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ENVIRONMENTAL STRATIFIED FLOWS

EDITED BY

VINCENZO ARMENIO
SUTANU SARKAR

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ENVIRONMENTAL STRATIFIED FLOWS

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PREFACE

Stratified flows, common in environmental and geophysical applications, are characterized by the variation of fluid density in the vertical direction that can result in qualitative and quantitative modifications of the flow patterns by buoyancy . Unstable stratification (dense water/air above light water/air) increases the vertical mixing by generation of convective cells while stable stratification generally suppresses vertical mixing of mass and momentum. Even so, a stably stratified fluid can support internal waves, instabilities and turbulence that play a critical role in transport and mixing.

The ocean is predominantly subject to stable stratification which, under external excitation, supports an environment of internal waves which may then break and generate turbulence. Wind forcing, currents and convective plumes are other sources of turbulence in the ocean. In the ocean, stratified turbulence mediates the upward transport of bottom water, nutrients, chemical and biological species, and pollutants. In the atmosphere, stratification affects the transport of pollutants released at ground level, a critical problem being the thermal inversion in urban areas that causes the stagnation of pollutants and small particulate (PM2.5 to PM10) in the lower part of the atmospheric boundary layer. In buildings, stratification governs the circulation of air and heat in natural ventilation systems. Stratification plays a key role in determining the environmental and human consequences of accidents such as the release of gases into the atmosphere, fires in urban areas and wildland, and oil spills in the ocean. In industrial applications, the presence of a heavier phase that settles to the bottom in a mixture introduces stratification and consequent buoyancy effects on the flow. In hydraulic applications, a river that merges into the ocean basin tends to give rise to an interface between light fresh water sliding and spreading over the salty sea water so that the ensuing transport is very different from that in neutrally buoyant flow. The above-mentioned examples show that the analysis of stratified flows is of broad interest in geophysical, industrial and environmental applications.

The main objective of the current volume is to provide insight into the fluid mechanics of stratified flows with particular emphasis on turbulence and internal waves. The volume is designed for doctoral students as well as experienced researchers in engineering, geophysics, applied mathematics and physics, who are interested in broadening their knowledge in the area of stratified flows. The material spans basic concepts to recent advances in theoretical, numerical and experimental techniques. The volume is composed of four chapters. Chapter 1 by V. Armenio contains a brief description of turbulence together with some basic mathematical tools. The governing equations are introduced and recent algorithms *for the numerical simulation of stratified flow are presented. Some insights on modeling stratified flows via large eddy simulation are given. Finally, a brief description of recent numerical results regarding stratified flows over topography are shown, in the contest of both atmospheric and ocean applications. Chapter 2 by C. Staquet deals with some basic notions on stably-stratified flows before focusing on the dynamics of internal gravity waves. The occurrence of stably-stratified flows in nature is illustrated and the Boussinesq approximation to the governing equations is derived. The properties of linearly-evolving waves are discussed together with the mechanisms that can lead the wave field to break. Parametric and buoyancy-induced instabilities, interaction with a shear flow, and interaction with a sloping boundary are also discussed. Finally, a briefly discussion about the statistical properties of the breaking wave field is given together with a brief introduction on mixing. Chapter 3 by S. Sarkar describes fundamental results on the properties of stratified turbulence and the associated mixing, obtained from direct numerical simulation (DNS) and large eddy simulation (LES) of building-block shear flows. The cases discussed include homogeneous turbulence evolving under the effect of linear stratification and linear shear, the shear layer, and channel flow. The chapter also deals with the novel situation where the mean shear is not aligned with the stratification, and the differences with the more classical case of alignment between shear and density gradient are highlighted. Finally, Chapter 4 by F. Nieuwstadt gives a review of the turbulent structure and dynamics of the atmospheric boundary layer. First, the equations governing the atmospheric boundary layer are given and discussed. The three main cases, namely the neutral, the stable, and the convective boundary layer are discussed in detail, and the appropriate scaling laws for each regime are identified. In addition, attention is paid to special topic such as wall roughness, the presence of vegetation, coherent structures, and clouds. The chapter concludes with a brief discussion of the non-stationary and inhomogeneous boundary layer evolving under different circumstances, from convective to stably stratified conditions.*

During the final composition of the present volume, Prof. F. T. M. Nieuwstadt, author of chapter 4, passed away. He was a leader in fluid mechanics with a wide range of interests including turbulence, the atmospheric boundary layer and multiphase flows. He also was a very friendly and brilliant person and we enjoyed his presence during the summer school. We wish to dedicate the present volume to his memory.

Vincenzo Armenio and Sutanu Sarkar

CONTENTS

Chapter 1: Mathematical modeling of Stratified flows

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AbstractThe present Chapter of the lecture notes is divided into three different sections. The first section is devoted to the description of the equations governing a stratified flow field. The Reynolds averaged equations are derived together with the transport equations for the mean and turbulent kinetic energies. A background discussion on the spectral characteristics of a turbulent field is given, aimed at helping the comprehension of the successive sections. The second section describes the direct numerical simulation, together with the numerical techniques currently in use for the integration of the governing equations. Section 2 also contains a brief discussion on recent achievements of DNS in the study of stratified turbulent flows. Section 2 also deals with Large-eddy simulation of stratified turbulent flows. Models widely in use for the closure of the subgrid scale stresses are described and recent achievements in the field of stratified flows discussed. Section 3 is devoted to the description of very recent numerical results for stratified flows over a topography.

1 Governing equations for stratified turbulent flows

The numerical simulation of environmental stratified flows (ESF) is relevant in many applicative fields. As an example for weather predictions, for understanding of the biological cycle in the ocean or in lakes, for short-term prediction of dispersion of plumes and jets in large reservoirs. In the present section we deal with modeling of stratified flow and turbulence closures. In particular, very briefly we describe the techniques currently in use for large-scale predictions (usually based on the solution of the Reynolds-averaged governing equations), whereas, with more details we talk about the techniques employed for the description and understanding of small-scale processes. The general equations we are going to write work for a fluid dynamic field, and thus can be used for the simulation of the atmospheric boundary layer as well as for the simulation of water reservoirs (including oceans, lakes etc.).

