# TECHNICAL REPORT:

# $THERMOALPHA$ - Two-phase System level Thermal-Hydraulics in $ChiTech$

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Rev 1.0

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# 1    Conservation equations

The overall objective of simulating system level thermal-hydraulics is to solve the following four field variables **for each phase**:

- Pressure, $P$

- Internal energy, $u$

- Velocity, $v$

- Density, $\rho$

In order to do this we apply the conservation equations to the control volume shown in Figure 1 below. In this configuration the conservation of momentum is calculated over the connection of adjoining control volumes in **staggered grid** fashion. This choice is convenient because it allows control volumes to be conveniently connected through pressure as well to allow for pressure loss devices to be incorporated at junctions instead of inside control volumes.
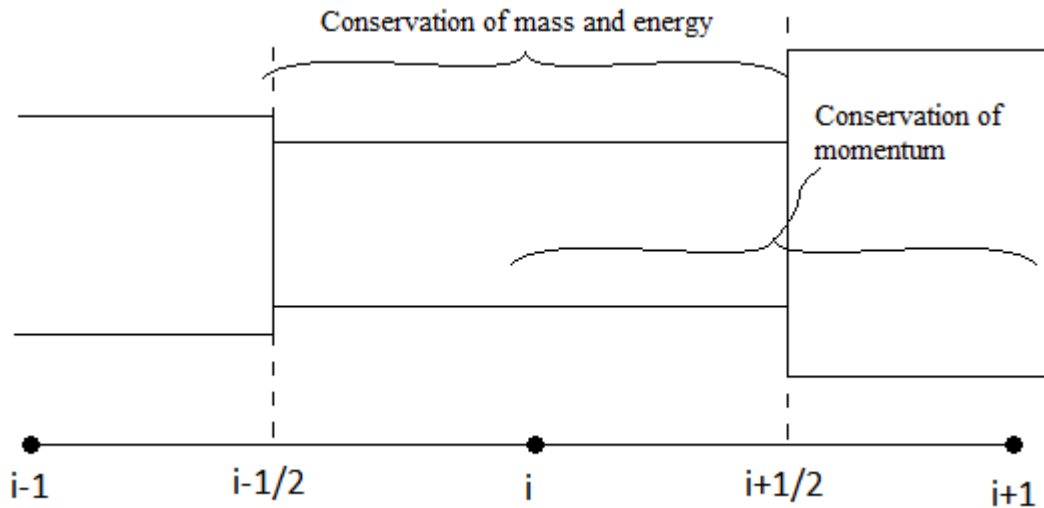


**Figure 1:** Simple layout of control volumes.

## 1.1 Conservation of Mass

The conservation of mass requires as a function of time, $t$, that the total mass of the system, $\alpha_g \rho_g + \alpha_f \rho_f$, be equal to that streaming in minus that streaming out (**subscript $g$ denotes steam and $f$ denotes liquid**):

$$\frac{d(\alpha_g \rho_g + \alpha_f \rho_f)}{dt} = \frac{1}{V} \int_S \alpha_g \rho_g . (\vec{v_g} \cdot \hat{n}).dA + \frac{1}{V} \int_S \alpha_f \rho_f . (\vec{v_f} \cdot \hat{n}).dA$$

And by applying it to the control volume:

$$\left( \frac{d(\alpha_g \rho_g + \alpha_f \rho_f)}{dt} \right)_i = \frac{1}{V_i} \left[ (\alpha_g \rho_g . A . v_g)_{i-\frac{1}{2}} - (\alpha_g \rho_g . A . v_g)_{i+\frac{1}{2}} \right]$$
$$+ \frac{1}{V_i} \left[ (\alpha_f \rho_f . A . v_f)_{i-\frac{1}{2}} - (\alpha_f \rho_f . A . v_f)_{i+\frac{1}{2}} \right] \tag{1}$$

Where:

$\alpha$ = phasic volume fraction

$\rho$ = density

$v$ = velocity.

$V$ = Volume.

$A$ = Area.

$\hat{n}$ = Surface normal.

## 1.2 Conservation of Momentum

The change in momentum, where momentum is the product of mass $m$ and velocity, $m_i . v_i$, in a control volume $i$ must balance the momentum of all the in and out flows as well as any forces applied. Additionally the momentum transfer during phase change, associated with vapor generation rate $\gamma_g$, gets applied in the balance:

$$\frac{d(m_f v_f)}{dt} + \frac{d(m_g v_g)}{dt} = \int_S \alpha_f \rho_f . (\vec{v_f}^2 \cdot \hat{n}).dA + m_f g_i - F_{f,\tau}$$
$$+ \int_S \alpha_g \rho_g . (\vec{v_g}^2 \cdot \hat{n}).dA + m_g g_i - F_{g,\tau}$$
$$+ \int_S P \cdot \hat{n}.dA - \Delta P_{loss} . A_{loss} - \gamma_g (v_g - v_f)$$

Where:

$P$ = Volume pressure

$\rho$ = Density

$\gamma_g$ = Vapor generation rate $[kg/s]$

$\Delta P_{loss}$ = Volume bulk pressure loss

$F_\tau$ is the wall friction force and $g_i$ is the gravitational component (i.e. $g_i = g.sin\theta_i$, $g = -9.81m.s^{-2}$). The volume bulk pressure loss, $\Delta P_{loss}$, is normally associated with a certain area, $A_{loss}$, making its application convenient for associating the loss with a junction or valve component.

