

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

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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:

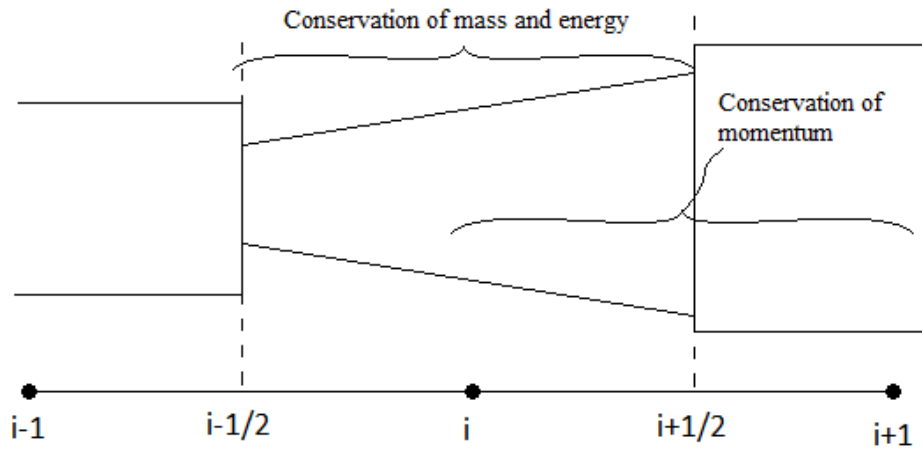


Figure 1: Simple layout of control volumes.

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:

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

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:

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

Here $\Delta x_{i+\frac{1}{2}}$ 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 :

$$\Delta P_{\tau} = \frac{1}{2} f \rho \frac{L}{D_H} v^2$$

Therefore:

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

In these equations L_i and $D_{H,i}$ are the length and hydraulic diameter of the i -th control volume. The Darcy friction factor is evaluated as shown below. The turbulent regime friction factor (i.e. $Re > 3000$) is calculated from the Zigrang and Sylvester correlation.

$$f = \begin{cases} g(Re) = \frac{64}{Re} & , Re \leq 2200 \\ h(Re) = \frac{1}{\sqrt{f}} = -2 \log \left(\frac{\epsilon}{3.7 D_H} + \frac{2.51}{Re \sqrt{f}} \right) & , Re > 3000 \\ g(2200) + \frac{h(3000) - g(2200)}{800} \cdot (Re - 2200) & , 2200 < Re \leq 3000 \end{cases}$$

The junction pressure loss $\Delta P_{loss,i+\frac{1}{2}}$ is calculated from a loss coefficient K as follows:

$$\Delta P_{loss,i+\frac{1}{2}} = \frac{1}{2} K_{i+\frac{1}{2}} \rho_{i+\frac{1}{2}} d_{i+\frac{1}{2}} v_{i+\frac{1}{2}}^2$$

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 (includes irreversible conversion of kinetic energy to internal energy).

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

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

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:

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

1.4 Equation of state

In addition to the conservation equations, there is the equation of state. ChiTech has the ability to use the IAPWS-95 steam tables which is captured within a function with the main entry specified as pressure [bar]. Therefore the property Y, which can be any thermal property (i.e. temperature, density, internal energy, enthalpy, entropy, heat capacity, dynamic viscosity, Prandtl number), can be determined from the equation below given X (a known quantity in the subset listed for Y):

$$Y_i = f(P_i, X_i) \quad (4)$$

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 $i + \frac{1}{2}$:

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

We use the following time notation:

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

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 $i - \frac{1}{2}$:

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

2.3 Conservation of Energy - finite difference formulation

We start with the original conservation of energy equation:

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

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

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

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 :

$$\frac{d(\rho_i^n u_i^n)}{d\rho} = \frac{\rho_{EOS}(P_i^n, T_i^n + \Delta T) u_{EOS}(P_i^n, T_i^n + \Delta T) - \rho_{EOS}(P_i^n, T_i^n - \Delta T) u_{EOS}(P_i^n, T_i^n - \Delta T)}{\rho_{EOS}(P_i^n, T_i^n + \Delta T) - \rho_{EOS}(P_i^n, T_i^n - \Delta T)}$$

Where ρ_{EOS} and u_{EOS} are determined from interpolating the steam tables. Also, ΔT is an arbitrary but small difference in temperature sufficient to locally linearize the equation of state. From this derivative we find the linearized equation of state:

