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The undersigned hereby certify that they have read and recommend to the Faculty of Aerospace Engineering for acceptance the thesis entitled **"Title"** by **Dikshant Sud** in fulfillment of the requirements for the degree of **Master of Science**.

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Chapter 1

Scalar Flux Modelling

In this chapter, an overview of the theory related to scalar flux and turbulence modelling is discussed. First, background on

1.1 Background on Navier Stokes and scalar fluxes

Fluid flows are governed by the Navier Stokes equations which can be expressed by equations 1.1 and 1.2 for incompressible flow of a Newtonian fluid without body forces. In these equations, u_i is the i-th component of the instantaneous velocity field, p is the instantaneous pressure field, ρ is the density and ν is the kinematic viscosity of the fluid.

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2} \tag{1.1}$$

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{1.2}$$

Along with these conservation of mass and momentum equations, simulations concerning the transport of a passive scalar quantity ϕ require an additional transport equation given in 1.3 without a source term. In equation 1.3, ϕ is considered a passive scalar because it has no effect on material and flow properties and Γ is the relevant molecular diffusivity parameter. For simulations concerning passive heat transfer, the instantaneous temperature (θ) can be identified as the scalar quantity with thermal diffusivity α as the relevant diffusivity constant [1].

$$\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} = \Gamma \frac{\partial^2 \phi}{\partial x_j^2} \tag{1.3}$$

The Navier Stokes equations can be solved exactly by resolving all time and length scales accurately by using a Direct Numerical Simulation (DNS) method. However, the computational effort to accurately resolve all fluid length and time scales for industry relevant flows is made impossible due to turbulence. Turbulence can be characterised as a collection of eddies over a range of different scales which are chaotic and unsteady in nature. The multi-scale properties of these turbulent eddies can be understood based on energy cascade and Kolmogorov's hypothesis for a fully turbulent flow at sufficiently high Reynold's number (Re) expressed in equation 1.4, with characteristic velocity $\mathcal{U}$ and length scale $\mathcal{L}$.

$$Re = \frac{\mathcal{U}\mathcal{L}}{\nu} \tag{1.4}$$

The largest eddies in the flow can be characterised with length scale l_0, characteristic velocity scale u_0 and time scale τ_0 for which the Reynolds number Re_0 is comparable to the flow Re. However, these large eddies are unstable and break-up to transfer energy to smaller eddies which undergo a similarly successive break-up process until a point of sufficiently small eddies with stable motion is reached where molecular viscosity acts to dissipate the kinetic energy of the eddies. According to Kolmogorov's hypothesis, these small scale eddies are statistically isotropic and exhibit universal behaviour that can be determined by ν and dissipation rate ϵ. Based on unit analysis, the characteristic length η, velocity u_η and time τ_η scales of these small scale Kolmogorov eddies are identified in equations 1.5-1.7 [2].

$$\eta = \left(\frac{\nu^3}{\epsilon}\right)^{1/4} \tag{1.5}$$

$$u_\eta = (\nu\epsilon)^{1/4} \tag{1.6}$$

$$\tau_\eta = \left(\frac{\nu}{\epsilon}\right)^{1/2} \tag{1.7}$$

The ratio between the largest and smallest turbulent scales can be expressed as a function of flow Re number as expressed in equations 1.8 and 1.9. As can be identified, the range of turbulent scales increase exponentially with flow Reynolds number. A DNS requires sufficiently small cell size and time step to accurately resolve the smallest eddies along with a suitable computational domain to capture the geometry and large eddies [2]. Therefore, with current computational resources, DNS of industry relevant flows, where Re can be in the order of 10^{6-8}, is impossible.

$$\frac{\eta}{l_0} = Re^{-3/4} \tag{1.8}$$

$$\frac{\tau_\eta}{\tau_0} = Re^{-1/2} \tag{1.9}$$

An alternative to DNS is the Large Eddy Simulation (LES) method where only the large energy containing eddies of turbulence are solved for and the effect of the small eddies is modelled. The velocity field is decomposed into the resolved component $\widetilde{\mathbf{u}}$ and unresolved subgrid-scale (SGS) component $\mathbf{u}^{\mathbf{sgs}}$ by using a filtering operation. The resolved component represents the motion of the large eddies for which the Navier Stokes equations are solved. The effect of the smaller scales is represented using the SGS tensor based on closure models that rely on assumptions of universal characteristics of small eddies [2].

