Conservation laws for one- and multi-component gases with and without source terms

Generalized Euler equations with non-equilibrium chemistry

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1 Generalized Euler equations

We consider the Euler equations in cartesian coordinates in N space dimensions with chemical reactive source terms (see [4, 5, 6] for detailed reviews). Conservation of K different gaseous species requires K continuity equations. We choose a symmetric formulation and write for the partial densities ρ_i:

$$\partial_t \rho_i + \sum_{n=1}^{N} \partial_{x_n}(\rho_i v_n) = W_i \, \dot{\omega}_i \qquad \text{for } \; i = 1, \ldots, K \tag{1}$$

$\dot{\omega}_i$ denotes the chemical production rate for each species and W_i is its molecular weight. Conservation of momentum yields

$$\partial_t(\rho v_m) + \sum_{n=1}^{N} \partial_{x_n}(\rho v_n v_m + \delta_{n,m}\, p) = 0 \qquad \text{for } \; m = 1, \ldots, N \tag{2}$$

where ρ is the total density, v is the velocity vector and p is the hydrodynamic pressure. $\delta_{n,m}$ denotes the Kronecker symbol. The energy equation is written as

$$\partial_t(\rho E) + \sum_{n=1}^{N} \partial_{x_n}\left[v_n(\rho E + p)\right] = 0 \tag{3}$$

with the total energy per unit mass E.

We assume that the flow is in thermal equilibrium (for all K species the same temperature T can be used) and that for each partial pressure the ideal gas law

$$p_i = \rho_i \frac{\mathcal{R}}{W_i} T \tag{4}$$

applies. The total pressure p is given by Dalton's law:

$$p = \sum_{i=1}^{K} p_i = \rho \frac{\mathcal{R}}{W} T \tag{5}$$

with

$$\rho = \sum_{i=1}^{K} \rho_i \quad , \qquad Y_i = \frac{\rho_i}{\rho} \quad , \qquad W = \left(\sum_{i=1}^{K} \frac{Y_i}{W_i} \right)^{-1}$$

Each gaseous specie is assumed to be *thermally perfect* and the specific heats $c_{pi} = c_{pi}(T)$ are functions of the temperature only. The enthalpies per unit mass are written as

$$h_i(T) = h_i^f + \int_{T_f}^{T} c_{pi}(s)ds$$

with h_i^f called the *heat of formation*. For the total enthalpy $h(T) = \sum_{i=1}^{K} Y_i \; h_i(T)$ holds. Inserting this into the thermodynamic relation $\rho h - p - \rho e = 0$ and applying (4), (5) as well as $E = e + v^2/2$ gives

$$\sum_{i=1}^{K} \rho_i \, h_i(T) - \mathcal{R}T \sum_{i=1}^{K} \frac{\rho_i}{W_i} - \rho E + \rho \, \frac{v^2}{2} = 0 \quad . \tag{6}$$

(6) is an implicit relation that allows the computation of the temperature T from the conserved quantities. With the aid of T the pressure p can be calculated. In contrast to the *calorically perfect* case, where the specific heats c_{pi} are constant, no explicit equation of state relating p directly to the conserved quantities can be obtained (see [1] for details).

The functions $c_{pi}(T)$ are usually approximated by polynoms of degree 4 of the form

$$c_{pi}(T) = \frac{\mathcal{R}}{W_i} \left(a_{1i} + a_{2i}T + a_{3i}T^2 + a_{4i}T^3 + a_{5i}T^4 \right) \qquad i = 1, \ldots, K \quad .$$

The constants a_{ji} and h_i^f can be taken from thermodynamic data bases [3].

2 Reaction mechanisms

The chemical production rates $\dot{\omega}_i$ are functions of temperature T and partial densities ρ_i:

$$\dot{\omega}_i = \dot{\omega}_i(\rho_1, \ldots, \rho_K, T) \qquad\qquad i = 1, \ldots, K$$

They are derived from a *reaction mechanism* that consists of M chemical reactions [2, 6]:

$$\sum_{i=1}^{K} \nu_{ji}^f S_i \rightleftharpoons \sum_{i=1}^{K} \nu_{ji}^r S_i \qquad\qquad j = 1, \ldots, M \tag{7}$$

Each reactant S_i is assigned a stoichiometric coefficient ν_{ji}^f for a particular forward reaction and a coefficient ν_{ji}^r for the corresponding backward reaction. Note that in (7) some coefficients are usually zero. Associated to a chemical reaction is a pre-exponential factor A_j, a temperature exponent β_j and an activation energy E_j. These are necessary to compute the temperature dependent forward reaction rate $k_j^f(T)$ with the empirical Arrhenius law

$$k_j^f(T) = A_j T^{\beta_j} \exp(-E_j/\mathcal{R}T) \quad . \tag{8}$$

Evaluation of the equilibrium constant $K_j^c(T)$ (see [2] for its definition) allows the calculation of the corresponding backward reaction rate

$$k_j^r(T) = k_j^f(T)/K_j^c(T) \quad . \tag{9}$$

The mass production rate of specie S_i is now given by

$$W_i \, \dot{\omega}_i = W_i \sum_{j=1}^{M} (\nu_{ji}^r - \nu_{ji}^f) \left[k_j^f \prod_{n=1}^{K} \left(\frac{\rho_n}{W_n} \right)^{\nu_{jn}^f} - k_j^r \prod_{n=1}^{K} \left(\frac{\rho_n}{W_n} \right)^{\nu_{jn}^r} \right] \quad i = 1, \ldots, K \quad . \qquad (10)$$

A chemical kinetics package (e.g. Chemkin) is usually utilized to compute (8)-(10) according to the particular reaction mechanism and given thermodynamic data [2].

References

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