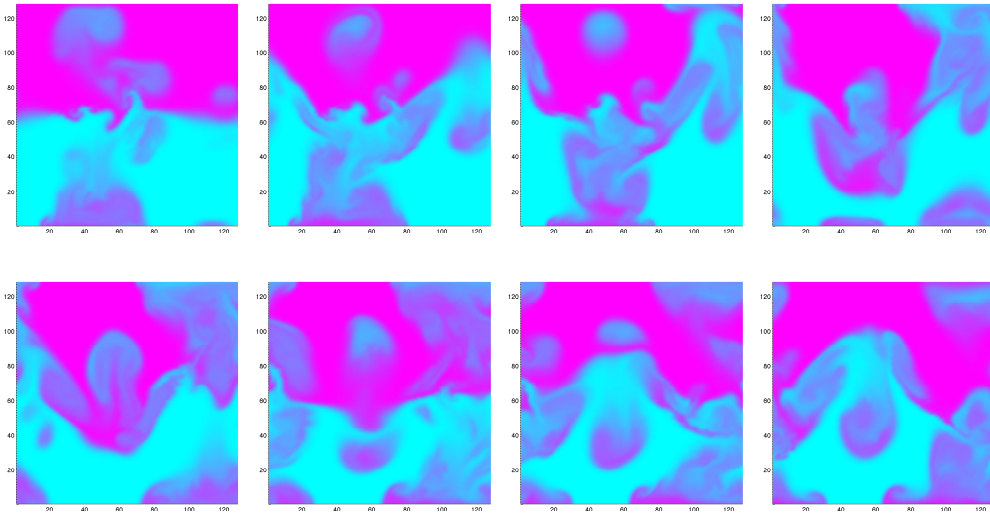


Figure 2: Slices at constant x through the scalar field at $t = 50$ displaying the detailed structure of the solution, including plume structures. We used a resolution 128^3 at $Re = 50$, $Fr = 2$ and $Sc = 10$.

To quantify the development of the unstably stratified mixing layer we evaluated the momentum thickness θ and the kinetic energy E , defined as

$$\theta = \int_{-L/2}^{L/2} \frac{1}{4}(1-u)(u+1) dz \quad ; \quad E = \int_{\Omega} \frac{1}{2} \mathbf{u} \cdot \mathbf{u} d\Omega \quad (4)$$

where u denotes the x -component of the velocity \mathbf{u} , and, the integration extends over the z -direction or the entire domain Ω . In Fig. 3 we compare results at three coarse resolutions to appreciate the convergence of the predictions. The grid-independent momentum thickness is approximated accurately already at a resolution of 64^3 while the resolution of the kinetic energy requires a slightly higher resolution. We notice that the kinetic energy shows oscillations on top of a general slow evolution - this is related to the confinement