Similar to the velocity field, LES of passive scalar transport involves filtering the scalar ϕ into resolved $\widetilde{\phi}$ component and subgrid-scale ϕ^{sgs} component. The SGS scalar flux σ_i, given by equation 1.10 is then closed by different models such as eddy diffusivity Smagorinsky model [3].

$$\sigma_i = \widetilde{u_i\phi} - \widetilde{u_i}\widetilde{\phi} \tag{1.10}$$

While LES models have grown in use for analysing fluid flows in recent years, they are still computationally intensive for industry relevant flows. Instead, solving the Reynolds Averaged Navier Stokes (RANS) equations is the most widely used method. The RANS equations can be obtained from the NS equations by (Reynolds) decomposing the velocity into a mean quantity $\bar{\mathbf{u}}$ and a fluctuating quantity $\mathbf{u}'$. The mean quantity represents the average value at a point over a fixed time interval. Similar decomposition is applied to the pressure and passive scalar to derive the full-form RANS equations [4].

$$\frac{\partial \overline{u}_j}{\partial x_j} = 0 \tag{1.11}$$

$$\frac{\partial \overline{u}_i}{\partial t} + \overline{u}_j \frac{\partial \overline{u}_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial^2 \overline{u}_i}{\partial x_j^2} - \frac{\partial \overline{u_i' u_j'}}{\partial x_j} \tag{1.12}$$

$$\frac{\partial \overline{\phi}}{\partial t} + \overline{u}_j \frac{\partial \overline{\phi}}{\partial x_j} = \Gamma \frac{\partial^2 \overline{\phi}}{\partial x_j^2} - \frac{\partial \overline{u_j' \phi'}}{\partial x_j} \tag{1.13}$$

Equations 1.11-1.13 represent the RANS equations wherein terms $\overline{u_i' u_j'}$ and $\overline{u_j' \phi'}$ represent the Reynolds stress tensor and scalar flux vector, respectively. The Reynold stress tensor R_{ij} represents six additional unknowns (symmetric tensor) that need to be modelled to close the RANS momentum equation. Similarly, the scalar flux vector leads to an additional three unknowns that represent turbulent scalar fluxed that need to be modelled for closure of the passive scalar transport equation (1.13).

As the focus of this thesis is on modelling of the heat transport equation, the scalar flux term is treated as the turbulent heat flux term (THF) for which the $\overline{u_i' \theta'}$ notation is adopted. Furthermore, Γ is treated as α whereby the thermal diffusivity is defined in equation 1.14, Pr is the molecular Prandtl number and θ represents the scalar temperature field. Finally, the focus of the thesis is on steady-state simulations and as such, the time-dependent gradient terms are dropped from the RANS equations for the rest of the report.

$$\alpha = \frac{\nu}{Pr} \tag{1.14}$$

1.2 Gradient diffusion models

The most widely adopted method for modelling the THF term is based on the gradient diffusion hypothesis wherein the scalar flux is linearly related to the mean temperature (scalar) gradient as given in equation 1.15. The diffusivity tensor ϵ_h^{ij} represents the most generalised form for these models but is typically reduced to a scalar value [5].

$$\overline{u_i' \theta'} = -\epsilon_h^{ij} \frac{\partial \overline{\theta}}{\partial x_i} \tag{1.15}$$

