

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

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

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} [\rho u_i u_j - \tau_{ij} + p] = S_u,$$

where ρ , 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. $\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - 2/3 \frac{\partial u_k}{\partial x_k} \delta_{ij} \right)$, μ is the dynamic viscosity. δ_{ij} is the Kronecker symbol: $\delta_{ij} = 1$ if $i = j$, 0 otherwise. S_ρ and S_u are the potential external source term for mass and momentum, respectively.

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

$$\frac{\partial (\rho Y_k)}{\partial t} + \frac{\partial (\rho (u_i + v_k^c) Y_k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho D_k \frac{M_k}{M} \frac{\partial X_k}{\partial x_i} \right) + \omega_k + S_Y,$$

$$\frac{\partial [\rho (h_s + K)]}{\partial t} + \frac{\partial [\rho u_i (h_s + K)]}{\partial x_i} = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \nabla \cdot \left(\rho \sum_k^N h_{sk} \left(\rho D_k \frac{M_k}{M} \frac{\partial X_k}{\partial x_i} + v_k^c Y_k \right) \right) + \omega_h + S_h,$$

$$v_k^c = \sum_{k=0}^{ns} D_k \frac{M_k}{M} \frac{\partial X_k}{\partial x_i},$$

where Y_k , X_k , M_k , h_{sk} , M , h_s , K , D_k , λ and C_p denote the mass fraction of species k , mole fraction of species k , molecular mass of species k , sensible enthalpy of species k , mean molecular weight of the mixture, sensible enthalpy of the mixture, turbulent kinetic energy, mass diffusivity of species k , thermal conductivity and heat capacity, respectively. N is the total species number. The third term in the right-hand side of energy conservation equation is the heat flux associated with species diffusion of different enthalpies. v_k^c is the correction velocity to ensure mass conservation and ns is the number of chemical species. In order to close the equation, two models are applied here. One is the mixture transport properties model, which is used to get the transport properties, e.g., species mass diffusion coefficients. Another is the chemical kinetic mechanism which describes the species formation rate and chemical heat release rate. S_Y and S_h are the potential external source term for species and energy, respectively. Here, the mixture-averaged model is used. The dependence of transport properties of species on temperature and pressure is prescribed by third-order logarithm ($N = 3$) polynomial fitting equations, as shown below:

$$\ln C_k = \sum_{n=1}^N a_{n,k} (\ln T)^{n-1},$$

$$\ln D_{kl} = (\sum_{n=1}^N b_{n,kl} (\ln T)^{n-1}) p/p_{\text{std}},$$

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 viscosity and thermal conductivity are calculated from the pure species. The Wilke formula for mixture viscosity is given by:

$$\mu = \sum_{k=1}^N \frac{X_k \mu_k}{\sum_{l=1}^K \frac{X_l \phi_{kl}}{\mu_l}}$$

where,

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

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

$$\lambda = \frac{1}{2} \left(\sum_{k=1}^N X_k \lambda_k + \frac{1}{\sum_{k=1}^N X_k / \lambda_k} \right)$$

where, X_k and M_k are the mole fraction and molecular mass of species k . D_k is calculated by:

$$D_k = \frac{\sum_{l \neq k}^N \frac{X_l M_l}{M}}{\sum_{l \neq k}^N \frac{X_l}{D_{kl}}}$$

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 $X_k = \frac{Y_k/M_k}{1/M} = MY_k/M_k$:

$$\frac{\partial}{\partial x_i} \left(\rho D_k \frac{M_k}{M} \frac{\partial X_k}{\partial x_i} \right) = \frac{\partial}{\partial x_i} \left(\rho D_k \left(\frac{\partial Y_k}{\partial x_i} + \frac{Y_k}{M} \frac{\partial M}{\partial x_i} \right) \right)$$

In addition, the derivation of h_s is:

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

Using this derivation in the thermal diffusion term in the energy conservation equation gives:

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

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