The equations governing the dynamics of a stratified flow field are the well-known continuity and Navier-Stokes equations that rule the evolution of the velocity and pressure fields. The momentum equation contains a gravitational term that accounts for the effect of the density variation in the flow field. The evolution of the fluid density is considered through an advection-diffusion equation for the density field, or, equivalently, for the temperature and concentration fields that affect the fluid density by means of the equation of state. In Chapter 2 of the present lecture notes the Boussinesq approximation of the equations for a stratified flow is discussed. Herein we only intend to remind that the Boussinesq form of the equations holds under the following circumstances:

- The density variations (due to the variation of the temperature and concentration field) are small if compared to the bulk density of the fluid;
- The inertial accelerations are small when compared to the gravitational acceleration.

It is noteworthy that such approximations are valid in most environmental applications. Hereafter we consider a Cartesian frame of reference having the z (or x_3) axis oriented vertically upward) and the x,y axes (or x_1, x_2) contained in the horizontal plane. The velocity components will be u, v, w (or u_1, u_2, u_3) respectively along x, y, z. The Boussinesq form of the Navier-Stokes equations reads as:

$$\frac{\partial u_i}{\partial x_i} = 0, \tag{1.1}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_j u_i}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial p}{\partial x_i} + \nu\frac{\partial^2 u_i}{\partial x_j \partial x_j} - \frac{\rho}{\rho_0} g \delta_{i3} - f_i \times u_i \tag{1.2}$$

where f_i are the components of the rotation vector. As already mentioned, the density variation:

$$\rho(x,y,z,t) = \rho_T(x,y,z,t) - \rho_0$$

is related to changes of temperature and concentration of a dissolved phase in the fluid. In Eqs. 1.1,1.2, ρ denotes the perturbation density that varies in time and in space and ρ_0 is the constant, bulk density. The Boussinesq approximation requires $\rho/\rho_0 = \epsilon << 1$. In particular, for water reservoirs, the density variations are related to changes in the temperature field and in the concentration of dissolved salt (hereafter referred to as salinity). As regards the atmosphere, temperature and specific humidity need to be considered. A more detailed discussion is in Chapter 4 of the present lecture notes. The set of equation is completed once the perturbation density field ρ is evaluated.

It is possible to follow two different strategies: The first one consists in writing the transport equation of *all* quantities affecting the density field and successively to calculate the perturbation density as a function of the quantities already evaluated. This step is possible once the equation of state for the fluid is known.

For example, let's consider the case of the ocean. The density variation is related to corresponding variations of salinity (percentage of salt dissolved in a unit volume of water) and temperature. The equations of transport of the temperature and salinity are:

$$\frac{\partial T}{\partial t} + \frac{\partial u_j T}{\partial x_j} = \frac{\nu}{Pr}\frac{\partial^2 T}{\partial x_j \partial x_j}, \tag{1.3}$$

$$\frac{\partial S}{\partial t} + \frac{\partial u_j S}{\partial x_j} = \frac{\nu}{Sc}\frac{\partial^2 S}{\partial x_j \partial x_j}, \tag{1.4}$$

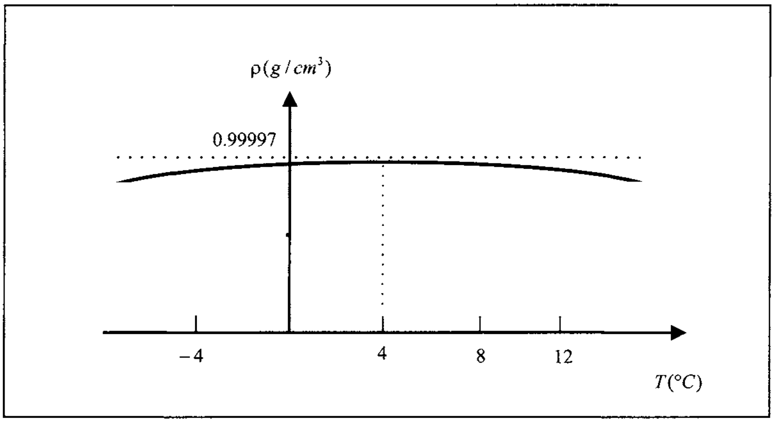

Figure 1. Variation of density of fresh water with temperature.

where T and S respectively denote the temperature and the salinity in the fluid, $Pr = \nu/k_T$, $Sc = \nu/k_c$ are the Prandtl and the Schmidt number. The Prandtl number is the ratio between the molecular diffusivity of momentum ν and that of temperature k_T, whereas the Schmidt number is the ratio between ν and the molecular diffusivity of the concentration (salinity) k_s. Now, the equation of state is needed that gives $\rho = f(T, S)$. For sea water the equation of state commonly used has been presented by Millero and Poisson (1981) and also given in the UNESCO Technical paper in Marine Science, Number 36 (UNESCO, 1981). A simplified (linearized) equation often used is the following:

$$\rho = \rho_0 + [-\alpha(T - T_0) + \beta(S - S_0)] \tag{1.5}$$

where α and β are respectively the coefficients of thermal and salinity expansion, and ρ_0 is the reference (bulk) density corresponding to the reference temperature T_0 and salinity S_0. Note that, in the range of values $T > 4^0C$, the increase of temperature gives a reduction of density (Fig.1), whereas the increase of salinity always produces the increase of density. Details on the complete equation of state for the ocean, for lakes, for dissolved gases in water and for the atmosphere can be found in Kantha and Clayson (2000).

