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The energy equation for modeling reacting flows on RANS, LES and DES approaches

La ecuación de la energía para modelar flujos reactivos con enfoques RANS, LES y DES

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ABSTRACT: Computational Fluid Dynamics (CFD), through high-performance computing and robust codes, has proven to be an invaluable tool for the simulation of combustion processes, ranging from low speed diffusive flames up to detonations. This work intends to provide a review of details needed in modeling as Reynolds-averaged Navier-Stokes (RANS), large eddy simulation (LES) or Detached eddy simulation (DES) energy equation in CFD codes used for solving chemically reacting turbulent flows. When the density is variable, traditional Reynolds averages introduce many open correlations between any quantity f and density fluctuations $\rho'f'$ which are difficult to close. Therefore, Favre's mass-weighted average technique must be preferred.

RESUMEN: La mecánica de fluidos computacional por medio del uso de computación de alto desempeño y códigos robustos ha probado ser una herramienta invaluable para la simulación de procesos de combustión que incluyen llamas difusivas con bajas velocidades hasta detonaciones. Este trabajo pretende ofrecer una revisión de detalles relacionados con la ecuación de la energía necesaria en los códigos de mecánica de fluidos computacional para resolver flujos turbulentos químicamente activos. Cuando la densidad varía, los promedios de Reynolds introducen diferentes correlaciones entre las variables de interés f y las fluctuaciones de la densidad $\rho'f'$ que son difíciles de cerrar. En consecuencia, resultan más adecuados los promedios ponderados por la masa de Favre.

1. Introduction

Chemically reacting flows have several applications in engineering [1–10]. To accurately solve chemically reacting turbulent flows is a current challenge of the Computational Fluid Dynamics (CFD). It is known that a direct numerical simulation (DNS) is the best tool for the analysis of

It allows solving the whole range of spatial and temporal scales of turbulence without being necessary to implement turbulence models. But this technique, at least for now, is out of reach for all engineering applications [11–18]. The large eddies simulation (LES) technique, developed relying on the spectral filtering of the turbulent energy, is a better form of dealing with turbulence normally found in engineering applications [19–21]. The most suggested type of filtering implies the decomposition into different zones of the energy spectrum, starting from a wave number k_c the grid size Δ can be successively

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used as a cutoff filter while the wave number remains lower than another wave number k_d , previously selected at the far end of the spectrum. The application of the filtering process on the instantaneous equations leads to the filtered equations of conservation of the flow and on which, the turbulent sub-grid scales must be modeled to close the system of equations. LES thus appears as a good compromise between DNS which solve all the turbulent scales and RANS statistical model in which the whole flow structure is modeled. However, LES that accurately solves the viscous region of wall-bounded flows is very costly in computer time because of the refined mesh required near the wall. The number of grids increases to such an extent, that the use of LES in practical applications is not always feasible with reasonable computational resources [17, 22–24].

On the other hand, the RANS methodology based on statistical averages (or in a time averaging that is sufficiently large in comparison with the turbulent time scales, although small enough compared with the evolution time of the mean flow), appears well adapted to typical flows of engineering with reasonable cost in computations. However, it shows weaknesses in situations where the mean flow quantities are strongly affected by the dynamics of large-scale eddies [5, 25]. RANS models perform well in flows where the time variations of their average values are of much lower frequency than the turbulence itself [26]. This is the field of applications of RANS and unsteady URANS [5, 15, 27–30].

Considering the limitations of RANS to treat unsteady flows and, the high computational cost with LES, a detached eddy simulation called DES has been developed as a hybrid approach to merge LES and RANS [31]. DES is an unsteady numerical simulation which functions as a sub grid scale (SGS) model in regions where the grid density is fine enough for LES, and as a RANS model where it is not. However, the main argument that allows building DES is that the RANS and LES averaged motion equations can take exactly the same mathematical form. The mass-weighted average technique proposed by Favre [32, 33], is used to derive the average equations of conservation of mass, momentum, energy, and species.

This work is intended to describe details about the equation of energy in modeling turbulent flows by different approaches, which later shall be implemented in CFD codes to compute chemically reactive flows. It should be noted that the turbulent energy equation to be developed will contain several additional unknown terms which must be modeled for closure of the equation prior to solving it.

2. The sensible energy of chemically reacting species

For a mixture of N reacting species Y_k , the sensible + chemical enthalpy h (Equation 1) is defined by [34]:

$$\begin{aligned} h &= \sum_{k=1}^N h_k Y_k \\ &= \sum_{k=1}^N \left(\int_{T_0}^T C_{p,k} dT + \Delta h_{f,k}^o \right) Y_k \\ &= \int_{T_0}^T C_p dT + \sum_{k=1}^N \Delta h_{f,k}^o Y_k \end{aligned} \quad (1)$$

where $C_{p,k}$ is the mass heat capacity at constant pressure of species k , and $C_p = \sum_{k=1}^N C_{p,k} Y_k$ is the mass heat capacity at constant pressure of the mixture. $\Delta h_{f,k}^o$ is the formation enthalpy of species k , and $\sum_{k=1}^N \Delta h_{f,k}^o Y_k$ is the chemical enthalpy related to the whole reacting process.