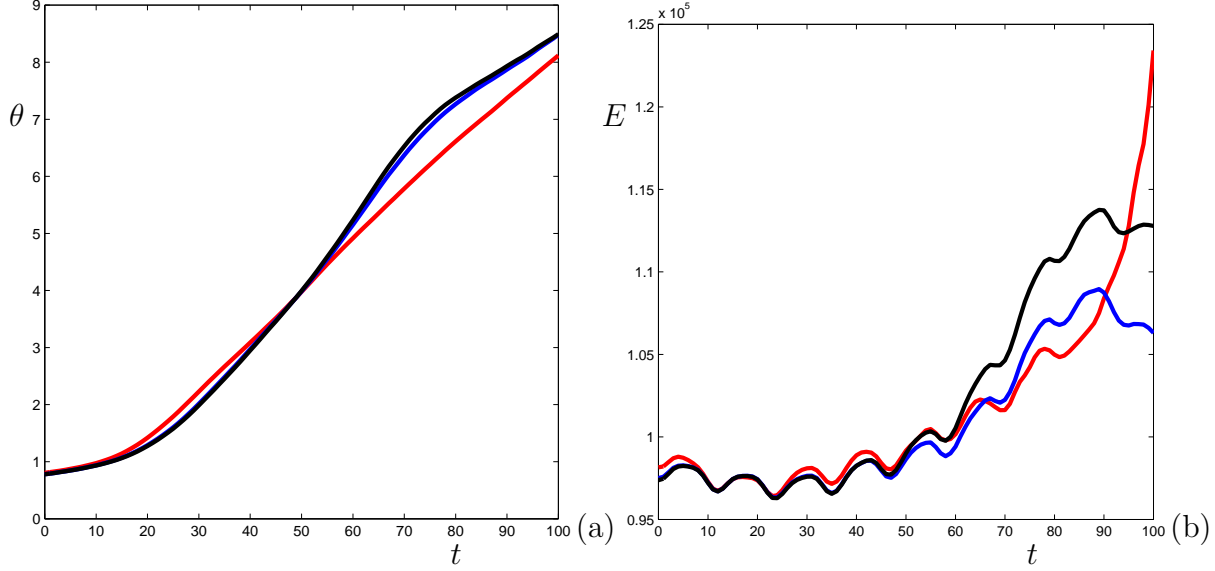


Figure 3: Evolution of the momentum thickness θ (a) and the kinetic energy E (b) in case $Fr = 4$, $Re = 50$ and $Sc = 10$, comparing results at different resolutions N^3 : $N = 32$ (red), $N = 64$ (blue) and $N = 96$ (black).

arising from the free-slip conditions adopted in the far field. These data present a point of reference for the assessment of large-eddy simulation momentarily.

The small-scale structure that develops in the scalar field can be characterized in various ways. We consider the evolution of the $c = 1/2$ iso-surface in more detail. This iso-surface is characteristic for the interface between the heavy and the light fluid. In particular, we measure the surface area A and wrinkling W of this iso-surface. These are defined in terms of integrals over the iso-surface. For a density f we define the integral quantity I as

$$I = \int_{S(a,t)} dA f(\mathbf{x}, t) = \int_{\Omega} d\mathbf{x} \delta(c(\mathbf{x}, t) - a) |\nabla c(\mathbf{x}, t)| f(\mathbf{x}, t) \quad (5)$$

where $S(a, t) = \{\mathbf{x} \in \mathbb{R}^3 \mid c(\mathbf{x}, t) = a\} \subset \Omega$. We use the value $a = 1/2$ in this paper and evaluate the integrals with a method developed in [4], based on Laplace transforms. The surface-area is obtained by selecting $f = 1$ while the wrinkling is defined by selecting $f = \nabla \cdot \mathbf{n}$ in which the normal is given by $\mathbf{n} = \nabla c / |\nabla c|$. In Fig. 4 we collected the evolution of A and W at $Sc = 10$ and a range of Froude numbers Fr . In case the Froude number increases, the growth of the surface area is reduced and delayed; this is consistent with the reduced influence of gravity in this case. Effectively, for $Fr \gtrsim 10$ the influence of gravity can be neglected. The wrinkling displays two characteristic stages of development; in the early stages a linear time-dependence is observed while a behavior between t^3 (at low Fr) and t^4 (at high Fr) is observed. These results provide additional points of reference for testing the LES models.