1.1 Reynolds-averaged equations for stratified flows

Basic definitions that can be useful in the following are *homogeneity* and *isotropy*. Turbulence is homogeneous if the statistics of the turbulent field are not a function of space. Turbulence can be homogeneous over the whole volume of fluid, over planes or along a direction. As an example, a turbulent field characterized by the presence of a *linear* mean shear can be easily shown to be homogeneous over the volume of fluid, turbulence in a channel flow (the flow confined between two parallel and infinite plates) is homogeneous over the planes parallel to the plates, turbulence in a spatial-evolving boundary layer is homogeneous along the cross-stream, spanwise direction.

Turbulence is isotropic when the statistics are not dependent on a rotation of the frame of reference. It can be easily shown that isotropy involves the absence of a mean shear. It is difficult to find an example of a *real* isotropic turbulent field. A typical isotropic turbulent field that can be reproduced in a laboratory experiment is the grid turbulence. In spite of the fact that isotropic turbulence is hardly found in real applications, the study of this simplified flow field has been very important in developing theories in turbulence.

In environmental applications the Reynolds number is typically of the order of $O(10^7-10^9)$, hence the flow field is in a turbulent regime. A well established way to deal with turbulent flow fields consists into the use of the Reynolds decomposition of the field variables. According to this approach the field variables are decomposed into a mean and a fluctuating part, and the mean value can be obtained using three different types of averaging procedures:

1. Time averaging: The field variables are averaged in time and are function of the spatial coordinates

$$U_i(x_i) = \frac{1}{T}\int_0^T u(x_i,t)dt$$

2. Spatial averaging: The field variables are averaged along one direction (along which turbulence is homogeneous) or over planes or volume of homogeneity. If, for example, turbulence is homogeneous over the $x-y$ plane, spatial averaging leads to:

$$U_i(z,t) = \frac{1}{L_x L_y}\int_0^{L_x}\int_0^{L_y} u_i(x,y,z,t)\, dx\, dy$$

3. Ensemble averaging: It consists in averaging over a number of samples N of a particular experiment.

$$U^e(x_i,t) = \frac{1}{N}\sum_{n=1}^{N} u_i^n(x_i,t)$$

We assume that the reader is familiar with operations involving average and fluctuating quantities.

If we:

1. Substitute the total field variables with the sum of the mean and the fluctuating parts ($u_i = U_i + u_i'$) into the governing equations (continuity, momentum and transport equation of the temperature and/or concentration),
2. Perform an averaging operation, according to one of the techniques above described,

it is possible to obtain the following Reynolds averaged equations governing the evolution of the mean velocity pressure and density (or temperature or concentration) field.

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{1.6}$$

$$\frac{\partial U_i}{\partial t} + \frac{\partial U_i U_j}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial p}{\partial x_i} + \nu\frac{\partial U_i}{\partial x_j \partial x_j} + \frac{g}{\rho_0}\overline{\rho} - \frac{\partial}{\partial x_j}\overline{u_i' u_j'} - f_i \times \overline{U}_i \tag{1.7}$$

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} U_j}{\partial x_j} = \frac{\nu}{Pr}\frac{\partial \overline{\rho}}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j}\overline{\rho' u_j'} \tag{1.8}$$

The Reynolds-averaged equations are formally similar to the governing equations for the instantaneous variables, apart the extra-terms on the right-hand side, that represent the contribution of turbulence to the mean velocity and density fields. The quantities $\rho_0\overline{u_i u_j}$ are the elements of the Reynolds stress tensor and represent transport of momentum due to turbulent fluctuations. Similarly, the quantities $\overline{\rho' u'}$ are transport of density by means of turbulent fluctuations, and they represent the contribution of the fluctuating field to the transport of the mean density. The momentum equation contains a gravitational term $\frac{1}{\rho_0} g\overline{\rho}$ that contributes to the enhancement or suppression of momentum depending on whether the flow is unstably or stably stratified.

Fluid flow involves conversion of energy from one form to another one. For example, kinetic energy is converted into heat by means of the molecular viscosity, consistently with the second principle of thermodynamics. When a gravitational term is present in the governing equations, due to the density variation in the flow field, conversion of kinetic energy into potential energy (or vice-versa) occurs in a stably (or unstably) stratified flow. In a stably stratified flow, for example kinetic energy is converted into potential one when a particle is displaced vertically in the fluid column. In order to understand how this conversion occurs, it is helpful to write the transport equation of the mean kinetic energy (MKE) K_M and of the turbulent kinetic energy (TKE) K:

$$K_M = \frac{1}{2} U_i U_i \, ,$$

$$K = \frac{1}{2}\overline{u_i' u_i'} \, .$$

The transport equation for the mean kinetic energy is obtained multiplying respectively by U_j and U_i the momentum equation for U_i and U_j, and summing the two equations in order to obtain a transport equation for $U_i U_j$. If we put $i = j$ and we sum over the three directions we obtain:

$$\frac{\partial K_M}{\partial t} + \frac{\partial U_j K_M}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial U_j P}{\partial x_j} + \frac{\partial}{\partial x_j}[2\nu U_i S_{ij} - \overline{u_i' u_j'} U_i] + \overline{u_i' u_j'} S_{ij} - 2\nu S_{ij} S_{ij} - \frac{g}{\rho_0} i_3 \overline{\rho} U_j \tag{1.9}$$

Equation 1.9 states that transport of mean kinetic energy in the flow field is due to the following contributions (the enumeration corresponds to the position of the terms of the right-hand side):

1. work done by the pressure forces (redistribution term);

2. transport by viscous forces and Reynolds stresses (redistribution term);
3. loss due to generation of turbulence (sink term);
4. energy dissipation due to viscosity (sink term);
5. work done by (or against) the gravitational field in unstably (stably) stratified flow. It represents a production (sink) term.

Terms 1 and 2 represent redistribution terms, in that they drop out when integrated over a closed volume; terms 3 to 5 are production-sink terms of MKE. Note that rotation of the frame of references does not contribute to production/destruction of MKE. Rather rotation leads to a redistribution of MKE among the three directions.