As mentioned, the most widely adopted gradient diffusion model assumes a singular scalar value to relate the THF to the mean scalar gradient called the gradient diffusion hypothesis (GDH). The underlying assumption of the GDH is that the turbulent transport of the scalar flux is down to the mean scalar gradient in the direction of $-\nabla \cdot \phi$ related with the turbulent diffusivity term α_t analogous to Fourier's law of heat conduction ([2]) which implies isotropic turbulence. A further simplification is also typically employed in the GDH model based on the Reynolds analogy that assumes a similarity between turbulent momentum exchange and turbulent heat transfer ([6]) described in equation 1.16.

$$\overline{u_i'\theta'} = -\alpha_t \frac{\partial \overline{\theta}}{\partial x_j} = \frac{Pr_t}{\nu_t}\frac{\partial \overline{\theta}}{\partial x_j} \tag{1.16}$$

In equation 1.16, Pr_t represents the turbulent Prandtl number and ν_t is the turbulent eddy viscosity. Pr_t can be characterised as a function of the turbulent shear stress, the turbulent heat flux, the velocity gradient and the temperature gradient ([7]). Based on these quantities, numerous experimental studies have been performed to obtain empirical relations for the Pr_t number.

The simplest model proposed by Reynolds assumes that heat and momentum are transferred by the same processes, and as such values of ν_t and α_t are the same leading to turbulent Prandtl number of unity ([8]). Kays ([7]) showed that such an assumption of a constant turbulent Prandtl number holds true for the unique case of turbulent flow over a flat plate (zero streamwise pressure gradient) and that a constant $Pr_t \approx 0.85$ number can be obtained based on curve fitting of the 'log-law' region of the thermal boundary layer. However, Kays also acknowledged the numerous limitation of applying this model for more complicated flow fields. Results from [9] and [10], evaluating the effect of pressure gradient on Pr_t, show that a favourable pressure gradient leads to an increase in Pr_t and an adverse pressure gradient leads to a decrease. Furthermore, Kays stated that the constant Pr_t only captures the log-law region of the thermal boundary layer but doesn't hold true for the sublayer and the 'wake' region at the outer edge of the thermal boundary layer. Instead, in the wake region, the Pr_t tends to decrease to 0.5-0.7 which represents the limitation of the model away from the wall. Alternatively, in the near-wall sublayer, empirical evidence shows a substantial increase in Pr_t ([11]). Kays also acknowledged that such a relation only holds true for moderate to high Pr number where molecular diffusivity is negligible in comparison to turbulent diffusivity.

To overcome these limitations, various algebraic equations have been proposed to calculate Pr_t analogous to the zero equation mixing length models for the closure of Reynolds stress tensor. A modification made to the constant Pr_t number was made by Jenkins who introduced the dependence of Pr_t on molecular Pr. Jenkins proposed a model based on heat conducting in or out of a turbulent eddy traversing orthogonal to the mean flow and proposed a relation based on the normalised turbulent eddy viscosity $\nu_t^+ = \frac{\nu_t}{\nu}$ and the Pr number. The Jenkins model showed good correlation with low to moderate Pr experimental flows but required additional factors for better correlation with empirical data at higher Prandtl number ($Pr = 0.7$) ([8]).

Cebeci ([8]) proposed a model for a wall-distance based turbulent Prandtl number inspired by Van Driest modelling of the viscous sublayer for Stokes flow and Prandtl's mixing length theory. The proposed model is defined by equation 1.17 and specified wall Pr_t prescribed by equation 1.18. In equation 1.17, expression for k_m, k_h, A and B are proposed based on analytical and experimental observations. In particular, expressions for k_m are based on Prandtl's mixing length concept for turbulent shear stress and value for A is empirically derived based on flat plate turbulent boundary layer data. Similarly, k_h and B are based on turbulent thermal boundary layer properties for incompressible flat plate flow.

$$Pr_t = \frac{k_m}{k_h}\frac{1-e^{-y/A}}{1-e^{-y/B}} \tag{1.17}$$

$$Pr_t = \frac{k_m}{k_h}\frac{B}{A} = \frac{k_m}{k_h}\frac{B^+}{A^{A+}} \tag{1.18}$$

