

TECHNICAL REPORT:
THERMOFLOW - System level Thermal-Hydraulics in *ChiTech*

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Contents

	Page
1 Conservation equations	2
1.1 Conservation of Mass	3
1.2 Conservation of Momentum	3
1.3 Conservation of Energy	5
1.4 Equation of state	6
2 Numerical solution	7
2.1 Conservation of Mass - finite difference formulation	7
2.2 Conservation of Momentum - finite difference formulation	7
2.3 Conservation of Energy - finite difference formulation	8
2.4 Equation of state numerical implementation	8
2.5 Unknowns in the available equations	9
2.6 Semi-implicit approach	10
2.7 Solution algorithm	11

List of Figures

Figure 1 Simple layout of control volumes.	2
Figure 2 Simple layout of multiple control volumes.	10

List of Tables

1 Conservation equations

The overall objective is that we want to solve the following four field variables:

- Pressure, P
- Internal energy, u
- Velocity, v
- Density, ρ

In order to do this we apply the conservation equations to the volume shown in Figure 1 below:

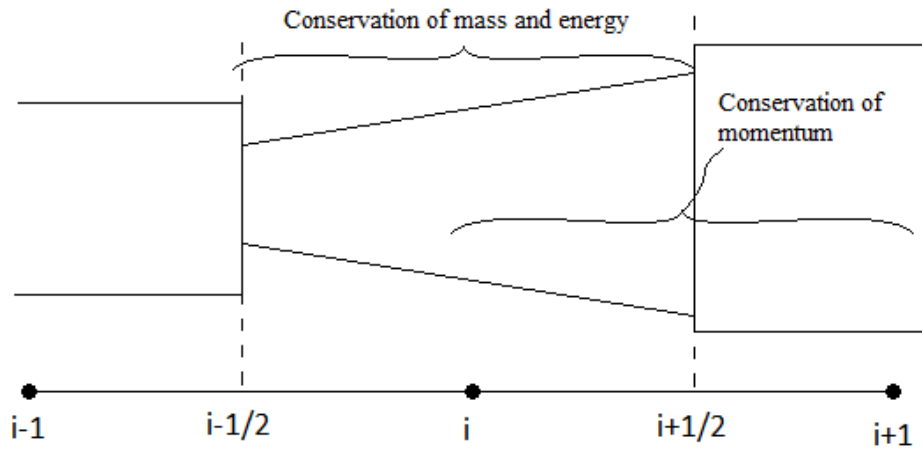


Figure 1: Simple layout of control volumes.

1.1 Conservation of Mass

Even though we will be dealing with incompressible liquids, the liquids can exist at different temperatures and therefore different densities, ρ . The conservation of mass requires as a function of time, t :

$$\frac{d\rho}{dt} = \frac{1}{V} \int_S \rho.(\vec{v} \cdot \hat{n}).dA$$

And by applying it to the control volume:

$$\frac{d\rho_i}{dt} = \frac{1}{V_i} \left[(\rho.A.v)_{i-\frac{1}{2}} - (\rho.A.v)_{i+\frac{1}{2}} \right] \quad (1)$$

Where:

v = velocity.

V = Volume.

A = Area.

\hat{n} = Surface normal.

1.2 Conservation of Momentum

The change in momentum, $m_i.v_i$, in a control volume must balance the momentum of all the in and out flows as well as any forces applied:

$$\frac{d(mv)_i}{dt} = \int_S \rho.|v|.((\vec{v}) \cdot \hat{n}).dA + \int_S P.\hat{n}.dA + mg - F_{friction}$$

For a control volume as shown in Figure 1 we have:

$$\begin{aligned} \frac{d(\rho v)_i}{dt} &= \frac{1}{V_i} \left[(\rho A v^2 d)_{i-\frac{1}{2}} + (\rho A v^2 d)_{i+\frac{1}{2}} \right] \\ &+ \frac{1}{V_i} \left[(PA)_{i-\frac{1}{2}} - (PA)_{i+\frac{1}{2}} \right] + \rho_i g_i - \frac{1}{V_i} F_\tau \end{aligned}$$

Where d is the direction value (either +1 or -1), F_τ is the wall friction force and g_i is the gravitational component (i.e. $g_i = g.\sin\theta_i$, $g = -9.81m.s^{-2}$). In later derivations of the numerical representation it is more convenient to define the conservation of momentum equation about a boundary by:

$$\frac{d(\rho v)}{dt} = -\rho \frac{d(v^2)}{dx} - \frac{dP}{dx} + \rho g - \frac{\tau}{L}$$

Applied to the boundary junction, $i + \frac{1}{2}$, we can write:

$$\begin{aligned} \frac{d(\rho v)_{i+\frac{1}{2}}}{dt} = & -\rho_{i+\frac{1}{2}} \cdot \frac{d_i \cdot (v_i^n)^2 + d_{i+1} \cdot (v_{i+1}^n)^2}{\Delta x_{i+\frac{1}{2}}} \\ & - \frac{P_{i+1} - P_i}{\Delta x_{i+\frac{1}{2}}} + \rho_{i+\frac{1}{2}} \cdot g_{i+\frac{1}{2}} - \frac{F_{\tau,i}}{2V_i} - \frac{F_{\tau,i+1}}{2V_{i+1}} \end{aligned} \quad (2)$$