By the use of a similar procedure it is possible to derive the transport equation of the TKE:

$$\frac{\partial K}{\partial t}+\frac{\partial U_j K}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial \overline{u_j p}}{\partial x_i}-\frac{\partial}{\partial x_j}(\frac{1}{2}\overline{u_j u_i u_i})+\frac{\partial}{\partial x_j}(2\nu\overline{u_j s_{ij}})-\overline{u_i u_j}S_{ij}-2\nu\overline{s_{ij}s_{ij}}-\frac{g}{\rho_0}\delta_{i3}\overline{u_j\rho'} \tag{1.10}$$

In Eq. 1.10 s_{ij} are the elements of the fluctuating strain-rate tensor. Equation 1.10 shows that turbulent kinetic energy is re-distributed by terms 1 to 3 of the right-hand side, whereas terms 4 to 6 represent production-sink terms of TKE.

In particular, term 4 of the RHS represents production of TKE. Note that $-\overline{u_i u_j}S_{ij}$ is in general positive and it appears in the equation of transport of MKE with the opposite sign. This means that what is subtracted from the mean flow for producing turbulence, appears in the TKE budget as a source term. Term 5 of the RHS of Eq. 1.10 is turbulent viscous dissipation whereas term 6 is a production (destruction) term in case of unstably (stably) stratified fluid column. In presence of the gravitational field, stratification in the fluid implies conversion between potential and kinetic energy. Figure 2a shows that, in case of unstable stratification vertical mixing of density is associated to negative values of the cross-correlation term $\overline{w'\rho'}$. In this case the buoyancy term 6 is positive, thus constituting a source term for TKE. Conversely, in case of stable stratification, the turbulent mixing of the density field is associated to a positive value of the cross-correlation term $\overline{w'\rho'}$ (Fig 2b); the buoyancy term 6 is in this case negative, thus acting as a sink term. To summarize:

- mean shear in the flow field always subtracts energy from the mean flow to sustain turbulence;
- the strain rate of the fluctuating field always gives rise to dissipation of turbulent kinetic energy; note that although the molecular viscosity is in general very small, the dissipation term $\epsilon = 2\nu\overline{s_{ij}s_{ij}}$ is such to be nearly in balance with the production term;
- stratification can give either production or destruction of TKE. In case of unstable stratification potential energy is converted into turbulent kinetic energy by means of the buoyancy term that acts as a source term in the TKE equation; In case of stable stratification, buoyancy term drains TKE that is thus converted into potential energy.

As already done for the kinetic energy, it is possible to derive a transport equation for the density variance. The procedure is similar to that already used for obtaining the transport equations for the Reynolds stresses. In particular:

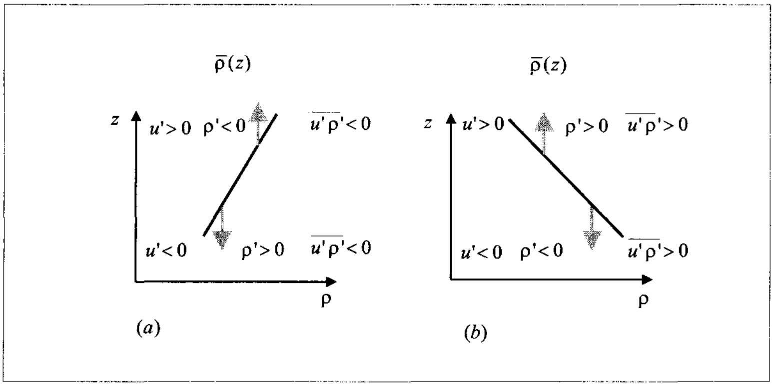

Figure 2. Schematic of turbulent density fluxes: (a) unstable stratification; (b) stable stratification.

- multiply the transport equation for the fluctuating density ρ' by ρ';
- Reynolds-average the terms of the equation.

We obtain the following equation:

$$\frac{\partial \overline{\rho'^2}}{\partial t} + \frac{\partial U_j \overline{\rho'^2}}{\partial x_j} = -\frac{\partial \overline{u_j \rho'^2}}{\partial x_j} - k_T \frac{\partial \overline{\rho'^2}}{\partial x_j \partial x_j} - 2\overline{u_j \rho'} \frac{\partial \overline{\rho}}{\partial x_j} - 2k_T \overline{\frac{\partial \rho'}{\partial x_j} \frac{\partial \rho'}{\partial x_j}} \tag{1.11}$$

The first two terms of the RHS give transport by density fluctuations and viscous diffusion of the density variance. The third term gives production of density variance by means of mean density gradient, whereas the fourth term gives turbulence dissipation. It is worth noting that the production term $-2\overline{u_j \rho'}\, \partial\overline{\rho}/\partial x_j$ is always positive. Indeed, the cross-correlation $\overline{u_j \rho'}$ is negative when the density gradient is positive (unstable stratification), and $\overline{u_j \rho'}$ is positive in case of stable stratification (negative density gradient).

Equations 1.6, 1.7 and 1.8 involve mean (in the Reynolds-averaging sense) quantities and their spatial distribution also related to the effect of the turbulent field. The contribution of turbulence to the evolution of the velocity field is given by the elements of the Reynolds stress tensor $\rho_0 \overline{u_i u_j}$, whereas the contribution of turbulence to the evolution of the mean density field is given by the density fluxes $\overline{\rho' u_i}$. These elements are not known *a priori*, rather they represent additional terms that need to be determined (or modeled) in order to close the system of equations. There is no way to determine such terms analytically. For example, if we write the transport equations for the Reynolds stresses and the density fluxes, we obtain new unknown terms in the form of triple correlation terms. Similarly, the transport equation of the triple correlation terms contains $IV-$order terms that need to be determined. This is known in literature as the *closure problem*. Assumption are required for modeling the Reynolds stress and the density fluxes, with the aim to arrive to a closed system of equations. In the present notes we do not discuss the RANS turbulence models used in environmental and geophysical applications. For a detailed review of these techniques, the reader is referred to Kantha and Clayson (2000).

