TransAT

Handbook Series

Turbulence Modelling & Simulation

Version 5.7.1

Overview

This document is meant to introduce the basic routes employed within TransAT for the modelling and simulation of turbulent fluid flow and scalar convection, without exploring the foundations and model derivations. We briefly present the transport equations and models for RANS and Scale-resolving strategies, including LES and V-LES. The document presents in addition a thorough description of near wall treatment on both approaches. Only the models that have been validated are presented in this document. The extension of these models for multiphase turbulent flows is not treated here. Examples of applications of the models and strategies can be found in internal reports available on the webpage.

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Chapter 1

Statistical Turbulence Modelling (RANS)

In this Chapter, the Reynolds-averaged equations for all quantities used in TransAT are presented. The initial equations, on which Reynolds averaging is applied, are presented in the Equations and Algorithms manual, Chapter Incompressible Navier-Stokes Equations .

1.1 Reynolds Averaging Procedure

According to the Reynolds flow-decomposition procedure, a flow variable ϕ can be expressed as the sum of an average and a fluctuating quantity:

$$\begin{aligned} \phi = \overline{\phi} + \phi'. \quad \phi = v_i,\, p,\, T\,, ...; \\ v_i = \overline{v_i} + u_i'\,; \quad p = \overline{p} + p'; \quad T = \overline{T} + \theta' \end{aligned} \tag{1.1}$$

where $\overline{\phi}$ is further taken to be the ensemble average of ϕ and ϕ' is the fluctuation around this mean ($\overline{\phi'} = 0$). Before proceeding further, it is necessary to recall the statistical rules of Reynolds averaging, often referred to as *Reynolds conditions*, which any two flow variables ϕ and ψ must obey:

$$\begin{aligned} \overline{\psi + \phi} = \overline{\psi} + \overline{\phi}; \quad \overline{a\,\psi} = a\,\overline{\psi} \quad (\text{a} = \text{const.}), \\ \overline{\frac{\partial \phi}{\partial t}} = \frac{\partial \overline{\phi}}{\partial t}; \quad \overline{\frac{\partial \phi}{\partial x_j}} = \frac{\partial \overline{\phi}}{\partial x_j}; \quad \overline{\phi}\,\overline{\psi} = \overline{\psi}\,\overline{\phi}, \end{aligned} \tag{1.2}$$

and

$$\begin{aligned} \overline{\phi'} = \overline{\psi'} = 0, \\ \overline{\phi\,\psi} = \overline{\phi}\,\overline{\psi} + \overline{\phi'\,\psi'}, \\ \overline{\phi'\,\overline{\psi}} = \overline{\psi'\,\overline{\phi}} = 0. \end{aligned} \tag{1.3}$$

1.2 The Reynolds Averaged Navier-Stokes Equations

For constant density and viscosity, Reynolds averaging, applied to the system of instantaneous equations of conservation yields the Reynolds averaged mass and momentum conservation equations, known as the Reynolds Averaged Navier-Stokes Equations (RANS):

$$\frac{\partial \overline{v_i}}{\partial x_i} = 0 \tag{1.4}$$

$$\frac{D\overline{v_i}}{Dt} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \nabla^2 \overline{v_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i; \quad i = 1,2,3 \tag{1.5}$$

where $\tau_{ij} \equiv \overline{u_i' u_j'}$ stands for the Reynolds-stress tensor (which is symmetric, i.e. $\tau_{ij} = \tau_{ji}$) representing the contribution of the turbulent motion generated by velocity fluctuations to the mean stress tensor in momentum equations. This turbulent motion will in turn result in an increase of momentum exchange and mixing. The off-diagonal components of τ_{ij}, or shear stresses ($\overline{u'v'}, \overline{v'w'}$, and $\overline{u'w'}$), prevail in theory in the transport of mean momentum by turbulent motion, while the diagonal terms, or normal stresses ($\overline{u'^2}, \overline{v'^2}$, and $\overline{w'^2}$), only play a minor role.

1.3 The Reynolds Averaged Energy Equation

The equation of energy conservation can be averaged with respect to time and solved together with the equations describing the mean flow and turbulence. If this equation is written for the temperature, the Reynolds-averaging procedure applied to T yields

$$\rho c_p \frac{D\overline{T}}{Dt} = \frac{\partial}{\partial x_j} \underbrace{\left(\lambda \frac{\partial \overline{T}}{\partial x_j} - \rho c_p \overline{u_j' \theta'} \right)}_{-q''_{total}} \tag{1.6}$$

where $q''_{total} = q''_j + Q''_j$ is the total rate of heat transfer due to both molecular and turbulent motions, and $Q''_j = -\rho c_p \overline{u_j' \theta'}$ represents the turbulent heat-flux.

To solve the system of RANS equations 1.4, 1.5 and 1.6, where each barred quantity represents a Reynolds average, we can take two avenues: Either the turbulent stresses and heat fluxes are determined individually by solving a set of transport equations for each component (a total of six + three), or one introduces proper closure relations for τ_{ij} and the turbulent heat-flux Q''_j. The closure relations must provide a physically coherent representation of turbulence mechanisms.

1.4 The Reynolds Averaged Scalar Equation

In the same way as Navier-Stokes equations, the scalar transport equations can be averaged using the Reynolds-averaging procedure. This gives the following equation

$$\frac{D\,\overline{C}}{Dt} \;=\; \frac{\partial}{\partial x_j}\left(\mathcal{D}\frac{\partial \overline{C}}{\partial x_j}\right) - \frac{\partial}{\partial x_j}\left(\overline{c'u'}\right) + \overline{F}_C \tag{1.7}$$

where $\mathcal{D}$ is the molecular diffusivity, $\overline{u'c'}$ is the turbulent scalar transport and $\overline{F}_C$ is the averaged source term applied to the scalar.

1.5 The Reynolds Stress Equations

The Reynolds stress, τ_{ij} can also be determined by solving its own transport equation. A special notation is introduced for this purpose, namely the Navier-Stokes operator $\mathcal{L}(u_i')$ producing the fluctuating–momentum equations

$$\mathcal{L}(u_i') \;=\; \frac{Du_i'}{Dt} + \frac{1}{\rho}\frac{\partial p'}{\partial x_i} - \nu\,\nabla^2 u_i' = 0 \tag{1.8}$$

This operator helps to directly derive an equation for the Reynolds stress tensor through construction of the following second order moment:

$$\overline{u_j'\,\mathcal{L}(u_i') \;+\; u_i'\,\mathcal{L}(u_j')} \;=\; 0 \tag{1.9}$$

After some calculations, one arrives at the Reynolds-stress transport equations:

$$\frac{D\tau_{ij}}{Dt} \;=\; P_{ij} + \Pi_{ij} - \varepsilon_{ij} + \frac{\partial}{\partial x_k}\left[\nu\frac{\partial \tau_{ij}}{\partial x_k} - C_{ijk}\right] \tag{1.10}$$

where

$$P_{ij} = -\,\tau_{ik}\,\frac{\partial \overline{v_j}}{\partial x_k} -\; \tau_{jk}\,\frac{\partial \overline{v_i}}{\partial x_k} \tag{1.11}$$

$$\Pi_{ij} \equiv \overline{p'\left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right)} \tag{1.12}$$

$$\varepsilon_{ij} \equiv \overline{2\mu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k}} \tag{1.13}$$

$$C_{ijk} \equiv \overline{\rho\, u_i' u_j' u_k'} + \overline{p' u_i'}\, \delta_{jk} + \overline{p' u_j'}\, \delta_{ik} \tag{1.14}$$

designate, respectively, the mechanical production of turbulence P_{ij}, or the source of Reynolds stress, the pressure-strain correlation or inter-component transfer term Π_{ij}, the dissipation (by the action of viscosity) rate tensor ε_{ij}, and the turbulent transport term (C_{ijk}), acting in addition to the molecular diffusion of τ_{ij} represented by $\nu \nabla^2 \tau_{ij}$.

The pressure-strain term Π_{ij}, gives rise to isotropy of the turbulence field by redistributing the turbulent kinetic energy among its three components and by reducing the shear stresses (Hinze, 1975).

1.6 The Dissipation Term

A typical practice in modelling the energy dissipation term ε_{ij} (Eq. 1.13) is to assume that the dissipative eddies are isotropic (Hinze, 1975) and thus

$$\varepsilon_{ij} = \frac{2}{3} \varepsilon \delta_{ij}\,; \quad \varepsilon \equiv \frac{1}{2} \varepsilon_{ii} = \nu \overline{\frac{\partial u_i'}{\partial x_k} \frac{\partial u_i'}{\partial x_k}} \tag{1.15}$$

This hypothesis, known as the Kolmogorov assumption of local isotropy, supposes that small turbulent structures associated with the rate of dissipation do not have a preferential direction. First, a transport equation for the dissipation rate tensor ε_{ij} has to be established. For the sake of brevity we restrict ourselves to the exact transport equation for ε itself (not for ε_{ij}), which can formally be obtained by constructing the moment:

$$2\nu \overline{\frac{\partial u_i'}{\partial x_j} \frac{\partial \mathcal{L}(u_i')}{\partial x_j}} = 0 \tag{1.16}$$

The equation takes the form

$$\frac{D\varepsilon}{Dt} = P_{\varepsilon 1} + P_{\varepsilon 2} + \Phi_\varepsilon + \mathcal{D}_\varepsilon + \nu \nabla^2 \varepsilon \tag{1.17}$$

where

$$P_{\varepsilon 1} = -2\,\nu\,\frac{\partial \overline{v_i}}{\partial x_j}\left(\overline{\frac{\partial u'_k}{\partial x_i}\frac{\partial u'_k}{\partial x_j} + \frac{\partial u'_i}{\partial x_k}\frac{\partial u'_j}{\partial x_k}}\right) \qquad (1.18)$$

$$-2\,\nu\,\overline{u'_k\frac{\partial u'_i}{\partial x_j}\frac{\partial^2 \overline{v_i}}{\partial x_j\,\partial x_k}}$$

$$P_{\varepsilon 2} = -2\,\nu\,\overline{\frac{\partial u'_k}{\partial x_i}\frac{\partial u'_k}{\partial x_j}\frac{\partial u'_i}{\partial x_j}} \qquad (1.19)$$

$$\Phi_\varepsilon = -2\,\nu^2\,\overline{\left(\frac{\partial^2 u'_i}{\partial x_j\,\partial x_k}\right)^2} \qquad (1.20)$$

$$\mathcal{D}_\varepsilon = -2\,\nu\,\frac{\partial}{\partial x_j}\left(\overline{\frac{\partial p'}{\partial x_i}\frac{\partial u'_j}{\partial x_i}} + \overline{\frac{u'_j}{2}\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_i}{\partial x_k}}\right) \qquad (1.21)$$

correspond to the following physical processes: The production by the mean motion (i.e by the mean velocity gradients) $P_{\varepsilon 1}$, the generation rate of vorticity fluctuations through the self-stretching of vortex tubes $P_{\varepsilon 2}$, the decay or destruction of the dissipation Φ_ε through the action of viscosity, and the turbulent diffusion of dissipation $\mathcal{D}_\varepsilon$ (diffusion by molecular effects is represented by $\nu\nabla^2\varepsilon$).

