Appendix-A  Solution of Unsteady Flow Equations

A.1 Benson Algorithm

In Chapter 3, the characteristic equations (3.1.8 and 3.1.10) and the compatibility equations (3.1.9 and 3.1.11) are expressed in terms of \( p, \rho, a \) and \( u \) for Zucrow-Hoffman algorithm. For Benson and the Modified algorithms, these equations are expressed in terms of the variables \( a, u \) and \( a^* \) where \( a^* \) is the speed of sound at the reference pressure due to an isentropic change of state from the pressure \( p \). \( a^* \) reflects the entropy level in the duct. \( U, A \) and \( A_a \) are the non-dimensional values of \( u, a \) and \( a_a \) and are defined as:

\[
U = \frac{u}{a_{ref}}, \quad \Lambda = \frac{a}{a_{ref}}, \quad A_a = \frac{a_a}{a_{ref}}
\]

Expressing \( U \) and \( A \) in terms of Riemann variables (\( \lambda \) & \( \beta \)) gives

\[
U = \frac{(\lambda - \beta) \gamma}{(\gamma - 1)}, \quad A = \frac{(\lambda + \beta)}{2}
\]

The characteristic and compatibility equations (3.1.8 – 3.1.11) may be rewritten in terms of above variables as:

1. **Pathline**

\[
\left( \frac{dX}{dZ} \right) = \left( \frac{\lambda - \beta}{\gamma - 1} \right)
\]

(A.1)

2. **Right running characteristic**

\[
\left( \frac{dX}{dZ} \right) = (b\lambda - a \beta)
\]

(A.2)

3. **Left running characteristic**

\[
\left( \frac{dX}{dZ} \right) = (a\lambda - b \beta)
\]

(A.3)

where \( X \) is non-dimensional distance = \( x/x_{ref} \)

\( Z \) is the non-dimensional time = \( a_{ref} t / x_{ref} \)

\( a \) and \( b \) are constants defined as

\[
a = \frac{(3 - \gamma)}{2(\gamma - 1)} \quad \text{and} \quad b = \frac{(\gamma + 1)}{2(\gamma - 1)}
\]
The compatibility equations

1. Along the pathline

\[
\delta A_a = \gamma - \frac{1}{2} \frac{A_a}{A^2} \left[ -q \frac{x_{ref}}{a^3_{ref}} + \frac{4f x_{ref}}{D} \right] \frac{U^3}{2} \Delta Z \tag{A.4}
\]

2. Along the right running Characteristic

\[
d\lambda = dA + \left( \gamma - \frac{1}{2} \right) dU = - \left( \gamma - \frac{1}{2} \right) \frac{A}{F} \frac{dF}{dx} dZ + \frac{A}{A_a} dA_a -
\left( \gamma - \frac{1}{2} \right) \frac{2f x_{ref}}{D} \frac{U^2}{|U|} \left[ 1 - (\gamma - 1) \frac{U}{A} \right] dZ +
\left( \frac{\gamma - 1}{2} \right)^2 \frac{q x_{ref}}{a^3_{ref}} \frac{1}{A} dZ \tag{A.5}
\]

3. Along the left running Characteristic

\[
d\beta = dA - \left( \gamma - \frac{1}{2} \right) dU = \left( \gamma - \frac{1}{2} \right) \frac{A}{F} \frac{dF}{dx} dZ + \frac{A}{A_a} dA_a +
\left( \gamma - \frac{1}{2} \right) \frac{2f x_{ref}}{D} \frac{U^2}{|U|} \left[ 1 + (\gamma - 1) \frac{U}{A} \right] dZ +
\left( \frac{\gamma - 1}{2} \right)^2 \frac{q x_{ref}}{a^3_{ref}} \frac{1}{A} dZ \tag{A.6}
\]

The solution of the characteristic and compatibility equations is performed in the Z-X field which is subdivided into a rectangular grid system as shown in Fig. (A.1). The grid pattern is chosen in the X-direction and the Z-coordinate is adjusted according to Courant et al (1928) stability criterion.

Determination of \( \lambda, \beta \) and \( A_a \) at the interior points

For the grid shown in Fig. (A.2), it is required to calculate the conditions at point R' at time step \( (Z + \Delta Z) \) from the conditions at time \( Z \). The characteristics are drawn from point R' to cut the X-axis at points P. The slope of \( \lambda \)-characteristic is given by Eqn. (A.2) and Eqn. (A.3.) gives the slope of \( \beta \)-characteristic. To obtain the Riemann variables at points P, the values are linearly interpolated between mesh points (L-1) and (L) for \( \lambda \) and between (L) and (L+1) for \( \beta \), i.e.,
\[ \lambda_p = \lambda_L - \frac{\delta x}{\Delta x} \left( \lambda_L - \lambda_{L-1} \right) \quad (A.7) \]
\[ \beta_p = \beta_L - \frac{\delta x}{\Delta x} \left( \beta_L - \beta_{L+1} \right) \quad (A.8) \]

The value of \( \lambda \) at point \( R' \) is then given by
\[ \lambda_{R'} = \lambda_p \cdot d\lambda \quad (A.9) \]

where, \( d\lambda \) is calculated from the compatibility equation along the right running characteristic, Eqn. (A.5).

\( \beta \) at \( R' \) is given by:
\[ \beta_{R'} = \beta_p + d\beta \quad (A.10) \]

\( d\beta \) is obtained from the compatibility equation valid along the left running characteristic, Eqn. (A.6).

For the pathline characteristic solution, non-mesh method is used as shown in Fig. (A.3). The location of the kth pathline at time step \( Z' = Z + \Delta Z \) is found from the direction condition for the pathline given by Eqn. (A.1). The change of \( A_a \) along the pathline, \( \delta A_{a_k} \), is given by the pathline compatibility Eqn. (A.4) as:
\[ A_{a_k'} = A_{a_k} + \delta A_{a_k} \quad (A.11) \]

The values of \( \lambda_k \) and \( \beta_k \) are obtained by linear interpolation from the known values of \( \lambda \) and \( \beta \) at the mesh points. The entropy level \( A_a \) at the mesh points are determined by linear interpolation of \( A_a \) at either side of the mesh point.

**Determination of \( \lambda, \beta \) and \( A_a \) at Boundaries**

The boundary conditions described in Section (3.2) are expressed in terms of the Riemann variables, \( \lambda_{in}, \lambda_{out} \) so that,

\[ U = \frac{\lambda_{in} - \lambda_{out}}{(\gamma - 1)} \quad (A.12) \]
\[ A = \frac{\lambda_{in} + \lambda_{out}}{2} \quad (A.13) \]
where
\[ \lambda_{in} \] is the known characteristic at the boundary.
\[ \lambda_{out} \] is the unknown characteristic at the boundary.

The known Riemann variable at the boundary is considered the incorrect value \( (\lambda_{in})_n \) and the correct values of both the characteristics, \( (\lambda_{in})_c \) and \( (\lambda_{out})_c \) are obtained from the solution of the appropriate boundary condition equations. Solutions of some of the boundary conditions are given below.

**Closed End Boundary Conditions**

For the closed end as in Section (3.2.1) the boundary condition is

\[ U = 0 \]

From Eqn. (A.12), this gives

\[ \lambda_{out} = \lambda_{in}. \] \hspace{1cm} (A.14)

**Open End Boundary Conditions**

From Section (3.2.2)

1. **For Subsonic Outflow**

\[ p = p_o \]

\[ \left( \frac{p_o}{p_{ref}} \right)^{\frac{\gamma-1}{2\gamma}} = \frac{a_o}{a_{ref}} = \frac{\lambda_{in} + \beta_{out}}{2} \]

\[ \beta_{out} = 2A_o - \lambda_{in} = 2 \left( \frac{p_o}{p_{ref}} \right)^{\frac{\gamma-1}{2\gamma}} - \lambda_{in} \] \hspace{1cm} (A.15)

2. **For Subsonic Inflow**

\[ A_o^2 = A^2 - \frac{\gamma - 1}{2} U^2 = \left( \frac{p_o}{p_{ref}} \right)^{(\gamma-1)/\gamma} \]

substituting for \( U \) and \( A \) from Eqns. (A.12) and (A.13) and after rearranging: gives

\[ \lambda_{out} = \left( \frac{3 - \gamma}{\gamma + 1} \right) \lambda_{in} + \frac{2}{\gamma + 1} \sqrt{(\gamma^2 - 1) A_o^2 + 2(1-\gamma) \lambda_{in}^2} \] \hspace{1cm} (A.16)
Nozzle Boundary Conditions

Nozzle boundary equations derived in Section (3.2.3) are expressed in terms of starred Riemann variables. This is of particular importance when nozzle boundary is used for the case of return flow in cylinder where the back pressure, $p_b$ (cylinder pressure) is not equal to the reference pressure $p_{ref}$.