The sensible energy $e_{s,k}$ (Equation 2) and sensible enthalpy $h_{s,k}$ of any species k , are related by [34]

$$e_{s,k} = h_{s,k} - \frac{p_k}{\rho_k} = \int_{T_0}^T C_{p,k} dT - \frac{RT}{W_k} \quad (2)$$

and then, the sensible + chemical energy e for the mixture of N reacting species becomes [34]

$$\begin{aligned} e &= \sum_{k=1}^N e_{s,k} Y_k \\ &= \sum_{k=1}^N \left(\int_{T_0}^T C_{p,k} dT - \frac{RT}{W_k} + \Delta h_{f,k}^o \right) Y_k \\ &= \sum_{k=1}^N \left(\int_{T_0}^T C_{v,k} dT - \frac{RT_0}{W_k} + \Delta h_{f,k}^o \right) Y_k \end{aligned} \quad (3)$$

To obtain Equation 3, the relation between the mass heat capacities (Equation 4) [34]

$$C_{p,k} - C_{v,k} = \frac{R}{W_k} \quad (4)$$

has also been used. Note that the R is the universal gas constant and W_k the molecular weight of species.

Finally, e (Equation 5) can be written as [34]

$$\begin{aligned} e &= \int_{T_0}^T C_v dT - \frac{RT_0}{W} + \sum_{k=1}^N \Delta h_{f,k}^o Y_k \\ &= e_s + \sum_{k=1}^N \Delta h_{f,k}^o Y_k \end{aligned} \quad (5)$$

where $C_v = \sum_{k=1}^N C_{v,k} Y_k$, and e_s is the non-chemical sensible energy involving all the species.

2.1 The total energy

Let's consider first the conservation equation for total energy [$e_t = e + \frac{1}{2}u_i u_i$] (Equation 6), as it is given by Kuo [34]:

$$\frac{\partial \rho e_t}{\partial t} + \frac{\partial (\rho u_i e_t)}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_i} (\sigma_{ij} u_j) \quad (6)$$

The heat flux q_i (Equation 7) is written [34]

$$q_i = -\lambda \frac{\partial T}{\partial x_i} + \rho \sum_{k=1}^N h_k Y_k V_{k,i} \quad (7)$$

and includes, first a heat diffusion term expressed by Fourier's law and a second term associated with different enthalpies which is specific to a gas with multi-species. Viscous and pressure tensors are combined into the σ_{ij} tensor [$\sigma_{ij} = \tau_{ij} - p \delta_{ij}$]. External heat source terms due, for example, to an electric spark, a laser or radiation flux whose rates usually written $\dot{Q}$, are not accounted. The power produced by volume forces f_k on any species ($\rho \sum_{k=1}^N Y_k f_{k,i} (u_i + V_{k,i})$), is also not accounted.

The above expression for total energy (Equation 6), is not always easy to implement in classical CFD codes because they use expressions for the energy, including chemical terms in addition to the sensible energy. Furthermore, the heat flux includes new transport terms. The use of only sensible energies (or enthalpies) are sometimes preferred [32, 34].

2.2 The use of a total non-chemical energy

The sum of sensible and kinetic energies leads to a total non-chemical energy [$E = e_s + \frac{1}{2}u_i u_i$, Equation 8], and the equation for E becomes [34]:

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_i} (\rho E u_i) = \dot{\omega}_T + \frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_i} (\sigma_{ij} u_j) \quad (8)$$

where

$$\dot{\omega}_T = -\sum_{k=1}^N \Delta h_{f,k}^o \dot{\omega}_k \quad (9)$$

is the total rate of heat release due to chemical activity (Equation 9) of all species. If the pressure p is added to ρE can be obtained Equation 10: [34]

$$\rho E + p = \rho \left(e_s + \frac{p}{\rho} + \frac{1}{2} u_i u_i \right) = \rho \left(h_s + \frac{1}{2} u_i u_i \right) = \rho H \quad (10)$$

being H the non-chemical total enthalpy. The left term of Equation 8 can now be written [34]

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_i} (\rho H u_i)$$

and the total energy equation for E (Equation 11) that will be used for now on is [34]:

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_i} (\rho H u_i) = \dot{\omega}_T + \frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_i} (\tau_{ij} u_j) \quad (11)$$

2.3 Reynolds and Favre averages

The time-averaged equations are obtained by decomposing each flow variable into a mean and a fluctuating part. In constant density flows, Reynolds averages consist in splitting any quantity f into a mean $\bar{f}$ and a fluctuating f' component [$f = \bar{f} + f'$]. However, Reynolds averages in variable density flows introduce many other unclosed correlations between any quantity f and density fluctuations $\rho' f'$. To avoid this difficulty, mass-weighted averages (Favre averages, Equation 12) are preferred [32, 34-37]:

$$\bar{\rho} \tilde{f} = \overline{\rho f} \quad (12)$$

Therefore, any quantity f splits into mean and fluctuating components as $f = \bar{f} + f''$. Note that time averages of double primed fluctuating quantities are not equal to zero. Instead, the time average of the double primed fluctuation multiplied by the density ($\overline{\rho f''}$) gives (Equation 13)

$$\overline{\rho f} = \overline{\rho (\bar{f} + f'')} = \overline{\rho \bar{f}} + \overline{\rho f''} \rightarrow \overline{\rho f''} = 0 \quad (13)$$

