Explicit algebraic turbulence modelling in buoyancy-affected shear flows

by

Werner M.J. Lazeroms

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Werner M.J. Lazeroms
Linné FLOW Centre, KTH Mekanik, Royal Institute of Technology
SE-100 44 Stockholm, Sweden

Abstract

Turbulent flows affected by buoyancy forces occur in a large amount of applications, from heat transfer in industrial settings to the effects of stratification in Earth's atmosphere. The two-way coupling between the Reynolds stresses and the turbulent heat flux present in these flows poses a challenge in the search for an appropriate turbulence model. The present thesis addresses this issue using the class of explicit algebraic models.

Starting from the transport equations for the Reynolds stresses and the turbulent heat flux, an explicit algebraic framework is derived for two-dimensional mean flows under the influence of buoyancy forces. This framework consists of a system of 18 linear equations, the solution of which leads to explicit expressions for the Reynolds-stress anisotropy and a scaled heat flux. The model is complemented by a sixth-order polynomial equation for a quantity related to the total production-to-dissipation ratio of turbulent kinetic energy. Since no exact solution to such an equation can be found, various approximation methods are presented in order to obtain a fully explicit algebraic model.

Several test cases are considered in this work. Special attention is given to the case of stably stratified parallel shear flows, which is also used to calibrate the model parameters. As a result of this calibration, we find a critical Richardson number of 0.25 in the case of stably stratified homogeneous shear flow, which agrees with theoretical results. Furthermore, a comparison with direct numerical simulations (DNS) for stably stratified channel flow shows an excellent agreement between the DNS data and the model. Other test cases include unstably stratified channel flow and vertical channel flow with either mixed convection or natural convection, and a reasonably good agreement between the model and the scarcely available, low-Reynolds-number DNS is found. Compared to standard eddy-viscosity/eddy-diffusivity models, an improvement in the predictions is observed in all cases.

For each of the aforementioned test cases, model coefficients and additional corrections are derived separately, and a general formulation has yet to be given. Nevertheless, the results presented in this thesis have the potential of improving the prediction of buoyancy-affected turbulence in various application areas.

Descriptors: Turbulence, RANS, explicit algebraic Reynolds-stress models, active scalars, stratified turbulence, stable and unstable stratification, mixed and natural convection

Explicit algebraisk turbulensmodellering i skjuvströmningar med flytkraftseffekter

Werner M.J. Lazeroms
Linné FLOW Centre, KTH Mekanik, Kungliga Tekniska Högskolan
SE-100 44 Stockholm, Sverige

Sammanfattning

Turbulenta strömningar som påverkas av flytkrafter är vanliga inom flera tillämpningsområden, från värmeöverföring i industriella sammanhang till effekterna av stratifiering i atmosfären. Kopplingen mellan de Reynoldska spänningarna och det turbulenta värmeflödet gör det ganska komplicerat att formulera adekvata turbulensmodeller för sådana strömningar. Avhandlingen behandlar detta problem med avseende på så kallade explicita algebraiska modeller.

Utgående från transportekvationerna för de Reynoldska spänningarna och det turbulenta värmeflödet härleds ett algebraisk ekvationssystem som är giltigt för strömningar med tvådimensionell medelhastighet under inverkan av flytkrafter. Systemet omfattar arton linjära ekvationer och dess lösning leder till explicita uttryck för de Reynoldska spänningarnas anisotropi och ett normaliserat värmeflöde. Modellen kompletteras av en sjätte gradens polynomekvation för en storhet som hänger ihop med förhållandet mellan den totala produktionen och dissipationen av turbulent kinetisk energi. Eftersom ingen exakt lösning till en sådan ekvation existerar, presenteras olika approximationsmetoder för att erhålla en fullständigt explicit modell.

Flera testfall betraktas i detta arbete. Särskild uppmärksamhet ägnas åt stabilt stratifierade parallella skjuvströmningar som även används i kalibreringen av modellparametrarna. Som ett resultat av kalibreringen erhåller vi ett kritiskt Richardsontal lika med 0.25 för en stabilt stratifierad homogen skjuvströmning, vilket överensstämmer med teoretiska resultat. En jämförelse med DNS-data för en stabilt stratifierad kanalströmning visar en utmärkt överensstämmelse mellan DNS och modellen. Andra testfall som beaktas är en instabilt stratifierad kanalströmning och en vertikal kanalströmning med antingen blandad konvektion eller naturlig konvektion. Modellresultaten i dessa fall överensstämmer någorlunda bra med DNS-data för låga Reynoldstal. I samtliga fall visar de erhållna resultaten en förbättring jämfört med standardmodeller som använder en virvelviskositet/diffusivitet.

Modellkoefficienterna härleds separat för vart och ett av de ovannämnda fallen tillsammans med vissa justeringar av modellen som krävs i vissa fall. Trots att en generell formulering fortfarande saknas har de resultat som presenteras i denna avhandling potential att förbättra beskrivningen av turbulens under inverkan av flytkrafter inom olika tillämpningsområden.

Preface

This thesis explores the possibilities of using explicit algebraic models to predict turbulent flows with stable stratification and other buoyancy-driven effects. The first part introduces some theoretical concepts of turbulence and turbulence modelling, and the effects of buoyancy on turbulence. The second part consists of one journal article and one internal report.

Paper 1. W.M.J. Lazeroms, G. Brethouwer, S. Wallin and A.V. Johansson, 2013
An explicit algebraic Reynolds-stress and scalar-flux model for stably stratified flows. *J. Fluid Mech.* **723**, 91-125

Paper 2. W.M.J. Lazeroms, G. Brethouwer, S. Wallin and A.V. Johansson, 2013
Explicit algebraic models for turbulent flows with buoyancy effects. *Internal Report*

Division of work between authors

The main advisor of the project is Prof. Arne V. Johansson (AJ) and the co-advisor is Dr. Geert Brethouwer (GB).

Paper 1

Model development, numerical simulations and writing of the article were carried out by Werner Lazeroms (WL). AJ and GB provided supervision and feedback on the article. The numerical solver used for the calculations was developed by Dr. Stefan Wallin (SW) and modified by WL with the help of SW. SW was also involved in discussions and provided feedback on the article.

Paper 2

Modification of the model and the resulting numerical simulations were carried out by WL. The article was written by WL with feedback given by AJ, GB and SW.

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Part I

Introduction

CHAPTER 1

Introduction

Turbulence is all around us. An illustrative (though very unhealthy) example is smoke coming from a cigaret, which nicely visualizes the typical chaotic structures of the turbulent flow surrounding it. On a larger scale, we can see similar flow structures in smoke coming out of a chimney. Going even further up into the sky, the typical shape of clouds reveals the presence of turbulence in the atmosphere, which is often experienced in airplanes.

Clearly, turbulent flows are associated with a vast range of different length (and time) scales, from everyday examples to the atmosphere. This makes the study of turbulent flow important for various applications. Within engineering, one can think of the reduction of turbulent drag on aircraft or other vehicles, or heat transfer through turbulent diffusion in heat exchangers. On the other hand, turbulence plays a significant role in the transfer of momentum and heat in the atmosphere, making its study relevant for weather and climate predictions as well.