Yokhot et al. [12] presented an analytical solution for the Pr_t based on the renormalisation group method to describe the process of heat transfer in turbulent pipe flow. They deduced a dependence of Pr_t on molecular Pr and the ratio $\frac{\nu_t}{\nu}$ and showed it's applicability to a wide range of Pr numbers where Pr_t converges to 0.85 for high values of $\frac{\nu_t}{\nu}$ ([13]). Further advancements in the modelling of the turbulent Prandtl number were proposed by [14]. With a modification introduced by [15], the extended formulation for the Pr_t was given in relation with the turbulent Peclet number (Pe_t) given in equation 1.19 where $Pr_{t,\infty}$ is given by expression 1.20. Furthermore, the Pe_t number is defined by equation 1.21 and constants C and D have values 0.31 and 100, respectively [13].

$$Pr_t = \frac{1}{\frac{1}{2Pr_{t,\infty}} + CPe_t\sqrt{\frac{1}{Pr_{t,\infty}}} - (CPe_t)^2\left(1 - e^{\frac{-1}{CPe_t\sqrt{Pr_{t,\infty}}}}\right)} \tag{1.19}$$

$$Pr_{t,\infty} = 0.85 + \frac{D}{PrRe^{0.888}} \tag{1.20}$$

$$Pe_t = Pr\frac{\nu_t}{\nu} \tag{1.21}$$

While these mixing length models improve the modelling of Pr_t for simple wall bounded flows, they are still poor for complex wall-free flows like scalar mixing due to jets. Furthermore, these models fail to account for transport phenomena like temperature fluctuations being transported from one area to another independent of the quality of locally modelled Pr_t [16].

Scalar variance models

Instead, one or two equation models can be adopted which solve additional transport equations to obtain turbulent thermal timescales to derive the appropriate turbulent diffusivity α_t as represented in equation 1.22. τ_m represents a hybrid time-scale which is a function of scalar time-scale for temperature fluctuation τ_θ and dynamic time-scale for turbulent eddies $\tau_u = \frac{k}{\epsilon}$.

$$\alpha_t = C_\lambda f_\lambda \tau_m \tag{1.22}$$

For turbulent heat transport, typically transport equations for thermal variance $k_\theta = \frac{\overline{\theta'^2}}{2}$ and thermal dissipation rate ϵ_θ are solved [17]. The thermal time-scale is resolved as $\tau_\theta = \frac{k_\theta}{\epsilon_\theta}$.

$$\frac{\mathcal{D}k_\theta}{\mathcal{D}t} = D_{k_\theta} + \mathcal{T}_{k_\theta} + \mathcal{P}_{k_\theta} - \epsilon_\theta \tag{1.23}$$

Equation 1.23 represents the full transport equation for k_θ. The left hand side term represents the advection of scalar variance represented using substantial derivative $\frac{\mathcal{D}()}{\mathcal{D}t} = \frac{\partial()}{\partial t} + u_j\frac{\partial()}{\partial x_j}$. The terms on the right hand side represent production $\mathcal{P}_{\theta_k}$, molecular diffusion D_{k_θ}, turbulent diffusion $\mathcal{T}_{k_\theta}$ and dissipation ϵ_θ given in equations 1.24 - 1.27, respectively.

$$\mathcal{P}_{k_\theta} = -\overline{u_j'\theta'}\frac{\partial\overline{\theta}}{\partial x_j} \tag{1.24}$$

$$\mathcal{T}_{k_\theta} = -\frac{\partial \overline{u'_j k'_\theta}}{\partial x_j} \tag{1.25}$$

$$D_{k_\theta} = \alpha \frac{\partial^2 k_\theta}{\partial x_j^2} \tag{1.26}$$

$$\epsilon_\theta = \alpha \overline{\frac{\partial \theta'}{\partial x_j} \frac{\partial \theta'}{\partial x_j}} \tag{1.27}$$