1.7 The Turbulent Kinetic Energy

A modelled version of the exact transport equation (1.10) can be derived, by letting $k \equiv \tau_{ii}/2$:

$$\frac{Dk}{Dt} = \underbrace{-\tau_{ij}\frac{\partial \overline{v_i}}{\partial x_j}}_{\mathcal{P}} - \varepsilon - \frac{\partial}{\partial x_j}\left(\tfrac{1}{2}\overline{u'_i u'_i u'_j} + \overline{p' u'_j}\right) + \nu\nabla^2 k \qquad (1.22)$$

In this equation, $\mathcal{P} \equiv P_{ii}/2$ represents the mechanical production of turbulence due to the interaction between turbulent stresses and mean velocity gradients. Note also that the contraction of τ_{ij} yields $\Pi_{ii} = 0$ by virtue of $\overline{u'_{i,i}} = 0$.

1.8 Chemical species equations

Chemical species transport equations are modelled using their respective mass fraction Y_k, where k represents the species index. When the species have different densities, the usual Reynolds average

gives new unclosed terms $\overline{\rho' u_j'}$ in the mass balance equation corresponding to the correlation between density and velocity fluctuations. To avoid this difficulty, mass-weighted averages (called Favre averages) are usually preferred

$$\widetilde{f} = \frac{\overline{\rho f}}{\overline{\rho}} \tag{1.23}$$

where f is a generic quantity. Splitting Y_i into a Favre mean $\widetilde{Y_i}$ and a fluctuation Y_i'' the transport equation can be written

$$\overline{\rho}\frac{D\widetilde{Y_k}}{St} = \frac{\partial}{\partial x_j}\left(\overline{(\rho D_k \nabla Y_k)}\right) - \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{\mathbf{v}''Y_k''}\right) + \overline{\rho}\widetilde{S_k} \tag{1.24}$$

where D_k is the molecular diffusion coefficient for species k and $\widetilde{S_k}$ is the Favre average of the source term.

Chapter 2

Two-Equation Turbulence Models

There are different ways to model the Reynolds–stress tensor τ_{ij} (when the transport equations of τ_{ij} are not solved explicitly). The best-known approach and the most practical one is based on the eddy viscosity concept or Boussinesq Hypothesis, which assumes that the Reynolds stress is decomposed into an isotropic and a deviatoric part,

$$\tau_{ij} = \frac{2}{3}\,\delta_{ij}k - 2\,\nu_t\,S_{ij}; \quad S_{ij} = \frac{1}{2}\,(\overline{v}_{i,j} + \overline{v}_{j,i}) \tag{2.1}$$

where $\delta_{ij} = 1$ for $i = j$, and zero otherwise. The deviatoric part (2nd term in the RHS of Eq. (2.1)) is a symmetric, traceless tensor and links τ_{ij} linearly to the rate–of–strain tensor S_{ij}. The coefficient of proportionality, ν_t, designates the eddy viscosity (or turbulent viscosity), which is a characteristic of the flow.

2.1 The Standard $k-\varepsilon$ Turbulence Model

In the $k-\varepsilon$ model (Launder & Spalding, 1974), the local state of turbulence is characterised by kinetic energy k and its dissipation rate ε. The combination of $\ell_0 \approx k^{3/2}/\varepsilon$ and $\tau_0 \approx k/\varepsilon$ (or ℓ_0 and $v_I \equiv \sqrt{k}$) leads to the generalised form of the isotropic eddy viscosity ν_t:

$$\nu_t \equiv \ell_0 v_I \equiv \ell_0^2/\tau_0 = C_\mu k^2/\varepsilon \tag{2.2}$$

where C_μ is a constant. The distribution of turbulent kinetic energy k and its rate of dissipation ε appearing in this relation are determined from the following model transport equations:

$$\frac{Dk}{Dt} = \frac{\partial}{\partial x_j}\left(\frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right) + \mathcal{P} - \varepsilon \tag{2.3}$$

$$\frac{D\varepsilon}{Dt} = \frac{\partial}{\partial x_j}\left(\frac{\nu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right) + C_{\varepsilon 1}\mathcal{P}\frac{\varepsilon}{k} - C_{\varepsilon 2}\frac{\varepsilon^2}{k} \tag{2.4}$$

The reader should refer to Launder & Spalding (1974) for a better understanding of the derivation of the model from the exact transport equations. The empirical constants are assigned the following standard values: $C_\mu = 0.09$; $C_{\varepsilon 1} = 1.44$; $C_{\varepsilon 2} = 1.92$; $\sigma_k = 1.$ and $\sigma_\varepsilon = 1.3$. The standard model (Eqs. 2.2 - 2.4) with its original coefficients is valid only in flow regions away from solid boundaries (high-Re-number flow regions), and depending on whether it is to be employed in low- or high-Re forms, special near-wall treatments are needed..

2.2 The RNG $k-\varepsilon$ Turbulence Model

The RNG $k-\varepsilon$ model, is more advanced than standard model and was derived from renormalization group theory. The distribution of turbulent kinetic energy k and its rate of dissipation ε appearing in this relation are determined from the following model transport equations:

$$\frac{Dk}{Dt} = \frac{\partial}{\partial x_j}\left(\frac{\nu_{eff}}{\sigma_k}\frac{\partial k}{\partial x_j}\right) + \mathcal{P} - \varepsilon \tag{2.5}$$

$$\frac{D\varepsilon}{Dt} = \frac{\partial}{\partial x_j}\left(\frac{\nu_{eff}}{\sigma_e}\frac{\partial \varepsilon}{\partial x_j}\right) + C_{\varepsilon 1}\mathcal{P}\frac{\varepsilon}{k} - C_{\varepsilon 2}\frac{\varepsilon^2}{k} - C_\mu \eta^3(1-\eta/\eta_0)/(1+\beta\eta^3)\frac{\varepsilon^2}{k} \tag{2.6}$$

where $\eta = Sk/\varepsilon$; $\eta_0 = 4.38$; $\beta = 0.012$ and S denotes strain rate $S = \sqrt{2S_{ij}S_{ij}}$. Effective viscosity instead of turbulent viscosity is used here:

$$\nu_{eff} = \nu\,(1 + k\sqrt{\frac{C_\mu}{\nu\varepsilon}})^2 \tag{2.7}$$

The empirical constants are assigned the following standard values: $C_\mu = 0.0845$; $C_{\varepsilon 1} = 1.42$; $C_{\varepsilon 2} = 1.68$; $\sigma_k = 0.71942$ and $\sigma_\varepsilon = 0.71942$. The RNG model (Eqs. 2.5 - 2.7) with its original coefficients is valid only in flow regions away from solid boundaries (high-Re-number flow regions), and depending on whether it is to be employed in low- or high-Re forms, special near-wall treatments are needed. In the energy/temperature equation a new formula for heat diffusion coefficient is employed which is also valid only for high-Re-number flow:

$$k_{eff} = 1.3929\, c_p \nu_{eff} \rho \tag{2.8}$$

In the mass transfer equations/concentration equations a new formula for mass diffusivity is employed:

$$D_{eff} = 1.3929\,\nu_{eff} \tag{2.9}$$

2.3 Extensions to $k-\varepsilon$ Turbulence Model

Depending on the flow conditions, different extensions to the basic $k-\varepsilon$ model have been proposed.

2.3.1 Yap correction

The Yap correction (Yap, 1987) consists of an additional source term of the form ρS_ε to the right hand side of the epsilon equation. The source term can be written as,

$$\rho\, S_\epsilon = 0.83\,\rho\,\frac{\varepsilon^2}{k}\left(\frac{k^{1.5}}{\varepsilon\, l_e} - 1\right)\left(\frac{k^{1.5}}{\varepsilon\, l_e}\right)^2 \tag{2.10}$$

where,

$$l_e = c_\mu^{-0.75}\,\kappa\, y_n \tag{2.11}$$

with y_n being the normal distance to the nearest wall.

The Yap correction is active in non-equilibrium flows and tends to reduce the departure of the turbulence length scale from its local equilibrium level. Yap (1987) showed improved results with the $k-\varepsilon$ model in separated flows when using this extra source term.

2.3.2 Swirl correction

The turbulent eddy viscosity is corrected for strongly swirling flows because the standard $k-\varepsilon$ models tend to overestimate turbulent diffusion for swirling flows. The eddy viscosity is modified using a swirl correction factor, f_{sw}, as follows (Shih *et al.*, 1997),

$$\nu_t = f_{sw} C_\mu \frac{k^2}{\varepsilon} \tag{2.12}$$

where,

$$f_{sw} C_\mu = \frac{1}{4.0 + A_S \dfrac{kU^*}{\varepsilon}} \tag{2.13}$$

and

$$A_S \;=\; \sqrt{6}\cos(\phi)$$

$$\begin{aligned}
\phi &= \frac{1}{3}\arccos(\sqrt{6}W^*) \\
W^* &= \frac{S_{ij}S_{jk}S_{ki}}{S^3} \\
U^* &= \sqrt{S^2+\Omega^2} \\
S &= \sqrt{S_{ij}S_{ij}} \\
\Omega &= \sqrt{\Omega_{ij}\Omega_{ij}}
\end{aligned}$$

2.3.3 Compressible correction

Initially turbulence models were designed for low-speed, isothermal flows. The compressibility correction is devised to deal with additional effects seen for higher Mach number flows, specifically, the effects of compressibility on the dissipation rate of the turbulence kinetic energy. For free shear flows, this is exhibited as the decrease in growth rate in the mixing layer with increasing Mach number. Standard turbulence models do not account for this Mach number dependence, and thus a compressibility correction is used. For compressible flows, two extra terms, known as the dilatation dissipation, ε_d, and the pressure-dilatation occur in the turbulence kinetic energy equation. The pressure-dilatation term is usually neglected because its contributions have been shown to be small (Wilcox, 1993).