Where $\Delta x_{i+\frac{1}{2}}$ is the distance between control volumes i and $i+1$, $g_{i+\frac{1}{2}}$ is the gravitational force component (function of inclination angle between control volume centroids). The wall friction force can be calculated from the Darcy Friction Factor, f :

$$F_{\tau} = \frac{1}{2} f \rho \frac{L}{D_H} A v^2$$

Therefore:

$$\begin{aligned} F_{\tau,i} &= \frac{1}{4} f_i \rho_i \frac{L_i}{D_{H,i}} A_i v_i^2 \\ F_{\tau,i+1} &= \frac{1}{4} f_{i+1} \rho_{i+1} \frac{L_{i+1}}{D_{H,i+1}} A_{i+1} v_{i+1}^2 \end{aligned}$$

In these equations L_i and $D_{H,i}$ are the length and hydraulic diameter of the i -th control volume

1.3 Conservation of Energy

The total energy of the system, E , must balance that of the in and out flow including the work performed and the heat transfer into the system:

$$\frac{dE}{dt} = \int_S \rho \cdot (\vec{v} \cdot \hat{n}) \cdot e \cdot dA + Q - W - E_{loss}$$

Where:

e = Specific energy of the system.

Q = Heat transfer into the system.

W = Work leaving the system.

E_{loss} = Dissipative energy losses.

The components of energy are internal energy, U , kinetic energy, $\frac{1}{2}mv^2$, and potential energy, mgz :

$$E = m \cdot e = m \cdot (u + \frac{1}{2}v^2 + gz)$$

For most control volume fluid flows where the control volume flow rate is small compared to its area it is often acceptable to neglect the kinetic energy term. Also, since it undergoes no change in elevation we can neglect the elevation change (but only for the control volume, not the junctions).

The heat transfer into the system is normally associated with some heat flux, \dot{q} , and the total heat transfer surface, A_s , therefore:

$$Q_i = \dot{q}_i \cdot A_{s,i}$$

The components of work include shaft work, W_{shaft} , and pressure work, $W_{pressure}$. For this case we will consider only pressure work:

$$W_{pressure} = (P \cdot A \cdot v)_{i-\frac{1}{2}} - (P \cdot A \cdot v)_{i+\frac{1}{2}}$$

From here the energy conservation equation becomes:

$$\begin{aligned} \frac{d}{dt} \left(m \cdot u \right) &= (\rho A v)_{i-\frac{1}{2}} \cdot (u + gz)_{i-\frac{1}{2}} - (\rho A v)_{i+\frac{1}{2}} \cdot (u + gz)_{i+\frac{1}{2}} \\ &+ \dot{q}_i \cdot A_{s,i} - \left[(P \cdot A \cdot v)_{i-\frac{1}{2}} - (P \cdot A \cdot v)_{i+\frac{1}{2}} \right] - E_{loss} \end{aligned}$$

Dividing by the volume we get:

$$\begin{aligned} \frac{d(\rho.u)_i}{dt} = & \frac{1}{V_i} \left[(\rho A v)_{i-\frac{1}{2}} \cdot (u + gz)_{i-\frac{1}{2}} - (\rho A v)_{i+\frac{1}{2}} \cdot (u + gz)_{i+\frac{1}{2}} \right] \\ & + \frac{A_{s,i}}{V_i} \dot{q}_i - \frac{1}{V_i} \left[(P.A.v)_{i-\frac{1}{2}} - (P.A.v)_{i+\frac{1}{2}} \right] - \frac{1}{V_i} \left[E_{loss,i-\frac{1}{2}} + E_{loss,i+\frac{1}{2}} \right] \end{aligned} \quad (3)$$

The energy loss term includes both dynamic losses at the junctions and those within the control volume, however, for simplicity we will only consider the loss associated with junction losses for which the pressure loss is given by:

$$\Delta P = \frac{1}{2} K \rho v^2$$

Where K is a dimensionless parameter dependent on the geometry. The energy loss associated with this factor is:

$$E_{loss,i-\frac{1}{2}} = \begin{cases} (\Delta P.A.v)_{i-\frac{1}{2}} = \frac{1}{2} K_{i-\frac{1}{2}} (\rho A v^3)_{i-\frac{1}{2}} & , v_{i-\frac{1}{2}} > 0 \\ 0 & , v_{i-\frac{1}{2}} < 0 \end{cases}$$

Similarly:

$$E_{loss,i+\frac{1}{2}} = \begin{cases} (\Delta P.A.v)_{i+\frac{1}{2}} = \frac{1}{2} K_{i+\frac{1}{2}} (\rho A v^3)_{i+\frac{1}{2}} & , v_{i+\frac{1}{2}} < 0 \\ 0 & , v_{i+\frac{1}{2}} > 0 \end{cases}$$

1.4 Equation of state

In addition to the conservation equations, there is the equation of state. For the incompressible liquids of this simulation we can approximate the equation of state as:

$$\begin{aligned} u &= -0.002053148 \rho^3 + 5.927524805 \rho^2 - 5710.176493 \rho + 1835863.516 \\ \rho &= 7.88656E-06 T^3 - 0.004477273 T^2 - 0.059652292 T + 1001.25303 \\ \mu &= 1.66762E-08 \rho^3 - 4.83243E-05 \rho^2 + 0.046680223 \rho - 15.03102921 \end{aligned} \quad (4)$$

2 Numerical solution

The conservation of momentum equations conveniently couples the pressure field and velocities and therefore is used implicitly to determine the pressures at time $n + 1$.