1.2 Governing equations in the spectral space

Herein, we give some definitions useful for introducing the concept of spectral analysis of turbulence. We define the general second-order correlation function as:

$$\overline{S_1 S_2}(X_1, X_2, t_1, t_2) = \overline{S_1(X_1, t_1) S_2(X_2, t_2)} \tag{1.12}$$

where S_1 and S_2 are two different (or the same) flow properties (for example velocity components, density, pressure), X_1 and X_2 can be different (or the same) spatial locations, and similarly t_1 and t_2. For stationary turbulence, the correlation function does not depend on the beginning time t_1 of the sampling; if turbulence is homogeneous over the direction X, the correlation is independent on the location X_1 but only varies with the distance $X_1 - X_2$. Correlation functions can be classified as:

- Point correlations, when $X_1 = X_2$. They are called direct- or cross-correlation functions, respectively in the case $S_1 = S_2$ or $S_1 \neq S_2$;
- Spatial correlations, when $t_1 = t_2$. They are called direct-spatial correlations or spatial cross-correlations in the case $S_1 = S_2$ or $S_1 \neq S_2$ respectively.

Correlation functions are important in turbulence because they appear in the transport equations of momentum, kinetic energy and density as momentum fluxes $\overline{u'_i u'_j}$ (the elements of the Reynolds stress tensor) and density fluxes $\overline{\rho' u'_i}$. Indeed, let's consider the direct point correlation of a velocity component (say u_1), calculated for $t_1 = t_2$ for $X_1 = X_2$, $\overline{u_1 u_1}(X)$. This quantity is the longitudinal Reynolds stress divided by the reference density ρ_0. Similarly, the point cross-correlation between u_1 and u_3 for $t_1 = t_2$ and $X_1 = X_2$, $\overline{u_1 u_3}(X)$ is the Reynolds shear stress divided by ρ_0. Similarly for the other turbulent fluxes. If turbulence is homogeneous over the volume of fluid, the correlation is a function of the distance r between two points in the three-dimensional space, and the correlation tensor can be written as:

$$R_{ij} = \overline{u_i(X,t) u_j(X + r, t)}.$$

It is possible to define the spectrum tensor as the Fourier transform of R_{ij}, such that:

$$R_{ij}(r) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_{ij}(k) e^{i\,k\,r} dk$$

where k is the wave number, and the integral has been extended over the whole range of wavenumbers. Obviously the following inverse Fourier transform holds:

$$F_{ij}(k) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} R_{ij}(r) e^{-i\,k\,r} dr$$

This way it is possible to go forth and back from the physical space to the Fourier (or wavenumber) space. Based on the above discussion, it can be easily shown that:

$$2K = R_{11}(0) + R_{22}(0) + R_{33}(0) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (F_{11} + F_{22} + F_{33}) dk$$

and, consequently the integral over the wave number of the sum of the spectra of the three velocity components is proportional to the turbulent kinetic energy. The function

$F_{ii}(k)$ (sum over i) gives the density of turbulent kinetic energy at the wavenumber k. Since $k_n = 2\pi/L_n$ with L_n a length-scale associated to the k_n-mode, the spectrum gives information on the energy content at different length-scales. If we consider a sphere of radius $k = |\bar{k}| = \sqrt{k_i k_i}$ and ds is the elementary surface of such sphere, the turbulent kinetic energy in the wavenumber space is:

$$E(k) = \frac{1}{2} \int_S F_{ii}(\bar{k}) ds,$$

where S is the surface of the sphere, and the turbulent kinetic energy is the integral of $E(k)$ over the whole range of wavenumbers.
Turbulence is characterized by the fact that energy is distributed over a wide range of scales (spatial and temporal). In particular, the shape of $E(k)$ informs on how energy is distributed over such scales. If we rewrite the transport equation of the TKE in the wavenumber space we can figure out the importance of the terms that contribute to the evolution of TKE over such scales.

Let's consider the equation of transport of kinetic energy (Eq. 1.10) and, for simplicity, let's assume the flow field to be homogeneous along the $x-y$-planes. This assumption is in general valid in the study of the atmospheric boundary layer, of the sea-bottom boundary layer and of the mixed layer in the upper part of the ocean. In case of homogeneity over the plane $x - y$ most terms of Eq. 1.10 drop out, and the equation simplifies to:

$$\frac{\partial K}{\partial t} = -\frac{\partial u_3' K}{\partial x_3} - \frac{\partial u_3' p}{\partial x_3} - \overline{u_1' u_3'}\frac{\partial U_1}{\partial x_3} + \frac{g}{\rho_0}\overline{\rho' u_3'} - \epsilon \tag{1.13}$$

where ϵ denotes the viscous dissipation. In order to understand how the terms that compose such equation are distributed over the different length-scales, it is convenient to recast such equation in the space of wave numbers. Such operation is quite complex and reported with details in Hinze (1976); Monin and Yaglom (1971). It gives:

$$\frac{\partial E(k)}{\partial t} = -\frac{\partial T_k(k,t)}{\partial k} + \tau(k)\frac{\partial U_1}{\partial x_3} + B(k) - 2\nu k^2 E(k) \tag{1.14}$$

In Eq. 1.14, $T_k(k,t)$ is the *spectral energy transfer rate* and represents the rate at which energy is transferred from a wave number k to $k + dk$ (from low to high modes). It has to be observed that the integral of $\partial T(k)/\partial k$ over the whole range of wave numbers gives 0. The second term of the RHS represents turbulent production of kinetic energy at the wave-number k, where $\tau(k)$ is the Fourier transform of the Reynolds stress tensor. The term $B(k)$ is the buoyancy production/destruction (depending on the sign of stratification) at the wave number k and, finally the last term is turbulent dissipation at the wave-number k. The following relationships hold:

$$\frac{g}{\rho_0}\overline{u_3\rho'} = \int_0^\infty B(k)\, dk \tag{1.15}$$

$$P_k = \overline{u_1 u_3}\frac{\partial U_1}{\partial x_3} = \int_{-\infty}^\infty \tau(k)\frac{\partial U_1}{\partial x_3} dk \tag{1.16}$$

Figure 3 shows the distribution of the different terms of Eq. 1.14 over the wave numbers.

