UNENE Graduate Course
Reactor Thermal-Hydraulics Design and Analysis

McMaster University

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Network Calculations

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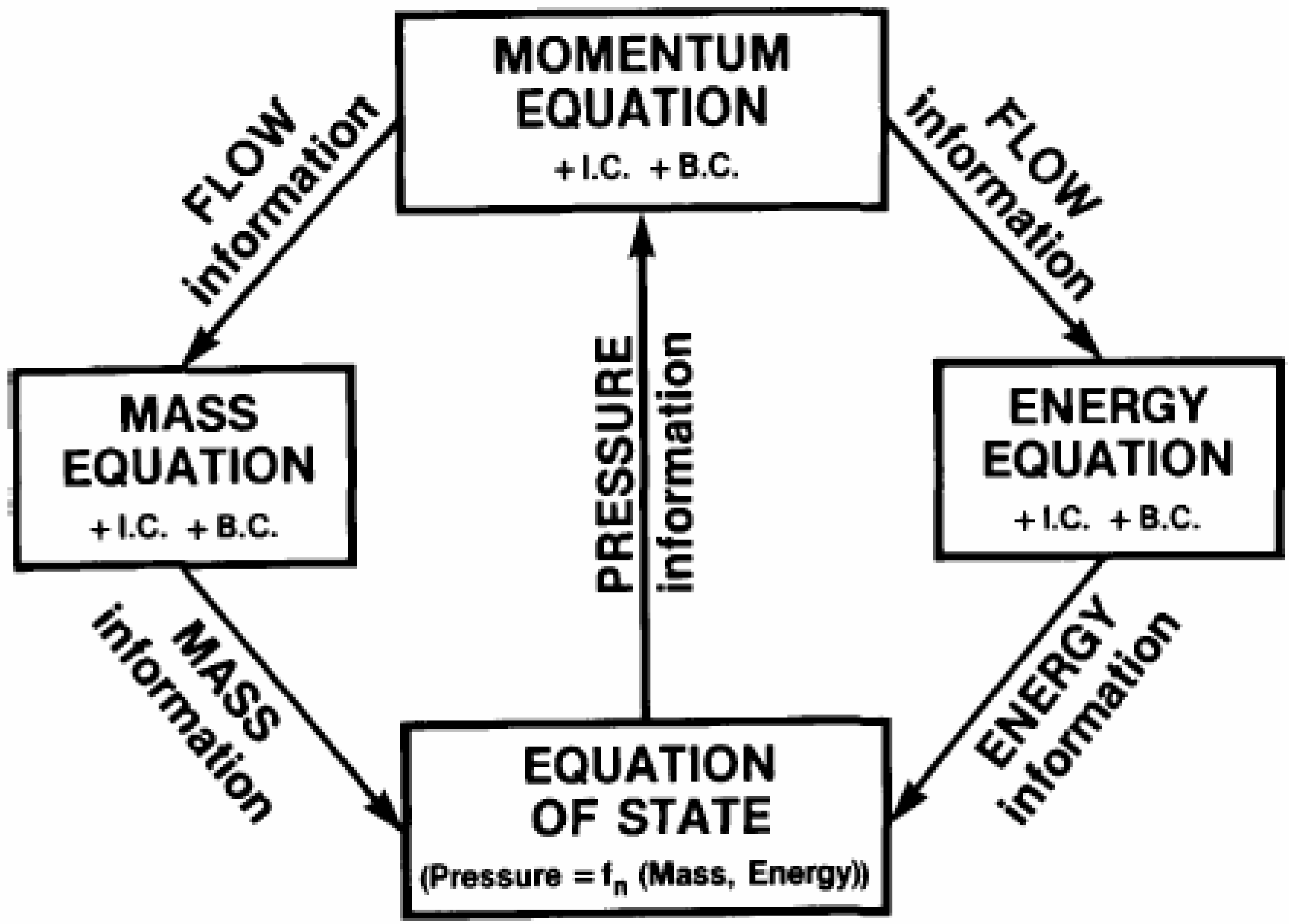
Outline