($\bar{f}$) averages. Comparisons between numerical simulations providing Favre averages $\tilde{f}$ with experimental data, are not obvious. Most experimental techniques provide Reynolds averages $\bar{f}$ (for example, when averaging thermocouple data). Differences between ($\bar{f}$) and ($\tilde{f}$) may be significant [32].

2.4 Favre's averages applied to the total energy equation

Substituting the decomposed variables in Equation 12 and Equation 13 into the energy Equation 11 and averaging the results, the desired time averaged energy equation (Equation. 14) can be written [32]:

$$\frac{\partial \bar{\rho} \tilde{E}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{H} \tilde{u}_i) = \frac{\partial}{\partial x_i} (-\bar{q}_i + \overline{\tau_{ij} \tilde{u}_j} + \overline{\tau_{ij} u_j''} - \bar{\rho} \widetilde{H'' u_i''}) + \bar{\omega}_T \quad (14)$$

For a Newtonian fluid, the average stress tensor ($\overline{\tau_{ij}}$, Equation. 15) is modeled as follows [38]:

$$\overline{\tau_{ij}} \approx \mu \left(\frac{\partial \tilde{u}_j}{\partial x_i} + \frac{\partial \tilde{u}_i}{\partial x_j} \right) - \frac{2}{3} \mu \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ji} \quad (15)$$

This approximation implies that the effects of turbulent fluctuations on the molecular viscosity (μ) are ignored, and the conventional ($\overline{u_i}$) and mass-weighted ($\tilde{u}_i$) average velocities are approximately equal.

The term $\overline{\tau_{ij} u_j''}$ is well approximated (Equation 16) for non-compressible flows by the following expression [38]

$$\overline{\tau_{ij} u_j''} \approx \mu \frac{\partial \tilde{k}}{\partial x_i} \quad (16)$$

where $\tilde{k}$ is the turbulent kinetic energy (Equation 17) [38]

$$\tilde{k} = \frac{1}{2} \widetilde{u_i'' u_i''} \quad (17)$$

For compressible flows, it can be assumed that this relationship remains valid.

The time average heat flux vector $\overline{q_i}$ contains contributions from heat conduction and an energy flux due to inter-species diffusion (Equation 7). If turbulent fluctuations effects are ignored when evaluating the thermal conductivity (λ), as it was done with the viscosity (μ), the contribution of heat conduction (Equation 18) can be written [38]

$$\overline{\lambda \frac{\partial T}{\partial x_i}} = \lambda \frac{\partial \overline{T}}{\partial x_i} \quad (18)$$

The energy flux due to inter-species diffusion will be considered later and its treatment will depend on the model chosen for the species diffusion velocity. So, the term to be next modeled is $\overline{\rho H'' u_i''}$.

The average mass-weighted total enthalpy (Equation 19) written regarding the static enthalpy h and kinetic energy terms, is [32]

$$\tilde{H} = \tilde{h} + \frac{1}{2} (\tilde{u_j u_j} + 2\tilde{k}) \quad (19)$$

and from its instantaneous expansion it is obtained

$$\tilde{H} + H'' = \tilde{h} + h'' + \frac{1}{2} (\tilde{u_j u_j} + \tilde{u_j u_j''} + \tilde{k} + k'') \quad (20)$$

Now, subtracting Equation. 19 from Equation 20, only the fluctuating component of the total enthalpy (Equation 21) remains, i.e.

$$H'' = h'' + \tilde{u_j u_j''} + k'' \quad (21)$$

The unclosed correlation $\overline{\rho H'' u_i''}$ given in Equation 14, can be expanded to yield [32]

$$\overline{\rho H'' u_i''} = \underbrace{\overline{\rho h'' u_i''}}_I + \underbrace{\overline{\rho \tilde{u_j u_j''} u_i''}}_{II} + \underbrace{\overline{\rho k'' u_i''}}_{III} \quad (22)$$

The first of the terms on the right side of Equation 22 is the Reynolds heat flux vector, which has historically been modeled using the gradient diffusion hypothesis (Equation 23). This model leads to the following expression for the Reynolds heat flux [32]

$$\overline{\rho h'' u_i''} = -\frac{\mu_t}{Pr_t} \frac{\partial \tilde{h}}{\partial x_i} \quad (23)$$

The turbulent Prandtl number (Pr_t), determines the ratio of the rate of turbulent momentum transport to rate of turbulent energy transport. Constant values for the Prandtl number are usually assumed, even though it has

been shown to vary spatially [39].