The dilatation dissipation term is included in addition to the solenoidal, or incompressible, dissipation, ε. Thus, the effect is that the growth rate of turbulence is inhibited when the correction is active. Sarkar *et al.* (1991) modeled the ratio of the dilatation dissipation to the solenoidal dissipation, $\varepsilon_d/\varepsilon$, as a function of the turbulence Mach number, M_t, defined as

$$M_t^2 = \frac{2k}{c^2} \tag{2.14}$$

where c is the speed of sound. For the model by Sarkar *et al.* (1991), the additional source term to the k equation is,

$$\rho\varepsilon_d = \rho\varepsilon\, M_t^2 \tag{2.15}$$

Chapter 3

Near–Wall Modelling

3.1 Near–Wall Treatment in High–Re Flows

The near-wall treatment to be presented next applies strictly to the standard $k-\varepsilon$ model (Eqs. 2.2 - 2.4), Their combination is referred to as the *high-Re* $k-\varepsilon$ *model*. This near-wall modelling consists in bridging the viscous sub layer, i.e. the first grid point must be located outside this zone.

3.1.1 Standard Wall–Function Approach

At a rigid boundary, the no-slip condition in setting the velocity of the fluid to zero (or to that of the wall to account for moving-boundaries) is used for laminar flows. In high-Re flows, the wall-function approach, whose theoretical basis is discussed next, is applied in place of the no-slip condition. This treatment is based on two assumptions: (i) The immediate near-wall region is in a state of local equilibrium ($\mathcal{P}=\varepsilon$), and (ii) the velocity profile merges with the "log-law" given by

$$U^+ = \frac{\overline{u}}{u_\tau} = \frac{1}{\kappa}\, ln\,(E\, y^+) \tag{3.1}$$

However one needs to make the extra assumption , that, the equilibrium layer near the surface, where production balances dissipation, is one-dimensional and the stress across is constant. In these circumstances, it can be demonstrated that

$$\frac{k_p}{u_\tau^2} = \frac{1}{C_\mu^{1/2}} \quad \text{or} \quad u_\tau = k_p^{1/2}\, C_\mu^{1/4} \tag{3.2}$$

where the subscript p refers to the first control volume centre relative to the wall. Laboratory data for flow over smooth surfaces indicate that $k_p/u_\tau^2 \approx 3.3$, and hence $C_\mu \approx 0.09$. In a second step and making use of (3.2) we can relate the induced retarding wall shear-stress $\vec{\tau}_w$ to the velocity vector $\vec{V}_p$ by

$$\vec{\tau}_w = -\lambda_w \vec{V}_p \tag{3.3}$$

where

$$\lambda_w = \begin{cases} \mu/y_p & \text{if } y_p^+ < 11.6 \\ \rho\, C_\mu^{1/4} \mathrm{k}_p^{1/2} \kappa / \ln(E y_p^+) & \text{otherwise} \end{cases} \tag{3.4}$$

with

$$y_p^+ = \rho\, C_\mu^{1/4} \mathrm{k}_p^{1/2} y_p/\mu, \qquad \kappa = 0.41 \tag{3.5}$$

Furthermore, the diffusive flux of k is equal to zero at the wall. In a second step, the wall shear-stress (supposed to be uniform and equal to that at the wall, $y \geq y_w$) acting at a distance $y_n = 2y_p$ from the wall induces a rate of turbulence production given by

$$\mathcal{P}_w = -\frac{1}{y_n} \int_{y_w}^{y_n} \tau_w \left.\frac{\partial \overline{u}}{\partial y}\right|_w dy = \frac{\tau_w^2}{\kappa \mu y_p^+} \tag{3.6}$$

This quantity ($\mathcal{P}_w$) has to replace the production term $\mathcal{P}$ in the transport equation of k (2.3). Likewise, over the fully turbulent region ($y_w \leq y \leq y_n$) where k was taken to be uniform (in the pace interval $y_w \leq y \leq d_p$), the mean value of ε_w can be obtained by the expression

$$\varepsilon_w = \frac{1}{y_n} \int_{y_w}^{y_n} C_\Delta \frac{k_p^{3/2}}{y} \cdot dy = \frac{C_\mu^{3/4} \mathrm{k}_p^{3/2}}{\kappa y_p} \tag{3.7}$$

It should be noted, however, that since the assumption of "local equilibrium" near the wall is not justifiable in the viscous sub layer ($y_p^+ < 11.6$), the wall-function approach requires the value of y_p^+ at the cell adjacent to the wall to fall in the range $11.6 \leq y_p^+ \leq 200 - 500$, otherwise, the result is systematically biased.

3.1.2 Two–layer turbulence models

The two–layer approach adopted here consists of resolving the viscosity–affected regions close to walls with a one–equation model, while the outer core flow is resolved with the standard $k - \epsilon$

model described above. In the one–equation model, the eddy viscosity is made proportional to a velocity scale and a length scale l_μ. The distribution of l_μ is prescribed algebraically while the velocity scale is determined by solving the k–equation (as in Eq. (2)). The dissipation rate ε appearing as sink term in the k–equation is related to k and a dissipation length scale l_ε which is also prescribed algebraically. The different two-layer versions available in the literature differ in the use of the velocity scale and the way l_μ and l_ε are prescribed. It should be mentioned that in the fully turbulent region the length scales l_μ and l_ε vary linearly with distance from the wall. However, in the viscous sublayer l_μ and l_ε deviate from the linear distribution in order to account for the damping of the eddy viscosity and the limiting behaviour of ε at the wall.

$k^{1/2}$ velocity scale based model Rodi (1991): TLK

The approach combines the standard $k-\epsilon$ model in the outer region with a one–equation model due to Norris and Reynolds Norris & Reynolds (1975) in the viscous–sublayer employing

$$\nu_t = C_\mu k^{1/2} l_\mu; \quad \varepsilon = k^{3/2}/l_\varepsilon \tag{3.8}$$

In this model, the length scale l_μ is damped in a similar way as the Prandtl mixing length by the Van Driest function, so that it involves an exponential reduction governed by the near–wall Reynolds number $R_y = U y_n/\nu$. However, in contrast to the original Van Driest function, R_y uses $k^{1/2}$ as a velocity scale U instead of U_τ which can go to zero for separated flows.

$$l_\mu = C_l\, y_n\, f_\mu \quad \text{with: } f_\mu = 1 - exp\left(-\frac{R_y}{A_\mu}\frac{25}{A^+}\right) \tag{3.9}$$

The constant C_l is set equal to $\kappa C_\mu^{-3/4}$ to conform with the logarithmic law of the wall. The empirical constants appearing in the f_μ–function are assigned the values $A_\mu = 50.5$ and $A^+ = 25$. The reader is referred to Rodi (1991) for a review and further details on the choice of the constants. For the dissipation scale the following distribution is used near the wall:

$$l_\varepsilon = \frac{C_l y_n}{1 + C_\varepsilon/(R_y C_l)}; \quad C_\varepsilon = 13.2 \tag{3.10}$$

The outer $(k-\epsilon)$ and the near–wall model are matched at a location where the damping function f_μ reaches the value 0.95, i.e. where viscous effects become negligible.

The combination of the Kato–Launder correction with the TLK model is hereafter labeled TLKK.

$(v'^2)^{1/2}$ velocity scale based model Rodi & Mansour (1993): TLV

The development of this model was motivated by the fact that the length scales-functions as proposed in Norris & Reynolds (1975) particularly the l_ε–function, are not in agreement with

direct numerical simulation (DNS) data, and that the normal fluctuations $(v'^2)^{1/2}$ are a more relevant velocity scale for the turbulent momentum transfer near the wall than is $k^{1/2}$. Therefore, the following model using $(v'^2)^{1/2}$ as a velocity scale was proposed in Rodi & Mansour (1993)

$$\nu_t = \sqrt{\overline{v'^2}}\, l_{\mu,\nu}, \quad \varepsilon = \sqrt{\overline{v'^2}}\, k/l_{\varepsilon,\nu} \tag{3.11}$$

$$\text{with } l_{\nu,\mu} = 0.33 y_n, \quad \text{and } l_{\varepsilon,\nu} = 1.3 y_n / \left[1. + 2.12\, \nu/\sqrt{\overline{v'^2}}\, y_n\right] \tag{3.12}$$

which is based on DNS data for fully developed channel flow. As an equation for k is solved, v'^2 needs to be related to k, which is done through the following DNS based empirical relation

$$\sqrt{\overline{v'^2}}/k = 4.65 \times 10^{-5} (R_y)^2 + 4.00 \times 10^{-4} R_y, \quad R_y = k^{1/2} y_n/\nu \tag{3.13}$$

valid only very near the wall. The matching between the outer and near–wall model is performed at a location where $R_y = 80$.

3.2 The Low-Re $k-\varepsilon$ Turbulence Model

The standard $k-\varepsilon$ model was developed for high Reynolds number flows and is therefore not valid in flow regions very close to the wall, i.e. within the viscous sub layer. In this approach, the following relation for ν_t was proposed; it includes a damping function, f_μ, varying from almost zero near the wall to ≈ 1 at the outer edge of the viscous sub layer:

$$\nu_t = C_\mu f_\mu k^2/\varepsilon \tag{3.14}$$

Experiments and DNS have also shown that the model constants $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ appearing in the source terms of the transport equation for ε need also to incorporate damping functions f_1 and f_2 in order to reproduce the steep gradient of ε near the wall, so that equation (2.4) takes the form

$$\frac{D\varepsilon}{Dt} = \frac{\partial}{\partial x_i}\left[\left(\nu + \frac{\nu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right] + C_{\varepsilon 1} f_1 \mathcal{P}\,\frac{\varepsilon}{k} - C_{\varepsilon 2} f_2\,\frac{\varepsilon^2}{k} + \Xi \tag{3.15}$$

where the molecular diffusion of ε is now re-introduced, unlike in (2.4) for high-Re-number flows. In this equation Ξ represents an additional term to account for the fact that dissipation processes are not isotropic within the viscous sub layer (Jones & Launder, 1972). The different low-Re models proposed so far differ either in the use of the model functions f_μ, f_1 and f_2 and the term Ξ, or the way the dissipation rate is obtained.

3.2.1 The Jones & Launder and Launder & Sharma Models

The Low-Re $k-\varepsilon$ model employed most frequently is due to Jones & Launder (1972). This model is

$$f_\mu = exp\left[-3.4/(1+R_t/50)^2\right]\;; \quad R_t = k^2/\nu\,\varepsilon \tag{3.16}$$

$$f_1 = 1.0\,; \quad f_2 = 1-0.3\,exp\left(-R_t^2\right)\;; \quad \Xi = 2\nu\nu_t(\overline{v}_{,yy})^2 \tag{3.17}$$

The model constants $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ are assigned the same values as those of the standard $k-\varepsilon$ model, i.e. $C_{\varepsilon 1}=1.44$ and $C_{\varepsilon 2}=1.92$ (as in Launder & Sharma (1974)) . This model is found to result in a very rapid growth of f_μ towards 1 (i.e. towards the edge of the viscous sub layer).