- Outline of Porsching method
- Development of fully-implicit back-substituted form (FIBS)
- Fully explicit scheme
- Semi-implicit scheme
- Fully implicit scheme
- Programming notes

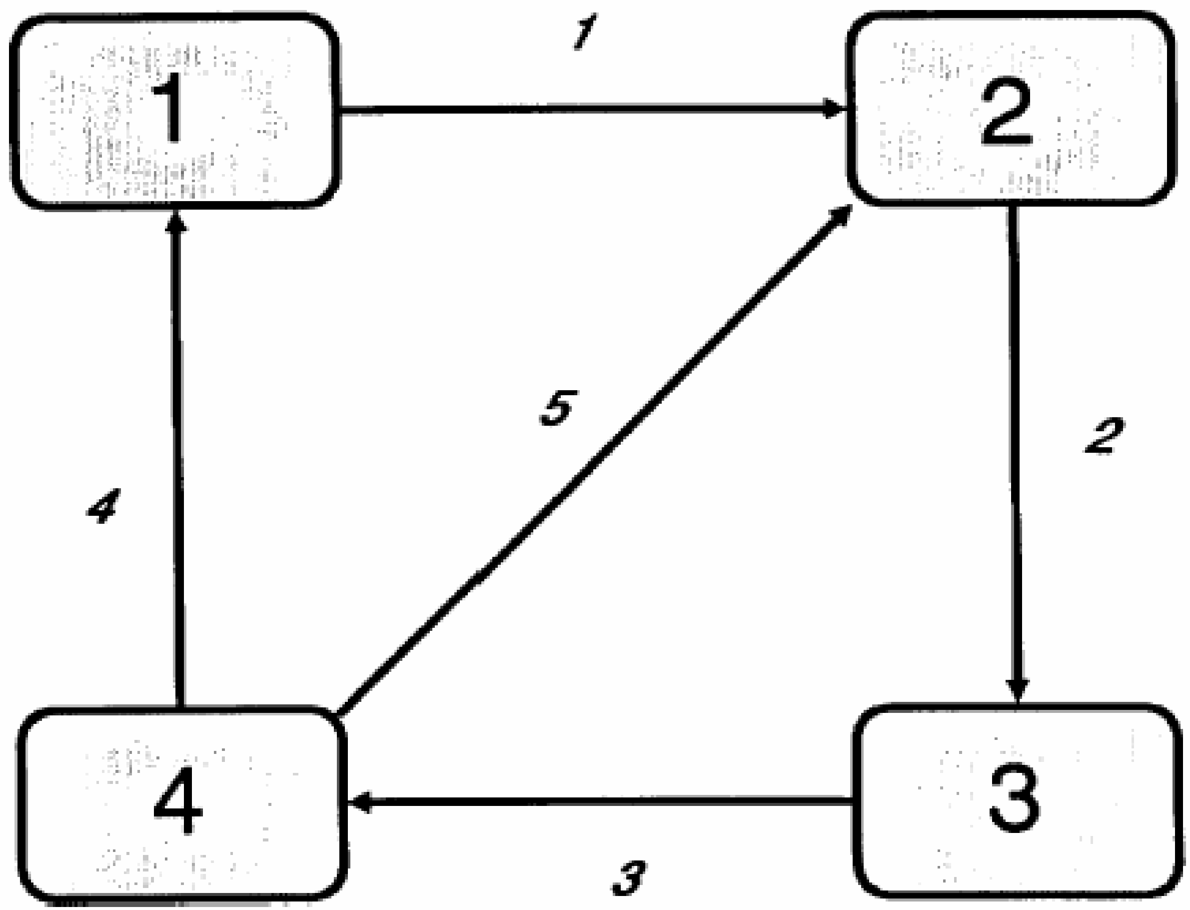
Porsching method

- This algorithm, involving the Jacobian (derivative of the system state matrix), is used originally in the computer code FLASH-4 and subsequently in the OPG code SOPHT, and evolved into forms used in RETRAN
- The strength of Porsching's approach lies in its recognition of flow as the most important dependent parameter and, hence, its fully implicit treatment of flow
- Based on system state matrix which contains all the system dynamics in terms of the dependent parameters of mass, energy and flow. Back substitution finally gives a matrix rate equation in terms of the system flow (the unknown) and the system derivatives.
- Porsching form is identical to the “Rate” form and is a subset of the fully implicit back-substituted form and is easily derived from it
- Some codes, but not all use this method