The third term $\overline{\rho k'' u_i''}$ (Equation 24) represents turbulent transport of the turbulent kinetic energy, and the gradient diffusion approximation is commonly used to model this term [32],

$$\overline{\rho k'' u_i''} = -\frac{\mu_t}{\sigma_k} \frac{\partial \tilde{k}}{\partial x_i} \quad (24)$$

where μ_t is the eddy viscosity and σ_k is a closure coefficient defined by the chosen model for turbulence.

The second term of the right side of Equation (22), is the dot product of the mean velocity with the Reynolds stress tensor. It is closed based on the model chosen for the Reynolds stress tensor. The most common closures used for the Reynolds stress tensor are linear models based on the Boussinesq approximation as shown in Equation 25 [32]

$$\begin{aligned} \overline{\rho u_j'' u_i''} = & \frac{2}{3} \left(\overline{\rho k} + \mu_t \frac{\partial \tilde{u_k}}{\partial x_k} \right) \delta_{ij} \\ & - \mu_t \left(\frac{\partial \tilde{u_j}}{\partial x_i} + \frac{\partial \tilde{u_i}}{\partial x_j} \right) \end{aligned} \quad (25)$$

This model assumes that the Reynolds stress components are related to the mean strain rate tensor through an isotropic eddy viscosity (μ_t). Models for the eddy viscosity vary from simple algebraic (zero equation) models [40], which require specification of a turbulent velocity and length scale, to two equations models [38, 41, 42]. In the two equations models, two partial differential equations are solved, one for the turbulent kinetic energy ($\tilde{k}$), and other for the dissipation rate per unit mass $\tilde{\varepsilon}$ or for an average turbulent dissipation rate $\tilde{\omega}$. In the former approach, the $\tilde{k} - \tilde{\varepsilon}$ model is achieved, and in the second one the $\tilde{k} - \tilde{\omega}$.

Algebraic models are numerically robust and easy to implement (at least for simple geometries). However, they require changes in their coefficients when applied to different types of flow fields and ambiguity often arise when defining turbulence scales for complex geometries. Two-equation models have a more extensive range of applicability into complex geometries where it may be challenging to determine applicable turbulent scales algebraically. Nevertheless, one equation models that involve solving a transport equation for a quantity that can be directly related to the eddy viscosity [43, 44] have gained popularity in recent years.

2.5 The RANS approach

For the RANS approach, closure models are based on a two-equation system that defines a transport equation for $\tilde{k}$ and an additional transport equation. This additional

equation is based either on the average dissipation rate per unit mass $\tilde{\varepsilon}$ or an average turbulence dissipation rate $\tilde{\omega}$ ($\tilde{k}-\tilde{\varepsilon}$ or $\tilde{k}-\tilde{\omega}$ models). The shear stress transport (SST) models developed by Menter, the SST from 1994 [41] and the SST from 2003 [45] are adopted and here are presented.

Standard Menter SST Two-Equations model (SST-1994)

The Menter basic idea, is to keep the formulation of Wilcox's $\tilde{k}-\tilde{\omega}$ [38, 41, 46] model applicable in inner parts of the boundary layer and all the way down to the wall, and take advantage of the Wilcox's $\tilde{k}-\tilde{\varepsilon}$ model [38] in areas where it performs better (free streams flows, especially in the presence of adverse pressure gradients and in separating flows). To achieve its objective, Menter transforms the $\tilde{k}-\tilde{\varepsilon}$ model into a variant of the Wilcox's $\tilde{k}-\tilde{\omega}$ model, adding a term called cross-diffusion and also, changing the closing constants as the distance from the contour wall increases. The procedure followed by Menter to obtain his $\tilde{k}-\tilde{\omega}-SST$ model is presented next [45].

Wilcox $\tilde{k}-\tilde{\omega}$ original model (Equation 26 and Equation 27) ¹ [41]:

$$\frac{\partial(\tilde{\rho}\tilde{k}_R)}{\partial t} + \frac{\partial(\tilde{\rho}\tilde{u}_i\tilde{k}_R)}{\partial x_i} = P - \beta^* \tilde{\rho}\tilde{\omega}\tilde{k}_R + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_{k1}\mu_{t,R}) \frac{\partial \tilde{k}_R}{\partial x_i} \right] \quad (26)$$

$$\frac{\partial(\tilde{\rho}\tilde{\omega})}{\partial t} + \frac{\partial(\tilde{\rho}\tilde{u}_i\tilde{\omega})}{\partial x_i} = \frac{\gamma_1}{\nu_t} P - \beta_1 \tilde{\rho}\tilde{\omega}^2 + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_{\omega 1}\mu_{t,R}) \frac{\partial \tilde{\omega}}{\partial x_i} \right] \quad (27)$$