2.1 Conservation of Mass - finite difference formulation

The finite difference formulation is as follows:

$$\frac{\rho_i^{n+1} - \rho_i^n}{\Delta t} = \frac{1}{V_i} \left[(\rho.A)_{i-\frac{1}{2}}^n v_{i-\frac{1}{2}}^{n+1} - (\rho.A)_{i+\frac{1}{2}}^n v_{i+\frac{1}{2}}^{n+1} \right] \quad (5)$$

2.2 Conservation of Momentum - finite difference formulation

Because no other future time equation has pressure as a variable we opt to include pressure at time $n + 1$ as an implicit variable. We manipulate the original conservation of mass equation for junction $i + \frac{1}{2}$:

$$\begin{aligned} \frac{d(\rho v)_{i+\frac{1}{2}}}{dt} &= -\rho_{i+\frac{1}{2}} \cdot \frac{d_i \cdot (v_i)^2 + d_{i+1} \cdot (v_{i+1})^2}{\Delta x_{i+\frac{1}{2}}} \\ &\quad - \frac{P_{i+1} - P_i}{\Delta x_{i+\frac{1}{2}}} + \rho_{i+\frac{1}{2}} \cdot g_{i+\frac{1}{2}} - \frac{F_{\tau,i}}{2V_i} - \frac{F_{\tau,i+1}}{2V_{i+1}} \end{aligned}$$

We use the following time notation:

$$\begin{aligned} \frac{\rho_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} - \rho_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^n}{\Delta t} &= -\rho_{i+\frac{1}{2}}^n \cdot \frac{d_i \cdot (v_i^n)^2 + d_{i+1} \cdot (v_{i+1}^n)^2}{\Delta x_{i+\frac{1}{2}}} \\ &\quad - \frac{P_{i+1}^{n+1} - P_i^{n+1}}{\Delta x_{i+\frac{1}{2}}} + \rho_{i+\frac{1}{2}}^n \cdot g_{i+\frac{1}{2}} \\ &\quad - \frac{1}{2V_i} F_{\tau,i}^n - \frac{1}{2V_{i+1}} F_{\tau,i+1}^n \end{aligned} \quad (6)$$

In the equations above we included implicit time instances to pressure in order to semi-implicitly couple the system.

We can find the same equation for junction $i - \frac{1}{2}$:

$$\begin{aligned} \frac{\rho_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - \rho_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^n}{\Delta t} &= -\rho_{i-\frac{1}{2}}^n \cdot \frac{d_{i-1} \cdot (v_{i-1}^n)^2 + d_i \cdot (v_i^n)^2}{\Delta x_{i-\frac{1}{2}}} \\ &\quad - \frac{P_i^{n+1} - P_{i-1}^{n+1}}{\Delta x_{i-\frac{1}{2}}} + \rho_{i-\frac{1}{2}}^n \cdot g_{i-\frac{1}{2}} \\ &\quad - \frac{1}{2V_{i-1}} F_{\tau,i-1}^n - \frac{1}{2V_i} F_{\tau,i}^n \end{aligned} \quad (7)$$

2.3 Conservation of Energy - finite difference formulation

We start with the original conservation of energy equation:

$$\begin{aligned} \frac{d(\rho \cdot u)_i}{dt} &= \frac{1}{V_i} \left[(\rho A v)_{i-\frac{1}{2}} \cdot (u + gz)_{i-\frac{1}{2}} - (\rho A v)_{i+\frac{1}{2}} \cdot (u + gz)_{i+\frac{1}{2}} \right] \\ &+ \frac{A_{s,i}}{V_i} \dot{q}_i - \frac{1}{V_i} \left[(P \cdot A \cdot v)_{i-\frac{1}{2}} - (P \cdot A \cdot v)_{i+\frac{1}{2}} \right] - \frac{1}{V_i} \left[E_{loss,i-\frac{1}{2}} + E_{loss,i+\frac{1}{2}} \right] \end{aligned}$$

We now discretize the left side and set the right side to correspond to time n .

$$\begin{aligned} \frac{(\rho_i^{n+1} \cdot u_i^{n+1} - \rho_i^n \cdot u_i^n)}{\Delta t} &= \frac{1}{V_i} \left[(\rho A u)_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - (\rho A u)_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} \right] \\ &+ \frac{1}{V_i} \left[(\rho A g z)_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - (\rho A g z)_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} \right] \\ &+ \frac{A_{s,i}}{V_i} \dot{q}_i^n - \frac{1}{V_i} \left[(P \cdot A)_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - (P \cdot A)_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} \right] \\ &- \frac{1}{V_i} E_{loss}^n \end{aligned} \tag{8}$$