Thermal-hydraulic System Simulation Equations



Sample Thermal-hydraulic Network



Fully-implicit back-substituted form (FIBS)

$$\dot{\mathbf{u}} = \mathrm{f}(\mathrm{t}, \mathbf{u})$$

$u = u(M_i, H_i, W_j)$

$$\dot{\mathbf{u}} = \mathbf{f}^{t} + \Delta t \ \mathbf{J} \ \dot{\mathbf{u}}$$

J is the Jacobian of the system of equations

$$\Delta \mathbf{u} = \Delta t \ \mathbf{f}^{t} + \Delta t \ \mathbf{J} \ \Delta \mathbf{u}$$

$$[\mathbf{I} - \Delta t \ \mathbf{J}]\Delta \mathbf{u} = \Delta t \ \mathbf{f}^{t}$$

FIBS (contd.)

$$\frac{dW_j}{dt} = \frac{A_j}{L_j}\left(P_u + S_{WP}\Delta P_u - P_d - S_{WP}\Delta P_d\right) + k_j\left(W_j + S_{WW}\Delta W_j\right)^2 + b_{wj}$$

$$= \frac{\Delta W_j}{\Delta t}$$

$$b_{wj} = (A_j/L_j)\,(h_j\rho_j g + \Delta P_{pump})$$

FIBS (contd.)

$$\frac{dM_i}{dt} = \sum_{j \forall d} (W_j + S_{MW}\,\Delta W_j) - \sum_{j \forall u} (W_j + S_{MW}\,\Delta W_j) \approx \frac{\Delta M_i}{\Delta t}$$

$$\begin{aligned}
\frac{dH_i}{dt} &= \sum_{j \forall d} (W_j + S_{HW}\,\Delta W_j)\frac{(H_j + S_{HH}\,\Delta H_j)}{(M_j + S_{HM}\,\Delta M_j)} - \sum_{j \forall u} (W_j + S_{HW}\,\Delta W_j)\frac{(H_j + S_{HH}\,\Delta H_j)}{(M_j + S_{HM}\,\Delta M_j)} + Q_i \\
&= \sum_{j \forall d} \left(\frac{W_j H_j}{M_j} + \frac{S_{HW} H_j}{M_j}\Delta W_j + \frac{S_{HH} W_j}{M_j}\Delta H_j - \frac{S_{HM}\, W_j\, H_j}{M_j^2}\Delta M_j \right) \\
&\quad - \sum_{j \forall u} \left(\frac{W_j H_j}{M_j} + \frac{S_{HW} H_j}{M_j}\Delta W_j + \frac{S_{HH} W_j}{M_j}\Delta H_j - \frac{S_{HM}\, W_j\, H_j}{M_j^2}\Delta M_j \right) + Q_i \\
&\approx \frac{\Delta H_i}{\Delta t}
\end{aligned}$$

$$\Delta P_i = \frac{\partial P_i}{\partial M_i}\Delta M_i + \frac{\partial P_i}{\partial H_i}\Delta H_i + \frac{\partial P_i}{\partial V_i}\Delta V_i$$

$$\frac{\Delta P_i}{\Delta t} = C_{1i}\frac{\Delta M_i}{\Delta t} + C_{2i}\frac{\Delta H_i}{\Delta t}$$ For constant volume

FIBS (contd.)

