Appendix B: Roe's Method for Finite-Rate Chemistry

As explained in Chapter 2 Roe's method was initially developed for perfect gases and later extended to flows with finite-rate chemistry. For the present treatment we follow Grossman and Cinnella (1990), which contains an unusually detailed and well-presented description of the procedure. However, they use as governing equations the N_S specie conservation equations; here, we use a global continuity and N_S-1 specie equations. The conversion is straightforward but long and laborious. In this Appendix the results of that conversion are given. For further details the reader should refer to the above-mentioned work, as well as to Hirsch (1990) for a general overview of the method.

It is assumed that at the interface where the flux $\vec{F}$ is to be calculated the left and right states $\vec{q}_L$ and $\vec{q}_R$ are known. Following are the steps necessary for the calculation of the correction $\Delta\vec{F}$ of equation 2.5.

- **Roe-average states**

Define the arithmetic-average operator

$$\langle \bullet \rangle = \frac{1}{2}\left[(\bullet)_L + (\bullet)_R\right]$$

and the **Roe-average** operator

$$\hat{\bullet} = \frac{\left\langle (\bullet)\sqrt{\rho} \right\rangle}{\left\langle \sqrt{\rho} \right\rangle}$$

All Roe-average variables $\hat{\bullet}$ in the following steps are calculated using the above operator **except** for the following variables:

$$\hat{\rho} = \sqrt{\rho_L \rho_R}$$

$$\hat{\rho}_i = \frac{\left\langle y_i \sqrt{\rho} \right\rangle}{\left\langle \sqrt{\rho} \right\rangle}$$

$$\hat{\gamma} = 1 + \frac{\hat{R}}{C_v^*}$$

$$\hat{e}_i' = \hat{e}_i - \frac{R_i}{\hat{\gamma}-1}\hat{T}$$

$$\hat{a}^2 = (\hat{\gamma}-1)\left[\hat{h}_t - \frac{u^2}{2} - \sum_{i=1}^{N_S} \hat{\rho}_i \left(\hat{e}_i - \frac{R_i}{\gamma-1}\hat{T}\right)\right]$$

$$\hat{a} = \sqrt{\hat{a}^2}\,.$$

In the above,

$$C_v^* = \sum_{i=1}^{N_S} \hat{\rho}_i C_{v_i}^*$$

$$C_{v_i}^* = \frac{1}{T_R - T_L} \int_{T_L}^{T_R} C_{v_i}(\tau)\, d\tau$$

- **Wave Strengths**

Define the jump operator

$$\|\bullet\| = (\bullet)_R - (\bullet)_L$$

Then the wave-strengths are given by

$$\alpha_1 = \|\rho\| - \frac{\|p\|}{\hat{a}^2}$$

$$\alpha_{i+1} = \|\rho_i\| - \frac{\|p\|}{\hat{a}^2}\frac{\hat{\rho}_i}{\hat{\rho}} \qquad (i = 1, \ldots, N_S - 1)$$

$$\alpha_{N_S+1} = \frac{1}{2\hat{a}^2}\left(\|p\| + \hat{\rho}\,\hat{a}\,\|u\|\right)$$

$$\alpha_{N_S+2} = \frac{1}{2\hat{a}^2}\left(\|p\| - \hat{\rho}\,\hat{a}\,\|u\|\right)$$

- **Eigenvalues**

$$\lambda_i = \begin{cases} \hat{u} & i = 1, \ldots, N_S \\ \hat{u} + \hat{a} & i = N_s + 1 \\ \hat{u} - \hat{a} & i = N_s + 2 \end{cases}$$

- **Eigenvectors**

$$\vec{E}_1 = \begin{bmatrix} 1 \\ \hat{u} \\ \hat{e}'_{N_S} + \frac{\hat{u}^2}{2} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \vec{E}_{i+1} = \begin{bmatrix} 0 \\ 0 \\ \hat{e}'_i - \hat{e}'_{N_S} \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \text{ --- 3+i row} \qquad (i = 1,\ldots,N_s\text{-}1)$$

$$\vec{E}_{N_S+1} = \begin{bmatrix} 1 \\ \hat{u} + \hat{a} \\ \hat{h}_t + \hat{u}\,\hat{a} \\ \hat{\rho}_1 \\ \vdots \\ \hat{\rho}_{N_S-1} \end{bmatrix} \qquad \vec{E}_{N_S+2} = \begin{bmatrix} 1 \\ \hat{u} - \hat{a} \\ \hat{h}_t - \hat{u}\,\hat{a} \\ \hat{\rho}_1 \\ \vdots \\ \hat{\rho}_{N_S-1} \end{bmatrix}$$

- **Flux Correction**

$$\Delta\vec{F} = \sum_{i=1}^{N_S+2} \alpha_i\,|\lambda_i|\,\vec{E}_i$$