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

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho u_{\mathrm{j}}}{\partial x_{\mathrm{j}}}=S_{\rho},$$

$$\frac{\partial \rho u_i}{\partial t}+\frac{\partial}{\partial x_{\mathrm{j}}}\left[\rho u_{\mathrm{i}} u_{\mathrm{j}}-\tau_{\mathrm{ij}}+p\right]=S_{\mathrm{u}},$$

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. $\tau_{\mathrm{ij}}=\mu(\frac{\partial \mathrm{u_i}}{x_{\mathrm{j}}}+\frac{\partial \mathrm{u_j}}{x_{\mathrm{i}}}-2/3\frac{\partial \mathrm{u_j}}{x_{\mathrm{j}}}\delta_{\mathrm{ij}})$, μ is the dynamic viscosity. δ_{ij} is the Kronecker symbol: δ_{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:

$$\frac{\partial(\rho Y_{\mathrm{k}})}{\partial t}+\frac{\partial(\rho(u_{\mathrm{i}}+v_{\mathrm{k}}^{\mathrm{c}})Y_{\mathrm{k}})}{\partial x_{\mathrm{i}}}=\frac{\partial}{\partial x_{\mathrm{i}}}\left(\rho D_{\mathrm{k}}\frac{M_{\mathrm{k}}}{M}\frac{\partial X_{\mathrm{k}}}{\partial x_{\mathrm{i}}}\right)+\omega_{\mathrm{k}}+S_{\mathrm{Y}},$$

$$\frac{\partial[\rho(h_{\mathrm{s}}+K)]}{\partial \mathrm{t}}+\frac{\partial[\rho u_{\mathrm{i}}(h_{\mathrm{s}}+K)]}{\partial x_{\mathrm{i}}}=\frac{\partial p}{\partial t}+\frac{\partial}{\partial x_{\mathrm{i}}}\left(\lambda\frac{\partial \mathrm{T}}{\partial x_{\mathrm{i}}}\right)+\nabla\cdot\left(\rho\sum_{\mathrm{k}}^{\mathrm{N}} h_{\mathrm{sk}}\left(\rho D_{\mathrm{k}}\frac{M_{\mathrm{k}}}{M}\frac{\partial X_{\mathrm{k}}}{\partial x_{\mathrm{i}}}+v_{\mathrm{k}}^{\mathrm{c}} Y_{\mathrm{k}}\right)\right)+\omega_{\mathrm{h}}+S_{\mathrm{h}},$$

$$v_{\mathrm{k}}^{\mathrm{c}}=\sum_{\mathrm{k}=0}^{\mathrm{N}} D_{\mathrm{k}}\frac{M_{\mathrm{k}}}{M}\frac{\partial X_{\mathrm{k}}}{\partial x_{\mathrm{i}}},$$

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. $v_{\mathrm{k}}^{\mathrm{c}}$ is the correction velocity to ensure mass conservation. 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:

$$\ln \mathrm{C_k} = \sum_{\mathrm{n=1}}^{\mathrm{N}} a_{\mathrm{n,k}}(\ln T)^{n-1},$$
$$\ln \mathrm{D_{kl}} = \left(\sum_{\mathrm{n=1}}^{\mathrm{N}} b_{\mathrm{n,kl}}(\ln T)^{n-1}\right)p/p_{\mathrm{std}},$$

where $\mathrm{C_k}$ is the viscosity or thermal conductivity of species i, and $\mathrm{D_{ij}}$ 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:

$$\mu = \sum_{\mathrm{k=1}}^{\mathrm{N}} \frac{X_{\mathrm{k}}\mu_{\mathrm{k}}}{\sum_{\mathrm{l=1}}^{\mathrm{K}} X_{\mathrm{l}}\phi_{\mathrm{kl}}}$$

where,

$$\phi_{\mathrm{kl}} = \frac{1}{\sqrt{8}}\left[\left(1+\frac{M_{\mathrm{k}}}{M_{\mathrm{j}}}\right)^{-0.5}\left(1+\left(\frac{\mu_{\mathrm{k}}}{\mu_{\mathrm{l}}}\right)^{0.5}+\left(\frac{M_{\mathrm{k}}}{M_{\mathrm{j}}}\right)^{0.25}\right)^{2}\right]$$

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

$$\lambda = \frac{1}{2}\left(\sum_{\mathrm{k=1}}^{\mathrm{N}} X_{\mathrm{k}}\lambda_{\mathrm{k}} + \frac{1}{\sum_{\mathrm{k=1}}^{\mathrm{N}} X_{\mathrm{k}}/\lambda_{\mathrm{k}}}\right)$$

where, X_{k} and M_{k} are the mole fraction and molecular mass of species k. $\mathrm{D_k}$ is calculated by:

$$D_{\mathrm{k}} = \frac{\sum_{\mathrm{k\neq l}}^{\mathrm{N}} X_{\mathrm{l}}M_{\mathrm{l}}}{M\sum_{\mathrm{k\neq l}}^{\mathrm{N}} X_{\mathrm{l}}/D_{kl}}$$

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 $X_{\mathrm{k}} = \frac{Y_{\mathrm{k}}/M_{\mathrm{k}}}{1/M} = MY_{\mathrm{k}}/M_{\mathrm{k}}$:

$$\frac{\partial}{\partial x_{\mathrm{i}}}\left(\rho D_{\mathrm{k}}\frac{M_{\mathrm{k}}}{M}\frac{\partial X_{\mathrm{k}}}{\partial x_{\mathrm{i}}}\right) = \frac{\partial}{\partial x_{\mathrm{i}}}\left(\rho D_{\mathrm{k}}\left(\frac{\partial Y_{\mathrm{k}}}{\partial x_{\mathrm{i}}}+\frac{Y_{\mathrm{k}}}{M}\frac{\partial \mathrm{M}}{\partial x_{\mathrm{i}}}\right)\right)$$

In addition, the derivation of h_{s} is:

$$\rho\frac{Dh_{\mathrm{s}}}{Dt} = \sum_{\mathrm{k=1}}^{\mathrm{N}} h_{\mathrm{sk}}\rho\frac{DY_{\mathrm{k}}}{Dt} + \rho C_{\mathrm{p}}\frac{D\mathrm{T}}{Dt}$$

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

$$\frac{\partial}{\partial x_{\mathrm{i}}}\left(\lambda\frac{\partial \mathrm{T}}{\partial x_{\mathrm{i}}}\right) = \frac{\partial}{\partial x_{\mathrm{i}}}\left(\frac{\lambda}{C_{\mathrm{p}}}\frac{\partial h_{\mathrm{s}}}{\partial x_{\mathrm{i}}} + \sum_{\mathrm{k=1}}^{\mathrm{N}} h_{\mathrm{sk}}\rho\frac{\partial Y_{\mathrm{k}}}{\partial x_{\mathrm{i}}}\right)$$

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