2.4 Equation of state numerical implementation

In order to implement a linear approximation to the equation of state we linearize the Equation of State by determine the derivative at the old time values. Specifically this applies to the relation of internal energy, u , to the density, ρ :

$$\begin{aligned} \frac{d(u_i^{n+1})}{d\rho} &= \frac{d}{d\rho} \left[-0.002053148 \rho^3 + 5.927524805 \rho^2 - 5710.176493 \rho + 1835863.516 \right] \\ &= -0.006159444 (\rho_i^n)^2 + 11.85504961 (\rho_i^n) - 5710.176493 \end{aligned}$$

From this derivative we find the linearized equation of state:

$$u_i^{n+1} = \frac{d(u_i^{n+1})}{d\rho} \cdot \rho_i^{n+1} - \frac{d(u_i^{n+1})}{d\rho} \cdot \rho_i^n + u_i^n \tag{9}$$

2.5 Unknowns in the available equations

The "new" time values that require solving are found in the following terms:

$$\rho_i^{n+1}, v_{i+\frac{1}{2}}^{n+1}, v_{i-\frac{1}{2}}^{n+1}, \text{ from equation 5}$$

$$v_{i+\frac{1}{2}}^{n+1}, P_{i+1}^{n+1}, P_i^{n+1}, \text{ from equation 6}$$

$$v_{i-\frac{1}{2}}^{n+1}, P_{i-1}^{n+1}, P_i^{n+1}, \text{ from equation 7}$$

$$\rho_i^{n+1}, u_i^{n+1}, v_{i-\frac{1}{2}}^{n+1}, v_{i+\frac{1}{2}}^{n+1}, \text{ from equation 8}$$

$$\rho_i^{n+1}, u_i^{n+1}, \text{ from equation 9}$$

However, the some unknowns in the old time variables also exist. we change $\rho_{i+\frac{1}{2}}^n$ according to:

$$\rho_{i+\frac{1}{2}}^n = \begin{cases} \rho_i^n & , v_{i+\frac{1}{2}}^n \geq 0 \\ \rho_{i+1}^n & , v_{i+\frac{1}{2}}^n < 0 \end{cases}$$

We then compute v_i^n from the arithmetic average of the junction velocities according to:

$$v_i^n = v_{i-\frac{1}{2}}^n \frac{A_{i-\frac{1}{2}}}{2A_i} + v_{i+\frac{1}{2}}^n \frac{A_{i+\frac{1}{2}}}{2A_i}$$

With this velocity known we can calculate the dimensionless Reynold's number, Re :

$$Re_i = \frac{\rho_i^n v_i^n D_{H,i}}{\mu_i^n}$$

The Reynold's number features in the calculation of the Darcy friction factor, f , which is contained in a different formula depending on the flow regime, i.e. the laminar flow regime at $Re < 2300$ and the turbulent flow regime at $Re > 4000$. In the laminar regime the factor is calculated from:

$$f = \frac{64}{Re}$$

In the turbulent regime the factor can be calculated from the Colebrook-White equation:

$$\frac{1}{\sqrt{f}} = -2 \log \left(\frac{\epsilon}{3.7 D_H} + \frac{2.51}{Re \sqrt{f}} \right)$$

This equation is a transcendental equation (i.e. no analytical solution), however, lookup tables can be generated as a function of Re for a given roughness ϵ using a Newton-Raphson numerical scheme. This lookup table generator needs to accommodate the transition between the laminar flow regime at $Re < 2300$

and the turbulent flow regime at $Re > 4000$. One such method is to calculate a spline fit between the two regimes. An example of such a generator is shown below.

2.6 Semi-implicit approach

From equation 5 we can solve for ρ_i^{n+1} and from equation 4 we can solve for u_i^{n+1} . From equation 7 we can solve for $v_{i+\frac{1}{2}}^{n+1}$. Now the only variables left unsolved is the pressures P_{i+1}^{n+1} and P_i^{n+1} .

Hence we are left with the conservation of momentum equation with the unknowns P_i and P_{i+1} . Therefore, in a single time step where we have I amount of control volumes as shown in Figure 2 below, we will have I unknowns and I amount of momentum equations.

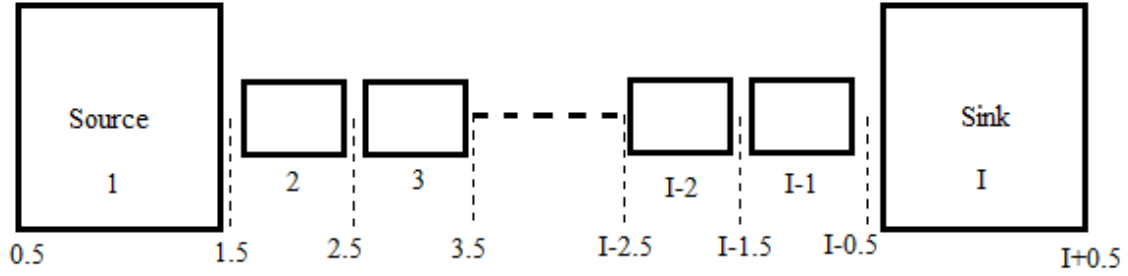


Figure 2: Simple layout of multiple control volumes.