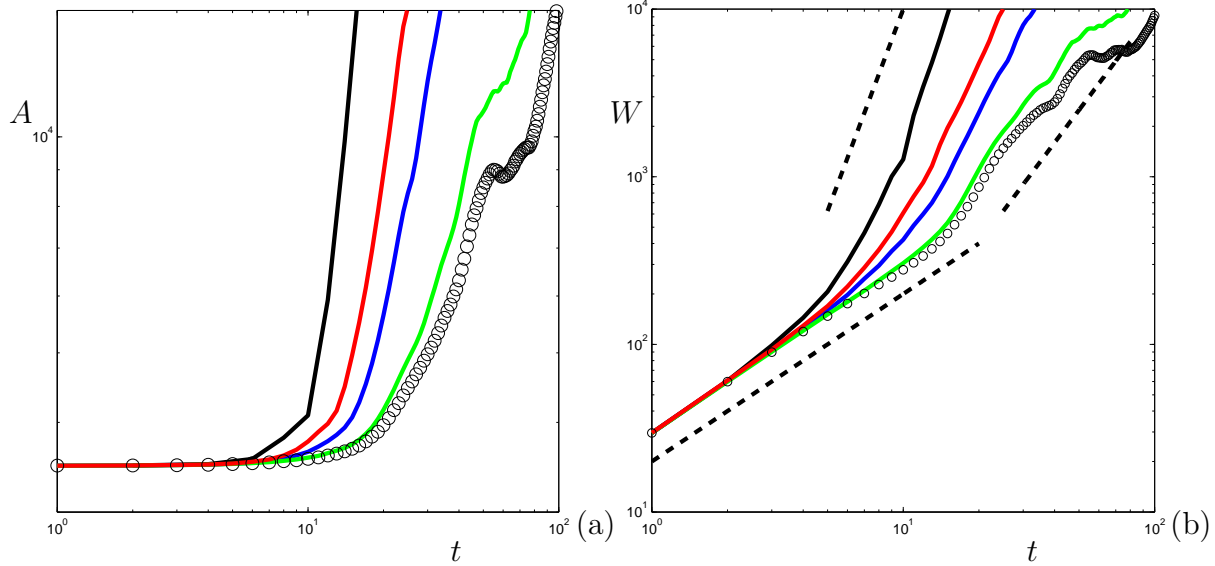


Figure 4: Evolution of the surface area A (a) and wrinkling W (b) in case $Re = 50$, $Sc = 10$ and $Fr = 1, 3/2, 2, 4, 8$ shown in solid black, red, blue, green and with markers respectively.

3 Large-eddy modeling of turbulent stratified mixing

In this section we briefly review the large-eddy approach to spatially filtered turbulence simulations. We discuss the closure of the momentum and the species equations. Filtering the Navier-Stokes equations requires a low-pass spatial filter. For incompressible fluids with stratification included the application of the filter to the continuity and Navier-Stokes equations leads to:

$$\partial_j \bar{u}_j = 0, \quad \text{and} \quad \partial_t \bar{u}_i + \partial_j (\bar{u}_j \bar{u}_i) + \partial_i \bar{p} - \frac{1}{Re} \partial_{jj} \bar{u}_i = -\partial_j (\overline{u_i u_j} - \bar{u}_j \bar{u}_i) - \frac{1}{Fr^2} \bar{c} \delta_{iz} \quad (6)$$

where $\delta_{iz} = 1$ if $i = z$ and 0 otherwise. In formulation (6) of the LES-template [1] we recognize the application of the Navier-Stokes operator to the filtered solution $\{\bar{u}_j, \bar{p}\}$ on the left-hand side. On the right-hand side, the terms expressing the central closure problem and filtered stratification are collected. The problem is to express the divergence of the turbulent stress tensor $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$ in terms of the filtered solution alone. The scalar field does not require modeling, as far as the contribution to the momentum equation is concerned.

Much of turbulence phenomenology is captured in the Kolmogorov picture, in which kinetic energy cascades in an average sense through an inertial range toward ever smaller scales, until its flow features are sufficiently localized that they may be effectively dissipated by viscosity. The continuous cascading of energy through the inertial range is often represented by an “extra” eddy-viscosity contribution. This may yield a computational model that at least retains large-scale information in the filtered solution. Dissipation of

turbulent kinetic energy was first parameterized by using the Smagorinsky model [5] in which one approximates:

$$\tau_{ij} \rightarrow m_{ij}^S = -(C_S \Delta)^2 |S| S_{ij} \quad (7)$$

where C_S denotes Smagorinsky's constant, $S_{ij} = \partial_i \bar{u}_j + \partial_j \bar{u}_i$ is the rate of strain tensor and $|S|^2 = S_{ij} S_{ij}$ is its magnitude. The Smagorinsky model often leads to excessive dissipation, especially near solid walls and in laminar flows with large gradients. This may even hinder a modeled flow from going through a complete transition to turbulence [2]. The central problem that now arises is how the eddy coefficient should be specified in accordance with the evolving flow. A well-known way to approach this without unduly introducing ad hoc parameters is based on Germano's identity [?] which provides the basis for the dynamic sub-grid modeling procedure. For further details we refer to [1].