Menter proposed variation of the Wilcox's $\tilde{k}-\tilde{\omega}$ original model (Equation 28 and Equation 29) [41]:

$$\frac{\partial(\tilde{\rho}\tilde{k}_R)}{\partial t} + \frac{\partial(\tilde{\rho}\tilde{u}_i\tilde{k}_R)}{\partial x_i} = P - \beta^* \tilde{\rho}\tilde{\omega}\tilde{k}_R + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_{k2}\mu_{t,R}) \frac{\partial \tilde{k}_R}{\partial x_i} \right] \quad (28)$$

$$\frac{\partial(\tilde{\rho}\tilde{\omega})}{\partial t} + \frac{\partial(\tilde{\rho}\tilde{u}_i\tilde{\omega})}{\partial x_i} = \frac{\gamma_2}{\nu_t} P - \beta_2 \tilde{\rho}\tilde{\omega}^2 + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_{\omega 2}\mu_{t,R}) \frac{\partial \tilde{\omega}}{\partial x_i} \right] + 2 \frac{\rho\sigma_{\omega 2}}{\tilde{\omega}} \frac{\partial \tilde{k}_R}{\partial x_i} \frac{\partial \tilde{\omega}}{\partial x_i} \quad (29)$$

Multiplying each term of Equation. 26 by a sort of blending function F_1 (later to be defined), and each term of Equation.

28 by $(1 - F_1)$ and after adding both, the equation for the energy k_R of the turbulence is obtained [41]:

$$\frac{\partial(\tilde{\rho}\tilde{k}_R)}{\partial t} + \frac{\partial(\tilde{\rho}\tilde{u}_i\tilde{k}_R)}{\partial x_i} = P - \beta^* \tilde{\rho}\tilde{\omega}\tilde{k}_R + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_k\mu_{t,R}) \frac{\partial \tilde{k}_R}{\partial x_i} \right] \quad (30)$$

Proceeding in the same way with Equations 27 and 29, it can be obtained [41]

$$\frac{\partial(\tilde{\rho}\tilde{\omega})}{\partial t} + \frac{\partial(\tilde{\rho}\tilde{u}_i\tilde{\omega})}{\partial x_i} = \frac{\gamma}{\nu_t} P - \beta \tilde{\rho}\tilde{\omega}^2 + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_{\omega}\mu_{t,R}) \frac{\partial \tilde{\omega}}{\partial x_i} \right] + 2(1 - F_1) \frac{\tilde{\rho}\sigma_{\omega 2}}{\tilde{\omega}} \frac{\partial \tilde{k}_R}{\partial x_i} \frac{\partial \tilde{\omega}}{\partial x_i} \quad (31)$$

The last two equations (Equations 30 and 31) are those of Menter model. The closing constant are obtained applying the relation given by Equations 32 [41]

$$\phi = F_1\phi_1 + (1 - F_1)\phi_2 \quad (32)$$

being ϕ_1 and ϕ_2 given by Equation 33 [41]

$$\phi_i = [\sigma_{ki}, \sigma_{\omega i}, \beta_i, \beta_i^*, \gamma_i] \quad (i = 1,2) \quad (33)$$

An illustrative example of the use of Equation 32 for calculating the constants in Equations 30 and 31 is here included:

First, the last term of Equation 26 is multiplied by F_1

$$\frac{\partial}{\partial x_i} \left\{ [F_1\mu + F_1\sigma_{k1}\mu_{t,R}] \frac{\partial \tilde{k}_R}{\partial x_i} \right\}$$

Second, the last term of Equation 28 is multiplied by $(1 - F_1)$, obtaining

$$\frac{\partial}{\partial x_i} \left\{ [(1 - F_1)\mu + (1 - F_1)\sigma_{k2}\mu_{t,R}] \frac{\partial \tilde{k}_R}{\partial x_i} \right\}$$

Adding the term coming from Equation 22 to the term coming from Equation 28, the result is [41]

$$\frac{\partial}{\partial x_i} \left\{ [\mu + (F_1\sigma_{k1} + (1 - F_1)\sigma_{k2}) \mu_{t,R}] \frac{\partial \tilde{k}_R}{\partial x_i} \right\}$$

and finally applying the relation defining ϕ (Equation 32), the above term reduces to

$$\frac{\partial}{\partial x_i} \left[(\mu + \sigma_k\mu_{t,R}) \frac{\partial \tilde{k}_R}{\partial x_i} \right]$$

which is the way it is, shown in Equation 30.

Constants of the set ϕ_1 – Wilcox and of the set ϕ_2 – Menter, are presented in Table 1.