The starred Reimann variables are defined as:

$$\lambda^* = \frac{\lambda}{A_a} \left( \frac{p_{ref}}{p_b} \right)^{\frac{\gamma - 1}{2\gamma}}, \quad \lambda^*_{in} = \frac{\lambda_{in}}{(A_a)_{out}} \left( \frac{p_{ref}}{p_b} \right)^{\frac{\gamma - 1}{2\gamma}}$$

$$\lambda^*_{out} = \frac{\lambda_{out}}{(A_a)_{out}} \left( \frac{p_{ref}}{p_b} \right)^{\frac{\gamma - 1}{2\gamma}}$$

$$U^* = \frac{\lambda^*_{in} - \lambda^*_{out}}{(\gamma - 1)} \quad \text{and} \quad \Lambda^* = \frac{\lambda^*_{in} + \lambda^*_{out}}{2} \quad (A.17)$$

For Subsonic outflow

The boundary condition for this case is given by Eqn. (3.2.8) rewritten below:

$$\frac{u^2}{a^2_a} = \frac{2}{\gamma - 1} \left[ \left( \frac{p}{p_a} \right)^{\frac{\gamma - 1}{\gamma}} - 1 \right] \quad \text{Eqn.}(3.2.8)$$

since,

$$\left( \frac{p}{p_a} \right) = \left( \frac{a}{a_a} \right)^{\frac{2\gamma}{\gamma - 1}} = A^{\frac{2\gamma}{\gamma - 1}}$$

and $U^* = u / a_a$

Eqn. (3.2.8) is rewritten as:

$$U^{*2} = \frac{2}{\gamma - 1} \left[ A^{*2} - 1 \right] \quad \frac{4}{\left( \frac{A}{\phi^2} \right)^{\frac{4}{\gamma - 1}} - 1}$$
substituting from Eqns. (A.17) for $U^*$ and $A^*$ in the above equation gives

$$\left( A^{\gamma - 1} - \phi^2 \right) \left( \lambda^* \right)^2 - \frac{\gamma - 1}{2} \phi^2 \left( A^* - 1 \right) = 0 \quad (A.18)$$

Eqn. (A.18) is solved by Newton Raphson method for $A^*$, and $\lambda_{\text{out}}^*$ is determined from Eqns. (A.17) as

$$\lambda_{\text{out}}^* = 2A^* - \lambda_{\text{in}}^*$$

The velocity at the throat $U_t$ in terms of the starred Riemann variables is given as:

$$U_t^* = \frac{A^*^{2(\gamma - 1)} U^*}{\phi} \quad (A.19)$$

2. **Sonic Outflow**

The boundary conditions for sonic outflow from Section (3.2.3) is

$$\left( \frac{u}{a} \right) = \phi \left( \frac{p_t}{p} \right)^{\frac{\gamma + 1}{\gamma - 1}} \quad (3.2.10)$$

and

$$\phi^2 = \left\{ \frac{\gamma + 1}{\gamma - 1} - \frac{2}{\gamma - 1} \left( \frac{p}{p_t} \right)^{\frac{\gamma - 1}{\gamma}} \left( \frac{p}{p_t} \right)^{\frac{2}{\gamma}} \right\} \quad (3.2.13)$$

expressed in terms of the starred Riemann variables as

$$\left( \frac{U^*}{\lambda^*} \right) = \phi / \left( A^* \right)^{\frac{\gamma - 1}{\gamma - 1}} \quad (A.20)$$

and

$$\phi^2 = \left\{ \frac{\gamma + 1}{\gamma - 1} - \frac{2}{\gamma - 1} \left( A^* \right)^{\frac{\gamma - 1}{\gamma}} \right\} \left( A^* \right)^{\frac{4}{\gamma - 1}} \quad (A.21)$$

where

$$A_{cr}^* = \left( \frac{a}{a_t} \right)_{cr} = \left( \frac{A}{A_t} \right)_{cr}$$

Eqn. (A.21) can be solved numerically by Newton Raphson method for $A_{cr}^*$ and $\lambda_{\text{out}}^*$ is obtained from Eqn. (A.20) using Eqns. (A.12 & A.13).
3. **Subsonic Inflow**

Boundary conditions similar to those described in Section (3.2.2) for subsonic inflow in an open end are used here.

**Cylinder Boundary Conditions**

The equations for cylinder boundary conditions are given in Section (3.2.4).

1. **Subsonic Outflow**

Eqn. (3.2.19) is solved as a quadratic to give:

\[
\frac{p}{p_c} = \left\{ \frac{1}{\gamma-1} \left[ 1 - \frac{\gamma-1}{2} \left( \frac{U}{A_c} \right)^2 \right] \right\}^2 \left[ \psi^2 + \frac{2 (\gamma-1) \left( \frac{U}{A_c} \right)^2}{1 - \frac{\gamma-1}{2} \left( \frac{U}{A_c} \right)^2} \right]^{-\frac{\gamma}{\gamma-1}}
\]

where \( A_c \) and \( p_c \) are the non-dimensional speed of sound and pressure in the cylinder, respectively.

An account has to be taken of the entropy change across the port which alters the value of the Riemann variable \( \lambda_{in} \) as it enters the boundary calculation. The corrected value, \( \beta_c \), of the Riemann variable entering the boundary, \( \beta_n \), due to entropy change is given by

\[
\beta_c = \beta_n + (\frac{A}{A_{a_c}})_c (A_{ac} - A_{an})
\]

where \( n \) denotes the incorrect value and \( c \) denotes the correct value

rearranging

\[
(A_{a_c})_c = \frac{A \cdot (A_{a_c})_n}{\beta_n - \beta_c + A}
\] (A.23a)

\( \beta_c \) may be written as

\[
\beta_c = A - (\gamma-1)/2 \ U
\]

substituting for \( \beta_c \) in Eqn. (A.23a) gives
(A_s)_c = \frac{A_s (A_s)_n}{\beta_n + \{(\gamma-1)/2\} U} \tag{A.23b}

since, \(\left(\frac{p}{p_a}\right)^\frac{\gamma-1}{2\gamma} = \left(\frac{A}{A_s}\right)\)

rewritten as:

\[
\left(\frac{p}{p_c}\right)^\frac{\gamma-1}{2\gamma} = \frac{A}{A_s} = \frac{\beta_n + (\gamma-1)/2 U}{(A_s)_n} \tag{A.24}
\]

substituting for \((p/p_c)\) from Eqn. (A.22) into Eqn. (A.24) yields

\[
f_1\left(\frac{U}{A_c}\right) = \left\{ \frac{1 - \frac{\gamma-1}{2} \left(\frac{U}{A_c}\right)^2}{(\gamma-1)^{1/2}} \right\} \psi \left[ \frac{2(\gamma-1) \left(\frac{U}{A_c}\right)^2}{\psi^{1/2} \left(1 - \frac{\gamma-1}{2} (U/A_c)^2\right)^{1/2}} \right]^{\gamma/2} \left(\frac{p_c}{p_a}\right)^{\gamma-1} 2\gamma
\]

\[
- \left(\frac{U}{A_c}\right) \left(\frac{\beta_n + \frac{\gamma-1}{2} U}{2 A_c (A_s)_n}\right) = 0 \tag{A.25}
\]

Eqn. (A.25) is solved by Newton Raphson method for \((U/A_c)\)

2. **Sonic flow in the Throat**

The boundary equation for this conditions from Section (3.2.4) is

\[
\left(\frac{p}{p_c}\right) = \psi \left(\frac{2}{\gamma+1}\right)^{2(\gamma-1)} \left\{ 1 - \frac{\gamma-1}{2} \left(\frac{U}{A_c}\right)^2 \right\} \tag{A.26}
\]

substituting for \((p/p_c)\) from Eqn. (A.26) into Eqn. (A.24) yields

\[
f_2\left(\frac{U}{A_c}\right) = \psi \left(\frac{p_c}{p_a}\right)^\frac{(\gamma-1)}{2\gamma} \left(\frac{2}{\gamma+1}\right)^{\frac{(\gamma+1)}{4\gamma}} \left\{ 1 - \frac{\gamma-1}{2} \left(\frac{U}{A_c}\right)^2 \right\} \tag{A.27}
\]

\[
- \left(\frac{\beta_n + \frac{\gamma-1}{2} U}{(A_s)_n}\right) = 0
\]
This equation is solved by Newton Raphson method for \((U/A_c)\). The corrected values of \(\lambda_{in}, \lambda_{out}, A_a\) are obtained as follows,

\[
A = \sqrt{A_c^2 - \frac{\gamma - 1}{2} U^2}
\]

\[
\beta_c = A - (\gamma - 1)/2 \cdot U
\]

\[
\lambda_c = 2A - \beta_c
\]

