Appendix A: Implicit Time-Integration

This Appendix presents the details for implicit time-integration. In particular the implementation of equation 2.15 at the CV level, its evaluation and solution will be described in some detail. Further information can be obtained from Pulliam (1993) and Hirsch (1990).

A.1. General Equation at the CV level

Rewriting equation 2.15 for CV i and with $\nu = 1$ and $\varphi = 0.5$ for second-order time accuracy,

$$\left[I + \frac{\Delta t}{15} \left(\frac{\partial R}{\partial Q} \right)^{n} \right] \Delta Q^{n}(i) = - \frac{\Delta t}{15} R^{n}(i) + \frac{0.5}{15} \Delta Q^{n-1}(i) \qquad (A.1)$$

(vector notation will be dropped unless otherwise specified). As mentioned in Section 2.8 only first-order schemes are unconditionally stable. Therefore equation A.1 has to be solved by an iteration procedure **at each time-level**. Replacing index n with a new iterative index p and linearizing about Q^{p} the final result is (Pulliam, 1993)

$$\left[I + \frac{\Delta t}{15} \left(\frac{\partial R}{\partial Q} \right)^{p} \right] \Delta Q^{p}(i) = - \frac{\Delta t}{15} R^{p}(i) - Q^{p}(i) + \frac{2}{15} Q^{n}(i) \quad \frac{0.5}{15} Q^{n-1}(i) \qquad (A.2)$$

Concentrating on the second term of the left-hand side and taking into account equation 2.10

$$\left(\frac{\partial R}{\partial Q} \Delta Q \right)(i) = \left[\left(\frac{\partial F}{\partial Q} \Delta Q \right)(i)\, A(i) - \left(\frac{\partial F}{\partial Q} \Delta Q \right)(i-1)\, A(i-1) - \frac{\partial W}{\partial Q}(i)\, \Delta Q(i) \right] \frac{1}{\Delta V(i)}$$

(A.3)

Evaluating the flux jacobians in equation A.3 with a flux-split scheme

$$\left(\frac{\partial F}{\partial Q}\Delta Q\right)(i) \quad = \quad \left(\mathrm{A}^{+}\Delta Q^{-} \quad + \quad \mathrm{A}^{-}\Delta Q^{+}\right)(i) \qquad (A.4)$$

where A is the $(N_s+2) \times (N_s+2)$ flux-jacobian matrix

$$\mathrm{A} \quad = \quad \frac{\partial F}{\partial Q} \qquad (A.5)$$

and where

- $\mathrm{A}^{+/-}$ means A evaluated with positive/negative eigenvalues
- $Q^{+/-}$ means Q interpolated mainly from the right/left.

Using first-order spatial interpolation

$$\begin{aligned}
\Delta Q^{-}(i) &= \Delta Q(i) \\
\Delta Q^{+}(i) &= \Delta Q(i+1) \\
\mathrm{A}^{+}(i) &= \mathrm{A}^{+}\left[Q(i)\right] \\
\mathrm{A}^{-}(i) &= \mathrm{A}^{-}\left[Q(i+1)\right]
\end{aligned} \qquad (A.6)$$

After lengthy but straightforward manipulation equation A.2 can be written as

$$\overline{\overline{A}}^{P}(i)\,\Delta Q^{P}(i-1) \quad + \quad \overline{\overline{B}}^{P}(i)\,\Delta Q^{P}(i) \quad + \quad \overline{\overline{C}}^{P}\,\Delta Q^{P}(i+1) \quad = \quad F(i) \qquad (A.7)$$

with

$$\begin{aligned}
\overline{\overline{A}}(i) &= -\,\mathrm{A}^{+}(i-1)\,A(i-1) \\
\overline{\overline{B}}(i) &= 1.5\,\frac{\Delta V(i)}{\Delta t}\,I \quad + \quad \mathrm{A}^{+}(i)\,A(i) \quad - \quad \mathrm{A}^{-}(i-1)\,A(i-1) \quad - \quad \frac{\partial W}{\partial Q}(i) \qquad (A.8) \\
\overline{\overline{C}}(i) &= \mathrm{A}^{-}(i)\,A(i) \\
F(i) &= -\,R^{p}(i) \quad - \quad \frac{\Delta V(i)}{\Delta t}\left[1.5\,Q^{p}(i) \quad - \quad 2\,Q^{n}(i) \quad + \quad 0.5\,Q^{n-1}(i)\right]
\end{aligned}$$

At convergence, $\Delta Q^p \rightarrow 0$, $Q^{p+1} \rightarrow Q^{n+1}$.