¹The subscript R stands for RANS

Table 1 Coefficients of turbulence closure models

	σ_k	σ_ω	β	β^*	γ
ϕ_1 – Wilcox	0.85	0.5	0.075	0.09	$\frac{\beta_1}{\beta^*} - \frac{\sigma_{\omega 1} \kappa^2}{\sqrt{\beta^*}}$
ϕ_2 – Menter	1.0	0.856	0.0828	0.09	$\frac{\beta_2}{\beta^*} - \frac{\sigma_{\omega 2} \kappa^2}{\sqrt{\beta^*}}$

Additional functions needed to complete the Menter model are given by Equations 34, 36 and 37 [41]

$$P = t_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} \quad (34)$$

being t_{ij} the turbulent stress tensor given by Equation 35 [46]

$$t_{ij} = \mu_{t,R} \left[\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right] - \frac{2}{3} \tilde{\rho} \tilde{k}_R \delta_{ij} \quad (35)$$

The function F_1 [41, 47], that it is used to couple the constants of the Wilcox and Menter models, is

$$F_1 = \tanh \left\{ \min \left[g, \frac{4 \tilde{\rho} \sigma_{\omega 2} \tilde{k}_R}{CD_{k\omega} d^2} \right] \right\}^4 \quad (36)$$

where g is given by:

$$g = \max \left(2 \frac{\sqrt{\tilde{k}_R}}{0.09 \tilde{\omega} d}, \frac{500 \mu}{\tilde{\rho} \tilde{\omega} d^2} \right)$$

and $CD_{k\omega}$ by

$$CD_{k\omega} = \max \left(2 \tilde{\rho} \sigma_{\omega 2} \frac{1}{\tilde{\omega}} \nabla \tilde{k}_R \cdot \nabla \tilde{\omega}, 10^{-20} \right) \quad (37)$$

and d is the distance from the field point to the nearest wall, it should be noted that the function F_1 has been designed so that its value is 1 in areas close to contour surfaces and 0 in distant areas.

The turbulent eddy viscosity $\mu_{t,R}$ [Equations 38] is given as [41]

$$\mu_{t,R} = \frac{\tilde{\rho} \alpha_1 \tilde{k}_R}{\max(\alpha_1 \tilde{\omega}, \Omega F_2)} \quad (38)$$

where $\alpha_1 = 0.31$, $\Omega = \sqrt{2 W_{ij} W_{ij}}$, $W_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i} \right)$ and the function F_2 [Equations 39], is defined as [47]

$$F_2 = \tanh \left[\max \left(2 \frac{\sqrt{\tilde{k}_R}}{0.09 \tilde{\omega} d}, \frac{400 \mu}{\tilde{\rho} \tilde{\omega} d^2} \right) \right] \quad (39)$$

Menter SST Two-Equations Model from 2003 (SST-2003)

The SST Menter from 2003 has introduced several changes to the SST from 1994. The main one is the definition of the eddy viscosity [Equation 40] which is now written [45]

$$\mu_t = \frac{\rho \alpha_1 \tilde{k}_R}{\max(\alpha_1 \tilde{\omega}, SF_2)} \quad (40)$$

where $S = \sqrt{2 S_{ij} S_{ij}}$ and $S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$. That is, in the definition of eddy viscosity, it is no longer used the magnitude of vorticity. The function P in both the $\tilde{k}$ and $\tilde{\omega}$ equations is replaced by $\min(P, 10 \beta^* \rho \tilde{\omega} \tilde{k})$, which implies the introduction of a limiter to P values. The definition of $CD_{k\omega}$ is changed by using in its second term 10^{-10} , instead of 10^{-20} . Finally, constants γ_1 and γ_2 are slightly different (the value γ_1 is $\sim 0.43\%$ higher than the original one and the value γ_2 is lower by 0.08%)

2.6 The LES approach

The closure problem in LES can be approached in a similar way as in RANS by defining an alternative to Equation 26. Following [48], one equation model is presented that defines the transport equation for $\tilde{k}_L$ as shown in Equation 41 (The subscript L stands for LES).

$$\frac{\partial(\tilde{\rho} \tilde{k}_L)}{\partial t} + \frac{\partial(\tilde{\rho} \tilde{u}_i \tilde{k}_L)}{\partial x_i} = P - C_d \frac{\tilde{\rho} \tilde{k}_L^{\frac{3}{2}}}{\Delta} + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_k \mu_{t,L}) \nabla \tilde{k}_L \right] \quad (41)$$

where t_{ij} [the turbulent stress tensor, Equation 35], is given substituting $\tilde{k}_R$ with $\tilde{k}_L$ and the eddy viscosity $\mu_{t,R}$ [Equation 42] with $\mu_{t,LES}$:

$$\mu_{t,L} = \rho C_s \Delta \sqrt{\tilde{k}_L} \quad (42)$$

where Δ is the characteristic length of cells. It implies the decomposition into different zones of the energy spectrum concerning a cutoff wave number k_c , given by the grid size. Yoshizawa's model assumes Δ to be the cubic root of the cell volume. In Equations 41 and 42, C_d and C_s constants are related to the Smagorinsky constant C_{smag} [Equation 43] [49].

$$C_{smag} = \left(\frac{C_s^3}{C_d} \right)^{0.25} \quad (43)$$

The Smagorinsky constant typically ranges from 0.065 to 0.2 and on any work, a constant value has to be assumed within the range given (Yoshizawa's values for the constant C_s and C_d are 0.046 and 1.0 respectively). Furthermore, the value for $\sigma_k = 1.0$.