The correct value of the entropy level is found from Eqn. (A.23b) as

\[
(A_s)_{bc} = \frac{A \cdot (A_s)_{bc}}{(\beta_n - \beta_c + A)}
\]

**Boundary Conditions at Joint of Two Pipes**

As described in Section (3.2.5), the boundary conditions at a joint of two pipes are:

1. \(P_2 = P_1\)

   or \(\left(\frac{P_2}{P_{ref}}\right) = \left(\frac{P_1}{P_{ref}}\right)\)

2. \(\left(\frac{A_2}{A_{a2}}\right)^{\frac{2\gamma}{\gamma - 1}} = \left(\frac{A_1}{A_{a1}}\right)^{\frac{2\gamma}{\gamma - 1}}\)

3. \(\left(\frac{\lambda_2 - \beta_2}{\gamma - 1}\right) = \left(\frac{\lambda_1 - \beta_1}{\gamma - 1}\right)\)

4. \(A_{a1} = A_{a2}\) \hspace{1cm} (A.30)

Substituting from Eqn. (A.30) into Eqn. (A.28) and solving along with Eqn. (A.29) gives
The values of $\lambda$, $\beta$, and $(A_n)_c$ depend on the direction of the flow. The following two conditions may prevail:

(i) Positive flow (from pipe 1 to pipe 2)

$\lambda_{1n}$, $(A_{a1})_n$ and $\beta_{2n}$ are known

$$(A_{a1})_c = (A_{a1})_n$$

$$(A_{a2})_c = (A_{a2})_n$$

and $\lambda_{1c} = \lambda_{1n}$

$\lambda_{2c} = \lambda_{1c}$

The correct value of $\beta_2$ is given by

$$\beta_{2c} = \beta_{2n} + \left(\frac{\lambda_{2c} + \beta_{2n}}{2A_{a2c}}\right) (A_{a2c} - A_{a2n})$$

From the condition of equal velocity and pressure

$$\beta_{1c} = \beta_{2c}$$

(ii) Reverse flow (Flow from pipe 2 to pipe 1)

$\lambda_{1n}$, $(A_{a2})_n$ and $\beta_{2n}$ are known

$$(A_{a2})_c = (A_{a2})_n$$

$$(A_{a1})_c = (A_{a1})_c$$

and $\beta_{2c} = \beta_{2n}$

$\beta_{1c} = \beta_{2c}$

and the value $\lambda_1$ is corrected in a similar manner as for $\beta_2$ and from equal velocity and pressure condition

$$\lambda_{2c} = \lambda_{1c}$$
A.2 Modified Algorithm

Payri et al (1986) reported that the algorithm given by Benson results in some parasitic discontinuities in pressure for the exhaust and inlet pipes. To overcome this difficulty they suggested some modifications. These modifications are based on assuming linear variation of the pressure $p$ and volumetric flow rate $V$ between grid points instead of linear variation of speed of sound $A$ and velocity $U$ as it is the case with Benson algorithm. The suggestion of linear variation of pressure between grid points rather than linear variation of speed of sound is based on the fact that pressure is a thermodynamic property that is transmitted at a high speed which is not the case with temperature. Consequently pressure tends to reach equilibrium state much faster than the temperature.

Linear distribution of the volumetric flow rate between grid points was proposed as an alternative to the linear distribution of the fluid velocity, since the velocity variation between two grid points depend mainly on the area variations. Therefore the fluid velocity distribution $U$ in each grid element will be a function of the volumetric flow rate at the grid points and the area variations across the grid points, so that,

$$U = \frac{V_L}{(\pi/4) D_L^2}$$

where : $V_L$ is volumetric flow rate at mesh point $L$

and $D_L$ is pipe diameter at mesh point $L$

The other important modification relates to the generation and elimination of pathlines. According to Benson (1964), pathlines and therefore entropy levels are generated at the pipe ends and this information is transmitted towards the inside of the pipe. If in the next time step a change is produced in the flow direction such that the fluid starts travelling into the pipe, a new pathline will be generated with an entropy level whose value depends on the fluid state at the boundary and then the entropy level of the fluid between both pathlines acquires an intermediate value between the two values of entropy. This sharp change of entropy level can cause serious incongruities in the calculations if the values of entropy levels are appreciably different which is frequently the case when the valves/ports open and when reverse flow exists in the open end of the exhaust pipe. Payri et al (1986) proposed creating a duplicated pathline
with an entropy of the previous time step. This pathline is positioned very close to
the new pathline introduced by the boundary at the pipe end so that the strong entropy
gradient appears only in the boundary and the interior fluid does not suffer an
instantaneous entropy level change.

**Determination of λ, β and A_a at Interior Points**

Fig. (A.4) represents a grid element which includes characteristics lines for
the grid points (L - 1) and L and for the interior points K and K - 1 through which
pathlines pass at time Z. To obtain the values of the characteristics passing through
point L at time (Z+ΔZ), denoted by point R'. it is necessary to find the position of
a point P through which the same characteristic line passes at time Z. The graphical
procedure for locating point P is represented in Fig. (A.5) for λ characteristic. It
includes the following steps.

1. An initial solution for the location of point P is point 1 which is obtained on
the line OR' at time Z. Where point O is defined as the intersection of the
characteristics lines \( \lambda_k \) and \( \lambda_{k+1} \) passing through the path points k and k+1 which
are the two closest pathlines to point R', as shown in Fig. (A.5a).

2. The slope of the characteristic \( \lambda_1 \) passing through point 1 is calculated and
point (1') is then determined as the intersection of the line \( \lambda_1 \) and the time
line (Z+ΔZ).

The slope of \( \lambda \) at point 1, \( \lambda_1 \), is determined as follows:

\[ A_1 \text{ and } U_1 \text{ are obtained by interpolating from the mesh points L and (L - 1).} \]

The slope is then estimated as:

\[ \frac{dX}{dZ} = (A_1 + U_1) \]

and the location of point 1', \( X_{1'} \), is found from the following equation

\[ X_{1'} = X_1 + \delta X_1 = X_1 + ΔZ (A_1 + U_1) \]

where

\[ \frac{dZ}{dX_1} |_{\lambda_1} = \frac{ΔZ}{\delta X_1} \]
3. The location of point 1' is checked whether it is to the right or to the left of point R' and thus the domain of the next estimation for point P, which is point 2 is determined. Point 2 is obtained on the line 1'R' at time Z, where point 1" is defined as the intersection of the characteristics \( \lambda_1 \) and \( \lambda_{k+1} \). Step 2 is repeated to locate point 2' as shown in Fig. (A.5b).

Steps 2 and 3 are repeated till a point is found which is located to the right of R', e.g., point 2' as may be seen in Fig. (A.5b).

4. Point 3 shown in Fig. (A.5b) is the location of the solution point P. This point represents the location along the time step Z, where the \( \lambda \) characteristics passess and intersect the time line \( (Z+\Delta Z) \) at point R'. It can been seen from Fig. (A.5b) that

\[
\frac{13}{12} = \frac{13}{12}.
\]

where dash (−) refers to the length of the line.

Once point P is located, interpolation is carried out for pressure \( p \), volumetric flow rate \( V \), diameter \( D \) and entropy level \( A_p \) as follows:

\[
p_P = p_L - \frac{(p_L - p_{L-1})}{\Delta X} \delta X_P
\]

\[
V_P = V_L - \frac{(V_L - V_{L-1})}{\Delta X} \delta X_P
\]

\[
D_P = D_L - \frac{(D_L - D_{L-1})}{\Delta X} \delta X_P
\]

and

\[
A_{ap} = A_k - \frac{(A_k - A_{k-1})}{X_k - X_{k-1}} \left[ X_k - \{(L-1) \Delta X - \delta X_P \} \right]
\]

Now \( A_P \) and \( U_P \) and \( \lambda_P \) can be obtained from the following expressions:

\[
A_P = A_{ap} \left( \frac{p_P}{p_a} \right)^{(r-1)/2}
\]

\[
U_P = \left( \frac{4V_P}{\pi D_P^2} \right)
\]
\[ \lambda_p = A_p + \left[ \frac{(y-1)}{2} \right] U_p \]

and \[ \lambda_p^\prime = \lambda_p + d\lambda_p \]

where \( d\lambda_p \) is determined from the compatibility Eqn. (A.5).

The same procedure is repeated for \( \beta \) characteristic.