Dynamic sub-grid models have contributed in many ways to the understanding of turbulent flow in complex situations. However, dynamic models are also known to be hampered by a number of drawbacks. First, the dynamic procedure is quite expensive in view of the relatively large number of additional explicit filter operations that need to be included. Moreover, the implementation contains various *ad hoc* elements or inaccurate assumptions such as the independence of the dynamic coefficient on the filter-level, or the well-known 'clipping' of negative eddy-viscosity, required to ensure stability of a simulation. The achieved accuracy in actual simulations remains quite limited, e.g., due to shortcomings in the assumed base models. Since the dynamic approach does not contain external parameters other than the ratio between the width of the explicit test-filter and the basic LES filter, there is no chance of improving the predictions by 'tinkering' with parameters. Finally, an extension to flows involving complex physics and/or developing in complex flow-domains is difficult since no systematic framework exists for this purpose. For these reasons, an alternative modeling approach is summoned and we turn to the recently proposed regularization modeling ([7]) next.

We consider two regularization principles for the Navier-Stokes equations and identify the associated sub-grid models in case the basic filter L has a formal inverse L^{-1} [7, 8]. We consider Leray regularization [?] and the Lagrangian averaged Navier-Stokes- α (LANS- α) approach [9]. In Leray regularization, one alters the convective fluxes into $\bar{u}_j \partial_j u_i$, i.e., the solution \mathbf{u} is convected with a smoothed velocity $\bar{\mathbf{u}}$. Consequently, the nonlinear effects are reduced by an amount governed by the smoothing properties of the filter operation, L . The governing Leray equations are [?, ?]

$$\partial_j \bar{u}_j = 0 \quad ; \quad \partial_t u_i + \bar{u}_j \partial_j u_i + \partial_i p - \frac{1}{Re} \Delta u_i = 0 \quad (8)$$

Leray solutions possess global existence and uniqueness with proper smoothness and boundedness, whose demonstration depends on the balance equation for $\int |\mathbf{u}|^2 d^3x$. Based on the Leray equations (8) we may eliminate \mathbf{u} by assuming $\bar{\mathbf{u}} = L(\mathbf{u})$ and $\mathbf{u} = L^{-1}(\bar{\mathbf{u}})$. We may derive the Leray model in terms of the LES template as:

$$\partial_t \bar{u}_i + \partial_j (\bar{u}_j \bar{u}_i) + \partial_i \bar{p} - \frac{1}{Re} \Delta \bar{u}_i = -\partial_j (m_{ij}^L) \quad (9)$$

where the Leray model m_{ij}^L involves both L and its inverse and may be expressed as:

$$m_{ij}^L = L\left(\overline{u_j L^{-1}(\overline{u_i})}\right) - \overline{u_j u_i} = \overline{\overline{u_j u_i}} - \overline{u_j u_i} \quad (10)$$

The reconstructed solution u_i is found from any formal or approximate inversion L^{-1} . For this purpose one may use a number of methods, e.g., polynomial inversion [?], geometric series expansions [?] or exact numerical inversion of Simpson top-hat filtering [?].

A regularization principle which additionally possesses correct circulation properties may be obtained by starting from the following Kelvin theorem:

$$\frac{d}{dt} \oint_{\Gamma(\mathbf{u})} u_j dx_j - \frac{1}{Re} \oint_{\Gamma(\mathbf{u})} \Delta u_j dx_j = 0 \quad (11)$$

where $\Gamma(\mathbf{u})$ is a closed fluid loop moving with the Eulerian velocity \mathbf{u} . The unfiltered Navier-Stokes equations may be derived from (11) [9, 1]. This provides some of the inspiration to arrive at an alternative regularization principle for Navier-Stokes turbulence [9]; in (11) we replace $\Gamma(\mathbf{u})$ by $\Gamma(\overline{\mathbf{u}})$; so the material loop Γ moves with the filtered transport velocity. From this filtered Kelvin principle, we may obtain the implied sub-grid model:

$$\partial_t \overline{u_i} + \partial_j (\overline{u_j \overline{u_i}}) + \partial_i \overline{p} - \frac{1}{Re} \Delta \overline{u_i} = -\partial_j \left(\overline{\overline{u_j u_i}} - \overline{u_j \overline{u_i}} \right) - \frac{1}{2} \left(\overline{u_j \partial_i \overline{u_j}} - \overline{\overline{u_j \partial_i u_j}} \right) \quad (12)$$

We observe that the Leray model (10) reappears as part of the implied LANS- α sub-grid model on the right-hand side of (12). Compared to the Leray model, the additional second term in the LANS- α model takes care of recovering the Kelvin circulation theorem for the smoothed solution. This formulation is given in terms of a general filter L and its inverse.