It should be noted that the sub-iteration scheme will give second-order time-accuracy regardless of the discretization choice for the left-hand side of equation A.2, **as long as the procedure converges**.

Equation A.7 represents a tri-diagonal system of equations. Furthermore it is a block system since each element in the main matrix is a $(N_s+2) \times (N_s+2)$ sub-matrix, and each element in the unknown and right-hand side vectors is an (N_s+2) sub-vectors. There are special algorithms for the inversion of this type of system (see for example Anderson et al., 1984).

A.2. Evaluation of the Flux Jacobian

Following the procedure of Grossman and Cinnella (1990) the flux-jacobian matrix for a system of reacting mixtures is

$$A = \tag{A.9}$$

$$\begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ e''_{N_s} + (\gamma-3)\frac{u^2}{2} & (3-\gamma)u & \gamma-1 & e''_1 - e''_{N_s} & \cdots & e''_{N_s-1} - e''_{N_s} \\ u\, e''_{N_s} + (\gamma-1)\frac{u^3}{2} - h_t u & h_t - (\gamma-1)u^2 & \gamma u & u\left(e''_1 - e''_{N_s}\right) & \cdots & u\left(e''_{N_s-1} - e''_{N_s}\right) \\ -\frac{\rho_1}{\rho}u & \frac{\rho_1}{\rho} & 0 & u & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\frac{\rho_{N_s-1}}{\rho}u & \frac{\rho_{N_s-1}}{\rho} & 0 & 0 & 0 & u \end{bmatrix}$$

where

$$e''_k = R_k T - (\gamma-1)\, e_k(T) \tag{A.9.1}$$

and

$$\gamma = \frac{C_p}{C_v} \tag{A.9.2}$$

(note C_P, C_V correspond to the **mixture** and can be obtained from equation 2.3.4)

As it is well known the flux jacobian can be diagonalized in terms of its eigenvalues and eigenvectors

$$A = T \Lambda T^{-1} \tag{A.10}$$

where Λ is the diagonal matrix of eigenvalues and T the matrix of right eigenvectors. In turn Λ can be decomposed into positive and negative eigenvalues

$$A = T\left(\Lambda^{+} + \Lambda^{-}\right)T^{-1} = A^{+} + A^{-} \tag{A.11}$$

The final expressions are

$$\Lambda^{\pm} = \mathrm{diag}\left(\lambda_i^{\pm}\right) \qquad (i = 1, \ldots, N_S + 2) \tag{A.12.1}$$

$$\lambda_i^{\pm} = \frac{1}{2}\left(\lambda_i \pm |\lambda_i|\right)$$

$$\lambda_1 = u$$

$$\lambda_2 = u + a$$

$$\lambda_3 = u - a$$

$$\lambda_k = u \qquad (k = 4, \ldots, N_S + 2)$$

$$
T = \begin{bmatrix} 1 & 1 & 1 & 0 & \cdots & 0 \\ u & u+a & u-a & 0 & \cdots & 0 \\ e'_{N_s} + \frac{u^2}{2} & h_t + u\,a & h_t - u\,a & e'_1 - e'_{N_s} & \cdots & e'_{N_s-1} - e'_{N_s} \\ 0 & \frac{\rho_1}{\rho} & \frac{\rho_1}{\rho} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \frac{\rho_{N_s-1}}{\rho} & \frac{\rho_{N_s-1}}{\rho} & 0 & \cdots & 1 \end{bmatrix} \qquad \text{(A.12.3)}
$$

In the above

$$
e'_i(T) = e_i(T) - \frac{R_i}{\gamma - 1} T
$$

and

$$
a^2 = \gamma \frac{p}{\rho}
$$

is the frozen speed of sound.

A.3. Source Jacobian

From all the terms that appear in the source vector (equation 2.4) we will consider as directly dependent on Q(i) the pressure term in F_{wall} (equation 2.28) and the chemical-production source terms. The inclusion of these terms is expected to enhance the stability of the iteration procedure.