2.7 Solution algorithm

Step 1

Load all control volumes. Input parameters:

- Area, A
- Length, L
- Pressure, P
- Temperature, T
- Elevation change, Δz
- Wall roughness, ϵ
- Hydraulic diameter, D_H
- Surface area, A_s

Step 2

Load all junctions. Input parameters:

- Junction velocity, v
- Area, A
- Loss factor, K

Step 3

Determine density, ρ_i , from:

$$\rho = 7.88656E - 06 T^3 - 0.004477273 T^2 - 0.059652292 T + 1001.25303$$

Internal energy, u_i , from:

$$u = -0.002053148 \rho^3 + 5.927524805 \rho^2 - 5710.176493 \rho + 1835863.516$$

Dynamic viscosity, μ_i , from:

$$\mu = 1.66762E - 08 \rho^3 - 4.83243E - 05 \rho^2 + 0.046680223 \rho - 15.03102921$$

Velocity, v_i , from:

$$v_i = v_{i-\frac{1}{2}} \frac{A_{i-\frac{1}{2}}}{2A_i} + v_{i+\frac{1}{2}} \frac{A_{i+\frac{1}{2}}}{2A_i}$$

Step 4

Determine all junction and control volume z values using control volume Δz values.

Step 5

Determine $\rho_{i-\frac{1}{2}}^n$ and $\rho_{i+\frac{1}{2}}^n$ as follows:

$$\rho_{i-\frac{1}{2}}^n = \begin{cases} \rho_{i-1}^n & , v_{i-\frac{1}{2}} \geq 0 \\ \rho_i^n & , v_{i-\frac{1}{2}} < 0 \end{cases}$$

$$\rho_{i+\frac{1}{2}}^n = \begin{cases} \rho_i^n & , v_{i+\frac{1}{2}} \geq 0 \\ \rho_{i+1}^n & , v_{i+\frac{1}{2}} < 0 \end{cases}$$

And similarly for $u_{i-\frac{1}{2}}^n$ and $u_{i+\frac{1}{2}}^n$ from:

$$u_{i-\frac{1}{2}}^n = \begin{cases} u_{i-1}^n & , v_{i-\frac{1}{2}} > 0 \\ u_i^n & , v_{i-\frac{1}{2}} < 0 \end{cases}$$

$$u_{i+\frac{1}{2}}^n = \begin{cases} u_i^n & , v_{i+\frac{1}{2}} > 0 \\ u_{i+1}^n & , v_{i+\frac{1}{2}} < 0 \end{cases}$$

Step 7

Determine the elements of equation 5:

$$\frac{\rho_i^{n+1} - \rho_i^n}{\Delta t} = \frac{1}{V_i} \left[(\rho.A)_{i-\frac{1}{2}}^n v_{i-\frac{1}{2}}^{n+1} - (\rho.A)_{i+\frac{1}{2}}^n v_{i+\frac{1}{2}}^{n+1} \right]$$

Where the elements are:

$$B_5 = \frac{\Delta t (\rho.A)_{i-\frac{1}{2}}^n}{V_i}$$

$$C_5 = \frac{\Delta t (\rho.A)_{i+\frac{1}{2}}^n}{V_i}$$

To get:

$$\rho_i^{n+1} = \rho_i^n + B_5 \cdot v_{i-\frac{1}{2}}^{n+1} - C_5 \cdot v_{i+\frac{1}{2}}^{n+1} \quad (10)$$

Step 8

Determine the elements of equation 6:

$$\begin{aligned} \frac{\rho_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} - \rho_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^n}{\Delta t} = & -\rho_{i+\frac{1}{2}}^n \cdot \frac{d_i \cdot (v_i^n)^2 + d_{i+1} \cdot (v_{i+1}^n)^2}{\Delta x_{i+\frac{1}{2}}} \\ & - \frac{P_{i+1}^{n+1} - P_i^{n+1}}{\Delta x_{i+\frac{1}{2}}} + \rho_{i+\frac{1}{2}}^n \cdot g_{i+\frac{1}{2}} \\ & - \frac{1}{2V_i} F_{\tau,i}^n - \frac{1}{2V_{i+1}} F_{\tau,i+1}^n \end{aligned}$$

Where the elements are:

$$\begin{aligned} B_6 &= \rho_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^n \\ C_6 &= \Delta t \rho_{i+\frac{1}{2}}^n \cdot \frac{d_i \cdot (v_i^n)^2 + d_{i+1} \cdot (v_{i+1}^n)^2}{\Delta x_{i+\frac{1}{2}}} \\ D_6 &= \frac{\Delta t}{\Delta x_{i+\frac{1}{2}}}, \quad E_6 = \Delta t \rho_{i+\frac{1}{2}}^n \cdot g_{i+\frac{1}{2}} \\ F_6 &= \frac{\Delta t}{2V_i} F_{\tau,i}^n, \quad G_6 = \frac{\Delta t}{2V_{i+1}} F_{\tau,i+1}^n \\ H_6 &= \frac{B_6 - C_6 + E_6 - F_6 - G_6}{\rho_{i+\frac{1}{2}}^n}, \quad I_6 = \frac{D_6}{\rho_{i+\frac{1}{2}}^n} \end{aligned}$$