Many textbooks on turbulence start with summarizing its complex nature. Quoting Pope (2000), “the flow is unsteady, irregular, seemingly random and chaotic, and surely the motion of every eddy or droplet is unpredictable.” Indeed, the governing equations of fluid motion, the Navier-Stokes equations, contain a number of nonlinear terms that lead to the chaotic dynamics of turbulent flows. A typical property of these flows is that they consist of larger eddies that break down into smaller eddies, leading to a large range of scales between the large-scale energy-containing flow structures and the smallest dissipative scales, the so-called Kolmogorov scales. Due to this large range of scales, it is very costly to accurately perform Direct Numerical Simulations (DNS) of turbulent flows, since an appropriate numerical grid needs to resolve everything down to the smallest scales. In fact, one can show that the required number of grid points scales with $Re_L^{9/4}$, where $Re_L = UL/\nu$ is the Reynolds number based on the large scales.[1] The Reynolds number typically ranges from 10^6 in engineering flows to 10^8 in the atmospheric boundary layer, which leads to grid requirements that are unfeasible for today’s computers.

In real-world applications, it is therefore impossible to perform full-scale DNS to study the effects of turbulence. These applications often rely on some

[1] In this definition, U and L are characteristic velocity and length scales of the large eddies and ν is the kinematic viscosity.

sort of modelling, for example Large-Eddy Simulations (LES), where only the larger eddies are resolved in combination with a model for the so-called subgrid scales. However, this still puts fairly high constraints on the required computer power, and sometimes modelling all the turbulent eddies is the only solution. This can be done by a statistical approach, in which one takes the average effect of all the eddies and solves equations for the mean flow quantities, the so-called Reynolds-averaged Navier-Stokes (RANS) equations. Appropriate models for the turbulence statistics are needed in order to close this system of equations, which is the focus of the field of RANS modelling.

Of particular interest are turbulent flows with heat transfer, which occur both in engineering and atmospheric applications. If changes in temperature and density are small enough, one can assume that the flow itself is not influenced by heat transfer. In such a case, we speak of the temperature as being a passive scalar. On the other hand, if the temperature gradients are significant, fluid particles experience a buoyancy force that influences the flow, in which case temperature acts as an active scalar. Finding an appropriate model for turbulent flows with buoyancy forces is important both for the atmospheric boundary layer and various industrial applications where such forces are no longer negligible.

The present thesis deals with the (RANS) modelling of turbulent flows with buoyancy forces. In particular, the work is based on the so-called explicit algebraic Reynolds-stress model (EARSM) by Wallin & Johansson (2000), which was extended to the explicit algebraic scalar-flux model (EASFM) for passive scalars by Wikström *et al.* (2000). In the case of buoyancy-affected flows, one needs to take into account the two-way coupling between velocity and temperature fluctuations, which is not present in the EARSM and EASFM. Various attempts have been made to devise an appropriate model for such flows (Mellor & Yamada 1982; Cheng *et al.* 2002; So *et al.* 2002, 2004; Violeau 2009), but a fully explicit, coordinate-free, self-consistent and robust formulation has not been found. The aim of the present work is to present a new model that satisfies these requirements.

The following chapters introduce basic theoretical and practical concepts and summarize the work. In chapter 2, we briefly present the governing equations of fluid motion and the RANS equations, and discuss some of the implications that the presence of buoyancy has for turbulent flows. Chapter 3 deals with the basic concepts of RANS modelling and puts the current work in the context of previously devised models. Chapter 4 provides a summary of the appended papers in Part II of the thesis. In chapter 5, we finish with some concluding remarks and an outlook of future research.

CHAPTER 2

Buoyancy effects in turbulent flows

In this chapter, we use the basic equations of fluid dynamics to introduce some concepts of the theory of turbulence. In particular, the focus will be on the effects of varying density and temperature, the buoyancy forces they exhibit, and the influence of such forces on turbulence.

2.1. Governing equations

The dynamics of fluids is based on three fundamental physical principles: conservation of mass, conservation of momentum and conservation of energy. In the case of a so-called Newtonian fluid, for which the shear stresses inside the fluid are proportional to the velocity gradient, these conservation laws can be described by the Navier-Stokes equations. Furthermore, we assume the flow to be incompressible, and density/temperature variations are considered to be small with respect to a reference state, so that the *Boussinesq approximation* can be used. The Navier-Stokes equations then take the following form:

$$\frac{\partial \widetilde{u}_j}{\partial x_j} = 0, \tag{2.1a}$$

$$\frac{\partial \widetilde{u}_i}{\partial t} + \widetilde{u}_j \frac{\partial \widetilde{u}_i}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial \widetilde{p}}{\partial x_i} + \nu \frac{\partial^2 \widetilde{u}_i}{\partial x_j \partial x_j} - \beta_T \widetilde{\theta} g_i, \tag{2.1b}$$

$$\frac{\partial \widetilde{\theta}}{\partial t} + \widetilde{u}_j \frac{\partial \widetilde{\theta}}{\partial x_j} = \kappa \frac{\partial^2 \widetilde{\theta}}{\partial x_j \partial x_j}, \tag{2.1c}$$

where $\widetilde{u}_i$ is the instantaneous velocity, $\widetilde{p}$ is the instantaneous pressure, and $\widetilde{\theta}$ is the instantaneous (potential) temperature. Moreover, g_i is the gravitational acceleration, ρ_0 is a (constant) reference density, ν is the kinematic viscosity, κ is the molecular heat diffusivity, and β_T is the thermal expansion coefficient. A detailed description of the equations above can be found in any fluid mechanics textbook (e.g. Kundu *et al.* 2012).

Equations (2.1) form a coupled system of second-order nonlinear partial differential equations, which makes the general description of fluid motion extremely complex. Of particular interest is equation (2.1b), describing conservation of momentum, and the nonlinear terms on its left-hand side that correspond to inertial forces. These nonlinear terms are responsible for the complicated chaotic nature of turbulent flows. Furthermore, one should note the last term on the right-hand side of (2.1b). This term corresponds to buoyancy forces, which couples the momentum equation to equation (2.1c) for the temperature. In other words, the temperature $\widetilde{\theta}$ acts as an *active scalar* that influences the flow field.

For modelling purposes, the chaotic motion of turbulent flows is best described by decomposing all instantaneous quantities into a mean part and a fluctuating part, the so-called *Reynolds decomposition.* This can be expressed as follows:

$$\widetilde{u}_i = U_i + u_i, \qquad \widetilde{p} = P + p, \qquad \widetilde{\theta} = \Theta + \theta, \tag{2.2}$$

in which (U_i, P, Θ) are the mean quantities and (u_i, p, θ) turbulent fluctuations. In theory, the mean quantities correspond to the ensemble average of (infinitely) many realizations of a turbulent flow. In the following, we shall denote this averaging procedure by an overbar, for example:

$$U_i = \overline{\widetilde{u}_i} = \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \widetilde{u}_i^{(k)}, \tag{2.3}$$

where $\widetilde{u}_i^{(k)}$ is a specific realization of the instantaneous flow field. This averaging operator is convenient for theoretical purposes because it has a number of mathematical properties, such as commutativity with differential operators (see, e.g., Nieuwstadt 1998; Wyngaard 2010). In practical situations, such as numerical simulations, one usually relies on (finite) time or space averages to calculate the mean quantities.