The triple correlation term in $\mathcal{T}_{k_\theta}$ (eq:1.25) and Reynolds averaging of fluctuating scalar field in ϵ_θ (eq:1.27) introduce additional unknowns that need to be modelled for the closure of the transport equation of k_θ. The turbulent diffusion term is typically approximated based on a gradient transport model which in a typical one or two equation model is given in equation 1.28 [17] [11]. For a second order closure model, the turbulent diffusion accounts for anisotropic turbulence by incorporating the resolved R_{ij} tensor as given in equation 1.29 [1].

$$\mathcal{T}_{k_\theta} = \frac{\partial}{\partial x_j}\left(\frac{\alpha_t}{\sigma_\theta}\frac{\partial k_\theta}{\partial x_j}\right) \tag{1.28}$$

$$\mathcal{T}_{k_\theta} = C_{k_\theta}\frac{\partial}{\partial x_j}\left(\frac{k}{\epsilon}\overline{u'_i u'_j}\frac{\partial k_\theta}{\partial x_j}\right) \tag{1.29}$$

For modelling the thermal variance dissipation, either a full transport equation for ϵ_θ is solved or an algebraic formulation based on a time scale ratio R given in equation 1.30. Based on the assumption that the ratio of thermal and dynamic time-scales is constant in an equilibrium boundary layer, a simple algebraic expression for ϵ_θ is proposed given in equation 1.31. Typically, a constant value of $R = 0.5$ is assumed [1]. However, the assumption of a constant time scale ratio through the whole domain doesn't hold true for even simple shear flows as shown by the DNS of passive scalar transport for turbulent channel flows [18] where R deviates significantly near-wall and at the channel centre. Furthermore, specifying wall and algebraic models for R can be as difficult as specifying Pr_t itself specially in flows where Pr differs from unity [16].

$$R = \frac{\tau_\theta}{\tau_u} \tag{1.30}$$

$$\epsilon_\theta = \frac{\epsilon}{R}\frac{k_\theta}{k} \tag{1.31}$$

To overcome the limitation of the constant time-scale ratio, a transport equation for ϵ_θ can be directly solved for given in equation 1.32. The transport equation for ϵ_θ has a similar structure to that of k_θ where D_{ϵ_θ} and $\mathcal{T}_{\epsilon_\theta}$ represent the molecular and turbulent diffusion of ϵ_θ. The equations for these terms has the same form as equations 1.26 and 1.25, respectively wherein k_θ can be replaced by ϵ_θ. The $\mathcal{P}^1_{\epsilon_\theta}$ - $\mathcal{P}^4_{\epsilon_\theta}$ represent the production terms. $\mathcal{P}^1_{\epsilon_\theta}$ represents production due to mean scalar gradient as shown in equation 1.33. Similarly, $\mathcal{P}^2_{\epsilon_\theta}$ represents production due to mean velocity gradient represented in equation 1.34. The other production terms, $\mathcal{P}^3_{\epsilon_\theta}$ and $\mathcal{P}^4_{\epsilon_\theta}$ represent the gradient and turbulent production, respectively shown in equations 1.35 and 1.36. Finally, $\Upsilon_{\epsilon_\theta}$ represents the destruction term given in equation 1.37 [19].

$$\frac{\mathcal{D}\epsilon_\theta}{\mathcal{D}t} = D_{\epsilon_\theta} + \mathcal{T}_{\epsilon_\theta} + \mathcal{P}^1_{\epsilon_\theta} + \mathcal{P}^2_{\epsilon_\theta} + \mathcal{P}^3_{\epsilon_\theta} + \mathcal{P}^4_{\epsilon_\theta} - \Upsilon_{\epsilon_\theta} \tag{1.32}$$

$$\mathcal{P}^1_{\epsilon_\theta} = -2\alpha \overline{\frac{\partial u'_j}{\partial x_k}\frac{\partial \theta'}{\partial x_k}}\frac{\partial \overline{\theta}}{\partial x_j} \tag{1.33}$$