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

2.5 Semi-implicit approach

From the set of equations 5 to 9 we can develop a system of unknowns. Before we depict how this is done, let us repeat these equations all together:

$$\begin{aligned}
 eq.5, \quad \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] \\
 &\dots \\
 eq.6, \quad \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{\Delta P_{\tau,i}^n}{2\Delta x_{i+\frac{1}{2}}} - \frac{\Delta P_{\tau,i+1}^n}{2\Delta x_{i+\frac{1}{2}}} - \frac{\Delta P_{loss,i+\frac{1}{2}}^n}{\Delta x_{i+\frac{1}{2}}} \\
 &\dots \\
 eq.7, \quad \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{\Delta P_{\tau,i-1}^n}{2\Delta x_{i-\frac{1}{2}}} - \frac{\Delta P_{\tau,i}^n}{2\Delta x_{i-\frac{1}{2}}} - \frac{\Delta P_{loss,i-\frac{1}{2}}^n}{\Delta x_{i-\frac{1}{2}}} \\
 &\dots \\
 eq.8, \quad \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] \\
 &\quad + \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] \\
 &\quad + \frac{A_{s,i}}{V_i} \dot{q}_i^n + \frac{1}{V_i} \left[(P.A)_{i-\frac{1}{2}}^n \cdot v_{i-\frac{1}{2}}^{n+1} - (P.A)_{i+\frac{1}{2}}^n \cdot v_{i+\frac{1}{2}}^{n+1} \right] \\
 &\quad - \frac{E_{loss,i}^n}{V_i} \\
 &\dots \\
 eq.9, \quad \rho_i^{n+1} u_i^{n+1} - \rho_i^n u_i^n &= \frac{d(\rho_i^n u_i^n)}{d\rho} \cdot (\rho_i^{n+1} - \rho_i^n)
 \end{aligned}$$

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

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

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

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

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

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

There are also the unknown junction quantities $\rho_{i+\frac{1}{2}}^n$ and $u_{i+\frac{1}{2}}^n$, however, these can be determined by a simple upwind scheme as follows:

$$\begin{aligned} \frac{d\rho_{i+\frac{1}{2}}}{dt} &= -v_{i+\frac{1}{2}} \cdot \frac{d\rho}{dx} \quad \text{and} \quad \frac{du_{i+\frac{1}{2}}}{dt} = -v_{i+\frac{1}{2}} \cdot \frac{du}{dx} \\ \therefore \rho_{i+\frac{1}{2}}^n &= \rho_{i+\frac{1}{2}}^{n-1} - v_{i+\frac{1}{2}}^n \cdot \frac{\Delta t}{\Delta x_{i+\frac{1}{2}}} \cdot (\rho_{i+1}^n - \rho_i^n) \\ u_{i+\frac{1}{2}}^n &= u_{i+\frac{1}{2}}^{n-1} - v_{i+\frac{1}{2}}^n \cdot \frac{\Delta t}{\Delta x_{i+\frac{1}{2}}} \cdot (u_{i+1}^n - u_i^n) \end{aligned}$$

By using simple mathematical manipulation we can reduce the set of equations (i.e. eq. 5 to 9) to a single equation in terms of P_{i-1}^{n+1} , P_i^{n+1} and P_{i+1}^{n+1} , a process indicated in the solution algorithm. We can then implicitly solve for the control volume pressure by constructing the system $Ax = b$ and solving it with a suitable sparse solver. After this has been done the junction velocities, $v_{i+\frac{1}{2}}^{n+1}$ can be determined from the advancement of the momentum equations (i.e. equation 6) and from those values one can determine ρ_i^{n+1} from the conservation of mass equation and finally u_i^{n+1} from the equation of state interpolation.

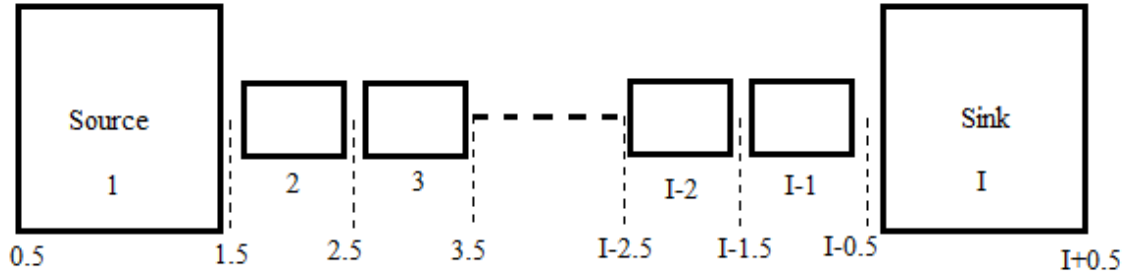


Figure 2: Simple layout of multiple control volumes.