**Determination of \( \lambda, \beta \) and \( A_a \) at Boundaries**

Using \( \lambda, \beta \) and \( A_a \) at interior points, the solution procedure for boundary conditions is same as that described for Benson algorithm in Section (A.1).
Fig. (A.1) Subdivision of Pipe into Meshes (Benson, 1982)

Fig. (A.2) Grid Notation for Non-homentropic Flow (Benson, 1982)
Fig. (A.3) Pathlines Superimposed on Mesh Grid for Benson Algorithm (Benson, 1982)

Fig. (A.4) Pathlines Superimposed on Mesh Grid for the Modified Algorithm (Payri et al, 1986)
Fig. (A.5) : Graphical Procedure for locating the Solution Points using Modified Algorithm (Payri et al, 1986)
Appendix-B  Combustion Initiation and Flame Geometry

B.1 Initiation of Combustion (Benson, 1975a)

After the combustion of small nucleus of the mixture during the delay period, the combustion chamber is divided into two zones, a burned zone and an unburned zone. Following Benson 1975a, combustion is initiated in three steps as shown in Fig. (B.1). It is assumed that in the first step, the unburned mixture undergoes compression from \( v_1 \) to \( v_2 \) with a heat loss \( q_m \). The temperature and pressure at the end of this step are given by:

\[
T'_m = T_{m1} \left( \frac{v_1}{v_2} \right)^{R_m/Cv_m} - \frac{q_m}{m_m Cv_m}
\]

\[
p' = \left( \frac{p_1 v_1 T'_m}{v_2 T_{m1}} \right)
\]

Subscripts 1 & 2 refer to the states at the beginning and end of the process, respectively.

In the second step, the flame nucleus appears which is formed due to constant volume adiabatic combustion from \( T'_m \) resulting in high pressure \( p'' \) and temperature \( T_p'' \) of the products in the nucleus. The adiabatic flame temperature \( T_p'' \) is calculated from the internal energy balance for unit mass of the mixture. The temperature of the products \( T_p'' \) is adjusted until the specific internal energy of the products = the specific internal energy of the reactants. The steps for calculations are shown in the flow chart in Fig. (B.2) and is called subroutine ADIA.

The corresponding pressure \( p'' \) is calculated as:

\[
p'' = \left( \frac{R_p T''_p}{R_m T'_m} \right) p'
\]

The mass of the products in nucleus is estimated as

\[
m_p = \left( \frac{2 \pi R_f^3 m_e}{3 v_1} \right) + 2 \times 10^{-10} \left( m_e / v_1 \right)
\]

where \( R_f \) is the flame radius and is given by
R_f = [3/2π (v_1 - v_2)]^{1/3} \quad (B.5)

and the last term in Eqn. (B.4) accounts for the increase in density of the products.

The unburned mixture mass and volume become:

\[ m_{m_2} = m_c - m_p \quad (B.6) \]

\[ v_{m_2} = \frac{m_{m_2}}{m_n v_2} \quad (B.7) \]

and the total energy in the cylinder is

\[ U = m_{m_2} u_{m_1} + m_p u_{p_2} \quad (B.8) \]

As a result of the second step, a pressure difference exists between the burned and the unburned zones therefore, the third step is carried on for equalization of the pressure. It is assumed that this step is an adiabatic constant volume process. The balance of internal energy before and after the third step gives:

\[ m_{m_2} u_{m_1} + m_p u_{p_2} = m_{m_2} u_{m_2} + m_p u_{p_2} \quad (B.9) \]

which after rearrangement results into

\[ m_{m_2} c_v m T_m \left( \frac{T_{m_2}}{T_m} - 1 \right) = m_p c_v p T_p \left( 1 - \frac{T_{p_2}}{T^n_p} \right) \quad (B.10) \]

where

\[ \left( \frac{T_{m_2}}{T_m} \right) = \left( \frac{p_2}{p'} \right)^{(\gamma_m - 1)/\gamma_m} \quad (B.11) \]

\[ \left( \frac{T_{p_2}}{T^n_p} \right) = \left( \frac{p_2}{p''} \right)^{(\gamma_p - 1)/\gamma_p} \quad (B.12) \]

\[ \frac{p_2}{p''} = \frac{p_2}{p'} \cdot \frac{p'}{p''} = \frac{p_2}{R_m} \cdot \frac{T_m}{R_p} \cdot \frac{T^n_m}{T^n_p} \quad (B.13) \]

and

- \( T_{m_2} \) is the mixture temperature at the beginning of the combustion process
- \( T_{p_2} \) is the products temperature at the beginning of the combustion process
- \( p_2 \) is the uniform pressure in cylinder at the beginning of combustion
- \( m_{m_2} \) is the mixture mass at beginning of combustion
- \( m_p \) is the products mass at beginning of combustion
Combining Eqns. (B.10 - B.13) and letting

\[ T_{m2} / T_m = \delta \]  \hspace{1cm} (B.14)

\[ \gamma_m / (\gamma_m - 1) \cdot (\gamma_p - 1) / \gamma_p = \alpha \]  \hspace{1cm} (B.15)

and

\[ \frac{m_p C_v T''_p}{m_m C_v T''_m} = A \]  \hspace{1cm} (B.16)

\[ \left( \frac{R_m T''_m}{R_p T''_p} \right)^{(\gamma_f - 1) / \gamma_p} = B \]  \hspace{1cm} (B.17)

we get

\[ \delta - 1 = A(1 - B \delta^a) \]  \hspace{1cm} (B.18)

Eqn. (B.18) is solved by Newton Raphson Technique for \( \delta \), where

\[ F(\delta) = \delta - 1 - A(1 - B \delta^a) = 0 \]  \hspace{1cm} (B.19)

and

\[ F'(\delta) = 1 + \alpha AB \delta^{(a-1)} = 0 \]  \hspace{1cm} (B.20)

The flow chart which describes the initiation of combustion is given in Fig. (B.3) and is called subroutine INIT.

**B.2 Flame Geometry**

During the combustion, where the cylinder is divided into two zones of burned gases and of unburned gases separated by the flame front, heat transfer areas of both gases to the chamber walls depend on the location of the flame front. The estimation of areas and volumes of both burned and unburned gases is carried out taking the spark plug to be located in the centre of the cylinder and the flame is assumed to propagate spherically from the spark plug. Following the notation shown in Fig. (B.4), there are five cases to be considered

1. \( R > R_f \leq X_p \)

\[ A_p = \pi R_f^2 \]

\[ A_m = 2\pi R^2 + \pi D R_f - A_b \]
\[ A_f = 2\pi R_f^2 \quad \text{(B.21)} \]
\[ V_p = (2/3)\pi R_f^3 \]
\[ V_m = V_c - V_p \]

where

- \( X_p \): piston displacement
- \( R \): cylinder radius
- \( A_p \): heat transfer area of burned gas (Products)
- \( A_m \): heat transfer area of unburned mixture
- \( A_f \): area of the flame front
- \( V_p \): volume of burned gases (Products)
- \( V_m \): volume of unburned mixture
- \( V_c \): total cylinder volume

2. \( X_p < R_f \leq R \)

Define \( a = \left( \frac{R_f}{X_p} \right)^{1/2} \)

\[ A_p = \pi a^2 + \pi R_f^2 \]
\[ A_m = 2\pi R_f^2 - \pi a^2 - \pi R_f^2 + \pi D X_p \]
\[ A_f = 2\pi R_f \cdot X_p \quad \text{(B.22)} \]
\[ V_p = \pi X_p \left( 12\pi R_f^2 + 12a^2 + 4X_p^2 \right) / 24 \]
\[ V_m = V_c - V_p \]

3. \( R < R_f < X_p \)

\[ a = \left( \frac{R_f^2 - R^2}{X_p} \right)^{1/2} \]

\[ A_p = 2\pi R_a a + \pi R^2 \quad \text{(B.23)} \]
\[ A_m = 2\pi R_f^2 - 2\pi R_f \cdot a \]
\[ A_f = A_m \]
\[ V_p = 2\pi R_f^2 \left( R_f - a \right) / 3 \]
\[ V_m = V_c - V_p \]

4. \( R < R_f > X_p \)

\[ a = \left( \frac{R_f^2 - R^2}{X_p} \right)^{1/2} \]
\( X = X_p - a \)
\( b = \left( R_f^2 - X_p^2 \right)^{1/2} \)
\( A_p = \pi R^2 + \pi Da + \pi b^2 \)
\( A_m = \pi D X + \pi (R^2 - b^2) \)
\( A_t = 2\pi R X_p + (\pi/4) R^2 \)
\( V_p = \pi R^2 a + (\pi X/24)(12R^2 + 12b^2 + 4X^2) \)
\( V_m = V_c - V_p \)