Therefore approximating the wall-force term as

$$
F_{wall} = p\,\Delta A \qquad \text{(A.13)}
$$

where p is the pressure **inside** the CV, the resulting source-jacobian matrix is

$$\frac{\partial W}{\partial Q} = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ \frac{\partial p}{\partial \rho}\Delta A & \frac{\partial p}{\partial \rho u}\Delta A & \frac{\partial p}{\partial \rho e_t}\Delta A & \frac{\partial p}{\partial \rho_1}\Delta A & \cdots & \frac{\partial p}{\partial \rho_{N_s-1}}\Delta A \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \frac{\partial \dot{\omega}_1}{\partial \rho}\Delta V & \frac{\partial \dot{\omega}_1}{\partial \rho u}\Delta V & \frac{\partial \dot{\omega}_1}{\partial \rho e_t}\Delta V & \frac{\partial \dot{\omega}_1}{\partial \rho_1}\Delta V & \cdots & \frac{\partial \dot{\omega}_1}{\partial \rho_{N_s-1}}\Delta V \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial \dot{\omega}_{N_s-1}}{\partial \rho}\Delta V & \frac{\partial \dot{\omega}_{N_s-1}}{\partial \rho u}\Delta V & \frac{\partial \dot{\omega}_{N_s-1}}{\partial \rho e_t}\Delta V & \frac{\partial \dot{\omega}_{N_s-1}}{\partial \rho_1}\Delta V & \cdots & \frac{\partial \dot{\omega}_{N_s-1}}{\partial \rho_{N_s-1}}\Delta V \end{bmatrix} \tag{A.14}$$

A.3.1. Pressure Terms

$$\frac{\partial p}{\partial \rho} = \left[R_{N_s} T \quad + \quad (\gamma - 1)\left(\frac{1}{2} u^2 - e_{N_s}\right)\right]$$

$$\frac{\partial p}{\partial \rho u} = -(\gamma - 1) u \tag{A.15}$$

$$\frac{\partial p}{\partial \rho e_t} = (\gamma - 1)$$

$$\frac{\partial p}{\partial \rho_i} = \left[\left(R_i - R_{N_s}\right) T \quad + \quad (\gamma - 1)\left(e_{N_s} - e_i\right)\right] \qquad (i = 1, \ldots, N_s)$$

A.3.2. Chemical Terms

For these terms we will restrict ourselves to a one-step reaction model ($N_s = 3$). From equations 2.24 and 2.26,

$$\frac{\partial \dot{\omega}_{fuel}}{\partial (\ )} = -\frac{\partial \dot{\omega}}{\partial (\ )}; \qquad \frac{\partial \dot{\omega}_{air}}{\partial (\ )} = -\upsilon \frac{\partial \dot{\omega}}{\partial (\ )} \tag{A.16}$$

where

$$\dot{\omega} = MW_{fuel}\, A \exp\left(\frac{-E_a / R_u}{T}\right)\left[C_x H_y\right]^m \left[O_2\right]^n \tag{A.17}$$

It is convenient to express $\dot{\omega}$ in terms of the main variables. After some manipulation

$$\dot{\omega} = C_1\, \rho^{m+n} \exp\left(\frac{C_2}{T}\right) y_{fuel}^m\, y_{air}^n \tag{A.18}$$

with

$$C_1 = 0.233^n \, 1000^{1-m-n} \frac{MW_{fuel}^{1-m}}{MW_{O_2}^{n}} A$$

$$C_2 = -\frac{E_a}{R_u}$$

where the factor C_1 accounts for several conversions: from concentrations to mass fractions; from O_2 to air mass-fraction and from CGS units to SI units in the pre-exponential factor A (usually given in CGS units).

Therefore it can be shown after laborious but straightforward manipulations

$$\begin{aligned}
\frac{\partial \dot\omega}{\partial \rho} &= \left[e_{N_s} - \frac{1}{2} u^2 \right] C_3 \, \dot\omega \\
\frac{\partial \dot\omega}{\partial \rho u} &= C_3 \, \dot\omega \, u \\
\frac{\partial \dot\omega}{\partial \rho e_t} &= -C_3 \, \dot\omega \\
\frac{\partial \dot\omega}{\partial \rho_{fuel}} &= m \frac{\dot\omega}{\rho_{fuel} + \varepsilon} - \left[e_{N_s} - e_{fuel} \right] C_3 \, \dot\omega \\
\frac{\partial \dot\omega}{\partial \rho_{air}} &= n \frac{\dot\omega}{\rho_{air} + \varepsilon} - \left[e_{N_s} - e_{air} \right] C_3 \, \dot\omega \\
C_3 &= \frac{C_2}{\rho \, C_v \, T^2} .
\end{aligned} \tag{A.19}$$

In the above, ε is a small factor introduced to avoid divisions by zero.

A.4. Boundary Conditions

In the present work use is made of explicit boundary conditions, i.e., the values of Q at i = 1 or $N_s + 2$ are imposed explicitly, rather than solved for implicitly. Therefore at those points $\Delta Q^p \equiv 0$. This approach was found to more robust for the present application.