3.2.2 The Abe-Kondoh-Nagano Model

Various new low–Re $k-\varepsilon$ have been proposed. One of them is proposed by Abe *et al.* (1994)

$$f_\mu = \left[1-exp\,(-y^*/14)\right]^2\left[1+5\,R_t^{-3/4}\,exp\left(-\left[R_t/200\right]^2\right)\right] \tag{3.18}$$

$$f_1 = 1; \quad f_2 = \left[1-exp\,(-y^*/3.1)\right]^2\left[1-0.3\,exp\left(-\left[R_t/6.5\right]^2\right)\right] \tag{3.19}$$

The wall boundary conditions used together with this type of model require the dissipation rate at the wall $\varepsilon|_{wall}$ to be adjusted so as to reproduce the correct asymptotic behaviour, i.e. $\varepsilon|_{wall}=2\nu k/y_p^2$. In contrast to the wall–function approach used with the standard $k-\varepsilon$ model for high–Re number flows, in the low-Re schemes the no-slip condition is to be employed for the velocity, along with the condition of zero turbulent kinetic energy at the wall. Additionally, the model should meet a criterion similar to the one required for the WF approach, i.e. $y_p^+ < 0.1-0.5$. In general, a typical layer of about 30 grid–points lying within the viscous sub layer (where $f_\mu < 0.95$) is necessary to correctly reproduce the steep gradient of the dissipation rate.

An alternative approach to the use of the damping function f_2 to avoid having to face a singularity in the destruction term $-C_{\varepsilon 2}\,\varepsilon^2/k$ consists in replacing this term by

$$-C_{\varepsilon 2}\frac{\varepsilon}{\mathcal{T}} \tag{3.20}$$

so as to allow the turbulent time scale $\mathcal{T}$ to recover $\tau_0 = k/\varepsilon$ far from boundaries – at high–Re

turbulence –, and makes it proportional to the Kolmogorov time scale $\sim \sqrt{\nu/\varepsilon}$ for low-Re near wall turbulence (Durbin, 1991, 1993):

$$\mathcal{T} = max\left[\frac{k}{\varepsilon}; C_K\left(\frac{\nu}{\varepsilon}\right)^{1/2}\right] \tag{3.21}$$

where C_K is a constant of order one.

3.2.3 The Lam-Bremhorst Model

Lam & Bremhorst (1981) extended the high Reynolds number form of the $k-\varepsilon$ model and tested by application to fully developed pipe flow. The relationship is of the form:

$$f_\mu = \left(1+\frac{20.5}{Re_t}\right)[1-exp\left(-0.0165Re_y\right)]^2 \tag{3.22}$$

$$f_1 = 1+\left(\frac{0.05}{f_\mu}\right)^2; \qquad f_2 = 1-exp\left(-Re_t^2\right) \tag{3.23}$$

$$Re_t = \frac{k^2}{\nu\varepsilon}; \qquad Re_y = \frac{k^{0.5}y_m in}{\nu} \tag{3.24}$$

Chapter 4

Turbulent Heat flux Modelling

In order to model the turbulent heat fluxes, the Reynolds Averaged Navier-Stokes equations (RANS) and the Reynolds Averaged Energy equation introduced in the first chapter need to be solved.

$$\frac{\partial \overline{v_i}}{\partial x_i} = 0 \tag{4.1}$$

$$\frac{D\overline{v}_i}{Dt} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \nabla^2 \overline{v}_i - \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i; \quad i = 1,2,3 \tag{4.2}$$

$$\rho\, c_p \frac{D\overline{T}}{Dt} = \frac{\partial}{\partial x_j} \underbrace{\left(\lambda \frac{\partial \overline{T}}{\partial x_j} - \rho\, c_p\, \overline{u_j' \theta'} \right)}_{-\, q''_{total}} \tag{4.3}$$

where $\tau_{ij} \equiv \overline{u_i' u_j'}$ stands for the Reynolds-stress tensor (which is symmetric, i.e. $\tau_{ij} = \tau_{ji}$) representing the contribution of the turbulent motion generated by velocity fluctuations to the mean stress tensor in momentum equations. This turbulent motion will in turn result in an increase of momentum exchange and mixing. The off-diagonal components of τ_{ij}, or shear stresses ($\overline{u'v'}, \overline{v'w'}$, and $\overline{u'w'}$), prevail in theory in the transport of mean momentum by turbulent motion, while the diagonal terms, or normal stresses ($\overline{u'^2}, \overline{v'^2}$, and $\overline{w'^2}$), only play a minor role. And $q''_{total} = q''_j + Q''_j$ is the total rate of heat transfer due to both molecular and turbulent motions, and $Q''_j = -\rho\, c_p\, \overline{u_j' \theta'}$ represents the turbulent heat-flux.

The different modelling approaches for turbulent heat flux modelling are presented in Fig. 4.1 wherein, the simplest approach is called the Simple Gradient Diffusion Hypothesis (SGDH) and the most complex one is the Turbulent Heat Flux Modelling (THFM) approach which requires the solution of 5 additional equations to model the turbulent heat flux.

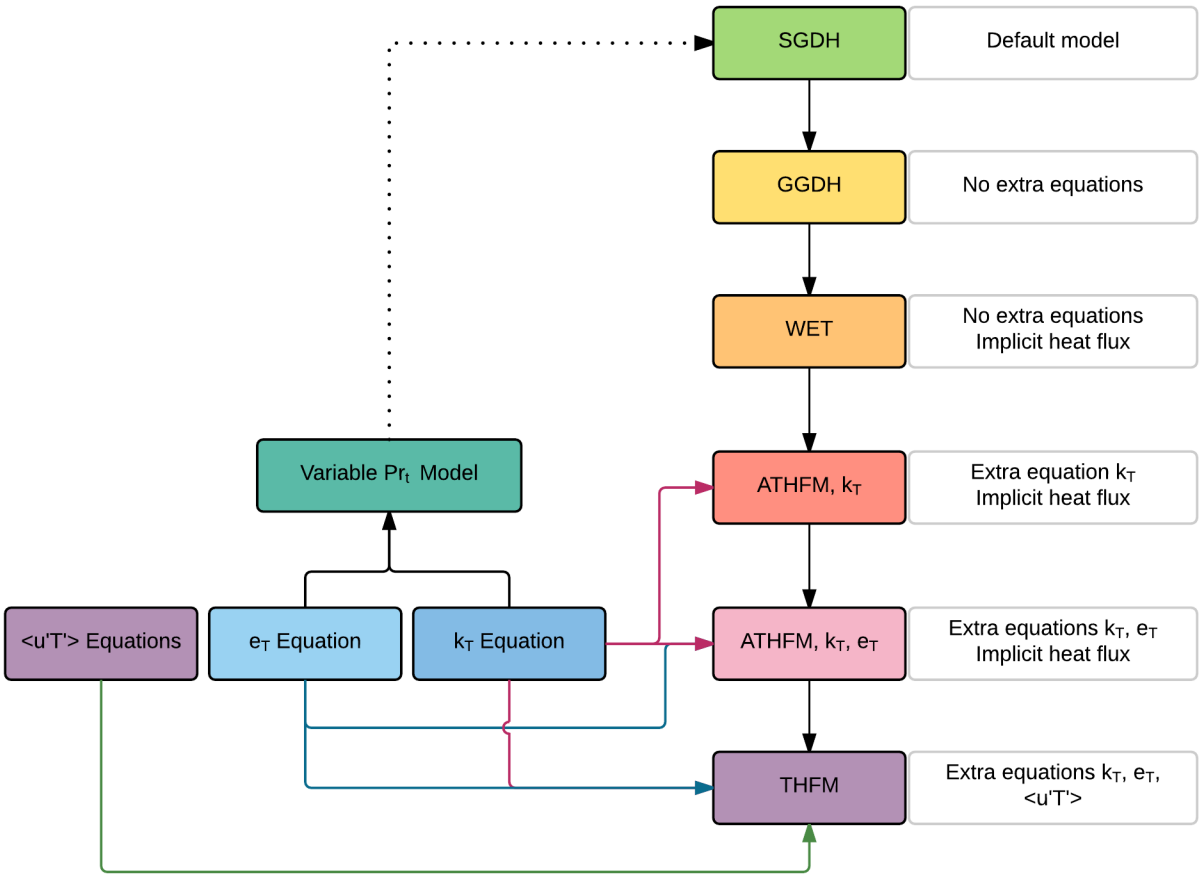

Figure 4.1: Turbulent heat flux modelling overview, where k_T represent the variance of the temperature fluctuations $\overline{\theta'^2}$ and e_T represent the dissipation rate of the heat fluxes $\varepsilon_{\theta'}$.

4.1 Turbulent Heat Flux Model (THFM)

The most accurate approach to account for thermal effects and heat transfer within the time-averaged context is to solve the transport equation for the turbulent heat fluxes $\overline{u_i'\theta'}$, by incorporating a detailed modelling of the buoyancy term. In this model, transport equations for the variance of the temperature fluctuations $\overline{\theta'^2}$ and its dissipation rate $\varepsilon_{\theta'}$ have to be solved in addition to close the set of equations.

The modeled transport equations for turbulent heat fluxes are given by: (for i=1,2,3) Carteciano & Grötzbach (2003)

$$\frac{D\overline{u_i'\theta'}}{Dt} = \frac{\partial}{\partial x_j}\left(\left[C_{TD}\frac{k^2}{\varepsilon}+\frac{\kappa+\nu}{2}\right]\frac{\partial\overline{u_i'\theta'}}{\partial x_j}\right) - \left(\overline{u_i'u_j'}\frac{\partial\overline{T}}{\partial x_j}+\overline{u_j'\theta'}\frac{\partial\overline{u_i}}{\partial x_j}\right) - G_{\overline{u_i'\theta'}} + \pi_i + \varepsilon_{\overline{u_i'\theta'}} \quad (4.4)$$

where κ is the thermal diffusivity: $\kappa = \frac{\lambda}{\rho c_p}$.

