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

March, 2016

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Rev 1.01

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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:

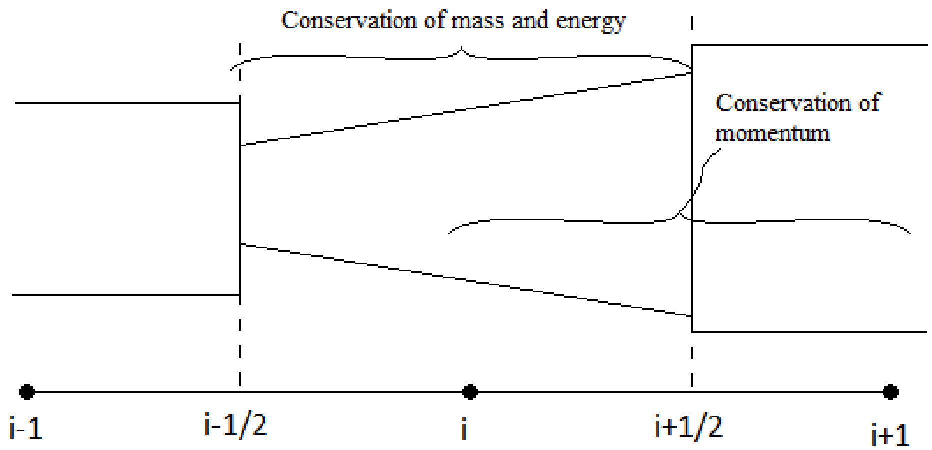

Figure 1: Simple layout of control volumes.

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:

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

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:

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

Where $VISC_{i+\frac{1}{2}}$ is an artificial viscosity term needed to correct for different junction velocities:

$$VISC_{i+\frac{1}{2}} = |v_{i+1}| \left[v_{i+\frac{3}{2}} \left(\frac{A_{i+\frac{3}{2}}}{A_{i+\frac{1}{2}}} \right) - v_{i+\frac{1}{2}} \right] - |v_i| \left[v_{i+\frac{1}{2}} - v_{i-\frac{1}{2}} \left(\frac{A_{i-\frac{1}{2}}}{A_{i+\frac{1}{2}}} \right) \right]$$

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

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

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:

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

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:

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

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

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

From here the energy conservation equation becomes:

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

Dividing by the volume we get:

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

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:

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

Similarly:

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

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:

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

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:

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

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

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

We use the following time notation:

$$\begin{aligned} \frac{\rho^n_{i+\frac{1}{2}}.v^{n+1}_{i+\frac{1}{2}} - \rho^n_{i+\frac{1}{2}}.v^n_{i+\frac{1}{2}}}{\Delta t} = &- \rho^n_{i+\frac{1}{2}} \cdot \frac{d_i.(v^n_i)^2 - d_{i+1}.(v^n_{i+1})^2}{\Delta x_{i+\frac{1}{2}}} \\ &- \frac{P^{n+1}_{i+1} - P^{n+1}_i}{\Delta x_{i+\frac{1}{2}}} + \rho^n_{i+\frac{1}{2}}.g_{i+\frac{1}{2}} \\ &- \frac{1}{2V_i} F^n_{\tau,i} - \frac{1}{2V_{i+1}} F^n_{\tau,i+1} + \rho^n_{i+\frac{1}{2}} \cdot \frac{VISC^n_{i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}} \end{aligned} \tag{6}$$

Where:

$$VISC^n_{i+\frac{1}{2}} = |v^n_{i+1}| \left[v^n_{i+\frac{3}{2}} \left(\frac{A_{i+\frac{3}{2}}}{A_{i+\frac{1}{2}}} \right) - v^n_{i+\frac{1}{2}} \right] - |v^n_i| \left[v^n_{i+\frac{1}{2}} - v^n_{i-\frac{1}{2}} \left(\frac{A_{i-\frac{1}{2}}}{A_{i+\frac{1}{2}}} \right) \right]$$