By using the Reynolds decomposition (2.2) in (2.1) and taking the average, one can derive the Reynolds-averaged Navier-Stokes (RANS) equations:

$$\frac{\partial U_j}{\partial x_j} = 0, \tag{2.4a}$$

$$\frac{\mathrm{D}U_i}{\mathrm{D}t} = -\frac{1}{\rho_0}\frac{\partial P}{\partial x_i} + \nu\frac{\partial^2 U_i}{\partial x_j \partial x_j} - \frac{\partial \overline{u_i u_j}}{\partial x_j} - \beta_T \Theta g_i, \tag{2.4b}$$

$$\frac{\mathrm{D}\Theta}{\mathrm{D}t} = \kappa\frac{\partial^2 \Theta}{\partial x_j \partial x_j} - \frac{\partial \overline{u_j \theta}}{\partial x_j}, \tag{2.4c}$$

in which $\mathrm{D}/\mathrm{D}t = \partial/\partial t + U_k \partial/\partial x_k$ is the material derivative along the mean flow. These equations form the basis of many turbulence models, but they also reveal some interesting theoretical facts. Comparing the RANS equations to the original Navier-Stokes equations (2.1), we see that they are almost identical except for two terms involving correlations between the velocity and temperature fluctuations, which appear due to the non-linear terms. The term involving $\overline{u_i u_j}$ in (2.4b) has the form of a stress term, and for this reason $\overline{u_i u_j}$ is referred to as the *Reynolds-stress tensor*. It describes the extra flux of momentum due to the turbulent velocity fluctuations. Similarly, $\overline{u_i \theta}$ in (2.4c) corresponds to the *turbulent heat flux* caused by the interaction of velocity and temperature fluctuations. However, both $\overline{u_i u_j}$ and $\overline{u_i \theta}$ are unknown quantities, which makes the set of RANS equations incomplete. This is the well-known closure problem of turbulence. For this reason, $\overline{u_i u_j}$ and $\overline{u_i \theta}$ need to be modelled, which will be discussed in more detail in the next chapter.

2.2. Scaling and dimensionless parameters

In fluid mechanics, one often makes use of scaling, dimensionless equations and dimensionless parameters that define different flow regimes. A widely applied scaling for wall-bounded turbulent flows uses the friction velocity u_τ, defined by:

$$u_\tau^2 = \frac{\tau_\mathrm{w}}{\rho_0} = \nu \left. \frac{\partial U}{\partial y} \right|_\mathrm{wall}, \tag{2.5}$$

where τ_w is the total shear stress at the wall, y is the wall-normal coordinate, and U is the mean velocity parallel to the wall. In this way, we can define dimensionless quantities in so-called *wall units*, e.g. $U_i^+ = U_i/u_\tau$ and $\overline{u_i u_j}^+ = \overline{u_i u_j}/u_\tau^2$. By also using a characteristic length scale δ (e.g. boundary-layer thickness in a boundary-layer flow or the half-width h in channel flow) and a characteristic temperature difference ΔT, equation (2.4b) can be put in the following dimensionless form:[1]

$$\frac{\mathrm{D}U_i^+}{\mathrm{D}\widetilde{t}} = -\frac{\partial P^+}{\partial \widetilde{x}_i} + \frac{1}{Re_\tau} \frac{\partial^2 U_i^+}{\partial \widetilde{x}_j \partial \widetilde{x}_j} - \frac{\partial \overline{u_i u_j}^+}{\partial \widetilde{x}_j} - Ri_\tau \widetilde{\Theta} \frac{g_i}{g}. \tag{2.6}$$

This scaling has given rise to two well-known dimensionless numbers within the field of wall-bounded stratified flows: the *friction Reynolds number* Re_τ and the *friction Richardson number* Ri_τ, defined as:

$$Re_\tau = \frac{u_\tau \delta}{\nu}, \qquad Ri_\tau = \frac{\beta_T g \Delta T \delta}{u_\tau^2}. \tag{2.7}$$

These parameters are often used to describe the strength of viscous forces and buoyancy forces, respectively (see, e.g., García-Villalba & del Álamo 2011). Another dimensionless parameter that often occurs in convection-dominated flows (Iida & Kasagi 1997; Kasagi & Nishimura 1997), and which is closely related to the aforementioned parameters, is the *Grashof number*:

$$Gr = \frac{\beta_T g \Delta T (2\delta)^3}{\nu^2} = 8 Re_\tau^2 Ri_\tau. \tag{2.8}$$

However, the viscous wall scaling described above is not appropriate in all wall-bounded flows. An alternative scaling for natural-convection flows is based on the molecular heat diffusivity κ, leading to a velocity scale κ/δ (Versteegh & Nieuwstadt 1999). Substituting this velocity scale for u_τ in (2.7) yields two new parameters governing the flow:

$$\frac{\kappa}{\nu} = Pr^{-1}, \qquad \frac{\beta_T g \Delta T \delta^3}{\kappa^2} = \tfrac{1}{8} H = \tfrac{1}{8} Pr\, Ra, \tag{2.9}$$

[1] We further define $\widetilde{x}_i = x_i/\delta$, $\widetilde{t} = u_\tau t/\delta$, $P^+ = P/(\rho_0 u_\tau^2)$, and $\widetilde{\Theta} = \Theta/\Delta T$.

in which Pr is the *Prandtl number* and Ra is the *Rayleigh number*. The parameter H is sometimes called the modified Rayleigh number. The Prandtl number also appears by applying viscous wall scaling to equation (2.4c).

2.3. Turbulent kinetic energy and temperature variance

Some aspects of turbulent flows can be conveniently described by a scalar quantity, the turbulent kinetic energy:

$$K = \tfrac{1}{2}\overline{u_k u_k}. \tag{2.10}$$

This quantity basically describes the total intensity of the velocity fluctuations. A transport equation for K can be derived by first considering the equations for the velocity fluctuations, which in turn are obtained by subtracting (2.4b) from (2.1b). After taking the inner product of these equations with u_i and averaging, the following is found:

$$\begin{aligned}\frac{\mathrm{D}K}{\mathrm{D}t} = &\underbrace{-\overline{u_i u_j}\frac{\partial U_i}{\partial x_j}}_{\mathcal{P}} \underbrace{- \nu\overline{\frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j}}}_{\varepsilon} \underbrace{-\beta_T g_j \overline{u_j \theta}}_{\mathcal{G}} \\ &\underbrace{-\frac{\partial}{\partial x_j}\left(\frac{1}{2}\overline{u_i u_i u_j} + \frac{1}{\rho_0}\overline{u_j p} - \nu\frac{\partial K}{\partial x_j}\right)}_{\mathcal{D}}.\end{aligned} \tag{2.11}$$

On the left-hand side of this equation, we have the advection term, whereas the right-hand side contains a shear production term $\mathcal{P}$ (which is usually positive), a dissipation term ε, a buoyancy production term $\mathcal{G}$, and a transport or diffusion term $\mathcal{D}$. Disregarding the transport term, which only redistributes kinetic energy in space, we see that the rate of change of K is governed by the interplay between (shear/buoyancy) production and (viscous) dissipation. Large-scale motions cause production of turbulent kinetic energy through mean shear (mean velocity gradients), while viscous dissipation takes place at small scales. This gives rise to the well-known energy cascade from large to small scales in (three-dimensional) turbulent flows.

In a similar fashion, we can describe the intensity of temperature fluctuations by defining the following quantity:

$$K_\theta = \tfrac{1}{2}\overline{\theta^2}, \tag{2.12}$$

which is half the variance of the temperature fluctuations. The equation for the temperature fluctuations, obtained by subtracting (2.4c) from (2.1c), can be used to derive the following transport equation for K_θ:

$$\frac{\mathrm{D}K_\theta}{\mathrm{D}t} = \underbrace{-\overline{u_j\theta}\frac{\partial \Theta}{\partial x_j}}_{\mathcal{P}_\theta} \underbrace{-\kappa\overline{\frac{\partial \theta}{\partial x_j}\frac{\partial \theta}{\partial x_j}}}_{\varepsilon_\theta} \underbrace{-\frac{\partial}{\partial x_j}\left(\frac{1}{2}\overline{u_j\theta^2} - \kappa\frac{\partial K_\theta}{\partial x_j}\right)}_{\mathcal{D}_\theta}. \tag{2.13}$$

From left to right, this equation contains an advection term, a production term $\mathcal{P}_\theta$, a dissipation term ε_θ and a transport/diffusion term $\mathcal{D}_\theta$. Once again, we can

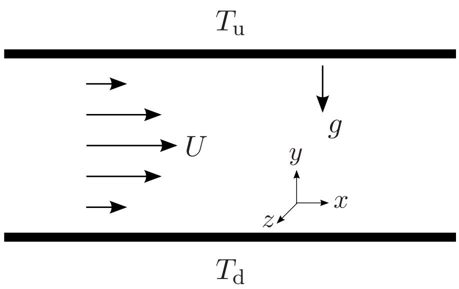

FIGURE 2.1. Geometry for the horizontal channel.

see that temperature fluctuations are produced due to the mean temperature gradient, which takes place at large scales, while the molecular diffusivity (in this case κ instead of ν) causes a dissipation at small scales.