A.5. Zonal Conditions

At the flow-division face of annular-flow burners the CV at the left is linked with three CVs to the right (see Fig. 3.2). This destroys the tri-diagonal nature of system A.2. Therefore the CVs will have to be uncoupled on the left-hand side of the equations. They will still remain coupled on the right-hand side, maintaining the spatial accuracy of the system.

For presentation purposes we will restrict ourselves to the situation shown in Fig. A.1, where it is desired for whatever reason to uncouple the two CVs shown adjacent to interface $i = i_{ZB}$. The following analysis can be extended to the flow-division interface.

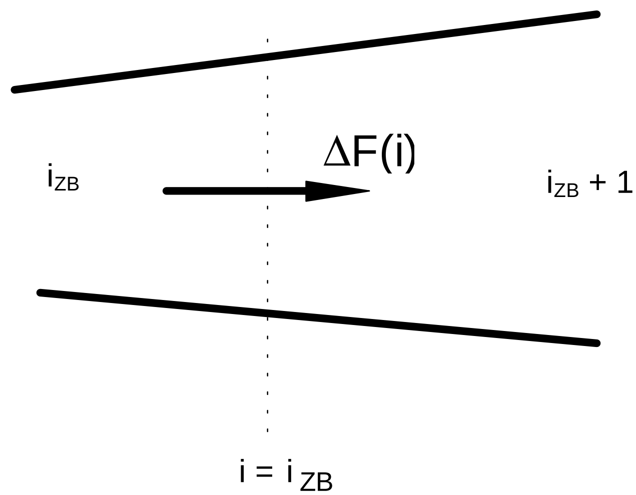

Figure A. 1: Zonal boundary

To uncouple $\Delta Q^p(i)$ from $\Delta Q^p(i+1)$ assume

$$\Delta F^P(i) \approx \Delta F^{P-1}(i). \tag{A.20}$$

Therefore equation A.3 as applied to CV $i = i_{ZB}$ can be rewritten as (taking into account A.4 and A.6 and including area terms in flux jacobians for convenience)

$$\left(\frac{\partial R}{\partial Q}\Delta Q\right)^p(i) \quad =$$

$$\Delta F^{p-1}(i)\,A(i) \quad - \quad \left[A^+(i-1)\,\Delta Q(i-1) + A^-(i-1)\,\Delta Q(i)\right]^p \quad - \quad \left(\frac{\partial W}{\partial Q}\right)^p(i)\,\Delta Q^p(i)$$

which ends up in

$$\overline{\overline{A}}^P(i)\,\Delta Q^p(i-1) \quad + \quad \overline{\overline{B}}^P(i)\,\Delta Q^p(i) \quad = \quad F^p(i) \qquad \text{(A.21.1)}$$

where

$$\overline{\overline{A}}(i) \quad = \quad -\,A^+(i-1)$$

$$\overline{\overline{B}}^p(i) \quad = \quad 1.5\,\frac{\Delta V(i)}{\Delta t} \quad - \quad A^-(i-1) \quad - \quad \left(\frac{\partial W}{\partial Q}\right)(i) \qquad \text{(A.21.2)}$$

$$F(i) \quad = \quad -\,\Delta F^{p-1}(i)\,A(i) - \; R^p(i) - \frac{\Delta V(i)}{\Delta t}\left[1.5\,Q^p(i) \quad - \quad 2\,Q^n(i) \quad + \quad 0.5\,Q^{n-1}(i)\right]$$

Similarly for CV i = $i_{ZB}+1$,

$$\overline{\overline{B}}^P(i)\,\Delta Q^p(i) \quad + \quad \overline{\overline{C}}^P(i)\,\Delta Q^p(i+1) \quad = \quad F^p(i) \qquad \text{(A.22.1)}$$

$$\overline{\overline{C}}(i) \quad = \quad A^-(i)$$

$$\overline{\overline{B}}^p(i) \quad = \quad 1.5\,\frac{\Delta V(i)}{\Delta t} \quad + \quad A^+(i) \quad - \quad \left(\frac{\partial W}{\partial Q}\right)(i) \qquad \text{(A.22.2)}$$

$$F(i) \quad = \quad \Delta F^{p-1}(i-1)\,A(i-1) - \; R^p(i) - \frac{\Delta V(i)}{\Delta t}\left[1.5\,Q^p(i) \quad - \quad 2\,Q^n(i) \quad + \quad 0.5\,Q^{n-1}(i)\right]$$