$$\mathcal{P}^2_{\epsilon_\theta} = -2\alpha \overline{\frac{\partial \theta'}{\partial x_k}\frac{\partial \theta'}{\partial x_j}}\frac{\partial \overline{u_j}}{\partial x_k} \tag{1.34}$$

$$\mathcal{P}^3_{\epsilon_\theta} = -2\alpha \overline{u_j\frac{\partial \theta'}{\partial x_k}}\frac{\partial^2 \overline{\theta}}{\partial x_j \partial x_k} \tag{1.35}$$

$$\mathcal{P}^4_{\epsilon_\theta} = -2\alpha \overline{\frac{\partial u'_j}{\partial x_k}\frac{\partial \theta'}{\partial x_k}\frac{\partial \theta'}{\partial x_j}} \tag{1.36}$$

$$\Upsilon_{\epsilon_\theta} = 2\alpha^2 \overline{\left(\frac{\partial^2 \theta'}{\partial x_k \partial x_j}\right)^2} \tag{1.37}$$

The transport of ϵ_θ introduces additional unknowns that need to be modelled for the closure of equation 1.32. Numerous scalar variance and dissipation models have been proposed that provide a complete model for the k_θ and ϵ_θ equations along with equations for the hybrid time-scale τ_m [11].

One of the early scalar variance models was proposed by Nagano and Kim [20] (NK model), wherein the hybrid time-scale is modelled as $\tau_m = \sqrt{\tau_\theta \tau_u} = \tau_u\sqrt{2R}$. The turbulent diffusion terms for both scalar variance and dissipation is modelled based on gradient-diffusion models similar to the form of equation 1.28. The $\mathcal{P}^1_{\epsilon_\theta}$, $\mathcal{P}^2_{\epsilon_\theta}$, $\mathcal{P}^4_{\epsilon_\theta}$ and $\Upsilon_{\epsilon_\theta}$ are modelled together based on a linear combination of mean flow gradients and time-scale ratios given in equation 1.38.

$$\begin{aligned}\mathcal{P}^1_{\epsilon_\theta} + \mathcal{P}^2_{\epsilon_\theta} + \mathcal{P}^4_{\epsilon_\theta} + \Upsilon_{\epsilon_\theta} = & -C_{P1}f_{P1}\frac{2\epsilon_\theta}{k_\theta}\overline{u'_j\theta'}\frac{\partial\overline{\theta}}{\partial x_j} - C_{P2}f_{P2}\frac{\epsilon_\theta}{k}\overline{u'_iu'_j}\frac{\partial\overline{u_i}}{\partial x_j} \\ & - C_{D1}f_{D1}\frac{2\epsilon_\theta^2}{k_\theta} - C_{D2}f_{D2}\frac{\epsilon\epsilon_\theta}{k}\end{aligned} \tag{1.38}$$

For the remaining gradient production $\mathcal{P}^3_{\epsilon_\theta}$, an approximation given in equation 1.39 is proposed with α_t defined by equation 1.22. The model function f_λ along with individual model function terms in equation 1.38 are introduced to model wall proximity effects and the model coefficients are optimised for the case of homogeneous scalar turbulence.

$$\mathcal{P}^3_{\epsilon_\theta} = \alpha\alpha_t\left(1 - f_\lambda\right)\left(\frac{\partial^2\overline{\theta}}{\partial x_j \partial x_k}\right)^2 \tag{1.39}$$

The NK model showed improvements over the GDH models specially in cases like thermal entry region of a pipe where the Reynold's analogy doesn't hold true and Pr_t varies significantly [20]. However, further studies highlighted the limitation of the model for cases with varying wall temperature [11] as the τ_m time-scale, which characterises large scale motion, is applied adjacent to walls where small scale dissipation is more dominant [21].