5. \( R < R_f > X_m \)

where

\( X_m = (R^2 + X_p^2)^{1/2} \)

\( V_p = \pi R^2 X_p \)
\( V_m = 0.0 \)
\( A_t = 0 \)
\( A_m = 0 \)
\( A_p = 2\pi R^2 + 2\pi R \cdot X_p \)
Fig. (B.1) Steps in Initiation of Combustion (Benson, 1975a)

Heat loss $q_m$

Initial state

Equilibration of pressure

Transform at fixed volume
Fig. (B.2) Flow Chart for Calculating the Adiabatic Flame Temperature, Subroutine ADIA

1.0 < \( T \) < 1.0

\[
T' = T + 2500 \times \phi \times RES - 700 (\phi - 1) RES
\]

\[
T' = T + 2500 \times RES \times \phi
\]

\( \Delta T' = T'/4.0 \)

Calculate internal energy of mixture \( u_m \), at \( T_m, p_e \)

Calculate internal energy of products \( u_p \), at \( T_p, p_e \)

\( 0 > u_p - u_m > 0 \)

\[
T = T + \Delta T'
\]

\[
T = T - \Delta T'
\]

\[
\Delta u = |u_p - u_m|
\]

\[
\Delta T' = \Delta T'/2
\]

1.0 < \( \Delta T' \) < 1.0

\[\Delta u \geq 1.0\]

\( T \) is the adiabatic flame temperature

EXIT
Fig. (B.3) Flow Chart for Initiation of the Combustion Process, Subroutine INIT.

**ENTRY**

- **$T_0$, $p_0$, $m_0$, $v_0$, $\alpha$, $\delta_0$**

  - $v_i = v(\alpha + \delta_0)$

  - **Calculate**: $T^\ast$, Eqn. (B.1)
    - $p'$, Eqn. (B.2)

  - Call subroutine ADIA to determine the adiabatic Flame temperature $T^\ast$.

  - **Calculate**: $p^\ast$, Eqn. (B.3)
    - $m^\ast$, Eqn. (B.4)
    - $R^\ast$, Eqn. (B.5)
    - $m_{n2}$, Eqn. (B.6)
    - $v_{n2}$, Eqn. (B.7)

  - $\delta = 1$

  - **Calculate**: $F(\delta)$, Eqn. (B.19)
    - $F(\delta)$, Eqn. (B.20)

  - $\delta_{n+1} = \delta_n - \left[\frac{E(\delta)}{F(\delta)}\right]_n$

  - **IF** $|\delta_{n+1} - \delta_n| > \text{limit}$ **THEN** $\delta_n = \delta_{n+1}$

  - **ELSE** $\delta = \delta_{n+1}$

  - **Calculate**: $T_{n2}$, Eqn. (B.14)
    - $T_2$, Eqn. (B.12)
    - $p_2$, Eqn. (B.13)

**EXIT**
Fig. (B.4) : Localization of the Flame Front
Appendix-C  Molar Composition of the Products and Thermal Properties

C.1  Determination of Molar Composition of the Products

At high temperature, complete combustion does not occur as there is a dissociation and the maximum temperature attained in the combustion is appreciably lower than that based upon complete combustion. In general, it is found that twelve combustion products are present in the cylinder, namely H₂O, H₂, OH, H, N₂, NO, N, CO₂, CO, O₂, O, AR. If the hydrocarbon (is-octane) is represented by the equivalent chemical formula C₇H₈O₄N₆, where W, Q, Y, Z, represent the number of atoms of C, H, O, and N, respectively in the reacting compound. The reaction is written as:

\[ A(C₇H₈O₄N₆) \rightarrow nH₂O + nH₂ + nOH + nH + nN₂ + nNO + nN + nCO₂ + nCO \]

where \( n_{H₂O}, n_{H₂}, \ldots \) etc. represent number of moles of the species, respectively. If \( A \) is defined as \( \frac{1}{n} \) where \( n \) is the total number of moles of products, the chemical reaction is then written as:

\[ A(C₇H₈O₄N₆) \rightarrow XH₂O + XH₂ + XOH + XH + XN₂ + XNO + XN + XCO₂ + XCO \]

where

\[ X_{H₂O}, X_{H₂}, \ldots \text{ etc.} = \frac{n_{H₂O}}{n}, \frac{n_{H₂}}{n} \ldots \ldots \ldots \text{etc.} \]

represent the mole fractions of species, respectively.

From mass balance of C, H₂, O and N₂ we get,

A. \( W = X_{CO₂} + X_{CO} \)  \hspace{2cm} (C.3)

A. \( Q = 2X_{H₂O} + 2X_{H₂} + X_{OH} + X_H \)  \hspace{2cm} (C.4)

A. \( Y = X_{H₂O} + X_{OH} + X_{NO} + 2X_{CO₂} + 2X_{O₂} + X_O \)  \hspace{2cm} (C.5)
A. \( Z = 2X_N + X_{NO} + X_N \)  \hspace{1cm} (C.6)

The fifth equation is written for mole fractions as:

\[
\sum_{i=1}^{12} X_i = 1.0
\]  \hspace{1cm} (C.7)

The equilibrium distribution of these species can be fully described by the following reactions:

\[
\begin{align*}
\frac{1}{2}H_2 & \rightarrow H \\ 
\frac{1}{2}O_2 & \rightarrow O \\ 
\frac{1}{2}N_2 & \rightarrow N \\ 
H_2 + \frac{1}{2}O_2 & \rightarrow H_2O \\ 
\frac{1}{2}H_2 + \frac{1}{2}O_2 & \rightarrow OH \\ 
\frac{1}{2}N_2 + \frac{1}{2}O_2 & \rightarrow NO \\ 
C + O_2 & \rightarrow CO_2 \\ 
C + \frac{1}{2}O_2 & \rightarrow CO
\end{align*}
\]  \hspace{1cm} (C.8-15)

The equilibrium constant \( K_p \) for the stoichiometric reaction between the substances \( A, B, C, D \):

\[
v_a A + v_b B \leftrightarrow v_c C + v_d D
\]

can be expressed as

\[
K_p = \frac{X_c^{v_c} X_d^{v_d} p^{(v_c + v_d - v_a - v_b)}}{X_a^{v_a} X_b^{v_b}}
\]

where,

\( v \) is the stoichiometric coefficient

\( X \) is the molar fraction and

\( p \) is the total pressure

The equilibrium equations for the above reaction can be described as

\[
K_1 = \frac{X_H}{\sqrt{X_{H_2}}} \sqrt{p}
\]  \hspace{1cm} (C.16)

\[
K_2 = \frac{X_O}{\sqrt{X_{O_2}}} \sqrt{p}
\]  \hspace{1cm} (C.17)
where $K, \ldots K_8$ represent equilibrium constants for the reaction described by Eqn. (C.8 – C.15). Also, the equilibrium constant for any species is expressed by a polynomial as function of temperature as:

$$\log K_p = A \ln T + B/T + C + DT + ET^2$$

where $T$ is the absolute temperature and $A, B, C, D$ and $E$ are constants given in Table (C.1) for different products.

Defining $B$ as:

$$B = \frac{X_{\text{H}_2\text{O}}}{X_{\text{H}_2}}$$

and arranging Eqns. (C.3 – C.7) and Eqns. (C.8 – C.15) and substituting for $B$, the equations for mole fractions can be written as:

$$X_{\text{H}} = \frac{K_1 \sqrt{X_{\text{H}_2}}}{\sqrt{p}}$$

$$X_{\text{O}} = \frac{K_2 \cdot B}{K_4 \cdot p}$$

$$X_{\text{N}} = \frac{K_3 \sqrt{X_{\text{N}_2}}}{\sqrt{p}}$$
\[ \begin{align*}
X_{O_2} & = \frac{B^2}{K_4^2 \cdot p} & (C.28) \\
X_{OH} & = \frac{K_5 \sqrt{X_{H2}} \cdot B}{K_4 \sqrt{p}} & (C.29) \\
X_{NO} & = \frac{K_6 \sqrt{X_{N2}} \cdot B}{K_4 \sqrt{p}} & (C.30) \\
X_{CO} & = \frac{K_8 \cdot X_{CO2} \cdot I}{K_7 \sqrt{X_{O2}}} \sqrt{p} & (C.31) \\
X_{CO2} & = \frac{A \cdot W \cdot K_7 \cdot \sqrt{X_{O2}} \cdot p}{K_7 \sqrt{X_{O2}}} \sqrt{p} + K_8 & (C.32) \\
X_{H2} & = \left[ -\frac{\alpha}{2} + \sqrt{\frac{\alpha^2}{4} + \frac{A \cdot Q}{2(B+1)}} \right]^2 & (C.33) \\
X_{N2} & = \left[ -\frac{\beta}{2} + \sqrt{\frac{\beta^2}{4} + \frac{A \cdot Z}{2}} \right]^2 & (C.35) \\
\text{and} & & \\
\beta & = \frac{B \cdot K_6 + K_3 \cdot K_4}{2 K_4 \cdot \sqrt{p}} & (C.36)
\end{align*} \]

where \( \alpha = \frac{B \cdot K_5 + K_1 \cdot K_4}{2(B+1) \cdot K_4 \cdot p} \) (C.34)

Eqns. (C.3 - C.7) along with Eqns. (C.24 - C.36) define the composition of a C-H-O-N system in terms of pressure, temperature and independent variables A and B.