2.6 Solution algorithm

Step 1 - Preliminaries

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

Load all junctions. Input parameters:

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

Step 2

Determine control volume connectivity to junctions. This step merely requires that control volumes know what they are connected to.

Step 3

Initialize control volume pressure, P_i^n , and junction velocities, $v_{i+\frac{1}{2}}^n$.

Determine density, ρ_i , from:

$$\rho = \rho_{EOS}(P, T)$$

Internal energy, u_i , from:

$$u = u_{EOS}(P, T)$$

Dynamic viscosity, μ_i , from:

$$\mu = \mu_{EOS}(P, T)$$

Initialize temperature and calculate control volume velocity, v_i , from:

$$v_i = \begin{cases} v_{i+\frac{1}{2}} \frac{A_{i+\frac{1}{2}}}{A_i} & , \text{left junction missing} \\ v_{i-\frac{1}{2}} \frac{A_{i-\frac{1}{2}}}{A_i} & , \text{right junction missing} \\ v_{i-\frac{1}{2}} \frac{A_{i-\frac{1}{2}}}{2A_i} + v_{i+\frac{1}{2}} \frac{A_{i+\frac{1}{2}}}{2A_i} & , \text{both junctions exist} \end{cases}$$

Step 4

Determine all junction and control volume z values using control volume Δz values. Also initialize the mass error and cumulative mass error.

***** End of Initialization phase *****

***** Repeat the steps below for each time step *****

Step 5

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

$$\rho_{i+\frac{1}{2}}^n = \rho_{i+\frac{1}{2}}^{n-1} - v_{i+\frac{1}{2}}^n \cdot \frac{\Delta t}{\Delta x_{i+\frac{1}{2}}} \cdot (\rho_{i+1}^n - \rho_i^n)$$

And similarly for $u_{i+\frac{1}{2}}$ from:

$$u_{i+\frac{1}{2}}^n = u_{i+\frac{1}{2}}^{n-1} - v_{i+\frac{1}{2}}^n \cdot \frac{\Delta t}{\Delta x_{i+\frac{1}{2}}} \cdot (u_{i+1}^n - u_i^n)$$

Step 6

Calculate control volume quantities, v_i , from: Velocity, v_i , from:

$$v_i = \begin{cases} v_{i+\frac{1}{2}} \frac{A_{i+\frac{1}{2}}}{A_i} & , \text{left junction missing} \\ v_{i-\frac{1}{2}} \frac{A_{i-\frac{1}{2}}}{A_i} & , \text{right junction missing} \\ v_{i-\frac{1}{2}} \frac{A_{i-\frac{1}{2}}}{2A_i} + v_{i+\frac{1}{2}} \frac{A_{i+\frac{1}{2}}}{2A_i} & , \text{both junctions exist} \end{cases}$$

Dynamic viscosity, μ_i , from:

$$\mu = \mu_{EOS}(P, T)$$

Reynolds number, Re_i , from:

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

Friction pressure drop, ΔP_τ , from:

$$\Delta P_{\tau,i} = \frac{1}{2} f_i \rho_i \frac{L_i}{D_{H,i}} v_i^2$$

With:

$$f = \begin{cases} 6.5 \times 10^6 & , Re = 0.0 \\ g(Re) = \frac{64}{Re} & , Re \leq 2200 \\ h(Re) = \frac{1}{\sqrt{f}} = -2 \log \left(\frac{\epsilon}{3.7 D_H} + \frac{2.51}{Re \sqrt{f}} \right) & , Re > 3000 \\ g(2200) + \frac{h(3000) - g(2200)}{800} \cdot (Re - 2200) & , 2200 < Re \leq 3000 \end{cases}$$

Junction pressure drop losses, E_{loss} , from:

$$E_{loss,i+\frac{1}{2}} = (\Delta P.A.v)_{i+\frac{1}{2}} = \frac{1}{2}K_{i+\frac{1}{2}}(\rho A v^3)_{i+\frac{1}{2}}$$

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:

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

Step 8

Determine the elements of equation 6:

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

Where the elements are:

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

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:

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

Where the elements are:

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

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:

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

Where the elements are:

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

To get:

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

And:

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

Step 11

Determine the elements of equation 9:

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

Where the elements are:

$$B_9 = \frac{d(\rho_i^n u_i^n)}{d\rho} = \frac{\rho_{EOS}(P_i^n, T_i^n + \Delta T)u_{EOS}(P_i^n, T_i^n + \Delta T) - \rho_{EOS}(P_i^n, T_i^n - \Delta T)u_{EOS}(P_i^n, T_i^n - \Delta T)}{\rho_{EOS}(P_i^n, T_i^n + \Delta T) - \rho_{EOS}(P_i^n, T_i^n - \Delta T)}$$

$$C_9 = B_9 \cdot \rho_i^n$$

To get:

$$\rho_i^{n+1}u_i^{n+1} - \rho_i^n u_i^n = B_9 \cdot \rho_i^{n+1} - C_9 \tag{14}$$

Step 12

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

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

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:

$$\begin{aligned}
\rho_i^{n+1} &= \rho_i^n + B_5.\left(H_7 - I_7.P_i^{n+1} + I_7.P_{i-1}^{n+1}\right) - C_5.\left(H_6 - I_6.P_{i+1}^{n+1} + I_6.P_i^{n+1}\right) \\
&= \rho_i^n + B_5H_7 - B_5I_7.P_i^{n+1} + B_5I_7.P_{i-1}^{n+1} - C_5H_6 + C_5I_6.P_{i+1}^{n+1} - C_5I_6.P_i^{n+1} \\
&= \rho_i^n + B_5H_7 - C_5H_6 + B_5I_7.P_{i-1}^{n+1} - B_5I_7.P_i^{n+1} - C_5I_6.P_i^{n+1} + C_5I_6.P_{i+1}^{n+1} \\
&= \left(\rho_i^n + B_5H_7 - C_5H_6\right) + \left(B_5I_7\right)P_{i-1}^{n+1} - \left(B_5I_7 + C_5I_6\right)P_i^{n+1} + \left(C_5I_6\right)P_{i+1}^{n+1}
\end{aligned}$$

More simplistically we define:

$$\begin{aligned}
B_{10} &= \rho_i^n + B_5H_7 - C_5H_6 \\
C_{10} &= B_5I_7 \\
D_{10} &= B_5I_7 + C_5I_6 \\
E_{10} &= C_5I_6
\end{aligned}$$

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 by inserting equation 14 into equation 13:

$$B_9 \cdot \rho_i^{n+1} - C_9 = K_8 + L_8 \cdot v_{i-\frac{1}{2}}^{n+1} - M_8 \cdot v_{i+\frac{1}{2}}^{n+1}$$

For simplicity we define:

$$B_{14} = \frac{K_8 + C_9}{B_9} \quad C_{14} = \frac{L_8}{B_9} \quad D_{14} = \frac{M_8}{B_9}$$

To get:

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

We need to also insert equations 11 and 12:

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

Again we define:

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

To get:

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

Now all that's left is to equate equation 15 and 16:

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

We now have a single equation for each control volume:

$$\left(C_{10} - F_{14} \right) P_{i-1}^{n+1} + \left(G_{14} - D_{10} \right) P_i^{n+1} + \left(E_{10} - H_{14} \right) P_{i+1}^{n+1} = E_{14} - B_{10} \quad (17)$$

Step 13

Using equation 17, in the form $a_i \cdot P_{i-1}^{n+1} + b_i \cdot P_i^{n+1} + c_i \cdot P_{i+1}^{n+1} = d_i$ we can construct a linear system $Ax = b$ as follows:

$$A = \begin{bmatrix} b_1 & c_1 & \cdots & \cdots & \cdots & 0 \\ a_2 & b_2 & c_2 & \cdots & \cdots & \vdots \\ \vdots & & \ddots & & & \vdots \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & a_{I-1} & b_{I-1} & c_{I-1} \\ 0 & \cdots & \cdots & \cdots & a_I & b_I \end{bmatrix} \quad x = \begin{bmatrix} P_1^{n+1} \\ P_2^{n+1} \\ \vdots \\ \vdots \\ P_{I-1}^{n+1} \\ P_I^{n+1} \end{bmatrix} \quad b = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ \vdots \\ d_{I-1} \\ d_I \end{bmatrix}$$

This system can be solved using a conjugate gradient numerical solver.

Step 14

Calculate junction velocities from equation 11:

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

Step 15

Calculate control volume new densities from equation 10:

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

Step 16

Calculate control volume new internal energies from equation 14:

$$\begin{aligned} \rho_i^{n+1} u_i^{n+1} - \rho_i^n u_i^n &= B_9 \cdot \rho_i^{n+1} - C_9 \\ \rho_i^{n+1} u_i^{n+1} &= \rho_i^n u_i^n - C_9 + B_9 \cdot \rho_i^{n+1} \\ \therefore u_i^{n+1} &= \frac{\rho_i^n u_i^n - C_9}{\rho_i^{n+1}} + B_9 \end{aligned}$$

Step 17

Advance the time values.

References