- The system unknowns to be solved for are ΔW, ΔM, ΔH and ΔP
- The mass equation is simple and is used to eliminate ΔM in terms of ΔW. Flow is chosen as the prime variable since it is the main actor in thermal-hydraulic systems.
- The enthalpy equation poses a problem as it is too complex to permit a simple substitution; Porsching surmounts this by setting $S_{HH} = S_{HM} = 0$, ie making the solution explicit in specific enthalpy.

$$\Delta \mathbf{M} = \Delta t \ \mathbf{A}^{MW}[\mathbf{W}^t + S_{MW} \ \Delta \mathbf{W}]$$

$$\mathbf{A}^{MW} = \begin{array}{c} \text{links} \rightarrow \\ \begin{pmatrix} -1 & 0 & 0 & 1 & 0 \\ 1 & -1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & -1 \end{pmatrix} \end{array} \begin{array}{c} \text{nodes} \\ \Downarrow \end{array}$$

FIBS (contd.)

$$\Delta \mathbf{W} = \Delta t\left\{\mathbf{A}^{WP}\left[\mathbf{P}^{t} + S_{WP}\Delta\mathbf{P}\right] + \mathbf{A}^{WW}\left[\mathbf{W}^{t} + 2S_{WW}\Delta\mathbf{W}\right] + \mathbf{B}^{W}\right\}$$

$$\mathbf{A}^{WW} = \begin{pmatrix} -k_1|W_1| & & 0 \\ & -k|W_2| & \\ 0 & & -k_5|W_5| \end{pmatrix} \qquad \mathbf{B}^{W} = \begin{pmatrix} A_1/L_1(h_1\rho_1 g + \Delta P_{pump1}) \\ A_2/L_2(h_2\rho_1 g + \Delta P_{pump2}) \\ \cdot \\ \cdot \end{pmatrix}$$

$$\mathbf{A}^{WP} = \begin{pmatrix} A_1/L_1 & -A_1/L_1 & 0 & 0 \\ 0 & A_2/L_2 & -A_2/L_2 & 0 \\ 0 & 0 & A_3/L_3 & -A_3/L_3 \\ -A_4/L_4 & 0 & 0 & A_4/L_4 \\ 0 & -A_5/L_5 & 0 & A_5/L_5 \end{pmatrix}$$

FIBS (contd.)

$$\mathbf{\Delta H} = \Delta t\left(\mathbf{A}^{HW}\left[\mathbf{W}^{t} + S_{HW}\mathbf{\Delta W}\right] + S_{HH}\mathbf{A}^{HH^*}\mathbf{\Delta H}^* - S_{HM}\mathbf{A}^{HM^*}\mathbf{\Delta M}^* + \mathbf{B}^{H}\right)$$

$$\mathbf{\Delta H}^* = \begin{pmatrix} \Delta H_1 \\ \Delta H_2 \\ \Delta H_3 \\ \Delta H_4 \\ \Delta H_4 \end{pmatrix} \quad , \quad \mathbf{\Delta M}^* = \begin{pmatrix} \Delta M_1 \\ \Delta M_2 \\ \Delta M_3 \\ \Delta M_4 \\ \Delta M_4 \end{pmatrix}$$

$$\mathbf{A}^{HW} = \begin{pmatrix} -H_1/M_1 & 0 & 0 & +H_4/M_4 & 0 \\ H_1/M_1 & -H_2/M_2 & 0 & 0 & H_4/M_4 \\ 0 & H_2/M_2 & -H_3/M_3 & 0 & 0 \\ 0 & 0 & H_3/M_3 & -H_4/M_4 & -H_4/M_4 \end{pmatrix}$$

FIBS (contd.)

$$\mathbf{A}^{HH*} = \begin{pmatrix} -W_1/M_1 & 0 & 0 & +W_4/M_4 & 0 \\ W_1/M_1 & -W_2/M_2 & 0 & & +W_5/M_4 \\ 0 & W_2/M_2 & -W_3/M_3 & 0 & 0 \\ 0 & 0 & W_3/M_3 & -W_4/M_4 & -W_5/M_4 \end{pmatrix}$$

$$\mathbf{A}^{HM} = \begin{pmatrix} -W_1H_1/M_1^2 & 0 & 0 & W_4H_4/M_4^2 & 0 \\ W_1H_1/M_1^2 & -W_2H_2/M_2^2 & 0 & 0 & W_5H_4/M_4^2 \\ 0 & W_2H_2/M_2 & -W_3H_3/M_3^2 & 0 & 0 \\ 0 & 0 & W_3H_3/M_3^2 & -W_4H_4/M_4^2 & -W_5H_4/M_4^2 \end{pmatrix}$$