The solution of above equations is based on Vickland modified method (Vick and et al, 1964) where values of A and B are selected and all the values of mole fractions \( X_i \) given by Eqns. (C.3 - C.7) and Eqns. (C.24 - C.36) are checked with these calculated values for balance. A is estimated as follows:

(i) For \( \phi \geq 1.0 \)

\[ A = \frac{1.3}{\left[ \left( w + 0.5Q + 1.863 \left( \frac{2W + 0.5Q - Y}{\phi} \right) \right) \right] \cdot \exp \left( \frac{0.13T}{1000} \right)} \]  

(C.37)
(ii) For \( \phi < 1.0 \)

\[
A = \frac{1.3}{\left[\left(0.25Q + 2.363 \left(\frac{2.0 + 0.5Q - Y}{\phi}\right)\right)\right]} \exp\left(\frac{0.13T}{1000}\right)
\]

where \( \phi \) is the equivalence ratio of the fuel

B is estimated as follows

(i) For \( T > 3000 \) K

\[
B = \exp\left[10.3 - (3.1 - 0.17 \log(p)) \left(\frac{T}{1000}\right)\right]
\]

(ii) For \( T \leq 3000 \) K

\[
B = \exp\left[-9.0 + 0.5 \log(p) + \left(\frac{3000}{T}\right)\right]
\]

Newton Raphson adjustment is made to A and B for balance and calculations are repeated till the required accuracy is obtained.

**C.2 Determination of Thermal Properties**

**Specific Heat at Constant Pressure**

\[
C_{p_i} = A + BT' + CT'^2 + DT'^3 + ET'^4 + FT'^5
\]

where \( T' = T - T_o \)

where \( C_{p_i} \) is the specific heat at constant pressure of the species \( i \) and \( T_o \) is the base temperature = 298 K. A, B, C, D, E, F are constants and listed in Table (C.2) for the twelve products of combustion and for fuel (iso-octane - \( C_{8}H_{18} \)).

**Specific heat of a mixture**

\[
C_p = \Sigma y_i C_{p_i}
\]

\[
y_i = \frac{N_i}{N}
\]

\[
N = \Sigma N_i
\]

where \( y_i \) is Mole fraction of species \( i \)

\( N_i \) = Number of moles of species \( i \) in the mixture

\( N \) = Total number of moles of the mixture

\( C_{p_i} \) = Specific heat at constant pressure of species \( i \)
Gas Constant of Mixtures

\[ R = \sum \frac{R_i}{m_i} \]  \hspace{1cm} (C.45)

\[ m_w = \sum y_i m_{wi} \]  \hspace{1cm} (C.46)

where \( R_i \) is the gas constant of species \( i \)
\( m_{wi} \) is molecular weight of species \( i \)
\( m_w \) is molecular weight of mixture

Specific Heat at Constant Volume of Mixture

\[ C_v = C_p - R \]  \hspace{1cm} (C.47)

Ratio of Specific Heats of the mixture

\[ \gamma = \frac{C_p}{C_v} \]  \hspace{1cm} (C.48)

Enthalpy of Species \( i \)

\[ h_i = \int_{T_o}^{T} C_{p_i} (T') \, dT' + \Delta H^o_{fi} \]  \hspace{1cm} (C.49)

where \( \Delta H^o_{fi} \) is the molar heat of formation at the base temperature \( T_o \)

Enthalpy of Mixture

\[ h = \sum y_i h_i \]  \hspace{1cm} (C.50)

where \( h_i \) is given by Eqn. (C.49)

Internal energy of Mixture

\[ u = h - pv = h - RT \]  \hspace{1cm} (C.51)

where \( h \) is given by Eqn. (C.50)

Viscosity

The calculation of viscosity and thermal conductivity of the fuel (iso-octane) and the products of combustion are obtained using relations given by Sherwood (1977).
The Champan-Enskog formula is used to calculate the viscosity as follows:

\[
\mu = \frac{(0.002669 \sqrt{MT})}{(\sigma^2 \Omega_v)} 
\]  
\[\text{(C.52)}\]

where:

\(\mu\) is viscosity in centipoise

\(M\) is the molecular weight

\(T\) is the temperature, K

\(\sigma\) is the characteristic dimension of the molecule, Å

\(\Omega_v\) is the collision integral and determined differently for polar and nonpolar gases

(a) \(\Omega_v\) For Nonpolar Gases

Neufeld proposed an empirical equation for determining \(\Omega_v\) as:

\[
\Omega_v = \frac{A}{T^b} + \frac{C}{\exp (DT^*)} + \frac{E}{\exp (FT^*)} 
\]  
\[\text{(C.53)}\]

and

\[T^* = \frac{KT}{\varepsilon} \]  
\[\text{(C.54)}\]

where:

\(K\) is the Boltzman's constant

\(\varepsilon\) is the characteristic energy

and the constants in Eqn. (C.53) are:

\(A = 1.16145\)

\(B = 0.14874\)

\(C = 0.52487\)

\(D = 0.77320\)

\(E = 2.16178\)

\(F = 2.43787\)

(b) \(\Omega_v\) For Polar Gases

\[
\Omega_v = \Omega_v \text{ (for non polar)} + \frac{0.28^2}{T^*} 
\]  
\[\text{(C.55)}\]
where $\delta$ is a polar parameter
values of $\epsilon/K$, $\sigma$ and $\delta$ are tabulated for various gases.

(c) For Hydrocarbons (Iso-octane)

The viscosity is calculated using the reduced properties as:

$$\mu \zeta = 4.61 T^{0.618} - 2.04 e^{-0.449 T_r} + 1.94 e^{-4.058 T_r} + 0.1$$  \hspace{1cm} (C.56)

where $\zeta = T_c^{1/6} \cdot M^{-1/2} \cdot p_c^{2/3}$  \hspace{1cm} (C.57)

$T_r = T / T_c$  \hspace{1cm} (C.58)

$T_c$ is the critical temperature, $K$

$p_c$ is the critical pressure, atm

**Thermal Conductivity**

(a) For polar and non-polar gases

Eucken Correlation for thermal conductivity is:

$$K = (C_v + 4.47) (\mu/M)$$  \hspace{1cm} (C.59)

where $K$ is the thermal conductivity

$C_v$ is the molar heat capacity in cal/(mole.K)

$\mu$ is the low pressure gas viscosity in poise

Another modified form of Eucken relation is

$$K = (1.32 C_v + 3.52) (\mu/M)$$  \hspace{1cm} (C.60)

Good results are obtained by averaging the two estimated values from Eqn. (C.59) and Eqn. (C.60).

(b) For Hydrocarbons (Iso-octane)

$$K = 10^{-6} (14.52 T_r - 5.14)^{2/3} (C_p/\Gamma)$$  \hspace{1cm} (C.61)

where, $\Gamma = T_c^{1/6} \cdot M^{1/2} \cdot p_c^{-2/3}$  \hspace{1cm} (C.62)

$C_p$ is molar heat capacity in cal/(mole.K)
C.2 Viscosity and Thermal Conductivity of Mixtures

The viscosity of the mixture is determined by Manson - Saxena method as follows:

\[
\mu_{\text{mix}} = \frac{\sum \mu_i}{(1+\sum \phi_{ij} (y_j/y_i))} \tag{C.63}
\]

\(y_i\) is the molar fraction of the \(i^{th}\) species.