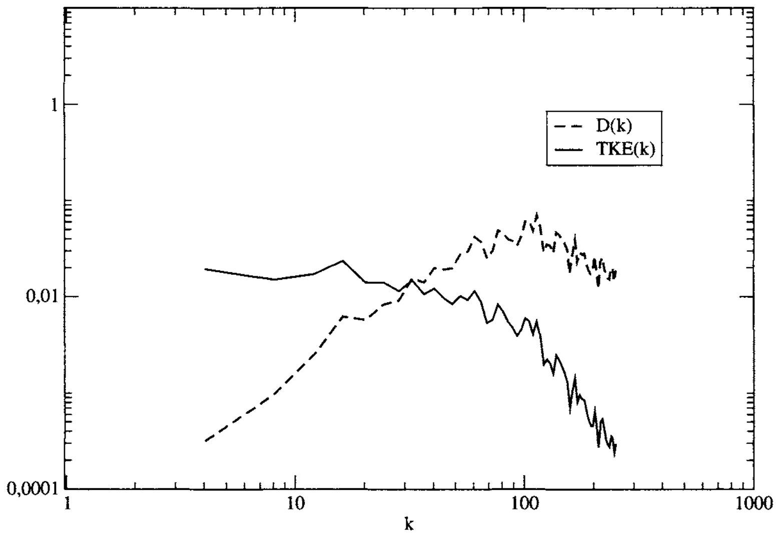

Figure 3. Distribution over the spatial wavenumbers of TKE and dissipation rate D of the turbulent kinetic energy. Data from a direct simulation of a turbulent channel flow at friction Reynolds number equal to 130.

It is worth observing that Fig. 3 refers to a case of large value of the Reynolds number. Turbulent kinetic energy is mainly concentrated in the range of low wavenumbers, corresponding to large length-scales. Hence, it clearly appears that the large scales carry most of turbulent kinetic energy. Dissipation is mainly concentrated in the region of large wavenumbers corresponding to small length-scales. Figure 3 also shows that the range of scales at which $E(k)$ is significant is well separated from that where dissipation occurs. Production of turbulent kinetic energy is significant at the small wavenumbers, since, such are the elements of the tensor $\tau(k)$. Finally, the intermediate range of scales over which both turbulence production and dissipation are negligible, is characterized by significant and nearly constant values of the spectral energy transfer rate. This range of scales, characterized by inviscid transfer of turbulent kinetic energy from the large to the small ones, is called *inertial subrange.* The classical theory of turbulence, corroborated by experimental evidence, states that the energy spectrum in the inertial range is proportional to $k^{-5/3}$. Finally, the buoyancy term (not shown in the Fig. 3) is significant at the small wave numbers, thus indicating that buoyancy production/destruction primarily affects the large, energy-carrying scales of motion.
The results discussed above confirm the theory of the universal equilibrium range postulated by Kolmogorov (1941b,a) on the basis of scaling arguments. The main points of such theory are:

1. At a Reynolds number large enough, there is a range of high wavenumbers where turbulence is statistically in equilibrium (production=dissipation) and determined by the dissipation rate ϵ and viscosity ν;

2. In the case of Reynolds number infinitely large, the energy spectrum at the intermediate scales (the above defined inertial subrange) is only dependent on the dissipation rate (ϵ) of TKE.

Based on the spectral analysis briefly described above, we try to give a short explanation and implications of the Kolmogorov theory. The largest scales of motion are responsible for the transport of momentum and generation of TKE. At these scales, the effective Reynolds number of the flow (based on the length of the largest scales and the characteristic velocity of these scales) is very large, and viscosity does not play a significant role. The non-linear terms of the Navier-Stokes equations prevent from the piling up of energy at the largest scales and are responsible of transferring energy from the largest scales toward the small scales. From a physical point of view this transfer occurs due to strong interaction and destruction of large-scale eddies into smaller and smaller eddies. This process would tend to go down in the length-scales (at infinitively large wave number), but there will be a certain length-scale η_k, characterized by a velocity scale v_k such that dissipative effects get dominant and supply complete dissipation of TKE. At these scales, the Reynolds number $Re_k = \eta_k v_k/\nu$ is expected to be of the order $O(1)$. Such scales are called the *Kolmogorov length- and velocity-scales.* The Kolmogorov theory assumes that the small-scales, characterized by small time scales, are statistically independent on the large and slow scales of motion. This hypothesis is confirmed by the analysis of the spectra of Fig. 3 that shows that the energy-carrying part of the spectrum is well separated by the part of the spectrum where dissipation takes place. When this assumption holds, the small scales of motion only depend on how they are fed by the energy coming down from the large scales and on the kinematic viscosity. Since in the intermediate-to-small scale turbulence is assumed to be in equilibrium, the rate of production of energy is equal to the rate of dissipation ϵ, and, hence, ϵ and ν are the key parameters that govern the smallest scales of the flow field. The application of the dimensional analysis suggests:

$$\eta_k \sim (\frac{\nu^3}{\epsilon})^{1/4} ,$$

$$v_k \sim (\nu\epsilon)^{1/4} ,$$

$$t_k \sim \frac{\nu}{\epsilon}^{1/4} .$$

Note that the above expressions give $Re_k = \eta_k v_k/\nu \sim O(1)$. Finally, the existence of the inertial subrange (postulated by Kolmogorov and verified experimentally in successive researches) suggests that within this range energy is neither produced nor dissipated, hence the dissipation rate ϵ at the small scales can be directly related to the production rate at the largest scales. At these scales, the amount of kinetic energy per unit mass is proportional to u^2 where u is a characteristic velocity scale of the largest scales, and the rate of transfer of such energy is of the order of L/u where L is the characteristic length scale of the energy carrying eddies, it follows that the rate of energy supplied by the large, energy carrying scales to the small ones is of order u^3/L. Hence,

$$\epsilon \sim u^3/L$$

that implies that the large eddies lose a significant part of energy by non-linear mechanism within one turnover time u/L.