To get:

$$\rho_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} = B_6 - C_6 - D_6 \cdot P_{i+1}^{n+1} + D_6 \cdot P_i^{n+1} + E_6 - F_6 - G_6$$

And:

$$v_{i+\frac{1}{2}}^{n+1} = H_6 - I_6 \cdot P_{i+1}^{n+1} + I_6 \cdot P_i^{n+1} \quad (11)$$

Step 9

Determine the elements of equation 7:

$$\begin{aligned} \frac{\rho_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - \rho_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^n}{\Delta t} = & -\rho_{i-\frac{1}{2}}^n \cdot \frac{d_{i-1} \cdot (v_{i-1}^n)^2 + d_i \cdot (v_i^n)^2}{\Delta x_{i-\frac{1}{2}}} \\ & - \frac{P_i^{n+1} - P_{i-1}^{n+1}}{\Delta x_{i-\frac{1}{2}}} + \rho_{i-\frac{1}{2}}^n \cdot g_{i-\frac{1}{2}} \\ & - \frac{1}{2V_{i-1}} F_{\tau,i-1}^n - \frac{1}{2V_i} F_{\tau,i}^n \end{aligned}$$

Where the elements are:

$$\begin{aligned}
 B_7 &= \rho_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^n \\
 C_7 &= \Delta t \rho_{i-\frac{1}{2}}^n \cdot \frac{d_{i-1} \cdot (v_{i-1}^n)^2 + d_i \cdot (v_i^n)^2}{\Delta x_{i-\frac{1}{2}}} \\
 D_7 &= \frac{\Delta t}{\Delta x_{i-\frac{1}{2}}}, \quad E_7 = \Delta t \rho_{i-\frac{1}{2}}^n \cdot g_{i-\frac{1}{2}} \\
 F_7 &= \frac{\Delta t}{2V_{i-1}} F_{\tau,i-1}^n, \quad G_7 = \frac{\Delta t}{2V_i} F_{\tau,i}^n \\
 H_7 &= \frac{B_7 - C_7 + E_7 - F_7 - G_7}{\rho_{i-\frac{1}{2}}^n}, \quad I_7 = \frac{D_7}{\rho_{i-\frac{1}{2}}^n}
 \end{aligned}$$

To get:

$$\rho_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} = B_7 - C_7 - D_7 \cdot P_i^{n+1} + D_7 \cdot P_{i-1}^{n+1} + E_7 - F_7 - G_7$$

And:

$$v_{i-\frac{1}{2}}^{n+1} = H_7 - I_7 \cdot P_i^{n+1} + I_7 \cdot P_{i-1}^{n+1} \quad (12)$$

Step 10

Determine the elements of equation 8:

$$\begin{aligned}
 \frac{(\rho_i^{n+1} \cdot u_i^{n+1} - \rho_i^n \cdot u_i^n)}{\Delta t} &= \frac{1}{V_i} \left[(\rho A u)_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - (\rho A u)_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} \right] \\
 &+ \frac{1}{V_i} \left[(\rho A g z)_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - (\rho A g z)_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} \right] \\
 &+ \frac{A_{s,i}}{V_i} \dot{q}_i^n - \frac{1}{V_i} \left[(P \cdot A)_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - (P \cdot A)_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} \right] \\
 &- \frac{1}{V_i} E_{loss}^n \\
 \rho_i^{n+1} \cdot u_i^{n+1} &= \rho_i^n \cdot u_i^n \\
 &+ \frac{\Delta t}{V_i} \left[(\rho A u)_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - (\rho A u)_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} \right] \\
 &+ \frac{\Delta t}{V_i} \left[(\rho A g z)_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - (\rho A g z)_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} \right] \\
 &+ \frac{\Delta t A_{s,i}}{V_i} \dot{q}_i^n - \frac{\Delta t}{V_i} \left[(P \cdot A)_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - (P \cdot A)_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} \right] \\
 &- \frac{\Delta t}{V_i} E_{loss}^n
 \end{aligned}$$

Where the elements are:

$$\begin{aligned}
B_8 &= \rho_i^n \cdot u_i^n \\
C_8 &= \frac{\Delta t (\rho A u)_{i-\frac{1}{2}}^n}{V_i}, \quad D_8 = \frac{\Delta t (\rho A u)_{i+\frac{1}{2}}^n}{V_i} \\
E_8 &= \frac{\Delta t (\rho A g z)_{i-\frac{1}{2}}^n}{V_i}, \quad F_8 = \frac{\Delta t (\rho A g z)_{i+\frac{1}{2}}^n}{V_i} \\
G_8 &= \frac{\Delta t A_{s,i}}{V_i} \dot{q}_i^n \\
H_8 &= \frac{\Delta t (P.A)_{i-\frac{1}{2}}^n}{V_i}, \quad I_8 = \frac{\Delta t (P.A)_{i+\frac{1}{2}}^n}{V_i} \\
J_8 &= \frac{\Delta t}{V_i} E_{loss,i}^n \\
K_8 &= B_8 - J_8 \\
L_8 &= C_8 + E_8 - G_8 \\
M_8 &= -D_8 - F_8 + I_8
\end{aligned}$$