\(\phi_{ij}\) is a parameter defined as

\[
\phi_{ij} = \frac{1 + \left(\frac{u_i}{u_j}\right)^{1/2} \left(\frac{M_j}{M_i}\right)^{1/4}}{\left[\sqrt{8} \left\{ 1 + \left(\frac{M_i}{M_j}\right)^{1/2} \right\} \right]} \tag{C.64}
\]

and \(\phi_{ji}\) is found by interchanging subscripts or by

\[
\phi_{ji} = \frac{\mu_j}{\mu_i} \cdot \frac{M_i}{M_j} \cdot \phi_{ij} \tag{C.65}
\]

for a binary system of (1) and (2)

\[
\mu_{\text{mix}} = \frac{\mu_1}{[1 + (y_2/y_1) \phi_{12}]} + \frac{\mu_2}{[1 + (y_1/y_2) \phi_{21}]} \tag{C.66}
\]

The thermal conductivity of gas mixture is determined in a similar way. In all the above calculations of viscosity and thermal conductivity, the effect of pressure is neglected.
Table (C.1) Coefficients Used for Calculating the Equilibrium Constants of Formation of Species from their Elements

\[
\text{LOG} \ (K_p) = A \ln T + \frac{B}{T} + C + D T + E T^2
\]

<table>
<thead>
<tr>
<th>Reaction</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\frac{1}{2} H_2 \rightarrow H)</td>
<td>0.432168</td>
<td>-11.2464</td>
<td>2.67269</td>
<td>-0.745744E-1</td>
<td>0.242484E-2</td>
</tr>
<tr>
<td>(\frac{1}{2} O_2 \rightarrow O)</td>
<td>0.310805</td>
<td>-12.954</td>
<td>3.21779</td>
<td>-0.738336E-1</td>
<td>0.344645E-2</td>
</tr>
<tr>
<td>(\frac{1}{2} N_2 \rightarrow N)</td>
<td>0.389716</td>
<td>-24.5828</td>
<td>3.14505</td>
<td>-0.963730E-1</td>
<td>0.585643E-02</td>
</tr>
<tr>
<td>(\frac{1}{2} H_2 + \frac{1}{2} O_2 \rightarrow OH)</td>
<td>-0.141784</td>
<td>-2.13308</td>
<td>0.853461</td>
<td>0.355615E-1</td>
<td>-0.310227E-2</td>
</tr>
<tr>
<td>(\frac{1}{2} N_2 + \frac{1}{2} O_2 \rightarrow NO)</td>
<td>0.150879E-1</td>
<td>-4.70959</td>
<td>0.646096</td>
<td>0.272805E-2</td>
<td>-0.15444E-02</td>
</tr>
<tr>
<td>(H_2 + \frac{1}{2} O_2 \rightarrow H_2O)</td>
<td>-0.752364</td>
<td>12.421</td>
<td>-2.60286</td>
<td>0.259556</td>
<td>-0.162687E-01</td>
</tr>
<tr>
<td>(CO + \frac{1}{2} O_2 \rightarrow CO_2)</td>
<td>-0.415302E-2</td>
<td>14.8627</td>
<td>-4.75746</td>
<td>0.124699</td>
<td>-0.900227E-02</td>
</tr>
</tbody>
</table>
Table (C.2) Coefficients for Computing Cp at Temperature T (K)

\[ \text{Cp} = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T^4 + F \cdot T^5 \text{ (Cal/Mol K)} \]

<table>
<thead>
<tr>
<th>Species</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>( \Delta H_{fo} ) (kJ/kg-mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>4.968</td>
<td>0.0000000</td>
<td>0.0000000</td>
<td>0.0000000</td>
<td>0.0000000</td>
<td>0.0000000</td>
<td>2.17986E5</td>
</tr>
<tr>
<td>O</td>
<td>5.346366</td>
<td>-0.6739781E-3</td>
<td>0.4481578E-6</td>
<td>-0.1411204E-9</td>
<td>0.2201334E-13</td>
<td>-0.1307902E-17</td>
<td>2.49195E5</td>
</tr>
<tr>
<td>N</td>
<td>4.958878</td>
<td>0.1942247E-4</td>
<td>0.461052E-8</td>
<td>0.197628E-10</td>
<td>0.8103602E-14</td>
<td>-0.6898808E-18</td>
<td>4.72646E5</td>
</tr>
<tr>
<td>OH</td>
<td>7.212435</td>
<td>-0.1005184E-02</td>
<td>0.1728465E-5</td>
<td>-0.6703618E-9</td>
<td>0.1080869E-12</td>
<td>0.63316047E-17</td>
<td>3.94634E4</td>
</tr>
<tr>
<td>H₂O</td>
<td>6.987605</td>
<td>0.2855784E-2</td>
<td>0.4082449E-6</td>
<td>-0.4530978E-9</td>
<td>0.9097223E-13</td>
<td>-0.58113041E-17</td>
<td>-2.41827E5</td>
</tr>
<tr>
<td>NO</td>
<td>6.30392</td>
<td>0.2603326E-2</td>
<td>-0.9660826E-6</td>
<td>0.1621015E-9</td>
<td>-0.9941074E-14</td>
<td>0.0000000</td>
<td>9.05924E4</td>
</tr>
<tr>
<td>CO₂</td>
<td>6.039775</td>
<td>0.1208784E-1</td>
<td>-0.6892165E-5</td>
<td>0.19769687E-8</td>
<td>-0.2758421E-12</td>
<td>0.1483168E-16</td>
<td>-3.93522E5</td>
</tr>
<tr>
<td>CO</td>
<td>6.133285</td>
<td>0.2579359E-2</td>
<td>-0.8839086E-6</td>
<td>0.1399667E-9</td>
<td>-0.8205784E-14</td>
<td>0.0000000</td>
<td>-1.10529E5</td>
</tr>
<tr>
<td>H₂</td>
<td>7.043649</td>
<td>-0.7481993E-3</td>
<td>-0.1414508E-6</td>
<td>0.5232309E-9</td>
<td>-0.8176101E-13</td>
<td>0.4673767E-17</td>
<td>0.0000000</td>
</tr>
<tr>
<td>O₂</td>
<td>6.014893</td>
<td>0.3832211E-2</td>
<td>-0.2106804E-5</td>
<td>0.6449786E-9</td>
<td>-0.95534103E-13</td>
<td>0.5355434E-17</td>
<td>0.0000000</td>
</tr>
<tr>
<td>N₂</td>
<td>6.170795</td>
<td>0.2272505E-2</td>
<td>-0.7181618E-6</td>
<td>0.1037995E-9</td>
<td>-0.5571979E-14</td>
<td>0.0000000</td>
<td>0.0000000</td>
</tr>
<tr>
<td>AR</td>
<td>4.968</td>
<td>0.000000000</td>
<td>0.0000000</td>
<td>0.0000000</td>
<td>0.0000000</td>
<td>0.0000000</td>
<td>0.0000000</td>
</tr>
<tr>
<td>C₈H₁₈</td>
<td>2.547736</td>
<td>0.1536359</td>
<td>-0.1333815E-4</td>
<td>-0.9377068E-7</td>
<td>0.7097913E-10</td>
<td>-0.1649594E-13</td>
<td>-2.08447E5</td>
</tr>
</tbody>
</table>
Fig. (D.1) Flow Chart for the Engine Simulation Program

 ENTRY

 Refering Fig. (3.1)
 Read Data

 \[ t = 0.0 \]

 Initialize conditions in the cylinder, crankcase, inlet system, transfer pipes and exhaust system

 Calculate, the time step \( \Delta t \) from the stability criterion at each mesh point for each pipe and find the minimum time step \( \Delta t \)

 \[ t = t + \Delta t \]

 Call subroutine 'INTER' at each mesh point of each pipe, except for the boundary points and determine \( p, u, p, \gamma, \) and \( R \)

 \( u_i = 0 \)

 \[ \begin{align*}
 (p_i), u &= (p_i), \\
 (\gamma_i), u &= (\gamma_i), \\
 (R_i), u &= (R_i), \\
 (R_i), u &= (R_i)
\end{align*} \]

 Call subroutine 'OPENL' and determine \( p_i, u_i, p_i, \gamma_i, \) and \( R_i \)

 No Flow

 \[ u_i < 0 \]

 Call subroutine 'CARB' and determine Properties upstream and downstream of carburettor \( p_i, u_i, p_i, \gamma_i, R_i \)

 \[ p_i, u_i, p_i, \gamma_i, R_i \]

 Call subroutine 'CCASE' to determine \( p_{i+}, T_{i+} \) and the fluid properties at points 3 & 4 \( p_i, u_i, p_i, \gamma_i, R_i, p_i, u_i, p_i, \gamma_i, R_i \)

 Call subroutine 'ENGINE' to determine \( p_{i+}, T_{i+} \) and the fluid properties at points 5 & 6 \( p_i, u_i, p_i, \gamma_i, R_i, p_i, u_i, p_i, \gamma_i, R_i \)