Therefore, model improvements have been proposed that aim to better capture near-wall turbulence characteristics by altering the function for τ_m or adding damping functions. Nagano et al. [22] proposed a new ratio for time-scale $\tau_m = \tau_u(2R)^2$ and added damping functions to improve near wall characteristics. Such a formulation allows for high variation in τ_m for a given time-scale ratio R and thus, allows for smaller hybrid time-scale if the τ_θ and τ_u time-scales are modelled accurately. Abe et al. [23] introduced the widely adopted AKN model which introduces a new relation for $\tau_m = \frac{2}{\frac{1}{\tau_u}+\frac{0.5}{\tau_\theta}}$ based on a harmonic average of thermal and dynamic time-scales such that the shorter time-scale is more weighted. The AKN model also introduces a new normalisation factor $u_\epsilon \equiv (\nu\epsilon)^{1/4}$ instead of the friction velocity u_τ to avoid singularities at points of separation and attachment. Abe et al. [23] showed the improvements in predicting heat tranfer using the AKN model for the case of heat transfer downstream of a backward facing step. The AKN model improved the prediction of Pr_t specially in recirculation regions downstream of the step where Pr_t varies significantly and cannot be captured by algebraic Pr_t log-laws.

While one or two equation scalar variance models have shown to improve heat transfer modelling, these models are still limited by the underlying assumptions of the GDH model. These models do not address either the assumption of isotropic diffusivity or the assumption of alignment between mean scalar gradient and the scalar flux vector.

1.3 Algebraic scalar flux models

An alternative approach to the gradient-diffusion models are algebraic scalar flux or Algebraic heat flux (AHF) models which are derived from the full second order transport equations of the scalar fluxes. The exact transport equation for THF in symbolic form is represented in equation 1.40. In equation 1.40, the $\mathcal{P}_{i\theta}$ represents the production term which can be obtained exactly from equation 1.41. The $\Pi_{i\theta}$ represents the pressure-temperature gradient correlation given by equation 1.42. The $\epsilon_{i\theta}$ term represents dissipation given in equation 1.43. Finally, the term $D_{i\theta}$ represents the combined viscous diffusion, turbulent transport and pressure transport as given in equation 1.44 [24]. The $\Pi_{i\theta}$, $\epsilon_{i\theta}$ and $D_{i\theta}$ terms all introduce additional higher order terms that require modelling to close the full second order tranport equation for scalar fluxes.

$$\frac{\mathcal{D}\overline{u_i'\theta'}}{\mathcal{D}t} = \mathcal{P}_{i\theta} + \Pi_{i\theta} - \epsilon_{i\theta} + D_{i\theta} \tag{1.40}$$

$$\mathcal{P}_{i\theta} = -\left(\overline{u_j'\theta'}\frac{\partial \overline{u_i}}{\partial x_j} + \overline{u_i'u_j'}\frac{\partial \overline{\theta}}{\partial x_j}\right) \tag{1.41}$$

$$\Pi_{i\theta} = \overline{\frac{p'}{\rho}\frac{\partial \theta'}{\partial x_i}} \tag{1.42}$$

$$\epsilon_{i\theta} = (\alpha+\nu)\overline{\frac{\partial \theta'}{\partial x_j}\frac{\partial u_i'}{\partial x_j}} \tag{1.43}$$

$$D_{i\theta} = \frac{\partial}{\partial x_j}\left(\alpha\overline{\frac{\partial \theta'}{\partial x_j}u_i'} + \nu\overline{\theta'\frac{\partial u_i'}{\partial x_j}}\right) - \frac{\partial\overline{\theta' u_i'u_j'}}{\partial x_j} - \frac{1}{\rho}\frac{\partial\overline{\theta' p'}}{\partial x_i} \tag{1.44}$$

Of the highlighted terms in equation 1.40, the $\Pi_{i\theta}$ is identified as an important agent in transport of the scalar fluxes as it is found to reduce the scalar flux [25] and primarily balances scalar production $\mathcal{P}_{i\theta}$ [26].

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