The term π_i represent the modeling of the pressure-temperature gradient correlation with Monin's and Launder's correlation.

$$\pi_i = -C_{T1}\frac{\varepsilon}{k}\overline{u_i'\theta'} + C_{T2}\overline{u_j'\theta'}\frac{\partial\overline{u_i}}{\partial x_j} + C_{T3}\beta g_i\overline{\theta'^2} - C_{T4}\frac{\varepsilon}{k}\overline{u_{[n]}'\theta'}\delta_{i[n]}\frac{k^{\frac{3}{2}}}{x_{[n]}\varepsilon} \quad (4.5)$$

where $\delta_{i[n]}$ is the Kronecker delta and the index n represent the normal direction to a wall.
The dissipation rate of the heat fluxes $\varepsilon_{\overline{u_i'\theta'}}$ can be modelled by:

$$\varepsilon_{\overline{u_i'\theta'}} = -\frac{1+Pr}{2\sqrt{Pr}\sqrt{R}}\left(\frac{\varepsilon}{k}\right)\exp\left[-C_{T5}\left(Re_t+Pe_t\right)\right]\overline{u_i'\theta'} \quad (4.6)$$

Where Re_t is the local turbulent Reynolds number, $Pe_t = Re_t \times Pr$ is the local Peclet number and R is the turbulent time-scale ratio. $\varepsilon_{\overline{u_i'\theta'}}$ is negligible in the transport equation (4.4) of the heat fluxes at high Peclet numbers but its contribution is important at low Peclet numbers.
Another expression for the dissipation rate is available for very low Peclet numbers:

$$\varepsilon_{\overline{u_i'\theta'}} = -\frac{1}{2}\left(1+\frac{1}{Pr}\right)\left(\frac{Pr}{R}\right)^{0.7}\left(\frac{\varepsilon}{k}\right)\overline{u_i'\theta'} \quad (4.7)$$

The buoyancy term $G_{u_i'\theta'}$ is expressed in terms of the variance of the temperature fluctuations $\overline{\theta'^2}$.

$$G_{u_i'\theta'} = \beta g_i\overline{\theta'^2} \quad (4.8)$$

For a detailed description of the buoyancy effects, a transport equation of the variance of the temperature fluctuations $\overline{\theta'^2}$ is solved:

$$\frac{\partial \rho \overline{\theta'^2}}{\partial t} + \frac{\partial \rho u_j \overline{\theta'^2}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\rho C_{TT}\frac{k^2}{\varepsilon} + \rho\kappa\right)\frac{\partial \overline{\theta'^2}}{\partial x_j}\right] - 2\rho\overline{u_j'\theta'}\frac{\partial \overline{T}}{\partial x_j} - 2\rho\varepsilon_{\theta'} - 2\rho\kappa\left(\frac{\partial\sqrt{\overline{\theta'^2}}}{\partial x_j}\right)^2 \quad (4.9)$$

The previous transport equation requires the dissipation rate of the temperature variance $\varepsilon_{\theta'}$ to be modeled using an other transport equation.

$$\begin{aligned}\frac{\partial \rho \varepsilon_{\theta'}}{\partial t} + \frac{\partial \rho u_j \varepsilon_{\theta'}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\rho C_{DD}\frac{k^2}{\varepsilon} + \rho\kappa\right)\frac{\partial \varepsilon_{\theta'}}{\partial x_j}\right] &- \rho\varepsilon_{\theta'}\left(C_{D1}\frac{\varepsilon_{\theta'}}{\overline{\theta'^2}} + C_{D2}\frac{\varepsilon}{k} + C_{P1}\frac{\overline{u_j'\theta'}}{\overline{\theta'^2}}\frac{\partial \overline{T}}{\partial x_j} - C_{P2}\frac{P_k}{k}\right) \\ &+ 2\rho\kappa\kappa_t\left(\frac{\partial^2 \overline{T}}{\partial x_k \partial x_j}\right)^2 \end{aligned} \quad (4.10)$$

with:

$$P_k = \nu_t\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right)\frac{\partial \overline{u_i}}{\partial x_j} \quad (4.11)$$

4.2 Full Algebraic Turbulent Heat Flux Model: $\overline{\theta'^2}$ - $\varepsilon_{\theta'}$

In this model, the turbulent heat flux $\overline{u_i'\theta'}$ is modelled algebraically instead of solving an additional set of partial differential equations. The model is referred to as the Algebraic Turbulent Heat Flux Model (ATHFM) (Launder, 1988). The turbulent heat flux ($\overline{u_i'\theta'}$) can be approximated by its production rate times the turbulent time scale. The production terms and turbulence fluctuations from the differential transport equations are locally in balance S. Kenjeres (2000).

$$\overline{u_i'\theta'} = -C^{\theta'}\frac{k}{\varepsilon}\left(\overline{u_i'u_j'}\frac{\partial \overline{T}}{\partial x_j} + \xi\overline{u_j'\theta'}\frac{\partial \overline{u_i}}{\partial x_j} + \eta\beta\, g_i\, \overline{\theta'^2}\right) \quad (4.12)$$

In order to close the above system, the values of $\overline{\theta'^2}$ and $\varepsilon_{\theta'}$ are needed. In the case where transport equations are solved for both the above quantities we obtain the ATHFM $-\overline{\theta'^2} - \varepsilon_{\theta'}$ model.

$$\frac{\partial \rho \overline{\theta'^2}}{\partial t} + \frac{\partial \rho u_j \overline{\theta'^2}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho\left(\kappa + \kappa_t\right)\frac{\partial \overline{\theta'^2}}{\partial x_j}\right) + 2\rho P_{\theta'} - 2\rho\varepsilon_{\theta'} \quad (4.13)$$

and

$$\begin{aligned}\frac{\partial \rho \varepsilon_{\theta'}}{\partial t} + \frac{\partial \rho u_j \varepsilon_{\theta'}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho\left(\kappa + \kappa_t\right)\frac{\partial \tilde{\varepsilon}_{\theta'}}{\partial x_j}\right) &+ C_{\varepsilon 1}^{\theta'}\rho P_{\theta'}\frac{\tilde{\varepsilon}_{\theta'}}{\overline{\theta'^2}} + C_{\varepsilon 3}^{\theta'}\rho P\frac{\tilde{\varepsilon}_{\theta'}}{k} \\ &- C_{\varepsilon 4}^{\theta'}\rho\frac{\tilde{\varepsilon}_{\theta'}^2}{\overline{\theta'^2}} - C_{\varepsilon 5}^{\theta'}\rho f_{\varepsilon\theta'}\frac{\tilde{\varepsilon}_{\theta'}\tilde{\varepsilon}}{k} + E_{\theta'}\end{aligned} \quad (4.14)$$

where:

$$P = -\overline{u_i'u_j'}\frac{\partial \overline{u_i}}{\partial x_j}, \qquad P_{\theta'} = -\overline{u_j'\theta'}\frac{\partial \overline{T}}{\partial x_j}, \qquad G = -\beta g_i \overline{u_i\theta'}, \qquad E_{\theta'} = 2\rho\kappa\kappa_t \left(\frac{\partial^2 T}{\partial x_j \partial x_k}\right)^2,$$

$$\tilde{\varepsilon} = \varepsilon - 2\nu\left(\frac{\partial\sqrt{k}}{\partial x_k}\right)^2, \qquad \tilde{\varepsilon}_{\theta'} = \varepsilon_{\theta'} - \kappa\left(\frac{\partial\sqrt{\overline{\theta'^2}}}{\partial x_k}\right)^2,$$

$$\kappa_t = C_\Phi f_\mu \frac{k^2}{\tilde{\varepsilon}}, \qquad f_\mu = \exp\left[\frac{-3.4}{\left(1+\frac{Re_t}{50}\right)^2}\right], \qquad f_{\varepsilon\theta'} = 1.$$

In Kenjereš *et al.* (2005), the model for the Reynolds stress was extended with a buoyancy and turbulent heat flux term given as,

$$\overline{u_i'u_j'} = \frac{2}{3}k\delta_{ij} - \nu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + C_\theta\tau\beta\left(g_i\overline{u_j'\theta'} + g_j\overline{u_i'\theta'} - \frac{2}{3}g_k\overline{u_k'\theta'}\delta_{ij}\right) \tag{4.15}$$

with $C_\theta = 0.15$.

This model was further developed and calibrated by Shams *et al.* (2014) where the eddy viscosity ν_t was given as,

$$\begin{aligned} \nu_t &= f_\mu C_\mu k\tau \\ \tau &= \max\left[\frac{k}{\varepsilon}, C_T\left(\frac{\nu}{\varepsilon}\right)\right], \quad \text{and} \\ f_\mu &= 1 - exp\left[-\left(C_{d_0}\sqrt{Re_d} + C_{d_1}Re_d + C_{d_2}Re_d^2\right)\right] \end{aligned} \tag{4.16}$$

Where $Re_d = \sqrt{k}d/\nu$ with d being the distance to the wall, and the constants being, $C_\mu = 0.09, C_T = 0.6, C_{d_0} = 0.091, C_{d_1} = 0.0042, C_{d_2} = 0.00011$.

The algebraic turbulent heat flux model used (Shams *et al.*, 2014; Kenjereš *et al.*, 2005) involves an additional term proportional to the Reynolds stress anisotropy. The algebraic turbulent heat flux is also redefined with different names for the model constants and is given as,

$$\overline{u_i'\theta'} = -C_{t_0}\tau\left(C_{t_1}\overline{u_i'u_j'}\frac{\partial T}{\partial x_j} + C_{t_2}\overline{u_j'\theta'}\frac{\partial u_i}{\partial x_j} + C_{t_3}\beta g_i\overline{\theta'^2}\right) + C_{t_4}a_{ij}\overline{u_j'\theta'} \tag{4.17}$$

with g_i the gravity vector and a_{ij} the Reynolds stress anisotropy tensor defined as,

$$a_{ij} = \frac{\overline{u_i'u_j'}}{k} - \frac{2}{3}\delta_{ij} \tag{4.18}$$

	C_{t_0}	C_{t_1}	C_{t_2}	C_{t_3}	C_{t_4}	R
AHFM-2005	0.15	0.6	0.6	0.6	1.5	0.5
AHFM-cc	0.2	0.25	0.6	2.5	0.0	0.5
AHFM-NRG if $RePr > 180$	0.2	0.053 x $\ln(RePr) - 0.27$	0.6	2.5	0.0	0.5

Table 4.1: Model constants for the algebraic heat flux model

The transport equation for $\overline{\theta'^2}$ is solved and $\varepsilon_{\theta'}$ is evaluated from the thermal to mechanical time-scale ratio (Eq. (4.23)) where an algebraic expression is used by Kenjereš *et al.* (2005) and a constant value of 0.5 by Shams *et al.* (2014). The assumption of the constant time-scale ratio R worked reasonably well in a number of flow regimes when compared with the respective reference DNS or experimental data.

In the work of Shams *et al.* (2014), the model proposed by Kenjereš *et al.* (2005) is referred to as AHFM-2005 which was calibrated for natural and mixed convection flow regimes close to unity Prandtl number. Shams *et al.* (2014) proposed a new calibration for forced convection and low Prandtl number fluids (liquid metal) referred to as AHFM-cc. The model was further extended by introducing a logarithmic dependence of coefficient C_{t_1} on the Reynolds and Prandtl numbers with a constraint to be positive for $RePr > 180$. This variant of AHFM-cc was called AHFM-NRG. The model constants for the above models are given in Table 4.1.

