DNS of reacting flows and mixture-averaged model

The continuity and momentum governing equations of DNS are given as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = S_\rho, \tag{2.1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho u_i u_j - \tau_{ij} + p\right] = S_{u_i}, \tag{2.2}$$

where ρ, $\boldsymbol{u}$ and p are the mixture density, flow velocity and pressure, respectively. u_i is the velocity component along Cartesian coordinate x_i direction. τ_{ij} is the stress tensor. $\tau_{ij} = \mu(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - 2/3\frac{\partial u_j}{\partial x_j}\delta_{ij})$, μ is the dynamic viscosity. δ_{ij} is the Kronecker symbol: $\delta_{ij} = 1$ if $i = j$, 0 otherwise. S denotes the potential external source term for corresponding variables.

The species and energy conservation equations of DNS on reacting flows can be written as:

$$\frac{\partial (\rho Y_k)}{\partial t} + \frac{\partial (\rho(u_i + V_{i,k})Y_k)}{\partial x_i} = \omega_k + S_Y, \tag{2.3}$$

$$\frac{\partial [\rho(h_s + K)]}{\partial t} + \frac{\partial [\rho u_i(h_s + K)]}{\partial x_i} = \frac{\partial p}{\partial t} + \nabla \cdot \boldsymbol{q} + \omega_h + S_h, \tag{2.4}$$

where Y_k, h_s, K, ω_k and ω_h denote the mass fraction, sensible enthalpy, turbulent kinetic energy, species formation rate and reaction heat release, respectively. $\boldsymbol{V}_k$ is the diffusion velocity of the k_{th} species. In the mixture-averaged formula, $\boldsymbol{V}_k$ is assumed to be composed of three parts:

$$\boldsymbol{V}_k = \boldsymbol{V}_{MD} + \boldsymbol{V}_{TD} + \boldsymbol{V}_C, \tag{2.5}$$

$\boldsymbol{V}_{MD}$ is the molecular diffusion velocity and is given in the Curtiss-Hirschfelder approximation:

$$\boldsymbol{V}_{MD} = -D_{km}\frac{1}{X_k}\frac{\partial X_k}{\partial x_i}, \tag{2.6}$$

where D_{km} is the mixture-averaged diffusion coefficient and X_k is the mole fraction. $\boldsymbol{V}_{TD}$ denotes the Ludwig–Soret effect, which represents the diffusion of lower molecular weight species from low to high temperature regions. It is given as:

$$\boldsymbol{V}_{TD} = -D_{kT}\frac{1}{T}\frac{\partial T}{\partial x_i}, \tag{2.7}$$

where D_{kT} is the Soret diffusion coefficient and T is the mixture temperature. $\boldsymbol{V}_C$ is the correction velocity to ensure the global mass conservation (the mass fractions sum to unity), which is often done by the formula:

$$\boldsymbol{V}_C = -\sum_k^N Y_k(\boldsymbol{V}_{MD} + \boldsymbol{V}_{TD}), \tag{2.8}$$

N is the total species number.

The q in the energy conservation equation is:

$$q = \lambda \frac{\partial T}{\partial x_i} + \sum_k^N h_{sk}(\rho Y_k V_k) + p \sum_k^N D_{kT} d_k, \tag{2.9}$$

where the first term is the heat conduction and the second term is heat flux associated with species diffusion of different enthalpies. The last term is the Dufour effect, in which d_k is given as:

$$d_k = \frac{\partial X_k}{\partial x_i} + (X_k - Y_k)\frac{1}{p}\frac{\partial p}{\partial x_i}. \tag{2.10}$$

Above equation permits simplification that the spatial pressure fluctuation is small for low-Mach flows so that the second term in the right-hand side can be neglected.

In order to close the equation system, two models are applied here. One is the mixture-averaged model, which is used to model the transport properties, e.g., species mass diffusion coefficients, mixture viscosity. Another is the chemical kinetic mechanism which describes the species formation rate and chemical heat release rate. Here, the dependence of transport properties of species on temperature and pressure is prescribed by third-order logarithm polynomial fitting equations, as shown below:

$$\ln C_k = \sum_{r=1}^3 a_{n,k}(\ln T)^{r-1}, \tag{2.11}$$

$$\ln D_{kl} = \left(\sum_{r=1}^3 b_{n,kl}(\ln T)^{r-1} \right)\frac{p}{p_{std}}, \tag{2.12}$$

where C_k is the viscosity or thermal conductivity of species i, and D_{ij} is the binary diffusivity of species i and species j. p_{std} denotes the standard atmosphere pressure. The mixture dynamic viscosity and thermal conductivity are calculated from the pure species. The Wilke formula for mixture viscosity is given by:

$$\mu = \sum_{k=1}^N \frac{X_k \mu_k}{\sum_{l=1}^K X_l \varphi_{kl}}, \tag{2.13}$$

$$\varphi_{kl} = \frac{1}{\sqrt{8}}\left[\left(1 + \frac{M_k}{M_l}\right)^{-0.5}(1 + (\frac{\mu_k}{\mu_l})^{0.5}\left(\frac{M_k}{M_l}\right)^{0.25})^2\right]. \tag{2.14}$$

The combination averaging formula is used for mixture-averaged thermal conductivity:

$$\lambda = \frac{1}{2}(\sum_{k=1}^N X_k \lambda_k + \frac{1}{\sum_{k=1}^N X_k/\lambda_k}), \tag{2.15}$$

where, X_k and M_k are the mole fraction and molecular mass of species k. D_{km} is calculated by:

$$D_{km} = \frac{\sum_{k \neq l}^N X_l M_l}{M \sum_{k \neq l}^N X_l/D_{kl}}. \tag{2.16}$$

It should be noted that the diffusion term in the species equation can be further

modified by using the relation between mole fraction and mass fraction $X_k = \frac{Y_k/M_k}{1/M} = MY_k/M_k$:

$$\frac{\partial}{\partial x_i}\left(\rho Y_k D_{km}\frac{1}{X_k}\frac{\partial X_k}{\partial x_i}\right) = \frac{\partial}{\partial x_i}\left(\rho D_{km}\left(\frac{\partial Y_k}{\partial x_i}+\frac{Y_k}{M}\frac{\partial M}{\partial x_i}\right)\right). \tag{2.17}$$

In addition, the derivation of h_s is:

$$\rho\frac{Dh_s}{Dt} = \sum_{k=1}^{N} h_{sk}\rho\frac{DY_k}{Dt} + \rho C_p\frac{DT}{Dt}. \tag{2.18}$$

Using this derivation in the heat conduction term in the energy conservation equation gives:

$$\frac{\partial}{\partial x_i}\left(\lambda\frac{\partial T}{\partial x_i}\right) = \frac{\partial}{\partial x_i}\left(\frac{\lambda}{C_p}\frac{\partial h_s}{\partial x_i} - \sum_{k=1}^{N} h_{sk}\frac{\lambda}{C_p}\frac{\partial Y_k}{\partial x_i}\right). \tag{2.19}$$

To do so, part of the diffusion term can be treated with an implicit scheme.

The thermal diffusion coefficient D_{kT} is calculated from the thermal diffusion ratio θ_k, as shown below:

$$D_{kT} = \frac{D_{km}\theta_k}{X_k}, \tag{2.20}$$

$$\theta_k = \sum_{j\neq k}^{N} \theta_{kj}, \tag{2.21}$$

where $\theta_{kj}/(X_k X_j)$ is prescribed by third-order polynomial fitting equations on temperature.