2.7 The DES approach

The detached eddy simulation (DES) was developed as a hybrid approach to merge LES and RANS. The reason behind the development of DES is to attempt to reduce the number of points required for accurately solve the flow close to the wall in 3D simulations. To solve with LES the flow close to the wall, that is in less than 10% the size of the computational domain, over 90% of the grid points are needed [50]. To overcome this difficulty, the RANS approach is used close to the wall where it is known to provide accurate mean boundary layer predictions.

Equations 26 and 41, RANS and LES models, can be blended together (Equation 44), resulting in the following $\tilde{k}$ transport equation [47]

$$\frac{\partial(\tilde{\rho}\tilde{k})}{\partial t} + \frac{\partial(\tilde{\rho}\tilde{u}_i\tilde{k})}{\partial x_i} = P - \left[\Gamma\beta^*\tilde{\rho}\tilde{\omega}\tilde{k} + (1-\Gamma)C_d\frac{\tilde{\rho}\tilde{k}^{\frac{3}{2}}}{\Delta} \right] + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_k\mu_t)\nabla\tilde{k} \right] \quad (44)$$

The eddy viscosity μ_t (Equation 45) is obtained by blending the $\mu_{t,R}$ and $\mu_{t,LES}$ in the following manner

$$\mu_t = \Gamma\mu_{t,R} + (1-\Gamma)\mu_{t,LES} \quad (45)$$

The blending function Γ (Equation 46) is defined as

$$\Gamma = \tanh \left[\max \left(\frac{\sqrt{\tilde{k}_R}}{0.09\tilde{\omega}d}, \frac{500\mu}{\tilde{\rho}\tilde{\omega}d^2} \right) \right]^4 \quad (46)$$

Depending on the value of Γ , there are three possible regions in the flow:

1. The RANS region, where $\Gamma = 1$. The closure is given by equations 30 and 31, and $k = \tilde{k}_R$.
2. The LES region where $\Gamma = 0$. Equation (41) recovers and leads to $k = \tilde{k}_{LES}$.
3. An intermediate region where Γ is less than 1, but greater than 0. In this region, equation (44) applies.

Note that the $\tilde{\omega}$ transport equation is solved everywhere in the computational domain to guarantee continuity, but it is not used in regions where LES is applicable.

2.8 The energy flux due to inter-species diffusion

The diffusion velocity of any species k is usually evaluated from Fick's law as shown in Equation 47 [32].

$$V_{k,i} = -\frac{D_k}{Y_k} \frac{\partial Y_k}{\partial x_i} \quad (47)$$

when the Reynolds averaged equation set is considered. It is usually accepted that the turbulent diffusion can also be

expressed through Fick's law. Further, it is also assumed that V_i and D are the same for all species, assumption justified by the premise that an "effective" turbulent diffusion dominates the molecular diffusion processes throughout most of the flow field. Then [32]

$$\overline{\rho Y_k V_i} = -\overline{\rho D} \frac{\partial \overline{Y_k}}{\partial x_i} \quad (48)$$

and

$$\sum_{k=1}^N \overline{\rho Y_k V_i h_{s,k}(T)} = -\sum_{k=1}^N \overline{\rho D h_{s,k}(T) \frac{\partial Y_k}{\partial x_i}} \quad (49)$$

These two expressions (Equations 48 and 49) simplify to the following (Equations 50 and 51) [32]:

$$\overline{\rho D} \frac{\partial \overline{Y_k}}{\partial x_i} \approx \overline{\rho D} \frac{\partial \widetilde{Y_k}}{\partial x_i} \quad (50)$$

$$\sum_{k=1}^N \overline{\rho D h_{s,k}(T) \frac{\partial Y_k}{\partial x_i}} \approx \sum_{k=1}^N \overline{\rho D h_{s,k}(\widetilde{T}) \frac{\partial \widetilde{Y_k}}{\partial x_i}} \quad (51)$$

which implies that turbulent fluctuations effects are neglected on the mixture diffusivity, and conventional averages assumed equivalent to mass weighted averages. It is worth noting that the effect of temperature fluctuations on species enthalpy has to be ignored to arrive at the above expression for the averaged interspecies diffusion terms. The turbulent transport of a scalar property has always been modeled using the gradient diffusion approach. For instance, the Reynolds mass flux (Equations 52) can be modeled as [32]

$$\overline{\rho Y_k'' u_j''} = -\frac{\mu_t}{S_{c_t}} \frac{\partial \widetilde{Y_k}}{\partial x_i} \quad (52)$$

The turbulent Schmidt (S_{c_t}) number defines the ratio of the turbulent momentum transport rate to the turbulent mass transport rate. Constant values for the Schmidt number are usually assumed in applications of engineering interest, even though values for this coefficient have been shown to vary spatially [39].

The terms that generally require most attention by model developers are: the Reynolds stress tensor ($\overline{\rho u_j'' u_i''}$), Reynolds heat flux vector ($\overline{\rho h'' u_i''}$), Reynolds mass flow vector ($\overline{\rho Y_k'' u_i''}$), and the chemical source term ($\dot{\omega}_k$). The turbulent diffusion rates are controlled by turbulent Prandtl (Pr_t) and Schmidt (S_{c_t}) numbers. Constant values for these numbers are usually assumed in applications (in low as well as in high speed reacting flows of engineering interest), even though values for these coefficients have been shown to vary spatially [Table 2, [39]].