For the scalar that is transported in a solenoidal velocity field $\partial_j u_j = 0$ we concentrate on the advection part:

$$\partial_t c + u_j \partial_j c = 0 \quad (13)$$

After spatial filtering we obtain:

$$\partial_t \overline{c} + \overline{u_j \partial_j c} = \partial_t \overline{c} + \overline{u_j \partial_j \overline{c}} + \left(\overline{u_j \partial_j c} - \overline{u_j \partial_j \overline{c}} \right) = \partial_t \overline{c} + \overline{u_j \partial_j \overline{c}} + \partial_j \zeta_j = 0 \quad (14)$$

where $\zeta_j = \overline{u_j c} - \overline{u_j} \overline{c}$. Motivated by the Leray approach we start with

$$\partial_t c + \overline{u_j} \partial_j c = 0 \quad (15)$$

As above for the momentum equation, this allows to derive the LES template:

$$\partial_t \overline{c} + \overline{u_j} \partial_j \overline{c} + \partial_j \zeta_j^L = 0 \quad (16)$$

from which we can read the implied scalar sub-filter model:

$$\zeta_j^L = L\left(\overline{u}_j L^{-1}(\overline{c})\right) - \overline{u}_j \overline{c} = \overline{\overline{u}_j c} - \overline{u}_j \overline{c} \quad (17)$$

This model requires an approximate inversion of the filter to recover c that occurs here. The LANS- α model will also be complemented with this Leray model for the scalar transport.

In the next section we consider the performance of the sub-filter models in simulations of stratified turbulent mixing.

4 Regularization prediction of stratified mixing

In this section we present some simulation results regarding the capturing of small-scale mixing by regularization models in LES. We consider mean flow properties and characteristics of the small-scale mixing.

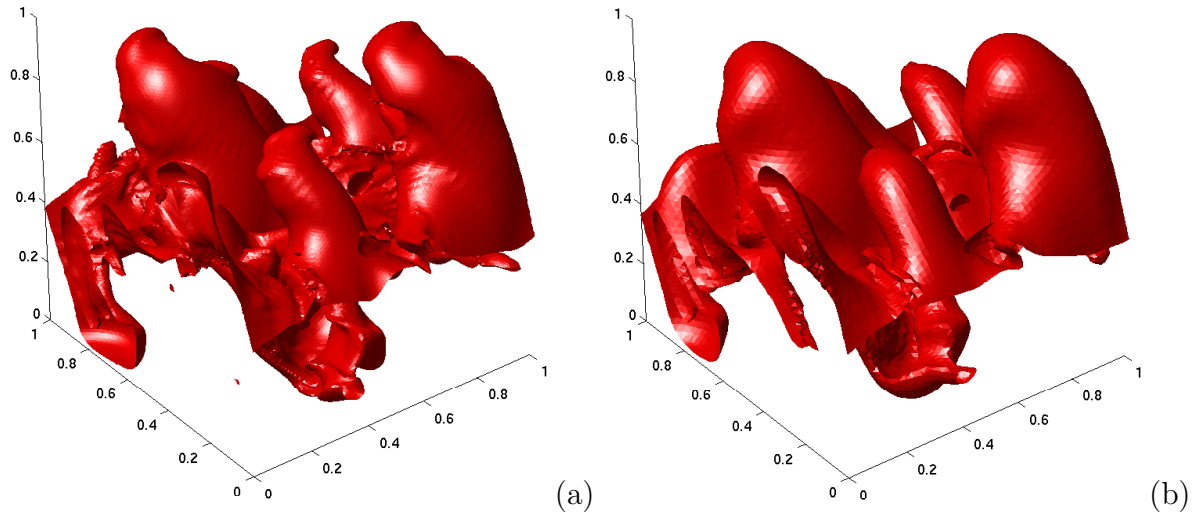


Figure 5: Snapshot of the $c = 1/2$ iso-surface at $t = 40$, comparing DNS (a) with Leray LES (b) predictions at $Re = 50$, $Fr = 2$ and $Sc = 10$. The filter-width $\Delta = \ell/16$.