Note that the nomenclature of the constants used by Shams *et al.* (2014) will be used in this report. In the model presented by Kenjereš *et al.* (2005), an additional coefficient C_{t_1} has been introduced as compared to S. Kenjeres (2000) which was by default set to one in earlier publications.

4.2.1 Equivalence between THFM and ATHFM heat flux modelling

The algebraic expression for the turbulent heat flux can be obtained from the partial differential model (Eq. 4.4) by simply dropping the unsteady, advection, and diffusion terms to obtain,

$$\overline{u_i'\theta'} = -\frac{1}{C_{T1}}\left(\frac{k}{\varepsilon}\right)\left[\overline{u_i'u_j'}\frac{\partial \overline{T}}{\partial x_j} + (1-C_{T2})\overline{u_j'\theta'}\frac{\partial \overline{u_i}}{\partial x_j} + (1-C_{T3})\beta g_i \overline{\theta'^2}\right] \tag{4.19}$$

where the near wall term in π_i and the dissipation rate of the turbulent heat fluxes have been ignored. By comparison with the algebraic model proposed by Kenjereš *et al.* (2005) in Eq. 4.17, we note that,

$$\begin{aligned} C_{t_0} &= \frac{1}{C_{T1}} \\ C_{t_1} &= 1 \\ C_{t_2} &= 1 - C_{T2} \end{aligned}$$

$\overline{u_i\theta'}$ tr. equation		$\overline{\theta'^2}$ tr. equation		$\varepsilon_{\theta'}$ tr. equation	
coeff.	value	coeff.	value	coeff.	value
C_{TD}	0.11	C_{TT}	0.13	C_{DD}	0.13
C_{T0}	3.0			C_{D1}	2.2
C_{T1}	0.0			C_{D2}	0.8
C_{T2}	0.33			C_{P1}	1.8
C_{T3}	0.5			C_{P2}	0.72
C_{T4}	0.5				

Table 4.2: Set of empirical coefficients for the equivalent THFM

$$C_{t_3} = 1 - C_{T3} \tag{4.20}$$

The work of Shams *et al.* (2014) has shown that C_{t_1} values are much different from 1.0. For example, Kenjereš *et al.* (2005) propose a value of 0.6 which is further reduced by Shams *et al.* (2014) for low Prandtl numbers to 0.25 in the so called AHFM-cc model. In the AHFM-NRG model proposed by them, C_{t_1} is made into a function of Reynolds and Prandtl numbers with values always below 1.0. With this in mind, the THFM model is extended by introducing a new coefficient and a new nomenclature where,

$$\begin{aligned} C_{t_0} &= \frac{1}{C_{T0}} \\ C_{t_1} &= 1 - C_{T1} \\ C_{t_2} &= 1 - C_{T2} \\ C_{t_3} &= 1 - C_{T3} \end{aligned} \tag{4.21}$$

such that a one-to-one equivalence is established between the algebraic model of Kenjereš *et al.* (2005) and the differential model of Carteciano & Grötzbach (2003). Due to this alteration the expression for π_i in the transport equations for the turbulent heat fluxes changes to,

$$\pi_i = -C_{T0}\frac{\varepsilon}{k}\overline{u_i'\theta'} + C_{T1}\overline{u_i'u_j'}\frac{\partial\overline{T}}{\partial x_j} + C_{T2}\overline{u_j'\theta'}\frac{\partial\overline{u_i}}{\partial x_j} + C_{T3}\beta g_i\overline{\theta'^2} - C_{T4}\frac{\varepsilon}{k}\overline{u_{[n]}'\theta'}\delta_{i[n]}\frac{k^{\frac{3}{2}}}{x_{[n]}\varepsilon} \tag{4.22}$$

The final set of model coefficients for the THFM model is given in Table 4.2.

4.3 Algebraic Turbulent Heat Flux Model: $\overline{\theta'^2}$

The ATHFM $-\overline{\theta'^2} - \varepsilon_{\theta'}$ model can be further simplified by calculating the dissipation rate of the temperature variance $\varepsilon_{\theta'}$ using the definition of the mechanical to thermal turbulent time-scale

ratio R. The time scale ratio R is either set to a constant value or prescribed algebraically. The dissipation rate of temperature fluctuation variance can then be directly obtained as,

$$\varepsilon_{\theta'} = \frac{1}{2R}\left(\frac{\varepsilon}{k}\right)\overline{\theta'^2} \tag{4.23}$$

This represents a measure of the relative importance of the relaxation timescales of the mechanical and thermal dissipation. With this simplification, the need to solve a transport equation for $\varepsilon_{\theta'}$ doesn't exist. This model is referred to as the ATHFM $-\ \overline{\theta'^2}$ model. Although the value and variation of R in most situations is not known, such an assumption has displayed remarkable success in a number of thermal flows driven by gravitational effects. Typically, a value of 0.5 is used.

4.4 WET Model

Further simplification is achieved by determining the turbulent heat flux by applying the WET (Wealth $\equiv$ Earnings $\times$ Time) theory, a syllogism applied by Launder (1988) to turbulent heat fluxes which lead to the expression: (Value of Second Moment $\equiv$ Production Rate of Second Moment $\times$ Turbulent Time Scale). This, together with the turbulent time k/ε, yields,

$$\overline{u_i'\theta'} = -C_{t_0}\frac{k}{\varepsilon}\left(C_{t_1}\overline{u_i'u_j'}\,\frac{\partial\overline{T}}{\partial x_j} + C_{t_2}\overline{u_j'\theta'}\,\frac{\partial\overline{u_i}}{\partial x_j}\right) \tag{4.24}$$

The WET model is supposed to remedy the drawback of simpler variants, in which the heat flux is only generated by temperature gradients; which is not always the case. For example, the mixed layer formed close to a heated wall featuring a uniform vertical temperature gradient is not necessarily linked to turbulence, so the heat flux is actually over-represented in the relative sense. The same is true when vertical temperature gradients are small: here it is the velocity gradients that cause the wall-to-flow heat transfer.

4.5 Generalized Gradient Diffusion Hypothesis (GGDH)

The WET model on further simplification yields the GGDH model. The turbulent heat-flux is modelled in an manner analogous to the turbulent transport term in the Reynolds stress equation, in particular by reference to Daly & Harlow (1970) model.

$$\overline{u_i'\theta'} = -C_{t_0}\frac{k}{\varepsilon}\left(C_{t_1}\overline{u_i'u_j'}\,\frac{\partial\overline{T}}{\partial x_j}\right) \tag{4.25}$$

This approach is known as the anisotropic eddy-diffusivity model, or the generalized gradient diffusion hypothesis (GGDH), a definition that points to the fact that heat transfer is driven by

C_{t_0}	C_Φ	$C_{\varepsilon 1}^{\theta'}$	$C_{\varepsilon 3}^{\theta'}$	$C_{\varepsilon 4}^{\theta'}$	$C_{\varepsilon 5}^{\theta'}$	C_{t_1}	C_{t_2}	C_{t_3}	C_{t_4}
0.2	0.09	1.3	0.72	2.2	0.8	0.25	0.6	2.5	0.0

Table 4.3: Coefficients for ATHFM

an anisotropic thermal diffusion (Λ_{ij}),

$$\Lambda_{ij} = C_{t_0} \frac{k}{\varepsilon} C_{t_1} \overline{u_i' u_j'} \tag{4.26}$$

This approach has the merit to conform to many experimental findings, including the measurements of turbulent heat transfer in pipes and boundary layer flows by Bremhorst & Bullock (1973), and by many others. Indeed, these authors demonstrated that turbulent heat flux in the flow direction are two to three times larger than in the direction normal to the wall while the streamwise temperature gradient is negligible compared to that normal to the surface.

4.6 Simple Gradient Diffusion Hypothesis (SGDH)

In the context of linear RANS modelling for convective heat transfer, the turbulent heat flux is linked to the temperature gradient via the expression below where the turbulent stress $\overline{u_i' u_j'}$ is replaced by the by its trace $\overline{u_i' u_i'}$ equal to $2k$, the turbulent kinetic energy. This gives rise to the isotropic thermal-diffusivity model, known as the Simple Gradient Diffusion Hypothesis (SGDH).

$$\overline{u_i' \theta'} = -\frac{\nu_t}{Pr_t} \frac{\partial T}{\partial x_i} \tag{4.27}$$

The turbulent Prandtl number Pr_t introduced in the above expression is typically set to a constant value of 0.9. However, two-equation models for thermal diffusivity have been developed in parallel with the $k - \varepsilon$ model of turbulence. This idea was motivated by the fact that turbulent heat diffusion should also be characterized by a scalar (thermal) time scale that varies in space and time, just like the turbulent time scale $\tau = k/\varepsilon$. Such models are also referred to as variable turbulent Prandtl number models.

The model coefficients for the whole chain for models from WET to ATHFM – $\overline{\theta'^2} - \varepsilon_{\theta'}$ is given in Table 4.3.

4.7 Variable Turbulent Prandtl Number Model

Within the Reynolds-averaged Navier Stokes model, where the turbulent heat flux is modelled by the SGDH model, the turbulent Prandtl number Pr_t is typically assumed to be a constant. This modelling approach limits the generality of these models because the turbulent Prandtl number

can alter the mean flow prediction. One approach to extend the applicability of the SGDH model is to model the variation of the turbulent Prandtl number.

The turbulent thermal diffusivity is defined using a composite time scale using both the mechanical and thermal turbulent time scales given by,

$$\kappa_t = C_\lambda f_\lambda k \sqrt{\frac{k}{\varepsilon}\frac{\overline{\theta'^2}}{\varepsilon_{\theta'}}} \tag{4.28}$$

where C_λ is a model constant and f_λ is a near-wall damping function for the turbulent thermal diffusivity applicable for low Reynolds number turbulence models. Using the standard expression for eddy diffusivity, the turbulent Prandtl number can be expressed as,

$$Pr_t = \frac{C_\mu f_\mu}{C_\lambda f_\lambda}\sqrt{\frac{k}{\varepsilon}\frac{\varepsilon_{\theta'}}{\overline{\theta'^2}}} \tag{4.29}$$

In order to close Eq. (4.29) the variance of the temperature fluctuations, and its dissipation rate are required. If transport equations of these quantities are solved, we obtain the 2-equation variable Pr_t turbulent heat flux model.