To get:

$$\rho_i^{n+1} \cdot u_i^{n+1} = B_8 + C_8 \cdot v_{i-\frac{1}{2}}^{n+1} - D_8 \cdot v_{i+\frac{1}{2}}^{n+1} + E_8 \cdot v_{i-\frac{1}{2}}^{n+1} - F_8 \cdot v_{i+\frac{1}{2}}^{n+1} + G_8 - H_8 \cdot v_{i-\frac{1}{2}}^{n+1} + I_8 \cdot v_{i+\frac{1}{2}}^{n+1} - J_8$$

And with the left hand side expanded:

$$\rho_i^n \cdot (u_i^{n+1} - u_i^n) + u_i^n (\rho_i^{n+1} - \rho_i^n) = K_8 + L_8 \cdot v_{i-\frac{1}{2}}^{n+1} + M_8 \cdot v_{i+\frac{1}{2}}^{n+1} \quad (13)$$

Step 11

Determine the elements of equation 9:

$$u_i^{n+1} = \frac{d(u_i^{n+1})}{d\rho} \cdot \rho_i^{n+1} - \frac{d(u_i^{n+1})}{d\rho} \cdot \rho_i^n + u_i^n$$

Where the elements are:

$$\begin{aligned}
B_9 &= \frac{d(u_i^{n+1})}{d\rho} = -0.006159444 (\rho_i^n)^2 + 11.85504961 (\rho_i^n) - 5710.176493 \\
C_9 &= u_i^n - B_9 \cdot \rho_i^n
\end{aligned}$$

To get:

$$u_i^{n+1} = B_9 \cdot \rho_i^{n+1} + C_9 \quad (14)$$

Step 11

Reduce the given equations to a single equation. This is possible because we have the following set of equations:

$$\begin{aligned}
 \text{eq 10, } \quad & \rho_i^{n+1} = \rho_i^n + B_5.v_{i-\frac{1}{2}}^{n+1} - C_5.v_{i+\frac{1}{2}}^{n+1} \\
 \text{eq 11, } \quad & v_{i+\frac{1}{2}}^{n+1} = H_6 - I_6.P_{i+1}^{n+1} + I_6.P_i^{n+1} \\
 \text{eq 12, } \quad & v_{i-\frac{1}{2}}^{n+1} = H_7 - I_7.P_i^{n+1} + I_7.P_{i-1}^{n+1} \\
 \text{eq 13, } \quad & \rho_i^n.(u_i^{n+1} - u_i^n) + u_i^n(\rho_i^{n+1} - \rho_i^n) = K_8 + L_8.v_{i-\frac{1}{2}}^{n+1} + M_8.v_{i+\frac{1}{2}}^{n+1} \\
 \text{eq 14, } \quad & u_i^{n+1} = B_9.\rho_i^{n+1} + C_9
 \end{aligned}$$

Now the reduction goal is find the unknowns in equation 13 by locally solving the set of equations until only the pressures remain, i.e. P_{i-1}^{n+1} , P_i^{n+1} and P_{i+1}^{n+1} .

We start by inserting equation 11 and 12 into 10:

$$\begin{aligned}
 \rho_i^{n+1} &= \rho_i^n + B_5.\left(H_7 - I_7.P_i^{n+1} + I_7.P_{i-1}^{n+1}\right) - C_5.\left(H_6 - I_6.P_{i+1}^{n+1} + I_6.P_i^{n+1}\right) \\
 &= \rho_i^n + B_5.H_7 - C_5.H_6 - B_5.I_7.P_i^{n+1} + B_5.I_7.P_{i-1}^{n+1} + C_5.I_6.P_{i+1}^{n+1} - C_5.I_6.P_i^{n+1} \\
 &= \left(\rho_i^n + B_5.H_7 - C_5.H_6\right) + \left(B_5.I_7\right)P_{i-1}^{n+1} - \left(B_5.I_7 + C_5.I_6\right)P_i^{n+1} + \left(C_5.I_6\right)P_{i+1}^{n+1}
 \end{aligned}$$

More simplistically we define:

$$\begin{aligned}
 B_{10} &= \rho_i^n + B_5.H_7 - C_5.H_6 \\
 C_{10} &= B_5.I_7 \\
 D_{10} &= B_5.I_7 + C_5.I_6 \\
 E_{10} &= C_5.I_6
 \end{aligned}$$

To arrive at:

$$\rho_i^{n+1} = B_{10} + C_{10}.P_{i-1}^{n+1} - D_{10}.P_i^{n+1} + E_{10}.P_{i+1}^{n+1} \tag{15}$$