FIBS (contd.)

$$\Delta \mathbf{H}^* = \mathbf{I}^{LN} \Delta \mathbf{H}$$

$$\mathrm{I}^{LN} = \begin{array}{c} \text{nodes} \rightarrow \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{array} \quad \begin{array}{c} \text{links} \\ \downarrow \end{array}$$

$$\mathbf{A}^{HH*} \Delta \mathbf{H}^* = \mathbf{A}^{HH*} \mathbf{I}^{LN} \Delta \mathbf{H}$$

$$\equiv \mathbf{A}^{HH} \Delta \mathbf{H}$$

$$\mathbf{A}^{HM*} \Delta \mathbf{M}^* = \mathbf{A}^{HM*} \mathbf{I}^{LN} \Delta \mathbf{M}$$

$$\equiv \mathbf{A}^{HM} \Delta \mathbf{M}.$$

FIBS (contd.)

$$\Delta \mathbf{H} = \Delta t \ \{\mathbf{A}^{HW} (\mathbf{W}^t + S_{HW}\, \Delta \mathbf{W}) + S_{HH}\, \mathbf{A}^{HH}\, \Delta \mathbf{H} - S_{HM}\, \mathbf{A}^{HM}\, \Delta \mathbf{M} + \mathbf{B}^H\}$$

$$\Delta \mathbf{H} = \Delta t \ \{\ \mathbf{A}^{HW} (\mathbf{W} + S_{HW}\, \Delta \mathbf{W}) + S_{HH}\, \mathbf{A}^{HH}\, \Delta \mathbf{H} - \Delta t\, S_{HM}\, \mathbf{A}^{HM}\, \mathbf{A}^{MW} (\mathbf{W}^t + \mathbf{W}^{MW}\, \Delta \mathbf{W}) + \mathbf{B}^H\ \}$$

$$\Delta \mathbf{H} = \Delta t[\mathbf{I} - \Delta t\, S_{HH}\, \mathbf{A}^{HH}]^{-1}\ \{\mathbf{A}^{HW} (\mathbf{W}^t + S_{HW}\, \Delta \mathbf{W}) - \Delta t\, S_{HM}\, \mathbf{A}^{HM}\, \mathbf{A}^{MW}(\mathbf{W}^t + S_{MW}\, \Delta \mathbf{W}) + \mathbf{B}^H\}$$

$$\Delta \mathbf{P} = \mathbf{C}_1\, \Delta \mathbf{M} + \mathbf{C}_2\, \Delta \mathbf{H},$$

$$\mathbf{C}_1 = \begin{pmatrix} C_{11} & & & \\ & C_{12} & 0 & \\ & & C_{13} & \\ 0 & & & C_{14} \end{pmatrix}$$

FIBS (contd.)

$$\Delta \mathbf{P} = \Delta t\, \mathbf{C}_1\, \mathbf{A}^{MW} (\mathbf{W}^t + S_{MW}\, \Delta\mathbf{W}) + \Delta t\, \mathbf{C}_2\, [\mathbf{I} - \Delta t\, S_{HH}\, \mathbf{A}^{HH}]^{-1} [\mathbf{A}^{HW} (\mathbf{W}^t + S_{HW}\, \Delta\mathbf{W})$$

$$- \Delta t\, S_{HM}\, \mathbf{A}^{HM}\, \mathbf{A}^{MW} (\mathbf{W}^t + S_{MW}\, \Delta\mathbf{W}) + \mathbf{B}^H]$$

$$\equiv \Delta t\, \mathbf{A}^{PW1}\, \mathbf{W}^t + \Delta t\, \mathbf{A}^{PW2}\, \Delta\mathbf{W} + \Delta t\, \mathbf{B}^P$$