To summarize, for large-Reynolds-number flows:

- The spectral analysis allows to identify the energy content of the different scales of a turbulent flow field;
- Small wave numbers corresponding to large length-scales in the physical space carry most of the turbulent kinetic energy;
- Large wave numbers that correspond to small length-scales are characterized by being strongly dissipative;
- The large-scales where turbulent production takes place are well separated from the small scales by the inertial subrange where both production and dissipation are negligible and transfer from the large to the small scales takes place;
- the inertial subrange has universal characteristics such that $E(k) \sim k^{-5/3}$;
- Viscosity is unimportant in the dynamics of the large scales. On the other hand, the small scales are governed by the viscosity and the dissipation rate of TKE;
- The dissipation rate can be found by the knowledge of the dynamics of the large, energy-carrying scales of motion.

Similar arguments can be used for the analysis of the density field.

Let's consider the transport equation of the density variance. In particular, we discuss the case of a passive scalar, namely a temperature or concentration field weak enough that the feed-back effect on the momentum equation is negligible. The passive scalar represents a case one-way coupling, in which the scalar is transported by the velocity field, and it does not affect the velocity field. A boundary layer heated from one boundary (either the top or the bottom), where the heating is very weak and not able to supply significant buoyancy, is a typical example of transport of a passive scalar. The transport equations of the mean passive scalar and of its variance are respectively Eq. 1.8 and Eq. 1.11 where $\overline{\rho}$ and ρ' have to be considered as mean and fluctuating parts of the passive scalar. Similarly to the case of energy spectra, the passive scalar has a three-dimensional spectrum. Let's consider a density fluctuation $\rho'(X,t)$ and the spatial autocorrelation function R_ρ defined as:

$$R_\rho = \overline{\rho(X,t)\rho(X+r,t)},$$

where r is the distance in the three-dimensional space from the point X to the point $X+r$. The Fourier transform of R_ρ is the spatial spectrum $F_\rho(k)$ such that:

$$R_\rho(r) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{ikr} F_\rho(k)\, dk.$$

The spatial spectrum $F_\rho(k)$ is obviously defined as:

$$F_\rho(k) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-ikr} R_\rho(r)\, dr.$$

Similarly to the velocity field, the density spectrum represents the *energy* of the density field associated to the wavenumber k. If we integrate over the surface S of the sphere of radius k the function $F_\rho(k)$, we obtain the three-dimensional spectrum:

$$E_\rho(k) = \frac{1}{2}\int_S F_\rho(\overline{k})\; ds,$$

where $k = |k| = \sqrt{k_i k_i}$ and ds is the elementary surface of the sphere of radius k. Obviously, the density variance is related to the three-dimensional spectrum by:

$$\frac{1}{2}\overline{\rho'\rho'} = \int_0^\infty E_\rho(k)\; dk.$$

An important point is that if an equilibrium range exists in the spectrum of the turbulent kinetic energy, there exists an equilibrium range in the spectrum of the density variance. This is reasonable since turbulence is responsible of the mixing of the scalar field and, thus the spectrum of the scalar field must have characteristics somewhat similar to those of the velocity field. The existence of an inertial subrange in the spectrum of the passive scalar has been first argued by Obukhov (1949) and Corrsin (1951). Similarly to the energy spectrum, such subrange (called inertial-convective subrange) is such that variance of passive scalar is neither produced nor dissipated, rather it is transferred from the large-scales to the small-scales of motion. The equation of transport of the density variance in spectral space gives terms equivalent to those of Eq. 1.14 . A production term is present that basically is fed by the large scales of motion and therefore is significant in the region of small wavenumbers. A dissipation term ϵ_ρ appears that is relevant in the range of small scales of motion, corresponding to high wavenumbers, and a transfer function appears that is significant at the intermediate scales, where both production and dissipation are negligible. Such inertial-convective subrange is present at intermediate wavenumbers in the following range:

$$\frac{1}{l_\rho} << k << \frac{1}{\eta_\rho},$$

where l_ρ is an integral scale at which the variance of passive scalar is produced, and η_ρ is the dissipation micro-scale, the smallest scale detectable in the spectrum. This scale is the counterpart of the Kolmogorov micro-scale of the energy spectrum, and it is called the Obukhov scale. Similarly to the inertial subrange, the inertial-convective subrange has been found to decrease with $k^{-5/3}$. Figure 4 shows the spectrum of passive scalar as derived from experimental data of Sreenivasan (1996) for cases characterized by large values of the Reynolds numbers.

A main difference between the spectrum of the velocity field and that of the density variance is that the latter is dependent on an additional parameter that is the Prandtl number (and/or the Schmidt number), namely the ratio between the fluid viscosity and the thermal (or concentration) diffusivity.

Dimensional arguments (see Tennekes and Lumley (1972)) suggest:

$$E_\rho = \epsilon_\rho \epsilon^{-1/3} k^{-5/3} f(k\eta, Pr)$$

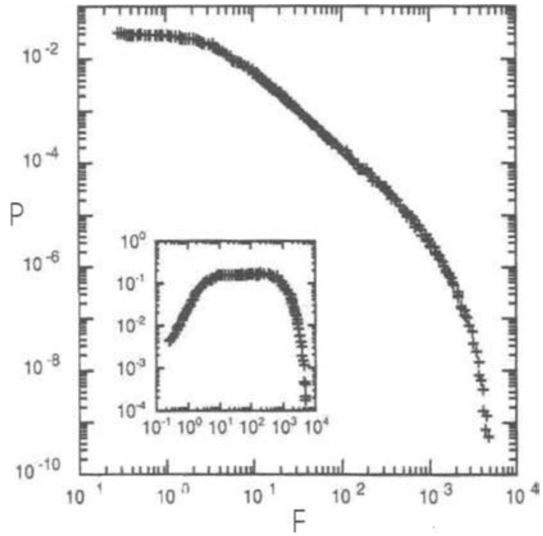

Figure 4. Spectrum of passive scalar obtained by experimental data. Reproduced with permission from Sreenivasan, (1996).