The study of the nature of turbulent flows, scale separation and energy cascades is an extensive topic, and equations (2.11) and (2.13) only reveal very basic truths. It is beyond the scope of this work to step into more details; the reader is referred to any textbook on turbulent flows (e.g. Nieuwstadt 1998; Pope 2000; Wyngaard 2010).

2.4. The effect of buoyancy forces

Buoyancy forces can affect turbulent flows in different ways. First of all, there is a direct buoyancy forcing affecting the mean velocity field, described by the last term in equation (2.4b). Secondly, there are buoyancy effects on the level of the turbulent fluctuations, which in part can be described by the buoyancy term $\mathcal{G}$ in equations (2.11). In some flow cases, for example (natural) convection, the direct forcing can be the only driving force of the mean flow, or it can function as an auxiliary force that aids or opposes a pressure-driven flow. In other situations, the buoyancy force is perpendicular to the mean flow. We shall first investigate the latter case.

Consider a parallel shear flow $U_i = U(y)\delta_{i,x}$ in the horizontal direction with a temperature gradient in the vertical direction, aligned with gravity $g_i = -g\delta_{i,y}$. An example of such a flow geometry is shown in figure 2.1, and it can also be thought of as a simplified version of the situation found in the atmosphere (disregarding the earth's rotation). In this case, a buoyancy force only appears in the y-component of (2.4b), where it determines the cross-flow pressure distribution, so the horizontal velocity component is only driven by a streamwise pressure gradient.

However, we do retain the buoyancy contribution in equation (2.11), which now becomes:

$$\mathcal{G} = \beta_T g \overline{v\theta}. \tag{2.14}$$

The nature of the flow is now determined by the sign of $\mathcal{G}$, which is related to the direction of the temperature gradient. If $\partial\Theta/\partial y > 0$, a fluid parcel moving up ($v > 0$) transfers a lower temperature to a region with a higher temperature, giving rise to a negative temperature fluctuation ($\theta < 0$). This causes the correlation $\overline{v\theta}$ to be negative. From (2.14), we conclude that $\mathcal{G} < 0$ in this case, which means that buoyancy damps the production of turbulent kinetic energy. An simple way to understand this is the fact that the fluid parcel just considered will experience a downward buoyancy force, since it has a lower temperature than the surroundings. Hence, upward moving fluid parcels are pushed down by buoyancy, and vice versa, which explains the damping of vertical motion. This situation is referred to as *stable stratification*.

Stably stratified flows are thus characterized by the damping of turbulent fluctuations. This particular effect makes it difficult to correctly predict such flows with standard turbulence models. Furthermore, in the same flow there can be regions where the stratification effects are very high and other regions where they are negligible. One example is stable stratification in a horizontal channel such as depicted in figure 2.1, for which the damping of turbulence is small near the wall but high in the centre of the channel (García-Villalba & del Álamo 2011). Stable stratification also occurs in the atmosphere during nighttime conditions (Stull 2009). However, the true nature of stably stratified turbulence is very complex and cannot be described by (2.11) alone. Various studies show that vertical motions are damped much more than horizontal motions, leading to highly anisotropic turbulence and so-called pancake structures. This gives rise to a debate whether this type of turbulence is still three-dimensional, as well as questions concerning the direction of the energy cascade (see, e.g., Lindborg 2006; Brethouwer *et al.* 2007).

As mentioned in section 2.2, the strength of the buoyancy force can be described by the friction Richardson number Ri_τ when using viscous wall scaling. A more general form of this parameter is the *gradient Richardson number*, which can be defined as follows for the parallel shear flow in figure 2.1:

$$Ri = \frac{\beta_T g \dfrac{\partial \Theta}{\partial y}}{\left(\dfrac{\partial U}{\partial y}\right)^2}. \qquad (2.15)$$

This parameter follows from the ratio of $\mathcal{G}$ and $\mathcal{P}$ in equation (2.11) when one assumes $\overline{uv} \sim \partial U/\partial y$ and $\overline{v\theta} \sim \partial \Theta/\partial y$. Hence, it is a local measure of the strength of buoyancy compared to shear production. For stably stratified flows, we can now define a *critical Richardson number* Ri_c above which turbulence is completely damped and the flow becomes laminar. A classical result of linear stability theory found by Miles (1961) and Howard (1961) shows that $Ri_c = 1/4$.

A different type of flow is found for $\partial\Theta/\partial y < 0$, and the same reasoning as applied above reveals that $\overline{v\theta} > 0$ in this case. Equation (2.14) then shows that $\mathcal{G} > 0$, i.e. the production of turbulent kinetic energy is increased by buoyancy. In other words, upward moving fluid parcels experience an upward

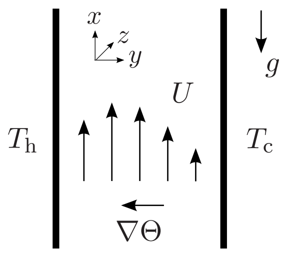

FIGURE 2.2. Geometry for the vertical channel.

buoyancy force, enhancing the vertical motions. In such *unstably stratified flows*, the convective motion caused by buoyancy enhances turbulent mixing. It typically occurs in the atmosphere during daytime conditions (Stull 2009). The convective effects caused by unstable stratification can be studied in the simplified geometry of a horizontal channel (Iida & Kasagi 1997).

We have seen that buoyancy can cause both an increase and a decrease of turbulent fluctuations. As mentioned, it can also act directly as a driving force of the flow. This can be illustrated in the case of a parallel shear flow $U_i = U(y)\delta_{i,x}$ in the vertical direction, with gravity $g_i = -g\delta_{i,x}$ perpendicular to the temperature gradient, as depicted in figure 2.2. For such a flow, the buoyancy force appears in the x-component of (2.4b), where it can act as a driving force of the mean flow together with the pressure gradient. In case buoyancy is the only driving force, we speak about *natural convection*, whereas *mixed convection* refers to a flow which is both pressure-driven and buoyancy-driven. The buoyancy production $\mathcal{G}$ in (2.11) is now determined by the streamwise turbulent heat flux $\overline{u\theta}$.

The case of mixed convection in a vertical channel with a heated and a cooled wall was studied by Kasagi & Nishimura (1997). In this case, one finds an upward, aiding buoyancy force on the heated side of the channel and a downward, opposing force on the cooled side. This causes a shift of the mean velocity maximum towards the heated wall as compared to channel flow without buoyancy. Furthermore, the streamwise heat flux $\overline{u\theta}$ is negative on the heated side and positive on the cooled side, resulting in damped velocity fluctuations ($\mathcal{G} < 0$) on the heated side and enhanced velocity fluctuations ($\mathcal{G} > 0$) on the cooled side. However, the opposite effect was found for the temperature fluctuations.

