

## 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  $\rho_i$ :

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

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

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

where  $\rho$  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

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

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

$$p_i = \rho_i \frac{\mathcal{R}}{W_i} T \quad (4)$$

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

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

with

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

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

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

(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

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

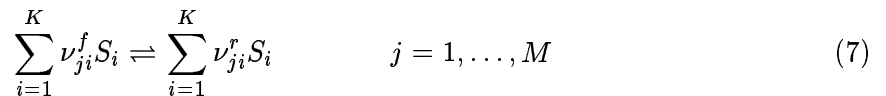
The constants  $a_{ji}$  and  $h_i^f$  can be taken from thermodynamic data bases [3].

## 2 Reaction mechanisms

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

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

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



Each reactant  $S_i$  is assigned a stoichiometric coefficient  $\nu_{ji}^f$  for a particular forward reaction and a coefficient  $\nu_{ji}^r$  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  $\beta_j$  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

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

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

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

The mass production rate of specie  $S_i$  is now given by

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

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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