$$\mathbf{A}^{PW1} = \mathbf{C}_1\, \mathbf{A}^{MW} + \mathbf{C}_2\, [\mathbf{I} - \Delta t\, S_{HH}\, \mathbf{A}^{HH}]^{-1} [\mathbf{A}^{HW} - \Delta t\, S_{HM}\, \mathbf{A}^{HM}\, \mathbf{A}^{MW}]$$

$$\mathbf{A}^{PW2} = S_{MW}\, \mathbf{C}_1\, \mathbf{A}^{MW} + \mathbf{C}_2\, [\mathbf{I} - \Delta t\, S_{HH}\, \mathbf{A}^{HH}]^{-1} [S_{HW}\, \mathbf{A}^{HW} - \Delta t\, S_{HM}\, S_{MW}\, \mathbf{A}^{HM}\, \mathbf{A}^{MW}]$$

$$\mathbf{B}^P = \mathbf{C}_2\, [\mathbf{I} - \Delta t\, S_{HH}\, \mathbf{A}^{HH}]^{-1}\, \mathbf{B}^H$$

$$\Delta\mathbf{W} = \Delta t\, \{\mathbf{A}^{WP}\, [\mathbf{P}^t + \Delta t\, S_{WP}\, (\mathbf{A}^{PW1}\, \mathbf{W}^t + \mathbf{A}^{PW2}\, \Delta\mathbf{W} + \mathbf{B}^P)] + \mathbf{A}^{WW}\, [W^t + 2S_{WW}\, \mathbf{A}^{WW}\, \Delta\mathbf{W}] + \mathbf{B}^W\, \}$$

$$[\mathbf{I} - \Delta t(2\, S_{WW}\, \mathbf{A}^{WW} + \Delta t\, S_{WP}\, \mathbf{A}^{WP}\, \mathbf{A}^{PW2})]\, \Delta\mathbf{W}$$

$$= \Delta t\, \{[\mathbf{A}^{WW} + \Delta t\, S_{WP}\, \mathbf{A}^{WP}\, \mathbf{A}^{PW1}]\, \mathbf{W}^t + \mathbf{B}^W + \mathbf{A}^{WP}\, [\mathbf{P}^t + \Delta t\, S_{WP}\, \mathbf{B}^P]\}$$

FIBS – Final Set of Equations

$$\mathbf{A}\,\Delta\mathbf{W} = \mathbf{B}$$

$$\mathbf{A}^{PW1} = \mathbf{C}_1\,\mathbf{A}^{MW} + \mathbf{C}_2\,[\mathbf{I} - \Delta t\, S_{HH}\,\mathbf{A}^{HH}]^{-1}\,[\mathbf{A}^{HW} - \Delta t\, S_{HM}\,\mathbf{A}^{HM}\,\mathbf{A}^{MW}]$$

$$\mathbf{A}^{PW2} = S_{MW}\,\mathbf{C}_1\,\mathbf{A}^{MW} + \mathbf{C}_2\,[\mathbf{I} - \Delta t\, S_{HH}\,\mathbf{A}^{HH}]^{-1}\,[S_{HW}\,\mathbf{A}^{HW} - \Delta t\, S_{HM}\,S_{MW}\,\mathbf{A}^{HM}\,\mathbf{A}^{MW}]$$

$$\mathbf{B}^{P} = \mathbf{C}_2\,[\mathbf{I} - \Delta t\, S_{HH}\,\mathbf{A}^{HH}]^{-1}\,\mathbf{B}^{H}$$

$$[\mathbf{I} - \Delta t(2\,S_{WW}\,\mathbf{A}^{WW} + \Delta t\,S_{WP}\,\mathbf{A}^{WP}\,\mathbf{A}^{PW2})]\,\Delta\mathbf{W}$$

