

Supplementary Material

1. Conservation equations

The evolution of a mixed-gas system is governed by the flow dynamics, the chemical reactions and the turbulence modeling. The set of transport equations represent the conservation of mass, momentum, energy and chemical species. These governing equations are briefly described in this section. For more in-depth scientific detail, the reader may consult for example [1].

The conservation equation for a generic variable ϕ (velocity components, enthalpy, energy, mass fractions...) that governs the fluid flow is

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho\phi\vec{v}) - \nabla \cdot (\Gamma_\phi \nabla\phi) = S_\phi , \quad (1)$$

where ∇ is a vector differential operator $(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$, ρ is the fluid density, $\vec{v} = (u, v, w)$ is the velocity vector, Γ_ϕ the diffusion coefficient and S_ϕ the source term. Both the fluid density and the diffusion coefficient are fluid properties. This conservation equation is also known as the transport equation. Hence, the first term is the temporal variation of ϕ , the second one is the convective term and the third one is the diffusive term.

1.1. Navier-Stokes equations

Mass and momentum conservation are described by the well-known Navier-Stokes equations. The PDE of the mass conservation is the so-called continuity equation,

$$\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\vec{v}) = 0 , \quad (2)$$

where ρ and \vec{v} are the density and the velocity vector of the mixture respectively. Usually, in most of the combustion problems, the density is calculated using the ideal gas law as

$$\rho = \frac{P\bar{M}}{RT} , \quad (3)$$

with R being the universal gas constant, P the total pressure, T the temperature and \bar{M} the average molecular weight of the mixture, defined as

$$\bar{M} = \left(\sum_{\alpha=1}^{N_\alpha} \frac{Y_\alpha}{M_\alpha} \right)^{-1} , \quad (4)$$

where Y_α and M_α are the mass fraction and the molecular weight of the species α respectively.

On the other hand, the momentum conservation is derived from the Newton's Second Law, and it is described by

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla P + \nabla \cdot \tau + \rho f , \quad (5)$$

where f are the body forces acting on the fluid and τ is the viscous stress tensor related with the surface forces. In this type of problems, gravitational acceleration (g) is the only body force that has to be taken into account.

Since the mixture of gases can be considered as a Newtonian fluid, the stress tensor is expressed as

$$\tau = \mu (\nabla \vec{v} + (\nabla \vec{v})') - \frac{2}{3} \mu (\nabla \cdot \vec{v}) I , \quad (6)$$

with μ being the dynamic viscosity and I the identity tensor.

1.2. Chemical species conservation

In a mixture of N_α species, the mass fraction of a single chemical species is defined by

$$Y_\alpha = \frac{m_\alpha}{m_T} , \quad (7)$$

where m_α is the mass of the species α and m_T is the total mass of the mixture. In terms of the mass fraction, the species conservation for a single species is described by

$$\frac{\partial}{\partial t}(\rho Y_\alpha) + \nabla \cdot (\rho \vec{v} Y_\alpha) = -\nabla \cdot J_\alpha + S_\alpha, \quad \alpha = 1, \dots, N_\alpha , \quad (8)$$

where J_α and S_α are the diffusive flux and the net formation rate of the species α respectively. The diffusive flux, J_α , has three components: the gradient of species, the gradient of temperature (Soret effect), and the gradient of pressure. The effect of temperature and pressure gradients is usually neglected in combustion fluxes [2]. Therefore, J_α only considers the mass diffusion due to the gradient of species, according to the Fick's Law. In terms of the Schmidt number, S_c , the diffusive flux of a species can be written as

$$J_\alpha = -\Gamma_\alpha \nabla Y_\alpha = -\frac{\mu}{S_{c_\alpha}} \nabla Y_\alpha , \quad (9)$$

where the Schmidt number of the species α , S_{c_α} , is defined by

$$S_{c_\alpha} = \frac{\mu}{D_\alpha \rho} , \quad (10)$$

being D_α the diffusion coefficient of the species α .