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

$$\begin{aligned}\frac{\rho^n_{i-\frac{1}{2}}.v^{n+1}_{i-\frac{1}{2}}-\rho^n_{i-\frac{1}{2}}.v^n_{i-\frac{1}{2}}}{\Delta t}=&-\rho^n_{i-\frac{1}{2}}\cdot\frac{d_{i-1}.(v^n_{i-1})^2+d_i.(v^n_i)^2}{\Delta x_{i-\frac{1}{2}}}\\&-\frac{P^{n+1}_i-P^{n+1}_{i-1}}{\Delta x_{i-\frac{1}{2}}}+\rho^n_{i-\frac{1}{2}}.g_{i-\frac{1}{2}}\\&-\frac{1}{2V_{i-1}}F^n_{\tau,i-1}-\frac{1}{2V_i}F^n_{\tau,i}+\rho^n_{i-\frac{1}{2}}\cdot\frac{VISC^n_{i-\frac{1}{2}}}{\Delta x_{i-\frac{1}{2}}}\end{aligned}\tag{7}$$

Where:

$$VISC^n_{i-\frac{1}{2}}=|v^n_i|\left[v^n_{i+\frac{1}{2}}\left(\frac{A_{i+\frac{1}{2}}}{A_{i-\frac{1}{2}}}\right)-v^n_{i-\frac{1}{2}}\right]-|v^n_{i-1}|\left[v^n_{i-\frac{1}{2}}-v^n_{i-\frac{3}{2}}\left(\frac{A_{i-\frac{3}{2}}}{A_{i-\frac{1}{2}}}\right)\right]$$

2.3 Conservation of Energy - finite difference formulation

We start with the original conservation of energy equation:

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

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

$$\begin{aligned}\frac{(\rho^{n+1}_i.u^{n+1}_i-\rho^n_i.u^n_i)}{\Delta t}=&\frac{1}{V_i}\left[(\rho Au)^n_{i-\frac{1}{2}}.v^{n+1}_{i-\frac{1}{2}}-(\rho Au)^n_{i+\frac{1}{2}}.v^{n+1}_{i+\frac{1}{2}}\right]\\&+\frac{1}{V_i}\left[(\rho Agz)^n_{i-\frac{1}{2}}.v^{n+1}_{i-\frac{1}{2}}-(\rho Agz)^n_{i+\frac{1}{2}}.v^{n+1}_{i+\frac{1}{2}}\right]\\&+\frac{A_{s,i}}{V_i}\dot{q}^n_i+\frac{1}{V_i}\left[(P.A)^n_{i-\frac{1}{2}}.v^{n+1}_{i-\frac{1}{2}}-(P.A)^n_{i+\frac{1}{2}}.v^{n+1}_{i+\frac{1}{2}}\right]\\&+\frac{1}{V_i}E^n_{loss}\end{aligned}\tag{8}$$

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:

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

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:

$$\rho_i^{n+1}, v_{i+\frac{1}{2}}^{n+1}, v_{i-\frac{1}{2}}^{n+1},\ from\ equation\ 5$$
$$v_{i+\frac{1}{2}}^{n+1}, P_{i+1}^{n+1}, P_i^{n+1},\ from\ equation\ 6$$
$$v_{i-\frac{1}{2}}^{n+1}, P_{i-1}^{n+1}, P_i^{n+1},\ from\ equation\ 7$$
$$\rho_i^{n+1}, u_i^{n+1}, v_{i-\frac{1}{2}}^{n+1}, v_{i+\frac{1}{2}}^{n+1},\ from\ equation\ 8$$
$$\rho_i^{n+1}, u_i^{n+1},\ from\ equation\ 9$$

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:

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

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:

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

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.