$$= \Delta t\,\{\,[\mathbf{A}^{WW} + \Delta t\,S_{WP}\,\mathbf{A}^{WP}\,\mathbf{A}^{PW1}]\,\mathbf{W}^{t} + \mathbf{B}^{W} + \mathbf{A}^{WP}\,[\mathbf{P}^{t} + \Delta t\,S_{WP}\,\mathbf{B}^{P}]\,\}$$

$$\Delta\mathbf{M} = \Delta t\,\mathbf{A}^{MW}\,[\mathbf{W}^{t} + S_{MW}\,\Delta\mathbf{W}]$$

$$\Delta\mathbf{H} = \Delta t\,\{\,\mathbf{A}^{HW}\,(\mathbf{W}^{t} + S_{HW}\,\Delta\mathbf{W}) + S_{HH}\,\mathbf{A}^{HH}\,\Delta\mathbf{H} - S_{HM}\,\mathbf{A}^{HM}\,\Delta\mathbf{M} + \mathbf{B}^{H}\,\}$$

$$\Delta\mathbf{P} = \mathbf{C}_1\,\Delta\mathbf{M} + \mathbf{C}_2\,\Delta\mathbf{H}$$

Fully Explicit Scheme (S=0)

$$\mathbf{A}^{PW1} = \mathbf{C}_1\ \mathbf{A}^{MW} + \mathbf{C}_2\ \mathbf{A}^{HW}$$

$$\mathbf{A}^{PW2} = 0$$

$$\mathbf{B}^{P} = \mathbf{C}_2\ \mathbf{B}^{H}$$

$$\therefore\ \Delta\mathbf{W} = \Delta t\ \{\ \mathbf{A}^{WW}\ \mathbf{W}^{t} + \mathbf{B}^{W} + \mathbf{A}^{WP}\ \mathbf{P}^{t}\ \}$$

$$\Delta\mathbf{M} = \Delta t\ \mathbf{A}^{MW}\ \mathbf{W}^{t}$$

$$\Delta\mathbf{H} = \Delta t\ \{\ \mathbf{A}^{HW}\ \mathbf{W}^{t} + \mathbf{B}^{H}\ \}$$

$$\Delta\mathbf{P} = \mathbf{C}_1\ \Delta\mathbf{M} + \mathbf{C}_2\ \Delta\mathbf{H},$$

Semi Implicit Scheme (S_{HH}, S_{HM} = 0)

$$\mathbf{A}^{PW1} = \mathbf{C}_1\ \mathbf{A}^{MW} + \mathbf{C}_2\ \mathbf{A}^{HW}$$

$$\mathbf{A}^{PW2} = \mathbf{C}_1\ \mathbf{A}^{MW} + \mathbf{C}_2\ \mathbf{A}^{HW}$$

$$\mathbf{B}^{P} = \mathbf{C}_2\ \mathbf{B}^{H}$$

$$[\mathbf{I} - \Delta t(2\ \mathbf{A}^{WW} + \Delta t\ \mathbf{A}^{WP}\ \mathbf{A}^{PW2})]\ \Delta\mathbf{W}$$

$$= \Delta t\ \{\ [\mathbf{A}^{WW} + \Delta t\ \mathbf{A}^{WP}\ \mathbf{A}^{PW1}]\ \mathbf{W}^{t} + \mathbf{B}^{W} + \mathbf{A}^{WP}\ [\mathbf{P}^{t} + \Delta t\ \mathbf{B}^{P}]\ \}$$

$$\Delta\mathbf{M} = \Delta t\ \mathbf{A}^{MW}\ [\mathbf{W}^{t} + \Delta\mathbf{W}]$$

$$\Delta\mathbf{H} = \Delta t\ \{\ \mathbf{A}^{HW}\ (\mathbf{W}^{t} + \Delta\mathbf{W}) + \mathbf{B}^{H}\ \}$$

$$\Delta\mathbf{P} = \mathbf{C}_1\ \Delta\mathbf{M} + \mathbf{C}_2\ \Delta\mathbf{H}$$