The development of the instantaneous scalar field is generally well captured by the Leray and dynamic sub-filter models. This is illustrated in Fig. 5 in which we compare instantaneous DNS and Leray LES results for the scalar field at a characteristic time $t = 40$. We notice the clear global resemblance, with the LES prediction lacking the smaller details of the iso-surface wrinkling. This is consistent with the use of a fixed filter-width $\Delta = \ell/16$. This global correspondence will next be complemented with predictions of the mixing layer thickness and the kinetic energy. These are collected in Fig. 6 for

the case $Fr = 4$. We compare DNS data with Leray and dynamic model predictions. The general correspondence for the momentum thickness is very close; even without sub-filter model this quantity can be predicted quite well. The sensitivity of the resolved kinetic energy is seen to be much stronger. We notice that the Leray model provides considerably higher levels of resolved kinetic energy, but still less than observed in the DNS. The improvement relative to the dynamic model is quite considerable. We also studied the use of the LANS- α model. On coarse meshes with $\alpha < h$ the simulations were found to become unstable. At higher resolutions, the results agreed well with Leray predictions.

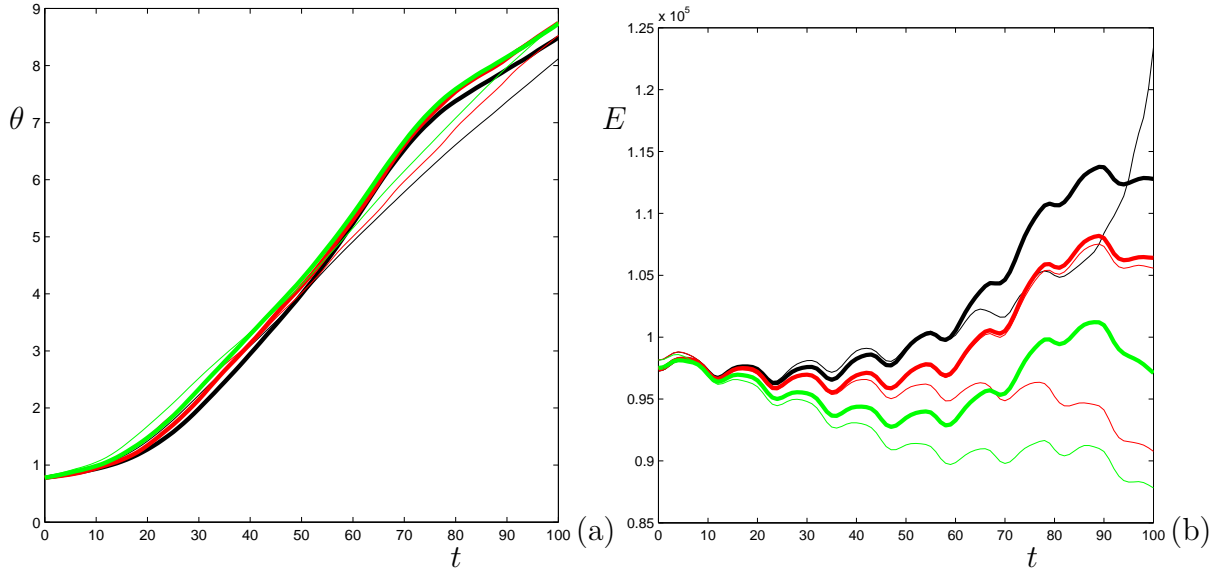


Figure 6: Evolution of the momentum thickness θ (a) and the kinetic energy E (b) in case $Fr = 4$, $Re = 50$ and $Sc = 10$, comparing results of LES with $\Delta = \ell/16$ for the Leray (red) and the dynamic (green) sub-filter model. We use different resolutions N^3 : $N = 32$ (thin), $N = 64$ (thin) and $N = 96$ (thick).