 Call subroutine 'JOIN' to determine fluid properties at point 7 \( p_i, u_i, p_i, \gamma_i, R_i \)

 Call subroutine 'JOIN' to determine fluid properties at point 8 \( p_i, u_i, p_i, \gamma_i, R_i \)
Call subroutine 'JOIN' to determine fluid properties at point 9, \( p_9, u_9, \rho_9, \gamma_9, R_9 \)

Call subroutine 'JOIN' to determine fluid properties at point 10, \( p_{10}, u_{10}, \rho_{10}, \gamma_{10}, R_{10} \)

Call subroutine 'JOIN' to determine fluid properties at point 11, \( p_{11}, u_{11}, \rho_{11}, \gamma_{11}, R_{11} \)

Call subroutine 'JOIN' to determine fluid properties at point 12, \( p_{12}, u_{12}, \rho_{12}, \gamma_{12}, R_{12} \)

\[ u_{11} = 0 \]

\[ (p_{11})_{n+1} = (p_9) \]

\[ (\rho_{11})_{n+1} = (\rho_9) \]

\[ (\gamma_{11})_{n+1} = (\gamma_9) \]

\[ (R_{11})_{n+1} = (R_9) \]

\[ 0 = u_{11} \]

\[ > 0 \]

Call subroutine OPENR and determine \( p_{11}, u_{11}, \rho_{11}, \gamma_{11}, R_{11} \)

Call subroutine INFLR and determine \( p_{11}, u_{11}, \rho_{11}, \gamma_{11}, R_{11} \)

Cycle is complete

\[ (\Delta p_c)^n = (p_c)^n - (p_c)^{n-1} \]

\[ |\Delta p_c| < \text{limit} \]

No

Yes

EXIT
Fig. (D.2) Flow Chart for Crankcase Calculations, Subroutine CCASE

**ENTRY**

**Input**
1. Engine Specifications.
2. Engine Operating conditions.
3. Fluid properties at boundary points adjacent to the ports.
4. $\Delta t$, $\alpha$, ICOR, ICC2

- $\alpha_i = \alpha + 180$

  **ICC2 > 1**
  - No: Calculation of constants and crankcase conditions at release, $p_{cc}$, $T_{cc}$, $m_{cc}$
  - Yes: $ICC2 = ICC2 + 1$

- $\delta\alpha_i = 6\times RPM\times\Delta t$

- $\alpha_i = \alpha_i + \delta\alpha_i$

- $\alpha_i \geq 360$
  - No: $\alpha_i = \alpha_i - 360$
  - Yes

Set area ratio of delivery port = 1

$\psi_i = $ coefficient of discharge

Call subroutine CBOUNDL to determine $u_i$, $p_u$, $p_d$, $p_r$, $R_i$

**Calculate**:
- $\delta m_i = \rho_d \psi_i u_i$
- $\delta m_i = \delta m_i \times \delta\alpha / 6N$

- $\delta m_i = \delta m_i \times $ no. of delivery ports

- $(m_i)^* = (m_i)^* + (\delta m_i)^*$

- $\alpha_i < 10$
  - Yes

- $\alpha_i > IC$
  - Yes: Inlet ports are closed
  - No: Inlet ports are open
Calculate the effective area ratio for inlet port \( \psi \).

Call subroutine CBOUND and determine \( u, p, p, \gamma, R \).

Calculate:
\[
\delta m_1 = \rho \psi u
\]
\[
\delta m_2 = \delta \delta m_1 \delta x / \delta N
\]

\[\delta m = \delta m_1 \times \text{no. of inlet ports} \]

\[(m_{\alpha})^y = (m_{\alpha})^y (\delta m)^y\]

No

\[(\delta m > 0) \& (\delta m < 0)\]

Yes

\[\delta T_{CC}, \text{Eqn. (3.2.29)}\]

No

\[(\delta m < 0) \& (\delta m > 0)\]

Yes

\[\delta T_{CC}, \text{Eqn. (3.2.30)}\]

No

\[(\delta m < 0) \& (\delta m < 0)\]

Yes

\[\delta T_{CC}, \text{Eqn. (3.2.31)}\]

No

\[(\delta m = 0) \& (\delta m > 0)\]

Yes

\[\delta T_{CC}, \text{Eqn. (3.2.32)}\]

No

\[(\delta m = 0) \& (\delta m < 0)\]

Yes

\[\delta T_{CC}, \text{Eqn. (3.2.33)}\]

No

\[\delta T_{CC}, \text{Eqn. (3.2.34)}\]

After replacing suffix 'c' by 'cc' and 'a' by 'a,' calculate:

\[T_{CC} \quad \text{Eqn. (3.2.48)}\]
\[\delta m_{CC} \quad \text{Eqn. (3.2.46)}\]
\[m_{CC} \quad \text{Eqn. (3.2.47)}\]
\[\delta T_{CC} \quad \text{Eqn. (3.2.34)}\]
Input 1. Engine Specifications.
2. Engine Operating conditions.
3. Conditions at boundary points adjacent to the ports.
4. $\Delta t, \alpha, ICOR, ICC1$

**ENTRY**

- $\alpha = EPO$
- **ICC1 > 1**
  - Yes: $ICC1 = ICC1 + 1$
  - No: $\delta \alpha = 6 \times RPM \times \Delta t$
    - $\alpha = \alpha + \delta \alpha$
      - $\alpha \geq 360$
        - Yes: $\alpha = \alpha - 360$
        - No: $\alpha < EO$
          - No: $\alpha > EC$
            - Yes: Exhaust port is closed
              - Call subroutine CLOSL and determine $u_s, p_s, \rho_s, Y_s, R_s$
            - No: Calculate effective exhaust port area ratio, $\psi_s$, Eqn. (3.2.45b)
              - Call subroutine CBOUNDL and determine $u_s, p_s, \rho_s, Y_s, R_s$
              - Calculate: $\delta m_s$, Eqn. (3.2.44)$\delta m, Eqn. (3.2.42)$
                - $\delta m_s = \delta m \times \text{no. of exhaust ports}$
                  - $(m_s)_p^n = (m_s)_p^{n-1} + (\delta m)_s^n$
- $\alpha < SO$
- $\alpha > SC$
- Scavenge ports are open
- Scavenge ports are closed
Call subroutine CBOUND and determine \( u, p, \rho, \gamma, R \).

Call subroutine CLOSR to determine \( u, p, \rho, \gamma, R \).

Calculate:
\[ \delta m_{a}, \text{ Eqn. (3.2.43)} \]
\[ \delta m_{s}, \text{ Eqn. (3.2.41)} \]

\[ \delta m = \delta m_{a} \times \text{no. of scavenge ports} \]
\[ (m_{a})^{*} = (m_{a})^{-1} + (\delta m_{a})^{*} \]

\( \text{EO} \rightarrow \text{GC} \)

Yes
Exhaust port is closed

No

\( \text{SC} \rightarrow \text{SO} \)

Yes

Call subroutine COMBUSTION to determine \( p_{c}, T_{c}, \rho_{c}, \gamma_{c}, R_{c} \).

No

Call subroutine SCAVENGE to determine \( \eta_{a}, \eta_{s}, \text{Res} \).

\( (\delta m_{a}, 0) \land (\delta m_{s}, 0) \)

Yes

\[ \delta T_{c}, \text{ Eqn. (3.2.28)} \]

No

\( (\delta m_{a}, 0) \land (\delta m_{s}, 0) \)

Yes

\[ \delta T_{c}, \text{ Eqn. (3.2.29)} \]

No

\( (\delta m_{a}, 0) \land (\delta m_{s}, 0) \)

Yes

\[ \delta T_{c}, \text{ Eqn. (3.2.30)} \]

No

\( (\delta m_{a}, 0) \land (\delta m_{s}, 0) \)

Yes

\[ \delta T_{c}, \text{ Eqn. (3.2.31)} \]

No

\( (\delta m_{a}, 0) \land (\delta m_{s}, 0) \)

Yes

\[ \delta T_{c}, \text{ Eqn. (3.2.32)} \]

No

\( (\delta m_{a}, 0) \land (\delta m_{s}, 0) \)

Yes

\[ \delta T_{c}, \text{ Eqn. (3.2.33)} \]

No

\[ \delta T_{c}, \text{ Eqn. (3.2.34)} \]

Calculate:
\[ T_{c}, \text{ Eqn. (3.2.48)} \]
\[ \delta m_{a}, \text{ Eqn. (3.2.46)} \]
\[ \delta m_{s}, \text{ Eqn. (3.2.47)} \]
\[ m_{a}, \text{ Eqn. (3.2.49)} \]
\[ p_{c}, \text{ Eqn. (3.2.50)} \]

EXIT