Fully Implicit Scheme

$$\mathbf{A}^{PW1} = \mathbf{C}_1\ \mathbf{A}^{MW} + \mathbf{C}_2\ [\mathbf{I} - \Delta t\ \mathbf{A}^{HH}]^{-1}\ [\mathbf{A}^{HW} - \Delta t\ \mathbf{A}^{HM}\ \mathbf{A}^{MW}]$$

$$\mathbf{A}^{PW2} = \mathbf{C}_1\ \mathbf{A}^{MW} + \mathbf{C}_2\ [\mathbf{I} - \Delta t\ \mathbf{A}^{HH}]^{-1}\ [\mathbf{A}^{HW} - \Delta t\ \mathbf{A}^{HM}\ \mathbf{A}^{MW}]$$

$$\mathbf{B}^{P} = \mathbf{C}_2\ [\mathbf{I} - \Delta t\ \mathbf{A}^{HH}]^{-1}\ \mathbf{B}^{H}$$

$$[\mathbf{I} - \Delta t(2\ \mathbf{A}^{WW} + \Delta t\ \mathbf{A}^{WP}\ \mathbf{A}^{PW2})]\ \Delta\mathbf{W}$$

$$= \Delta t\ \{\ [\mathbf{A}^{WW} + \Delta t\ \mathbf{A}^{WP}\ \mathbf{A}^{PW1}]\ \mathbf{W}^{t} + \mathbf{B}^{W} + \mathbf{A}^{WP}\ [\mathbf{P}^{t} + \Delta t\ \mathbf{B}^{P}]\ \}$$

$$\Delta\mathbf{M} = \Delta t\ \mathbf{A}^{MW}\ [\mathbf{W}^{t} + \Delta\mathbf{W}]$$

$$\Delta\mathbf{H} = \Delta t\ \{\ \mathbf{A}^{HW}\ (\mathbf{W}^{t} + \Delta\mathbf{W}) + \mathbf{A}^{HH}\ \Delta\mathbf{H} - \mathbf{A}^{HM}\Delta\mathbf{M} + \mathbf{B}^{H}\ \}$$

$$\Delta\mathbf{P} = \mathbf{C}_1\ \Delta\mathbf{M} + \mathbf{C}_2\ \Delta\mathbf{H}$$

Programming Notes

- System geometry is contained in $\mathbf{A}^{MW}$
  - All other matrices are derived from this matrix and node/link properties
- The fully-implicit method is more complicated than the semi-implicit method
  - it requires the addition and multiplication of more matrices as well as a matrix inversion, especially when a large number of nodes is required
  - In one case study, for 9 nodes and links, the cost is a 50% increase in iteration time. But this becomes a 250% increase as one approaches the 36 node/link case.

Programming Notes

- Usually the matrices contain mostly zeros and, in the case of a circular loop, may be diagonally dominant in nature (i.e. non-zero elements occupy one, two or three stripes through the matrix).
- If the multiplication of two large matrices is desired, say NxN in dimension, the time to carry out the operation (N^3 multiplications and N^3 additions) can be very significant. However, it is possible to reduce the number of individual operations without losing the generality of the method.
- Suffice it to say that, in general, the semi-implicit method has a Courant limit on the maximum time step that can be taken in order to ensure stability. The fully-implicit method does not have this limitation.
- As the Courant time step limit is determined by the nodal residence time, the time step limit is dependant on the node sizes and the flows through the nodes.

Programming Notes

- Usually the matrices contain mostly zeros and, in the case of a circular loop, may be diagonally dominant in nature (i.e. non-zero elements occupy one, two or three stripes through the matrix).
- For example, for a 9 node case, the semi-implicit method required 0.10 seconds per iteration and required 2 iterations to meet the report time of 1.0 seconds. The fully-implicit method meet the report time in one iteration which took 0.14 seconds. At 36 nodes however, the semi-implicit method took 2 x 0.71 seconds while the fully-implicit method took 2.12 seconds.
- Clearly, one method is not superior to the other in all cases.
- Pressure determination involves the use of property derivatives. To avoid the numerical problems associated with discontinuities, smooth functions for properties, and other thermal-hydraulic correlations must be used