The prediction of small scale mixing features using LES is illustrated in Fig. 7. We compare the evolution of the surface area and wrinkling of the $c = 1/2$ iso-surface, representing the ‘interface’ between the heavy and light layers. At $Fr = 2$ we notice that all LES compare almost equally well for the surface-area with a slight preference for the Leray model. This preference is more outspoken when turning to the wrinkling - we observe that the overall agreement between the DNS and the Leray results is closest among the models studied. The fact that merely adhering to a regularization principle is no guarantee for accurate results is illustrated by the LANS- α model which is found to exaggerate small scales. This was also reported elsewhere [10]. The dynamic model is seen to be roughly comparable to, but slightly less accurate than, the Leray model.

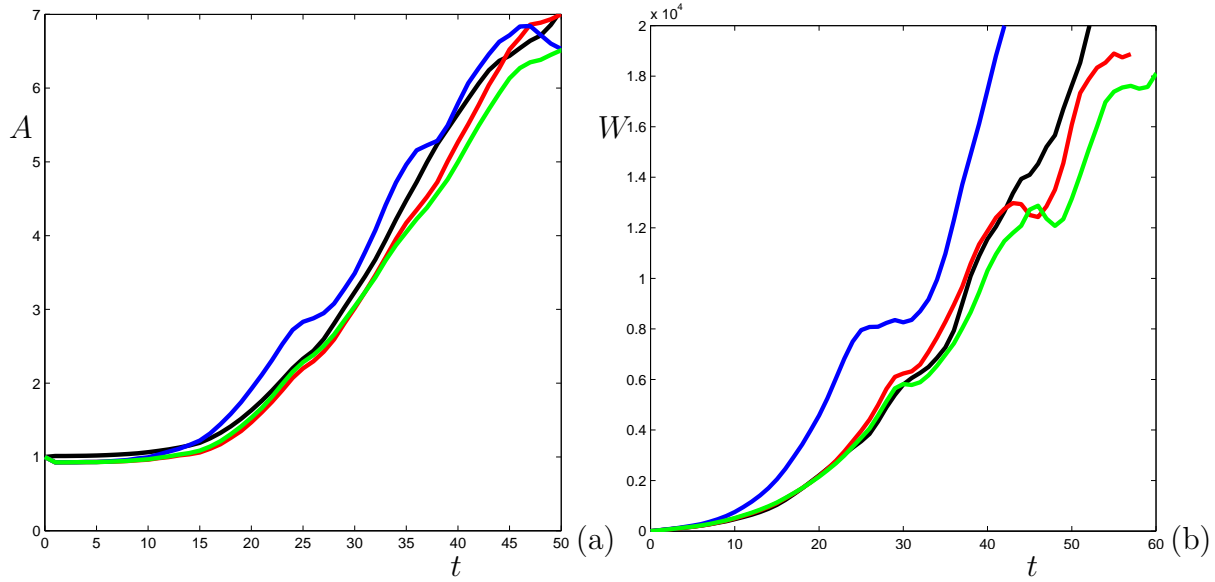


Figure 7: Evolution of the surface area A (a) and wrinkling W (b) in case $Re = 50$, $Sc = 10$ and $Fr = 2$ for DNS (black), Leray (red), LANS- α (blue) and the dynamic model (green).

5 Concluding remarks

We presented large-eddy simulations of unstably stratified turbulent mixing, based on regularization models for the turbulent stress tensor and the scalar field. It was shown that robust and accurate representations of the small-scale turbulence were obtained when the Leray regularization model was adopted for the momentum and the scalar equation. This regularization approach provides a systematic framework for deriving sub-filter closures. The use of the dynamic eddy-viscosity model was found to yield LES results that were quite comparable with those obtained on the basis of the Leray model. However, in this case the evaluation of the model is more complex, requires more computational effort and lacks a systematic background, particularly for more complex flow domains. This general impression was substantiated with predictions for the fluid flow, e.g., the thickness of the mixed layer and the resolved kinetic energy, and predictions for the scalar mixing, e.g., surface-area and wrinkling of the interface between the heavy and the lighter fluid domains. The LES predictions were found to capture the dependence of the turbulent mixing efficiency on the Froude number quite well. The use of the LANS- α model was found to lead to exaggerated small scale contributions. Moreover, at coarse resolutions simulations based on this model were found to become unstable.

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