On the other hand, the same geometry with natural convection was investigated by Versteegh & Nieuwstadt (1998, 1999). Again, we have an upward buoyancy force at the heated wall and a downward buoyancy force at the cooled wall. In the absence of a streamwise pressure gradient, this causes a fully antisymmetric velocity profile, with an upflow on the heated side and a downflow on the cooled side. The streamwise heat flux $\overline{u\theta}$ is now positive throughout the channel, causing a positive buoyancy production $\mathcal{G}$. There is, however, a small region near the wall where the shear production $\mathcal{P}$ becomes negative.

Obviously, the presence of buoyancy in turbulent flows has many different features. For this reason, it is a challenge to devise a turbulence model that correctly describes all physical phenomena caused by buoyancy forces. The main concepts of turbulence modelling and the issues associated with it are the focus of the next chapter.

CHAPTER 3

Explicit algebraic turbulence models

The previous chapter introduced some of the basic concepts of the theory of turbulence that are needed for devising turbulence models. In particular, we presented the RANS equations (2.4) and explained that these equations are essentially incomplete. The only way to calculate the mean flow and mean temperature from these equations is to determine the Reynolds stresses $\overline{u_i u_j}$ and the turbulent heat flux $\overline{u_i \theta}$, for which we need suitable models. This is the topic of the current chapter, in which we also present a summary of our own work.

3.1. Model hierarchy

The search for an appropriate model for the Reynolds stresses and turbulent heat flux has had a long history, and numerous types of models with varying complexity exist today. The most simple formulation, which is still widely used, is the eddy-viscosity approach. Such models are based on a hypothesis postulated by Boussinesq (1877), who introduced the concept of an eddy viscosity ν_t as a coefficient of proportionality between the Reynolds shear stress $\overline{uv}$ and the mean strain rate, in analogy with the kinematic viscosity ν appearing in the viscous stress term. Similarly, one can introduce an eddy diffusivity κ_t to describe the turbulent heat flux as aligned with the mean temperature gradient, in analogy with the molecular heat diffusivity κ. Following this approach, the models can be expressed as follows:

$$\overline{u_i u_j} = -\nu_\mathrm{t} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + \tfrac{2}{3} K \delta_{ij}, \tag{3.1a}$$

$$\overline{u_i \theta} = -\kappa_\mathrm{t} \frac{\partial \Theta}{\partial x_i}. \tag{3.1b}$$

Unlike the constants ν and κ, which are fluid properties, ν_t and κ_t are non-constant coefficients that depend on the flow. Finding a closed formulation for $\overline{u_i u_j}$ and $\overline{u_i \theta}$ now amounts to modelling ν_t and κ_t. Standard eddy-viscosity/eddy-diffusivity models (EDM) are often classified according to the number of additional transport equations that are used. For example, a well-known two-equation model is the K-ω model by Wilcox (1993), which uses a transport equation for K based on (2.11) and a transport equation for the quantity ω, an inverse time scale related to the dissipation rate ε. The eddy viscosity is then modelled as $\nu_\mathrm{t} = K/\omega$. For the eddy-diffusivity one often takes $\kappa_\mathrm{t} = \nu_\mathrm{t}/Pr_\mathrm{t}$, where the turbulent Prandtl number Pr_t is given a constant value.

Even though the simplicity of EDMs makes them popular in various applications, the Boussinesq hypothesis is generally not valid. The anisotropic part of $\overline{u_i u_j}$ is not necessarily aligned with the mean strain-rate tensor, and the eddy-viscosity approach has been shown to fail in more complex flow situations. A more sophisticated class of models can be obtained by considering the transport equations of $\overline{u_i u_j}$ and $\overline{u_i \theta}$ themselves, which are obtained in a way similar to the derivation of (2.11) and (2.13). Symbolically, these transport equations can be written as:

$$\frac{\mathrm{D}\overline{u_i u_j}}{\mathrm{D}t} - \mathcal{D}_{ij} = \mathcal{P}_{ij} + \Pi_{ij} - \varepsilon_{ij} + \mathcal{G}_{ij}, \tag{3.2a}$$

$$\frac{\mathrm{D}\overline{u_i \theta}}{\mathrm{D}t} - \mathcal{D}_{\theta i} = \mathcal{P}_{\theta i} + \Pi_{\theta i} - \varepsilon_{\theta i} + \mathcal{G}_{\theta i}. \tag{3.2b}$$

In each of the equations above, we have terms describing, from left to right, advection, diffusion, (shear) production, pressure redistribution, dissipation, and buoyancy. Models that make use of (3.2) are called differential Reynolds-stress models (DRSM). Since some of these terms contain more unknown correlations (as a result of the closure problem), new model expressions are required, namely for the diffusion terms ($\mathcal{D}_{ij}$ and $\mathcal{D}_{\theta i}$), the pressure-redistribution terms (Π_{ij} and $\Pi_{\theta i}$), and the dissipation terms (ε_{ij} and $\varepsilon_{\theta i}$). For example, a widely used model for Π_{ij} was proposed by Launder *et al.* (1975), derived from the Poisson equation for the pressure fluctuations. Furthermore, in order to close the formulation of a DRSM, it should be used in conjunction with a suitable formulation for the dissipation rate ε of turbulent kinetic energy (e.g. the Wilcox (1993) K-ω model),[1] as well as equations for K_θ and ε_θ (see (2.13)).

Differential Reynolds-stress models are clearly more general than EDMs, and they have been shown to give a better description of the physics in more complex flow situations. However, the fact that many partial differential equations need to be solved makes it hard to handle a DRSM numerically. Therefore, we search for a compromise between the good physical description of DRSM and the simplicity of EDM, which is the main topic of the current work.

3.2. Explicit algebraic models

The transport equations (3.2) are differential equations by virtue of the advection and diffusion terms on the left-hand sides. Therefore, one way of dealing with the numerical issues of DRSMs would be to appropriately model these advection and diffusion terms in order to turn equations (3.2) into algebraic equations. Pioneering work for this modelling approach was performed by Rodi (1972, 1976), who postulated that the advection and diffusion of the dimensionless quantity $\overline{u_i u_j}/K$ could be neglected, assuming that dimensionless

[1] Note that the turbulent kinetic energy $K = \overline{u_k u_k}/2$ follows from the diagonal components of (3.2a).

quantities only vary slowly in space and time. This so-called *weak-equilibrium assumption* is a natural way of finding algebraic approximations of (3.2). More recently, the weak-equilibrium assumption has been applied to the Reynolds-stress anisotropy a_{ij}, defined as:

$$a_{ij} = \frac{\overline{u_i u_j}}{K} - \frac{2}{3}\delta_{ij}. \tag{3.3}$$

By rewriting the transport equations of an existing DRSM in terms of this quantity and neglecting the corresponding advection and diffusion terms, one obtains algebraic equations of the following form:[2]

$$N\boldsymbol{a} = \boldsymbol{\mathcal{L}}\left(\boldsymbol{a}; \boldsymbol{S}, \boldsymbol{\Omega}\right) \tag{3.4}$$

in which the right-hand side is a linear tensor function of $\boldsymbol{a}$, the mean strain-rate tensor $\boldsymbol{S}$ and the mean rotation-rate tensor $\boldsymbol{\Omega}$ (see, e.g., Wallin & Johansson 2000).