Next we aim to eliminate the internal energy from equation 13 by inserting equation 14:

$$\begin{aligned}
\rho_i^n \cdot \left((B_9 \cdot \rho_i^{n+1} + C_9) - u_i^n \right) + u_i^n (\rho_i^{n+1} - \rho_i^n) &= K_8 + L_8 \cdot v_{i-\frac{1}{2}}^{n+1} + M_8 \cdot v_{i+\frac{1}{2}}^{n+1} \\
\rho_i^n \cdot B_9 \cdot \rho_i^{n+1} + \rho_i^n \cdot C_9 - \rho_i^n \cdot u_i^n + u_i^n \cdot \rho_i^{n+1} - u_i^n \cdot \rho_i^n &= K_8 + L_8 \cdot v_{i-\frac{1}{2}}^{n+1} + M_8 \cdot v_{i+\frac{1}{2}}^{n+1} \\
\left(\rho_i^n \cdot B_9 + u_i^n \right) \rho_i^{n+1} &= \left(K_8 - \rho_i^n \cdot C_9 + \rho_i^n \cdot u_i^n + u_i^n \cdot \rho_i^n \right) + L_8 \cdot v_{i-\frac{1}{2}}^{n+1} + M_8 \cdot v_{i+\frac{1}{2}}^{n+1}
\end{aligned}$$

For simplicity we define:

$$\begin{aligned}
B_{14} &= \rho_i^n \cdot B_9 + u_i^n \\
C_{14} &= K_8 - \rho_i^n \cdot C_9 + \rho_i^n \cdot u_i^n + u_i^n \cdot \rho_i^n
\end{aligned}$$

To get:

$$B_{14} \cdot \rho_i^{n+1} = C_{14} + L_8 \cdot v_{i-\frac{1}{2}}^{n+1} + M_8 \cdot v_{i+\frac{1}{2}}^{n+1}$$

We need to also insert equations 11 and 12:

$$\begin{aligned}
B_{14} \cdot \rho_i^{n+1} &= C_{14} + L_8 \cdot \left(H_7 - I_7 \cdot P_i^{n+1} + I_7 \cdot P_{i-1}^{n+1} \right) + M_8 \cdot \left(H_6 - I_6 \cdot P_{i+1}^{n+1} + I_6 \cdot P_i^{n+1} \right) \\
B_{14} \cdot \rho_i^{n+1} &= \left(C_{14} - L_8 H_7 + M_8 H_6 \right) + \left(L_8 I_7 \right) \cdot P_{i-1}^{n+1} + \left(M_8 I_6 - L_8 I_7 \right) \cdot P_i^{n+1} - \left(M_8 I_6 \right) \cdot P_{i+1}^{n+1}
\end{aligned}$$

Again we define:

$$\begin{aligned}
D_{14} &= C_{14} - L_8 H_7 + M_8 H_6 \\
E_{14} &= L_8 I_7 \\
F_{14} &= M_8 I_6 - L_8 I_7 \\
G_{14} &= M_8 I_6
\end{aligned}$$

To get:

$$B_{14} \cdot \rho_i^{n+1} = D_{14} + E_{14} \cdot P_{i-1}^{n+1} + F_{14} \cdot P_i^{n+1} - G_{14} \cdot P_{i+1}^{n+1} \quad (16)$$

Now all thats left is to insert equation 15 into 16:

$$\begin{aligned}
B_{14} \cdot \left(B_{10} + C_{10} \cdot P_{i-1}^{n+1} - D_{10} \cdot P_i^{n+1} + E_{10} \cdot P_{i+1}^{n+1} \right) &= D_{14} + E_{14} \cdot P_{i-1}^{n+1} + F_{14} \cdot P_i^{n+1} - G_{14} \cdot P_{i+1}^{n+1} \\
B_{14} B_{10} + B_{14} C_{10} \cdot P_{i-1}^{n+1} - B_{14} D_{10} \cdot P_i^{n+1} + B_{14} E_{10} \cdot P_{i+1}^{n+1} &= D_{14} + E_{14} \cdot P_{i-1}^{n+1} + F_{14} \cdot P_i^{n+1} - G_{14} \cdot P_{i+1}^{n+1} \\
\left(B_{14} \cdot C_{10} - E_{14} \right) P_{i-1}^{n+1} - \left(B_{14} D_{10} + F_{14} \right) P_i^{n+1} + \left(B_{14} E_{10} + G_{14} \right) P_{i+1}^{n+1} &= D_{14} - B_{14} B_{10}
\end{aligned}$$

References

- [1] *Safety Evaluation Report on High-Uranium Content, Low-Enriched Uranium-Zirconium Hydride Fuels for TRIGA Reactors*, NUREG-1282, Docket number 50-163, GA Technologies, August 1987.
- [2] Ginnings D.C., Corruccini R.J., *Heat Capacities at High Temperatures of Uranium, Uranium Trichloride, and Uranium Tetrachloride*, Journal of Research of the National Bureau of Standards, Research Paper RP1831, Volume 39, October 1947.
- [3] Douglas T.B., Victor A.C., *Heat Content of Zirconium and of Five Compositions of Zirconium Hydride from 0° to 990°C*, Journal of Research of the National Bureau of Standards, Research Paper RP2878, Volume 61, July 1958.