The equations governing the transport of temperature variance and its dissipation rate are given as, N. Chidambaram & Kenzakowski (2001)

$$\frac{\partial \rho\overline{\theta'^2}}{\partial t} + \frac{\partial \rho u_j \overline{\theta'^2}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho\left[\kappa + \frac{\kappa_t}{\sigma_{\overline{\theta'^2}}}\right]\frac{\partial \overline{\theta'^2}}{\partial x_j}\right) + 2\rho\kappa_t\left(\frac{\partial T}{\partial x_j}\right)^2 - 2\rho\varepsilon_{\theta'} \tag{4.30}$$

$$\begin{aligned}\frac{\partial \rho\varepsilon_{\theta'}}{\partial t} + \frac{\partial \rho u_j \varepsilon_{\theta'}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho\left[\kappa + \frac{\kappa_t}{\sigma_{\varepsilon_{\theta'}}}\right]\frac{\partial \varepsilon_{\theta'}}{\partial x_j}\right) &+ \left(C_{p_1}\frac{\varepsilon_{\theta'}}{\overline{\theta'^2}} + C_{p_2}\frac{\varepsilon}{k}\right)\rho\kappa_t\left(\frac{\partial T}{\partial x_j}\right)^2 + C_{p_3}\frac{\varepsilon_{\theta'}}{k}\underline{P} \\ &- C_{d_1}\frac{\hat{\varepsilon}_{\theta'}}{\overline{\theta'^2}}\rho\varepsilon_{\theta'} - C_{d_2}\frac{\hat{\varepsilon}}{k}\rho\varepsilon_{\theta'} + \xi_{\varepsilon_{\theta'}}\end{aligned} \tag{4.31}$$

where the operator $\hat{}$ denotes the low Reynolds number modifications, $\xi_{\varepsilon_{\theta'}}$ is the near-wall correction function, and $\underline{P}$ is the turbulent kinetic energy production term. According to T.P. Sommer & Lai (1993), different values of C_{p_1} can be used: a value of 1.8 for boundary layers and 2.0 for internal flows

$$\underline{P} = \mu_t\left(\frac{\partial \overline{u_i}}{\partial x_j}\right)^2 \tag{4.32}$$

The near-wall correction function is given as,

$$\xi_{\varepsilon_{\theta'}} = f_w\rho\left[\left(C_{d_1}-4\right)\frac{\hat{\varepsilon}_{\theta'}}{\overline{\theta'^2}}\varepsilon_{\theta'} + C_{d_2}\frac{\hat{\varepsilon}}{k}\varepsilon_{\theta'} - \frac{\varepsilon^{*2}_{\theta'}}{\overline{\theta'^2}} - \left(2 - C_{p_1} - C_{p_2}Pr\right)\frac{\varepsilon_{\theta'}}{\rho\overline{\theta'^2}}P_{\theta'}\right] \tag{4.33}$$

C_{p_1}	C_{p_2}	C_{p_3}	C_{d_1}	C_{d_2}	$\sigma_{\overline{\theta' 2}}$	$\sigma_{\varepsilon_{\theta'}}$	C_λ	A^+	$C_{1\lambda}$
2.0	0.0	0.72	2.2	0.8	1.0	1.0	0.14	45	0.1

Table 4.4: Coefficients for Variable turbulent Prandtl number model

where $P_{\theta'}$ is the production due to the mean temperature gradient in the streamwise direction to account for a wall heat-flux boundary, the damping function is defined as,

$$f_w = \exp\left[-\left(\frac{Re_t}{80}\right)^2\right], \qquad \hat{\varepsilon}_{\theta'} = \varepsilon_{\theta'} - \kappa\left(\frac{\partial\sqrt{\overline{\theta' 2}}}{\partial x_j}\right)^2, \qquad \hat{\varepsilon} = \varepsilon - 2\nu\left(\frac{\partial\sqrt{k}}{\partial x_j}\right)^2 \qquad \varepsilon^*_{\theta'} = \varepsilon_{\theta'} - \frac{\kappa\overline{\theta' 2}}{d^2} \tag{4.34}$$

The near-wall damping function f_λ is given as,

$$f_\lambda = \frac{f_w C_{1\lambda}}{Re_t^{\frac{1}{4}}} + \left[1 - \exp\left(-\frac{y^+}{A^+}\right)\right]^2 \tag{4.35}$$

Chapter 5

Buoyancy–Driven Turbulent Flows

5.1 The Equations of Motion

The buoyancy effects give rise to an additional body-force term $\mathbf{f_i} = -\beta\, g_i\, (T - T_0)$ proportional to the perturbations in the temperature,

$$\frac{D\overline{v_i}}{Dt} \;=\; -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu\,\nabla^2\mathbf{u}' - \frac{\partial \tau_{ij}}{\partial x_j} + \mathbf{f_i}\,; \quad i = 1,2,3 \tag{5.1}$$

this body force per unit volume, applied to a fluid element, has the potential of modifying the turbulent structure through a production (or destruction) of Reynolds stress at a rate proportional to $(\,\overline{f_i' u_j'} + \overline{f_j' u_i'}\,)$, where f_i' is the turbulent perturbation superimposed on $\overline{f_i}$. The effects of this body force will change according to the physical processes in question, i.e. through the coupling with the flow or scalar fields.

Chapter 6

Scale Resolving Strategies: LES and V-LES

6.1 The filtered Navier-Stokes equations (bases of LES)

In Large Eddy Simulation (LES) the motion of the super-grid turbulent eddies is directly captured whereas the effect of the smaller scale eddies is modelled or represented statistically by means of simple models, very much the same way as in Reynolds-averaged models (RANS); i.e. the usual practice is to model the sub-grid stress tensor by an eddy viscosity model. In terms of computational cost, LES (Sagaut, 2005) lies between RANS and DNS and is motivated by the limitations of each of these approaches. Since the large-scale unsteady motions are represented explicitly, LES is more accurate and reliable than RANS. In the present work, use was made to the Dynamic sub-grid scale model of (Moin *et al.*, 1991); both in the single-phase and boiling flow case. LES involves the use of a spatial filtering operation

$$\overline{F_k}(x,t) = \int_{-\infty}^{+\infty} F(\mathbf{x}',t)G(\mathbf{x}-\mathbf{x}^{'})d\mathbf{x}' \tag{6.1}$$

where the fluctuation of any variable F from its filtered value is denoted by $f^{'} = \overline{F_k} - \mathbf{F}_k$. Filter function $G(\mathbf{x}-\mathbf{x}^{'})$ is invariant in time and space, and is localized, obeying the properties:

$$G(\mathbf{x}) = G(-\mathbf{x}) \tag{6.2}$$

$$\int_{-\infty}^{+\infty} G(\mathbf{x})dx = 1 \tag{6.3}$$

Applying the filtering operation to the instantaneous Navier-Stokes equations under incompressible flow conditions leads to the system of filtered transport equations for turbulent convective flow:

$$\nabla \cdot \overline{\mathbf{u}} = 0 \tag{6.4}$$

$$\frac{\partial}{\partial t}(\rho\overline{\mathbf{u}}) + \nabla \cdot (\rho\overline{\mathbf{u}}\overline{\mathbf{u}}) = \nabla \cdot (\overline{\pi} - \tau) + F_b + F_c \tag{6.5}$$

where $\mathbf{u}$ is the velocity vector, ρ is the density, π=$(-p.\mathbf{I} + \sigma)$ is the Cauchy stress embedding pressure and viscous terms. The source terms in the RHS of the momentum equation represents the body force, F_b, and the convolution-induced, F_c. Further, filtering introduces the SGS stress tensor defined as $\tau = \rho(\overline{\mathbf{u}\mathbf{u}} - \overline{\mathbf{u}}\,\overline{\mathbf{u}})$, of which the deviatoric part is to be statistically modeled. This way, turbulent scales larger than the filter width imposed by filter function $G(\mathbf{x}-\mathbf{x}^{'})$ are directly solved, whereas the diffusive effects of the SGS scales are modeled.

6.2 Sub-grid Scale (SGS) Modelling

In turbulent flows, small-scale eddies are known to be simpler to model than the entire spectrum, since, in this high-wave number zone turbulence is likely to be homogeneous and isotropic (Kolmogorov, 1942). In other words, the subgrid-scale turbulence is much less problem–dependent than the resolvable one. Use is generally made of the Eddy Viscosity Concept, linking linearly the SGS eddy viscosity and thermal diffusivity to the gradients of the filtered velocity and temperature, respectively:

$$\tau_{ij} = -2\mu_{sgs}\overline{S_{ij}} + \frac{1}{3}\delta_{ij}\tau_{ll}; \quad \mu_{sgs} = (Cs\Delta)^2\,\overline{\rho}|\overline{S}|^2 \tag{6.6}$$

$$q_j^{"} = -\alpha_\theta \frac{\partial \overline{T}}{\partial x_j}; \quad \alpha_\theta = \frac{\mu_{sgs}}{Pr_t} \tag{6.7}$$

where Pr_t is the turbulent Prandtl number, the strain rate tensor $\overline{S}_{ij}$ and the temperature gradients are determined from the large-scale turbulence. In the above two relations, the eddy viscosity μ_t and thermal diffusivity α_θ parameterise locally the non-resolvable dynamic stresses and the heat flux in terms of the local rate of strain tensor $\overline{S}_{ij}$ and the temperature gradients, calculated from the large-scale turbulence. The model constant (Cs) is either fixed or made dependent on

the flow; this latter option is precisely the spirit of the dynamic model, known as DSM (Moin *et al.*, 1991). A damping function is often introduced for the model constant Cs to accommodate the asymptotic behavior of near-wall turbulence. Similarly, the same strategy could be used to close the turbulent SGS heat flux, where the thermal diffusivity could be determined either based on the resolved thermal-flow field, or alternatively based on the eddy viscosity (defined dynamically) and a fixed Pr_t. In the present simulations, we have tested two variants based on fixed and variable model coefficient Cs, namely the DSM and the WALE sgs models (Nicoud & Ducros, 1999), the latter has been shown to behave very well in wall-bounded flows, and to be less dissipative, capable to capture the thin-shear layer accurately.

6.2.1 The Smagorinsky Model

The Smagorinsky model (Smagorinsky, 1963) is based on the Boussinesq approach, Eqs. (6.6 and 6.7). It is nothing more than a mixing-length theory

$$\nu_t = \ell^2 \left| \frac{d\overline{v}}{dy} \right| = \ell^2 \ | \overline{S} | = \ (C_s \overline{\Delta})^2 \ | \overline{S} | \text{ with: } | \overline{S} | = \ (2 \overline{S}_{ij} \overline{S}_{ij})^{1/2} \tag{6.8}$$

where the length scale ℓ is based on the cell size $\overline{\Delta}^3 = (\Delta_1 \Delta_2 \Delta_3)$ rather than on the distance to the wall, i.e. on the mixing length $\ell_0 = \kappa \cdot y_n$. The constant C_s is referred to as the Smagorinsky constant.