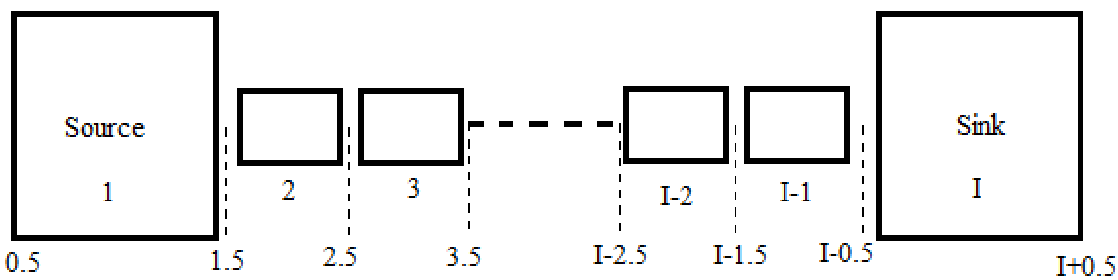

Figure 2: Simple layout of multiple control volumes.

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 - Repeat from for new time steps

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

$$\rho^n_{i-\frac{1}{2}} = \begin{cases} \rho^n_{i-1} & , v_{i-\frac{1}{2}} \geq 0 \\ \rho^n_i & , v_{i-\frac{1}{2}} < 0 \end{cases}$$

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

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

$$u^n_{i-\frac{1}{2}} = \begin{cases} u^n_{i-1} & , v_{i-\frac{1}{2}} > 0 \\ u^n_i & , v_{i-\frac{1}{2}} < 0 \end{cases}$$

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

Step 6

Calculate control volume quantities. First, velocity, v_i, from:

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

Dynamic viscosity, μ_i, from:

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

Reynolds number, Re_i, from:

$$Re_i = \frac{\rho^n_i v^n_n D_{H,i}}{\mu^n_i}$$

Drag force, F_τ, from:

$$F_{\tau,i} = \frac{1}{4} f_i \rho_i \frac{L_i}{D_{H,i}} A_i v_i^2$$

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

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

Similarly:

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

Step 7

Determine the elements of equation 5:

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

Where the elements are:

$$B_5 = \frac{\Delta t(\rho.A)^n_{i-\frac{1}{2}}}{V_i}$$
$$C_5 = \frac{\Delta t(\rho.A)^n_{i+\frac{1}{2}}}{V_i}$$

To get:

$$\rho_i^{n+1} = \rho_i^n + B_5.v^{n+1}_{i-\frac{1}{2}} - C_5.v^{n+1}_{i+\frac{1}{2}} \tag{10}$$

Step 8

Determine the elements of equation 6:

$$\frac{\rho^n_{i+\frac{1}{2}}.v^{n+1}_{i+\frac{1}{2}} - \rho^n_{i+\frac{1}{2}}.v^n_{i+\frac{1}{2}}}{\Delta t} = - \rho^n_{i+\frac{1}{2}} \cdot \frac{d_i.(v^n_i)^2 - d_{i+1}.(v^n_{i+1})^2}{\Delta x_{i+\frac{1}{2}}} - \frac{P^{n+1}_{i+1} - P^{n+1}_i}{\Delta x_{i+\frac{1}{2}}} + \rho^n_{i+\frac{1}{2}}.g_{i+\frac{1}{2}} - \frac{1}{2V_i}F^n_{\tau,i} - \frac{1}{2V_{i+1}}F^n_{\tau,i+1}$$

Where the elements are:

$$B_6 = \rho^n_{i+\frac{1}{2}}.v^n_{i+\frac{1}{2}}$$

$$C_6 = \Delta t \rho^n_{i+\frac{1}{2}} \cdot \frac{d_i.(v^n_i)^2 - d_{i+1}.(v^n_{i+1})^2}{\Delta x_{i+\frac{1}{2}}}$$

$$D_6 = \frac{\Delta t}{\Delta x_{i+\frac{1}{2}}}, \quad E_6 = \Delta t \rho^n_{i+\frac{1}{2}}.g_{i+\frac{1}{2}}$$

$$F_6 = \frac{\Delta t}{2V_i}F^n_{\tau,i}, \quad G_6 = \frac{\Delta t}{2V_{i+1}}F^n_{\tau,i+1}$$

$$H_6 = \frac{B_6 - C_6 + E_6 - F_6 - G_6}{\rho^n_{i+\frac{1}{2}}}, \quad I_6 = \frac{D6}{\rho^n_{i+\frac{1}{2}}}$$