It is noteworthy that the shape of the spectrum depends on the characteristics of the fluid, due to the presence of Pr. If the Reynolds number is large enough for the development of an inertial subrange, and the thermal diffusivity is small enough, there is a large part of the spectrum where thermal diffusivity is unimportant and an inertial-convective range is detectable. In this case the spectrum of this range is:

$$E_\rho = \beta \epsilon_\rho \epsilon^{-1/3} k^{-5/3}$$

Recent measurements of Sreenivasan (1996) show values of $\beta \sim 0.4 - 0.5$. This is indeed the case of a passive scalar like salinity, characterized by $Sc \sim 500$.

When the thermal diffusivity is to be taken into account, we must consider separately fluids with $Pr < 1$ (like diffusion of temperature in air) and fluids with $Pr > 1$ like , for example, temperature diffusion in water ($Pr \sim 5$). The case $Pr < 1$ is such that the thermal diffusivity gets importance within the inertial-convective range where viscosity is still unimportant. The Obhukov scale is larger than the Kolmogorov scale and the spectrum of density variance decays much faster than the $k^{-5/3}$ law. The region of wavenumbers $1/\eta_\rho < k < 1/\eta_k$ is called the *inertial-diffusive region.*

The case $Pr > 1$ is characterized by the fact that viscosity becomes important in a region of the spectrum where the effect of thermal diffusivity is still negligible. The range of wavenumbers where $k\eta > 1$ and $k\eta_\rho << 1$ is called *viscous-convective* subrange and here $E_\rho \sim k^{-1}$. In this case there is also a region where $k\eta_k >> k\eta_\rho > 1$ called *viscous diffusive* range. The ranges above illustrated are shown in Fig. 5

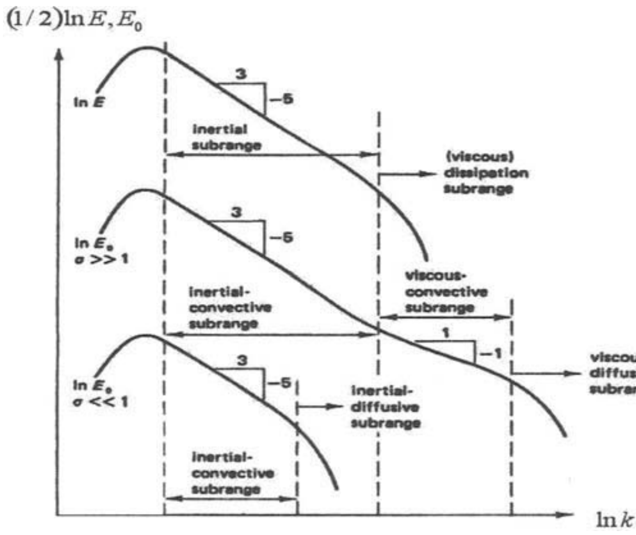

Figure 5. Examples of spectra of passive scalar for different values of the Prantl number. Reproduced with permission from Tennekes and Lumley, (1972).

When buoyancy effects become important the spectrum turbulent kinetic energy an that of the density variance exhibit different characteristics. This aspect is exploited in Chapter 2 of the present lecture notes.

2 Numerical simulation of turbulent stratified flows

In the previous section, we have presented the equations governing the motion of a stratified flow, and shown some results from classical theories of turbulence. The few information given above will be useful for understanding how to tackle turbulence using numerical simulations. We will discuss in two separate subsections, the direct use of the primitive variable equations and the primitive variable equations with a subgrid-scale closure. The use of the Reynolds-averaged equations, together with description and discussion of models for the closure of the Reynolds stress, have been widely treated in other courses, advanced schools and books (see for example Kantha and Clayson (2000) and will not be repeated here.

2.1 Modeling turbulence using direct numerical simulation

As already discussed, Reynolds averaged equations are able to give an estimation of the mean velocity and density field provided that the contribution of the fluctuating field (the Reynolds stresses and the density fluxes) be properly modeled. Such model supplies a parameterization of the Reynolds stress and density flux tensors. The main drawback of turbulence models for Reynolds averaged equations is in the dependence of the results on a series of empirical parameters to be tuned case by case. On the other hand, the advantage of using RANS, consists in the possibility to deal with values of Reynolds number of practical significance.

On the opposite side, one may be tempted to simulate a turbulent flow, solving *all* the scales of turbulence directly, by direct simulation of the NSEs without the use of any turbulent closure. Such an approach is called *direct numerical simulation* (DNS). In order to understand how this operation can be performed, and the limits of such simulations, we need to go back and discuss some issues on the characteristics of a turbulent flow field.

As discussed in a previous section, turbulence is characterized by a cascade of energy from the large, energetic scales toward the small ones. The large scales are energetic and anisotropic. The evolution of such scales is strongly related to the boundary condition on the flow field, and hence their structure is strongly dependent on the physical problem under investigation. As an example the shape and the temporal evolution of the spatial large scales in a boundary layer are very different from those developing in a shear layer, or in a turbulent jet. Conversely, the small scales of turbulence tend to be more universal, in that they tend to be more and more isotropic and strongly dissipative. Figure 6 shows a typical energy spectrum for a large class of neutrally stratified turbulent flows (Saddoughi and Veeravalli (1994)). Figure 6 contains the spectra calculated from data obtained for a wide range of values of the Reynolds number and for different kinds of experiments (for example, grid turbulence, shear flows, boundary layers...). The energetic part of the spectrum is observable at the left side of the spectrum, corresponding to small wavenumbers (large spatial scales). In some of the experiments (those carried out at large Reynolds numbers) the presence of the inertial subrange is well detectable in the range of moderate wavenumbers. Finally, the large wavenumbers are characterized by fast decay of energy spectrum. The analysis of Fig. 6 also shows that:

- different flow conditions are characterized by different levels of energy content at