The (scalar) factor N on the left-hand side of (3.4) is related to the production-to-dissipation ratio of turbulent kinetic energy ($\mathcal{P}/\varepsilon = -\mathrm{tr}\{\boldsymbol{aS}\}$). Hence, the resulting (implicit) algebraic equations for $\boldsymbol{a}$ are nonlinear and generally have multiple roots, of which only one is the valid physical solution. This fact can lead to severe problems when using iterative numerical methods to solve the equations. In practice, therefore, a fully explicit solution of the algebraic equations is needed, i.e.:

$$\boldsymbol{a} = \boldsymbol{a}\left(\boldsymbol{S}, \boldsymbol{\Omega}\right). \tag{3.5}$$

A systematic method of finding such a solution was first proposed by Pope (1975), who used a linear expansion of $\boldsymbol{a}$ into ten tensor groups involving $\boldsymbol{S}$ and $\boldsymbol{\Omega}$. In this way, one can solve the linear part of (3.4) by further assuming the factor N to be known. The result is an expression of the following form:

$$\boldsymbol{a} = \beta_1 \boldsymbol{S} + \sum_{i=2}^{10} \beta_i \boldsymbol{T}^{(i)}, \tag{3.6}$$

in which the tensors $\boldsymbol{T}^{(i)}$ are symmetric, traceless combinations of $\boldsymbol{S}$ and $\boldsymbol{\Omega}$. Equation (3.6) clearly shows the advantage of an explicit algebraic model over a standard EDM. Except for the first term, the expansion contains terms that are not aligned with the mean strain-rate tensor. Furthermore, the coefficients β_i depend on scalar (or invariant) combinations of $\boldsymbol{S}$ and $\boldsymbol{\Omega}$, as well as N.

Since Pope (1975), the class of explicit algebraic models has been improved. A recently succesful example is the explicit algebraic Reynolds-stress model (EARSM) by Wallin & Johansson (2000) (also to be found in Johansson & Wallin 1996). The EARSM is derived from a DRSM with the pressure-redistribution model of Launder *et al.* (1975) and an isotropic dissipation term. The main advantage of this model is the use of the exact solution of N, resulting from a third-order polynomial equation, where previous models mainly

[2]Here we use matrix notation for tensors and vectors, i.e. $\boldsymbol{a} = (a_{ij})$, etc.

used ad-hoc assumptions for this quantity to obtain an explicit model. A similar result was obtained independently by Girimaji (1996). Using the exact expression for N results in a self-consistent formulation of the production-to-dissipation ratio $\mathcal{P}/\varepsilon$ and a correct asymptotic behaviour of this quantity for large strain rates.

In the case of passive scalars, the EARSM can be solved without any knowledge of the turbulent heat flux. An explicit algebraic model for the turbulent heat flux can then be found by considering the normalized heat flux ξ_i, defined as:

$$\xi_i = \frac{\overline{u_i\theta}}{\sqrt{KK_\theta}}. \tag{3.7}$$

Applying the weak-equilibrium assumption to this quantity leads to a new implicit algebraic equation for ξ_i, which also depends on a_{ij}. Wikström *et al.* (2000) presented an explicit algebraic scalar-flux model (EASFM) that can be obtained directly from $\boldsymbol{a}$ and the temperature gradient $\boldsymbol{\Theta}$ by inverting a matrix, leading to the following expression:

$$\boldsymbol{\xi} = -\boldsymbol{A}^{-1}\left(\boldsymbol{a} + \tfrac{2}{3}\boldsymbol{I}\right)\boldsymbol{\Theta}, \tag{3.8}$$

where $\boldsymbol{A}$ is a matrix involving $\boldsymbol{S}$ and $\boldsymbol{\Omega}$ and a scalar factor N_θ playing a role similar to N in the EARSM. As shown by Wikström *et al.* (2000), N_θ can be obtained either from a fourth-order polynomial equation, or directly from N by using a non-linear model for the terms $\Pi_{\theta i} - \varepsilon_{\theta i}$ in (3.2b). Compared to a standard EDM, equation (3.8) clearly gives a more general model for the heat flux that is not aligned with the temperature gradient.

In summary, the EARSM and EASFM yield fully explicit, coordinate-free, algebraic expressions for $\overline{u_iu_j}$ and $\overline{u_i\theta}$ that can be used to solve the RANS equations, together with suitable models for K, ε, K_θ and ε_θ. A correct treatment of the factors N and N_θ leads to a self-consistent formulation with a correct asymptotic behaviour for $\mathcal{P}/\varepsilon$. The explicit algebraic models capture most of the physics contained in a DRSM, but are easier to handle numerically. Nevertheless, the weak-equilibrium assumption is not generally valid, and explicit algebraic models may fail in regions with significant advection and diffusion (e.g. the near-wall region in wall-bounded flows). Several corrections exist to overcome such problems (also discussed by Wallin & Johansson 2000). Another important issue is the fact that approximating PDEs by algebraic equations may lead to singularities in the model, which puts certain constraints on model parameters (see Wikström *et al.* 2000).

3.3. Modelling buoyancy-affected flows

The discussion above focussed on passive scalars. For active scalars, there is a two-way coupling between equations (3.2a) and (3.2b) caused by the buoyancy term $\mathcal{G}_{ij}$. This coupling remains in the algebraic equations and it makes the search for an explicit algebraic solutions more complicated. A classical model of this type for atmospheric flows is the one by Mellor & Yamada (1982), who obtained a non-coordinate-free algebraic model based on scaling arguments.

More recently, coordinate-free expressions have been obtained by So *et al.* (2002, 2004) and Violeau (2009), which suffer from some important drawbacks. These are discussed in Lazeroms *et al.* (2013*b*), in which we devise a new explicit algebraic model by rewriting equations (3.2), including the buoyancy contributions, in terms of a_{ij} and ξ_i, and applying the weak-equilibrium assumption. This approach is a natural extension of the passive-scalar EARSM and EASFM, and it leads to implicit algebraic equations of the form:

$$N\boldsymbol{a} = \boldsymbol{\mathcal{L}}^{(a)}\left(\boldsymbol{a}, \boldsymbol{\xi}; \boldsymbol{S}, \boldsymbol{\Omega}, \boldsymbol{\Theta}, \boldsymbol{\Gamma}\right), \tag{3.9a}$$

$$N_\theta\boldsymbol{\xi} = \boldsymbol{\mathcal{L}}^{(\xi)}\left(\boldsymbol{a}, \boldsymbol{\xi}; \boldsymbol{S}, \boldsymbol{\Omega}, \boldsymbol{\Theta}, \boldsymbol{\Gamma}\right), \tag{3.9b}$$

which, in analogy to (3.4), contain linear functions on the right-hand sides, and non-linear terms on the left-hand sides. The vector $\boldsymbol{\Gamma}$ is related to the gravitational acceleration ($\Gamma_i \sim \beta_T g_i$). The factors N and N_θ are now related to the *total* production-to-dissipation ratio $(\mathcal{P} + \mathcal{G})/\varepsilon$.

Since equations (3.9) are mutually coupled, we need to solve for $\boldsymbol{a}$ and $\boldsymbol{\xi}$ simultaneously. This involves writing both quantities as a linear combination of basis tensors and basis vectors, respectively, in analogy to Pope (1975). As shown in Lazeroms *et al.* (2013*b*), a correct non-singular formulation for two-dimensional mean flows can be obtained by using ten tensor groups and eight vectors in the expansions, i.e.:

$$\boldsymbol{a} = \sum_{i=1}^{10} \beta_i \boldsymbol{T}^{(i)}, \qquad \boldsymbol{\xi} = \sum_{i=1}^{8} \lambda_i \boldsymbol{V}^{(i)}, \tag{3.10}$$

in which the symmetric, traceless tensors $\boldsymbol{T}^{(i)}$ and the vectors $\boldsymbol{V}^{(i)}$ involve the mean strain-rate tensor $\boldsymbol{S}$, the mean rotation-rate tensor $\boldsymbol{\Omega}$, the temperature gradient $\boldsymbol{\Theta}$, and the scaled gravitational vector $\boldsymbol{\Gamma}$. This approach is an improvement as compared to the model by Violeau (2009), who only used three basis tensors and two basis vectors, leading to singular coefficients in the limit of zero strain-rate. The coefficients β_i and λ_i are solved from a system of 18 linear equations, and they depend on invariant combinations of $\boldsymbol{S}$, $\boldsymbol{\Omega}$, $\boldsymbol{\Theta}$ and $\boldsymbol{\Gamma}$, as well as the unknown factors N and N_θ.