To get:

$$\rho^n_{i+\frac{1}{2}}.v^{n+1}_{i+\frac{1}{2}} = B_6 - C_6 - D_6.P^{n+1}_{i+1} + D_6.P^{n+1}_i + E_6 - F_6 - G_6$$

And:

$$v^{n+1}_{i+\frac{1}{2}} = H_6 - I_6.P^{n+1}_{i+1} + I_6.P^{n+1}_i \tag{11}$$

Step 9

Determine the elements of equation 7:

$$\begin{aligned}\frac{\rho^n_{i-\frac{1}{2}}.v^{n+1}_{i-\frac{1}{2}} - \rho^n_{i-\frac{1}{2}}.v^n_{i-\frac{1}{2}}}{\Delta t} =& - \rho^n_{i-\frac{1}{2}} \cdot \frac{d_{i-1}.(v^n_{i-1})^2 - d_i.(v^n_i)^2}{\Delta x_{i-\frac{1}{2}}} \\ &- \frac{P^{n+1}_i - P^{n+1}_{i-1}}{\Delta x_{i-\frac{1}{2}}} + \rho^n_{i-\frac{1}{2}}.g_{i-\frac{1}{2}} \\ &- \frac{1}{2V_{i-1}} F^n_{\tau,i-1} - \frac{1}{2V_i} F^n_{\tau,i}\end{aligned}$$

Where the elements are:

$$\begin{aligned}B_7 &= \rho^n_{i-\frac{1}{2}}.v^n_{i-\frac{1}{2}} \\ C_7 &= \Delta t \rho^n_{i-\frac{1}{2}} \cdot \frac{d_{i-1}.(v^n_{i-1})^2 - d_i.(v^n_i)^2}{\Delta x_{i-\frac{1}{2}}} \\ D_7 &= \frac{\Delta t}{\Delta x_{i-\frac{1}{2}}}, \quad E_7 = \Delta t \rho^n_{i-\frac{1}{2}}.g_{i-\frac{1}{2}} \\ F_7 &= \frac{\Delta t}{2V_{i-1}} F^n_{\tau,i-1}, \quad G_7 = \frac{\Delta t}{2V_i} F^n_{\tau,i} \\ H_7 &= \frac{B_7 - C_7 + E_7 - F_7 - G_7}{\rho^n_{i-\frac{1}{2}}}, \quad I_7 = \frac{D7}{\rho^n_{i-\frac{1}{2}}}\end{aligned}$$

To get:

$$\rho^n_{i-\frac{1}{2}}.v^{n+1}_{i-\frac{1}{2}} = B_7 - C_7 - D_7.P^{n+1}_i + D_7.P^{n+1}_{i-1} + E_7 - F_7 - G_7$$

And:

$$v^{n+1}_{i-\frac{1}{2}} = H_7 - I_7.P^{n+1}_i + I_7.P^{n+1}_{i-1} \tag{12}$$

Step 10

Determine the elements of equation 8:

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

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

Where the elements are:

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

To get:

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

And with the left hand side expanded:

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

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:

$$B_9 = \frac{d(u_i^{n+1})}{d\rho} = -0.006159444\ (\rho_i^n)^2 + 11.85504961\ (\rho_i^n) - 5710.176493$$
$$C_9 = u_i^n - B_9.\rho_i^n$$

To get:

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

Step 12

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

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

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:

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

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 from equation 13 by inserting equation 14:

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

For simplicity we define:

$$B_{14}=\rho_i^n.B_9+u_i^n$$
$$C_{14}=K_8-\rho_i^n.C_9+\rho_i^n.u_i^n+u_i^n.\rho_i^n$$

To get:

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

We need to also insert equations 11 and 12:

$$B_{14}.\rho_i^{n+1}=C_{14}+L_8.\left(H_7-I_7.P_i^{n+1}+I_7.P_{i-1}^{n+1}\right)+M_8.\left(H_6-I_6.P_{i+1}^{n+1}+I_6.P_i^{n+1}\right)$$
$$B_{14}.\rho_i^{n+1}=\left(C_{14}-L_8H_7+M_8H_6\right)+\left(L_8I_7\right).P_{i-1}^{n+1}+\left(M_8I_6-L_8I_7\right).P_i^{n+1}-\left(M_8I_6\right).P_{i+1}^{n+1}$$

Again we define:

$$D_{14}=C_{14}-L_8H_7+M_8H_6$$
$$E_{14}=L_8I_7$$
$$F_{14}=M_8I_6-L_8I_7$$
$$G_{14}=M_8I_6$$

To get:

$$B_{14}.\rho_i^{n+1}=D_{14}+E_{14}.P_{i-1}^{n+1}+F_{14}.P_i^{n+1}-G_{14}.P_{i+1}^{n+1} \tag{16}$$

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

$$B_{14}.\Bigg(B_{10}+C_{10}.P_{i-1}^{n+1}-D_{10}.P_i^{n+1}+E_{10}.P_{i+1}^{n+1}\Bigg)=D_{14}+E_{14}.P_{i-1}^{n+1}+F_{14}.P_i^{n+1}-G_{14}.P_{i+1}^{n+1}$$
$$B_{14}B_{10}+B_{14}C_{10}.P_{i-1}^{n+1}-B_{14}D_{10}.P_i^{n+1}+B_{14}E_{10}.P_{i+1}^{n+1}=D_{14}+E_{14}.P_{i-1}^{n+1}+F_{14}.P_i^{n+1}-G_{14}.P_{i+1}^{n+1}$$
$$\Bigg(B_{14}.C_{10}-E_{14}\Bigg)P_{i-1}^{n+1}-\Bigg(B_{14}D_{10}+F_{14}\Bigg)P_i^{n+1}+\Bigg(B_{14}E_{10}+G_{14}\Bigg)P_{i+1}^{n+1}=D_{14}-B_{14}B_{10}$$

We now have a single equation for each control volume:

$$\Bigg(B_{14}.C_{10}-E_{14}\Bigg)P_{i-1}^{n+1}-\Bigg(B_{14}D_{10}+F_{14}\Bigg)P_i^{n+1}+\Bigg(B_{14}E_{10}+G_{14}\Bigg)P_{i+1}^{n+1}=D_{14}-B_{14}B_{10} \tag{17}$$

Step 13

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

$$A=\begin{bmatrix} b_1 & c_1 & \cdots & \cdots & \cdots & 0 \\ a_2 & b_2 & c_2 & \cdots & \cdots & \vdots \\ \vdots & & \ddots & & & \vdots \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & a_{I-1} & b_{I-1} & c_{I-1} \\ 0 & \cdots & \cdots & \cdots & a_I & b_I \end{bmatrix} x=\begin{bmatrix} P_1^{n+1} \\ P_2^{n+1} \\ \vdots \\ \vdots \\ P_{I-1}^{n+1} \\ P_I^{n+1} \end{bmatrix} b=\begin{bmatrix} d1 \\ d2 \\ \vdots \\ \vdots \\ d_{I-1} \\ d_I \end{bmatrix}$$

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

Step 14
Calculate junction velocities from equation 11:

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

Step 15
Calculate control volume new densities from equation 10:

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

Step 16
Calculate control volume new internal energies from equation 14:

$$u_i^{n+1} = B_9.\rho_i^{n+1} + C_9$$

Step 17
Advance the time values.

References