Numerical studies have suggested that when attempting to characterize high-speed devices (that contain a variety of different mechanisms) with constant turbulent transport coefficients, care is required.

Table 2 Turbulent Prandtl and Schmidt number values

Flow Fields	Pr _t	Sc _t
Planar Jets	0.2 - 3.0	0.1 - 2.2
Round Jets	0.7 - 2.0	0.1 - 2.0
Backward Facing Step	0.7 - 3.0	NA
Jet into Cross Flow	NA	0.1 - 0.5
Injection behind a Blunt Body	NA	0.2 - 0.7

3. Chemical production rates

The most common species production rates used for reacting flows are built based on a laminar chemistry formulation. This approach based on laminar chemistry assumption ignores turbulence-chemistry interactions by evaluating the chemical source terms based only on mean flow properties. Any of the reactions between the N species, can be written in a compact form as shown in Equations 53 and 54 [51]

$$\sum_{k=1}^N \nu_{kl}^R [C_k] \xrightarrow{k_l^f} \sum_{k=1}^N \nu_{kl}^P [C_k] \quad (53)$$

$$\sum_{k=1}^N \nu_{kl}^P [C_k] \xrightarrow{k_l^b} \sum_{k=1}^N \nu_{kl}^R [C_k] \quad (54)$$

where ν_{kl}^R and ν_{kl}^P are the reactant and product stoichiometric coefficients for species k , k_l^f and k_l^b the forward and backward rate constants of any reaction l from the total number of reactions nR . $[C_k]$ is the molar concentration of species k involved. After introducing the mass reaction rates $(\rho Y_k / W_k)$, being W_k the molecular weight of the species, the rate progress $(RP)_l$ [Equation 55] of reaction l can now be written as follows [34]:

$$(RP)_l = k_l^f \prod_{k=1}^N \left(\rho \frac{Y_k}{W_k} \right)^{\nu_{kl}^R} - k_l^b \prod_{k=1}^N \left(\rho \frac{Y_k}{W_k} \right)^{\nu_{kl}^P} \quad (55)$$

If forward rates and the equilibrium constants are used to determine backward rates [32, 34], the rate production of species k due to reaction l , is written in the form shown in Equation 56

$$\dot{\omega}_{kl} = W_k \alpha_l (\nu_{kl}^P - \nu_{kl}^R) (RP)_l \quad (56)$$

Note that on the rate production $\dot{\omega}_{kl}$ for species k , the factor α_l accounts for third body effects. Finally, the total rate of species k is the nR sum of rates $\dot{\omega}_{kl}$ [Equation 57] produced by each reaction, therefore [34]

$$\dot{\omega}_k = \sum_{l=1}^{nR} \dot{\omega}_{kl} \quad (57)$$

This value $\dot{\omega}_k$ is used when the heat released $\dot{\omega}_T$, due to chemical activity of all the species is computed [Equation 9]. The matrix of stoichiometric coefficients resulting from any chemical system has dimension $N \times nR$, and from this matrix, a set of N stiff ODES in each control volume and time step, must be assembled and solved [52].

4. The model for the equation of state

It is assumed that the fluid behaves as a mixture of perfect gas (Equation 58). Therefore the pressure p is given by [32]

$$p = \sum_{k=1}^N p_k = \sum_{k=1}^N \rho_k \frac{R}{W_k} T = \rho R \left(\sum_{k=1}^N \frac{Y_k}{W_k} \right) T \quad (58)$$

Since the mixture gas constant (Equations 59) is defined by [34]

$$R_{mix} = R \sum_{k=1}^N \frac{Y_k}{W_k} \quad (59)$$

the equation of state (Equations 60) can now be written as [34]

$$\bar{p} = \overline{\rho R_{mix} T} = \bar{\rho} R_{mix} (\bar{Y}_k) \bar{T} \quad (60)$$

where to minimize closure difficulties, the effects of composition fluctuations on the equation of state are neglected

5. Conclusions

In this paper, essential aspects of RANS, LES, and DES methodologies for turbulence modeling are described. The needed theoretical formalism to develop and closure an energy equation applicable to turbulent reactive flows was discussed. This work was motivated because the authors consider that models built based on theoretical arguments are more satisfactory than models built from practical arguments, even if a practical model provides better results for one specific case. However, in industrial as well as in academic environments, the available computational framework has a strong influence when decisions are to be made.

6. Declaration of competing interest

I declare that I have no significant competing interests including financial or non-financial, professional, or personal interests interfering with the full and objective presentation of the work described in this manuscript.

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8. Authors contributions

Tamagno J.P, Elaskar S.A and Gutiérrez Marcantoni L. F performed the research, data collection, analysis and writing.

9. Data availability statement

The author confirms that the findings of this study are available within the article.

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