1.3. Energy conservation

Total energy in a fluid volume is, in general, the sum of internal energy u , kinetic energy k , and potential energy p :

$$e = u + k + p . \quad (11)$$

By introducing the relationship between internal energy u and enthalpy H , described as

$$u = \frac{H + PV}{m_T} , \quad (12)$$

where V is the total volume of the mixture, the conservation equation for the energy can be described with the following enthalpy transport equation:

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho v h) = \frac{\partial P}{\partial t} + v \cdot \nabla P - \nabla \cdot J_h + \Phi_v + S_h . \quad (13)$$

Enthalpy h can be defined in terms of the specific enthalpy h_α of each species α , as:

$$h = \sum_{\alpha=1}^{N_\alpha} Y_\alpha h_\alpha \quad (14)$$

$$h_\alpha = h_\alpha^0 + \int_{T_0}^T C_{p,\alpha}(T) dT , \quad (15)$$

where $C_{p,\alpha}$ is the specific heat at constant pressure of species α and h_α^0 the specific enthalpy of formation at the reference temperature, T_0 .

Pressure terms in Eq. 13 can be neglected in the context of this thesis because they are only relevant when large pressure gradients are present (e.g. detonation problems [2]). Besides, the term Φ_v , which represents the viscous dissipation, can be also neglected. Hence, Eq. 13 is simplified as:

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \vec{v} h) = -\nabla \cdot J_h + S_h , \quad (16)$$

where J_h represents the heat diffusive flux and S_h accounts for any additional volumetric source term of enthalpy. The heat diffusive flux, J_h , has also three components: the gradient of temperature (Fourier's Law), the gradient of concentrations (Dufour effect) and the last one related with the diffusive flux of the chemical species. In combustion problems, the last two terms are often neglected [2]. Thus, the term J_h is expressed by the Fourier's Law as

$$J_h = -\kappa \nabla T , \quad (17)$$

being κ the thermal conductivity of the mixture.

2. Passive transported scalar

The definition of a passive transported scalar in a CFD code can be used to track any stream that enters the system. This marker physically follows the flow coming from the corresponding inlet boundary condition by solving an additional transport equation similar to Eq. 1. This equation captures all the phenomena (unsteadiness, convection, and diffusion) of a scalar ϕ , which stands for the concentration of a generic species. The so-called 'passive' term implies that it does not undergo any creation or destruction process in the flow, so the source terms (S_ϕ) are null. The procedure can be summarized in the following steps:

1. Enable a generic transport equation (Eq. 1) for the whole fluid zone.
2. Specify the boundary conditions of the scalar (ϕ) as:
 - primary stream (in this case, partially premixed air-fuel inlet) \rightarrow Scalar marker $\phi = 1$,
 - secondary air stream (air coflow) \rightarrow Scalar marker $\phi = 0$.
3. Define the effective diffusivity of the scalar ϕ as

$$\Gamma_\phi = \Gamma + \Gamma_t, \quad (18)$$

which takes into account both the molecular (Γ) and the turbulent (Γ_t , if applicable) contribution. Both diffusion terms can be estimated by invoking the Schmidt number S_c definition as in Eqs. 9 and 10.

4. Solve the transport equation, enabling the location of the spatial distribution of primary and secondary air:
 - $\phi = 1 \rightarrow$ 100% primary air, 0% secondary air.
 - $\phi = 0 \rightarrow$ 0% primary air, 100% secondary air.
5. Given the local mass fraction of oxygen (Y_{O_2}), obtain the corresponding fractions that come from either the primary or the secondary streams:
 - $(Y_{O_2})_{prim} = Y_{O_2} * \phi$
 - $(Y_{O_2})_{sec} = Y_{O_2} * (1 - \phi)$

References

- [1] T. Poinsot, D. Veynante, Theoretical and Numerical Combustion: Second Edition, Edwards, 2005.
- [2] J. Warnatz, U. Maas, R. Dibble, Combustion: Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation, Springer-Verlag Berlin Heidelberg, 2006.