As in the model of Wallin & Johansson (2000) without buoyancy, the exact expressions for N and N_θ are needed to obtain a consistent formulation for the production-to-dissipation ratio. However, one can show that the equation for N is a sixth-order polynomial, for which no analytical solution exists. So *et al.* (2002, 2004) do not discuss this issue and solve the non-linear equations for $\mathcal{P}/\varepsilon$ and $\mathcal{G}/\varepsilon$ iteratively, which undermines the advantage of explicit algebraic models compared to DRSMs. In fact, one could argue that such a model is not explicit. Therefore, a fully explicit model for N and N_θ is preferred, and in Lazeroms *et al.* (2013*a*,*b*) we present methods to approximate the sixth-order polynomial equation for N such that an explicit expression can be found.

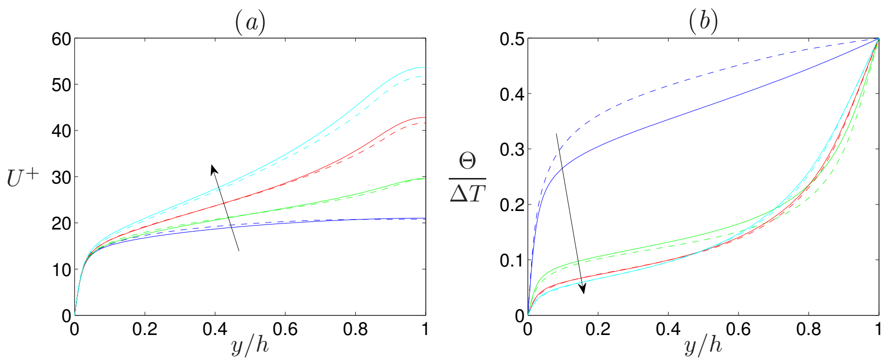

Figure 3.1. Comparison of the explicit algebraic model (dashed lines) with DNS by García-Villalba & del Álamo (2011) (solid lines) in stably stratified channel flow, for $Re_\tau = 550$ and $Ri_\tau = 0$ (blue), 120 (green), 480 (red), 960 (cyan). The arrows point in the direction of increasing Richardson number. Shown are (*a*) the mean velocity profile scaled with the friction velocity u_τ, and (*b*) the mean temperature profile scaled with the temperature difference between the walls ΔT. (Taken from Lazeroms *et al.* 2013*b*)

The result of this derivation is a fully explicit, coordinate-free and self-consistent algebraic model for the Reynolds stresses $\overline{u_i u_j}$ and the turbulent heat flux $\overline{u_i \theta}$ in the case of active-scalar flows. Taking into account some requirements for the model parameters in order to avoid singularities, the resulting model is robust for stably stratified parallel shear flows (Lazeroms *et al.* 2013*b*). Comparison with available DNS data shows that the model is well adapted to capture the effects of stable stratification in turbulent channel flow (figure 3.1).[3] For other flow cases in which convection plays a role, the robustness of the model is not guaranteed (Lazeroms *et al.* 2013*a*), posing a limit on the strength of the buoyancy forces. Nevertheless, the model is able to give reasonably good predictions in such flows, for example, a vertical channel with natural convection (figure 3.2), with moderate levels of convection, and some improvement over a standard EDM is obtained.

A more detailed discussion and further results can be found in the appended papers, which are summarized in the following chapter.

[3]The calculations have been performed with explicit algebraic models in combination with the Wilcox (1993) K-ω model, a transport equations for K_θ and, where appropriate, near-wall corrections. A description of the numerical solver is given in appendix A.

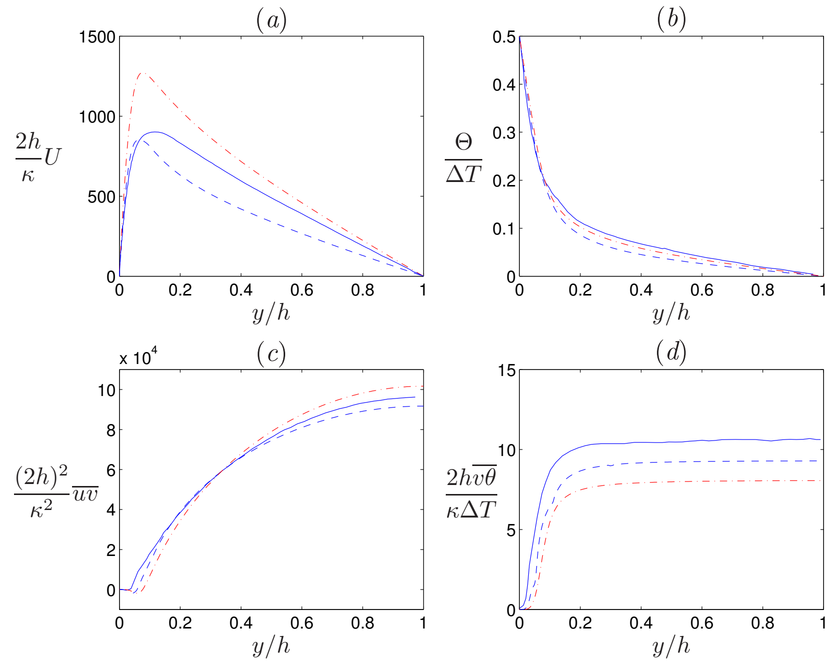

FIGURE 3.2. Comparison of the explicit algebraic model (dashed) with an eddy-diffusivity model (dashed-dotted) and the DNS by Versteegh & Nieuwstadt (1998, 1999) (solid) for the vertical channel with natural convection and $H = 4.254 \times 10^6$. Shown are: (a) mean velocity, (b) mean temperature, (c) Reynolds shear stress, (d) wall-normal heat flux. Only the heated half of the channel is shown. (Taken from Lazeroms *et al.* 2013*a*)

CHAPTER 4

Summary of the papers

Paper 1

An explicit algebraic Reynolds-stress and scalar-flux model for stably stratified flows.

Starting from the transport equations for the Reynolds stresses and the turbulent heat flux, we derive a framework for obtaining explicit algebraic turbulence models in the case of two-dimensional mean flows with buoyancy. The formulation consists of expanding the Reynolds-stress anisotropy and a normalized heat flux in terms of ten basis tensors and eight basis vectors, which are shown to give a complete, non-singular model. The coefficients in these expansions can be obtained from a system of 18 linear equations, presented in the paper.

The full expressions for the 18 coefficients are found in the specific case of parallel shear flows, in which the temperature gradient is aligned with gravity. These expressions are applied to stably stratified flows. In order to obtain a fully explicit, self-consistent model, the non-linear part of the algebraic equations needs to be solved through a sixth-order polynomial equation. Since an exact expression for the root of such an equation does not exist, we devise a method to approximate the root specifically for stably stratified flows. Furthermore, we discuss the use of a K-ω model to close the formulation, and the need for near-wall corrections to improve the model's predictions in wall-bounded flows.