Other options for near-wall treatment are also available. The Deardorff model is given as (Deardorff, 1970)

$$\ell = \min(C_s \overline{\Delta}, \kappa d_w) \tag{6.9}$$

where d_w is the minimum distance to the wall. In addition to this the Schmidt and Schumann model (Schmidt & Schumann, 1989) is given as,

$$\ell = \min(C_s \overline{\Delta}, \ell_{mix}) \tag{6.10}$$

$$\ell_{mix} = \left(\frac{1}{c_2 \overline{\Delta}} + \frac{1}{\kappa d_w} \right)^{-1} \tag{6.11}$$

where c_2 is taken to be $c_2 = 0.1$.

Assuming a direct analogy between momentum and heat flux diffusion by turbulence, one can determine the thermal diffusivity α_θ by reference to the eddy viscosity given by $\alpha_\theta = \nu_t / Pr_t$, as is usually done in turbulence modelling. This practice is quite robust in the context of the Smagorinsky model.

6.2.2 The Dynamic Approach (DSM)

In this approach developed by Germano *et al.* (1991), *A priori* adjustment of the Smagorinsky constant C_s is not needed. Instead, the dynamic model is used to determine this unknown variable C_s from the information contained in the resolved velocity field.

The main idea consists of introducing a test filter with a larger width than the original one, i.e. $\widetilde{\overline{\Delta}} > \overline{\Delta}$. This test filter is then applied to the filtered Navier-Stokes equations (the NS equations are filtered twice), yielding a sub–test–scale stress tensor T_{ij} similar in form to τ_{ij} that takes the following form:

$$T_{ij} = \widetilde{\overline{u_i' u_j'}} - \widetilde{\overline{u_i}}\,\widetilde{\overline{u_j}} \tag{6.12}$$

By virtue of the Germano identity, the two SGS stress tensors τ_{ij} and T_{ij} are connected through the following relation

$$T_{ij} - \widetilde{\tau}_{ij} \equiv \mathcal{L}_{ij} = \widetilde{\overline{u_i'}\,\overline{u_j'}} - \widetilde{\overline{u_i}}\,\widetilde{\overline{u_j}} \tag{6.13}$$

Assuming now the Smagorinsky functional form to hold and a variable coefficient C_s to be used to close the deviatoric parts of τ_{ij} and T_{ij}, we get

$$\tau_{ij} = -2(C_s\,\overline{\Delta})^2 \;\mid \overline{S} \mid \overline{S}_{ij} \tag{6.14}$$

$$T_{ij} = -2(C_s\,\widetilde{\overline{\Delta}})^2 \;\mid \widetilde{\overline{S}} \mid \widetilde{\overline{S}}_{ij} \tag{6.15}$$

where $\widetilde{\overline{S}} = (\widetilde{\overline{v}}_{i,j} + \widetilde{\overline{v}}_{j,i})/2$ is the rate–of–strain tensor of the test–filtered velocity field. Rearranging the last three equations results in

$$\mathcal{L}_{ij} = -2\,(C_s\,\overline{\Delta})^2 \left[\frac{\widetilde{\overline{\Delta}}^2}{\overline{\Delta}^2} \;\mid \widetilde{\overline{S}} \mid \widetilde{\overline{S}}_{ij} - \widetilde{\mid \overline{S} \mid \overline{S}_{ij}} \right] \tag{6.16}$$

A variant of this model (Lilly, 1992) uses a least–squares approach to obtain values for $(C_s\,\overline{\Delta})^2$, leading to

$$(C_s\,\overline{\Delta})^2 = -\frac{1}{2}\,\frac{\mathcal{L}_{ij}\mathcal{M}_{ij}}{\mathcal{M}_{ij}\mathcal{M}_{ij}} \tag{6.17}$$

where $\mathcal{M}_{ij}$ is the term in brackets in Eq. (6.16).

Following the procedure employed to derive the dynamic parameter C_s, we can arrive at a relation for C_θ, the equivalent parameter for the thermal diffusivity, through

$$\alpha_\theta = (C_\theta \overline{\Delta})^2 \mid S \mid \tag{6.18}$$

We get

$$(C_\theta \overline{\Delta})^2 = - \frac{\mathcal{L}^\theta{}_j \mathcal{M}^\theta{}_j}{\mathcal{M}^\theta{}_j \mathcal{M}^\theta{}_j} \tag{6.19}$$

where

$$\mathcal{L}^\theta{}_j = - (C_\theta \overline{\Delta})^2 \left[\frac{\widetilde{\overline{\Delta}}^2}{\overline{\Delta}^2} \mid \widetilde{\overline{S}} \mid \widetilde{\frac{\partial \overline{T}}{\partial x_j}} - \mid \overline{S} \mid \widetilde{\frac{\partial \overline{T}}{\partial x_j}} \right] \tag{6.20}$$

6.2.3 Turbulent Prandtl Number

The thermal diffusivity can be determined within the Newtonian closure framework using $\alpha_\theta = \nu_t / Pr_t$, but with the turbulent Prandtl number Pr_t, not α_θ, derived via the dynamic procedure of Germano (Moin *et al.*, 1991). Here as well, information on the resolvable flow and temperature fields serve to determine the dynamic Pr_t. The turbulent Prandtl number takes the following form:

$$Pr_t = (C_s \overline{\Delta})^2 \left[\frac{\widetilde{\overline{\Delta}}^2}{\overline{\Delta}^2} \mid \widetilde{\overline{S}} \mid \widetilde{\frac{\partial \overline{T}}{\partial x_j}} \frac{\partial \overline{T}}{\partial x_j} - \mid \overline{S} \mid \widetilde{\mid \overline{T} \mid} \right] \tag{6.21}$$

where

$$\mid \overline{T} \mid = \frac{\partial \overline{T}}{\partial x_j} \frac{\partial \overline{T}}{\partial x_j} \tag{6.22}$$

and $(C_s \overline{\Delta})^2$ is determined from Eq. (6.17).

Alternatively, a constant turbulent Prandtl number can be assumed, typically ($Pr_t \approx 0.85$). The turbulent Prandtl number can be also calculated based on the model proposed by Kays (1994) given as,

$$Pr_t = 0.85 + \frac{0.7}{Pr} \frac{\nu}{\nu_t} \tag{6.23}$$

where $Pr = \mu C_p/\lambda$ is the molecular Prandtl number, nu is the kinematic viscosity. As the grid is refined Pr_t tends towards large values. This is acceptable since the eddy thermal diffusivity tends to zero. However, it can be shown that the thermal diffusivity tends to zero much faster than the eddy kinematic viscosity.

6.2.4 The WALE Model

In the WALE concept (Nicoud & Ducros, 1999), the eddy viscosity is given as

$$\nu_t = (C_w \Delta)^2 \frac{(\mathcal{S}_{ij}^d \mathcal{S}_{ij}^d)^{3/2}}{(\bar{S}_{ij}\bar{S}_{ij})^{5/2} + (\mathcal{S}_{ij}^d \mathcal{S}_{ij}^d)^{5/4}} \tag{6.24}$$

where, $C_w = \sqrt{10.6\, C_s^2}$ and $\mathcal{S}_{ij}^d$ is defined as,

$$\mathcal{S}_{ij}^d = \frac{1}{2}(\bar{g}_{ij}^2 + \bar{g}_{ji}^2) - \frac{1}{3}\delta_{ij}\bar{g}_{kk}^2 \tag{6.25}$$

$$\bar{g}_{ij} = \frac{\partial \bar{u}_i}{\partial x_j} \tag{6.26}$$

where, $\bar{g}_{ij}^2 = \bar{g}_{ik}\bar{g}_{kj}$ and δ_{ij} is the Kronecker symbol.

6.3 Variable Turbulence Prandtl Number

Turbulent Prandtl number is given by Kays (Churchill, 2002)

$$Pr_t = 0.85 + \frac{0.7}{Pr}\left(\frac{\nu}{\nu_t}\right) \tag{6.27}$$

where ν_t is limited by

$$\nu_t = max(\nu_t, \frac{\nu}{F}) \tag{6.28}$$

$$F = \left(\frac{85 - 0.85}{0.7}\right) Pr \tag{6.29}$$

6.4 Wall treatment in LES

At high Reynolds number, resolving eddies in the near-wall region would require the use of a very fine mesh close to the wall. To avoid this, Near-wall treatment is available in TransAT.

6.4.1 The Werner-Wengle model

The Werner-Wengle wall law (Werner & Wengle, 1991) consists in a two-layer approximation, with an assumption that a $1/7^t h$ power law holds outside the viscous sub-layer. It can then be written

$$u^+ = \begin{cases} y^+ & \text{if} \quad y^+ \leq 11.8 \\ 8.3\,(y^+)^{1/7} & \text{if} \quad y^+ > 11.8 \end{cases} \tag{6.30}$$

with

$$y^+ = \frac{y u_\tau}{\nu} \tag{6.31}$$

$$u^+ = \frac{u}{u_\tau} \tag{6.32}$$

being the dimensionless wall distance and dimensionless velocity, respectively. ν is the kinematic viscosity and $u_\tau = \sqrt{\tau_w/\rho}$ is the wall shear stress velocity, with τ the shear at the wall and ρ the density. The wall shear stress is then computed using the instantaneous velocity in the flow.

6.5 Very-Large Eddy Simulation Concept (V-LES)

Very Large Eddy Simulation (V-LES) is based on the concept of filtering a larger part of turbulent fluctuations as compared to LES. This necessitates the use of a more complex sub–grid modelling strategy. The V-LES used in TransAT based on the use of the $k-\epsilon$ model as a sub–filter model. The filter width can be chosen by the user; it must be larger than the grid size. Increasing the filter width beyond the largest length scales in the flow, will lead to a standard RANS simulation, whereas in the limit of a small filter width the model will tend towards a large eddy simulation (although with a different sub–grid scale model).

The V-LES concept is based on the $k-\varepsilon$ model. A filter is applied to this model, so that turbulent structures smaller than the filter width are not solved. A length-scale limiting function f has been derived (Johansen *et al.*, 2004) and can be written

$$f\left(C_3 \frac{\Delta\varepsilon}{k^{3/2}}\right) = \text{Min}\left(1, C_3 \frac{\Delta\varepsilon}{k^{3/2}}\right) \tag{6.33}$$

where Δ is the filter width and

$$C_3 = \frac{\gamma}{4C_\mu\sqrt{3/2}} = 1.0 \tag{6.34}$$

is a new constant defined by Johansen *et al.* (2004), with $\gamma \leq 1$ the anisotropic factor and $C_\mu = 0.09$ the $k-\varepsilon$ constant. Applying this function to the $k-\varepsilon$ model gives the following expression for turbulent viscosity

$$\nu_t = C_\mu \text{Min}\left[1, C_3 \frac{\Delta\varepsilon}{k^{3/2}}\right] \frac{k^2}{\varepsilon} \tag{6.35}$$

Near the wall boundaries, the length-scale limiting function is equal to one, which means that the standard $k - \varepsilon$ model is applied. This enables one to use standard wall-function of RANS models for V-LES.

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