The model is applied to two test cases: stably stratified homogeneous shear flow and stably stratified channel flow. Some parameters in the model are calibrated in order to optimize the results in these test cases, while others have been given specific values to avoid the occurrence of singularities. In the case of homogeneous shear flow, the model predicts a critical Richardson number of 0.25 above which turbulence decays, which is in good agreement with theoretical results. A comparison between the model results and DNS data is made for the channel-flow test case, and a very good agreement is obtained. We also show that the modelled root of the aforementioned sixth-order equation leads to an appropriate, self-consistent formulation. Finally, the realizability of the model is confirmed by means of the Lumley triangle.

Paper 2

Explicit algebraic models for turbulent flows with buoyancy effects.

This work considers two different geometries for parallel shear flows with buoyancy: the horizontal channel in which the temperature gradient is aligned with gravity (in the cross-flow direction), and the vertical channel in which the temperature gradient and gravity are perpendicular, with gravity in the streamwise direction. In both cases, explicit algebraic models for the Reynolds stresses and heat flux are derived, based on the framework established in Paper 1, and using a K-ω model to close the formulation.

The case of the horizontal channel was already considered in the previous paper specifically for stable stratification. Here we also investigate unstable stratification, for which some features of the model need to be modified. In particular, a different method is used for approximating the sixth-order polynomial equation. Comparisons with DNS data are shown for both stable and unstable stratification. Reasonably good predictions of the DNS are found for the unstably stratified case, which are also slightly better than the results of a standard EDM. Furthermore, the model is shown to be self-consistent.

For the vertical channel, we consider two test cases: mixed convection and natural convection. The 18 model coefficients for this geometry can be obtained directly from the linear system presented in the previous paper. Again, we show how to approximate the sixth-order polynomial equation, and some additional corrections to the model are presented. A comparison with DNS data reveals that the model predictions are reasonably good and there is some improvement over a standard eddy-viscosity/eddy-diffusivity model.

CHAPTER 5

Conclusion and outlook

The explicit algebraic models presented in this thesis give results that are promising for many important application areas. In particular, the results obtained for stably stratified channel flow show a very good agreement with the DNS data. Apparently, the damping of turbulence in the centre of the channel is well described by the model. This indicates that the model has great potential for improving, for example, atmospheric models with stably stratified conditions, in which the correct description of turbulence is still an issue.

Apart from stable stratification, the model was also applied to three other test cases that are characterized by convection (unstable stratification, and mixed and natural convection in a vertical channel). In general, the model results agreed reasonably well with the DNS data in these cases, and the results were slightly better than a standard EDM. However, one should note that the DNS data used for the unstably stratified horizontal channel and the two convection cases have a low Reynolds number, which means that the near-wall region consitutes a large part of the full width of the channel. For this reason, no near-wall corrections have been used in these cases, since they would be active in the entire channel. For higher Reynolds numbers, including such corrections will possibly improve the model predictions. Therefore, new DNS data for higher Reynolds numbers is needed for a proper model validation.

The aim of every modeller is, of course, to find the "perfect" model that is widely applicable. In the present work, we only considered specific cases of two-dimensional mean flows. An important issue is the approximation of the sixth-order equation for the factor N, which has been modelled using different methods for different test cases. A general formulation applicable to all test cases would be preferred, and this should be the subject of future research. The current approximations could already be implemented for use in a more general context if the different cases are selected in terms of the invariants that define the geometry.

Furthermore, the model parameters currently have been chosen to avoid singularities in the stably stratified cases. We also indicated that a singular behaviour for the three convective cases might be inevitable if the buoyancy forces are strong enough. One should, however, look into the equations and search for an analytical result in order to confirm this, which has not been done so far. Of further interest is the case of general two-dimensional mean flows, for which the model coefficients can be directly derived from the linear system presented in Lazeroms *et al.* (2013*b*), and which most probably will lead to more a complicated formulation and modified behaviour of the model.

As far as the applications are concerned, an interesting topic of future investigations is the implementation of the model in an existing atmospheric framework, and the comparison of the outcome to atmospheric data. In its current form, the model is suitable for a so-called single-column model in which the atmosphere is represented by a vertical column. Such a geometry is similar to the horizontal channel-flow cases represented in this thesis. It will also be interesting to investigate the behaviour of the model when rotational effects are included. The case of a vertical channel is mainly relevant for industrial applications with vertical boundary layers. These flows contain some particular features, especially in the near-wall region, and the ability of the model to capture these features needs to be investigated once DNS data for a higher Reynolds number is available.

APPENDIX A

Description of the numerical solver for 1-D PDEs

The calculations of which the results are presented throughout this work have been performed using the 1-D solver code, courtesy of Dr Stefan Wallin. Within this code, model equations can be conveniently expressed in Maple in a symbolic form. Specially written procedures discretize the implemented partial differential equations, and the FORTRAN code describing the numerical solver is automatically generated. Using this package, any system of PDEs of the form

$$\frac{\partial \boldsymbol{q}}{\partial t} = \boldsymbol{f}\left(\boldsymbol{q}, \frac{\partial \boldsymbol{q}}{\partial y}, \frac{\partial^2 \boldsymbol{q}}{\partial y^2}, \dots\right) \tag{A.1}$$

can be solved numerically for the vector of unknowns $\boldsymbol{q} = (q^1, q^2, \dots)$. Equation (A.1) is discretized using second-order central differences in the spatial domain and a second-order Crank-Nicholson scheme for time integration. This leads to the following discrete system:

$$\frac{\mathbf{q} - \mathbf{q}^{\text{old}}}{\Delta t} = s\mathbf{A}^*(\mathbf{q})\mathbf{q} + (1-s)\mathbf{A}^*\left(\mathbf{q}^{\text{old}}\right)\mathbf{q}^{\text{old}}, \tag{A.2}$$

where the Crank-Nicholson method is obtained for $s = 1/2$. For steady-state calculations, a first-order implicit Euler scheme ($s = 1$) is sufficient. At each timestep, $\mathbf{q}$ is obtained from the previous solution $\mathbf{q}^{\text{old}}$ by an interative method, which entails decomposing the matrix $\mathbf{A}^*$ in a (tridiagonal) implicit part $\mathbf{A}^{\text{impl}}$ and an explicit part $\mathbf{A}^{\text{expl}}$, i.e.:

$$\mathbf{A}^*(\mathbf{q})\mathbf{q} \to \mathbf{A}^{\text{impl}}(\mathbf{q}^j)\mathbf{q}^{j+1} + \mathbf{A}^{\text{expl}}(\mathbf{q}^j)\mathbf{q}^j,$$

for each iteration step j (within the same timestep). By including an underrelaxation $r < 1$, the iterative procedure can be written as follows:

$$\mathbf{q}^{j+1} = r\mathbf{A}^{-1}\mathbf{R} + (1-r)\mathbf{q}^j \tag{A.3}$$

with

$$\mathbf{A} = \mathbf{I} - s\Delta t\mathbf{A}^{\text{impl}}(\mathbf{q}^j),$$

$$\mathbf{R} = \mathbf{q}^{\text{old}} + s\Delta t\mathbf{A}^{\text{expl}}(\mathbf{q}^j)\mathbf{q}^j + (1-s)\Delta t\left\{\mathbf{A}^{\text{impl}}(\mathbf{q}^{\text{old}}) + \mathbf{A}^{\text{expl}}(\mathbf{q}^{\text{old}})\right\}\mathbf{q}^{\text{old}}.$$

The simulations are performed on a collocated grid $(y_0, \dots, y_{N+1})$ with the boundaries at y_1 and y_N. The solution vector $\mathbf{q} = (q^1_0, \dots, q^1_N, q^2_0, \dots, q^2_N, \dots)$ is specified in between gridpoints. Typically, $N = 201$ gridpoints clustered in the near-wall region have been used in the present work.

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