The format of the momentum flux, $\int_S \rho.(\vec{v}^2 \cdot \hat{n}).dA$, can be altered according Gauss's divergence theorem to the following (the half arises from the fundamentals of the theorem):

$$\int (\hat{d}.v^2 \cdot \hat{n}).dA = \int \frac{1}{2} \cdot \hat{d} \cdot \frac{d(v^2)}{dx}.dV$$

Since this modification loses the sense of direction we add the variable $\hat{d}$, where $\hat{d}$ is the direction value (either $+1$ or $-1$).

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

$$
\begin{aligned}
\frac{d(\alpha_g\rho_g v_g)_{i+\frac{1}{2}}}{dt} + \frac{d(\alpha_f\rho_f v_f)_{i+\frac{1}{2}}}{dt} = & \frac{1}{2}\alpha_g\rho_{g,i+\frac{1}{2}} \cdot \frac{d_{g,i}.(v_{g,i})^2 - d_{g,i+1}.(v_{g,i+1})^2}{\Delta x_{i+\frac{1}{2}}} \\
& + \frac{1}{2}\alpha_f\rho_{f,i+\frac{1}{2}} \cdot \frac{d_{f,i}.(v_{f,i})^2 - d_{f,i+1}.(v_{f,i+1})^2}{\Delta x_{i+\frac{1}{2}}} \\
& - \frac{P_{i+1} - P_i}{\Delta x_{i+\frac{1}{2}}} + \alpha_g\rho_{g,i+\frac{1}{2}}.g_{i+\frac{1}{2}} + \alpha_f\rho_{f,i+\frac{1}{2}}.g_{i+\frac{1}{2}} \\
& - \frac{\Delta P_{\tau,i}A_{\tau,i}}{2V_i} - \frac{\Delta P_{\tau,i+1}A_{\tau,i+1}}{2V_{i+1}} \\
& - \frac{\Delta P_{loss,i+\frac{1}{2}}A_{loss,i+\frac{1}{2}}}{V_{i+1}} - \Gamma_g(v_{g,i+\frac{1}{2}} - v_{f,i+\frac{1}{2}})
\end{aligned}
\tag{2}
$$

$\Gamma_g$ = Volumetric vapor generation rate $[kg/m^3.s]$

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 friction related losses $\Delta P_\tau.A_\tau$ is associated with the wall friction, this together with the volume bulk pressure loss, $\Delta P_{loss}$, is discussed in later section. Here the wall friction over a junction is taken as the arithmetic average of two adjoining volumes whilst the bulk loss remains isolated to the junction.

## 1.3   Conservation of Energy

The total phasic 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. Additionally, phase change will also include a component. The governing equation for each phase is therefore:

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

Where:

$e/E$   = Total/Specific energy of the system.

$h$   = Heat of formation.

$Q$   = 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, $mgz$:

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

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 (stationary) 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, $A_s$. Also, the interface between phases is also subject to heat transfer, therefore:

$$Q_i = \dot{q}_{w,i}.A_{s,i} + \dot{q}_{\sigma,i}.A_{\sigma,i}$$

The components of work include shaft work, $W_{shaft}$, and pressure work, $W_{pressure}$. The pressure work originates from moving boundaries experience pressure differences. For a single phase control volume this would only include the pressure at the boundaries. For two phase flow however, one also needs to consider the change in volume fraction and hence the volume pressure multiplied by the rate of change of volume fraction needs to be added:

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

From here the energy conservation equation becomes:

$$\frac{d}{dt}\left(m.u\right) = (\rho Av)_{i-\frac{1}{2}}.(u+gz)_{i-\frac{1}{2}} - (\rho Av)_{i+\frac{1}{2}}.(u+gz)_{i+\frac{1}{2}}$$

$$+ \dot{q}_i.A_{s,i} + \dot{q}_{\sigma,i}.A_{\sigma,i} + \left[(P.A.v)_{i-\frac{1}{2}} - (P.A.v)_{i+\frac{1}{2}}\right] - P_iV_i\frac{d\alpha}{dt} + E_{loss} + \gamma h$$

Dividing by the volume we get:

$$\frac{d(\rho.u)_i}{dt} = \frac{1}{V_i}\left[(\rho Av)_{i-\frac{1}{2}}.(u+gz)_{i-\frac{1}{2}} - (\rho Av)_{i+\frac{1}{2}}.(u+gz)_{i+\frac{1}{2}}\right]$$

$$+ \frac{A_{s,i}}{V_i}\dot{q}_{w,i} + \frac{A_{\sigma,i}}{V_i}\dot{q}_{\sigma,i} + \frac{1}{V_i}\left[(P.A.v)_{i-\frac{1}{2}} - (P.A.v)_{i+\frac{1}{2}}\right] - P_i\frac{d\alpha}{dt} + \frac{E_{loss}}{V_i} + \Gamma h$$

We can now proceed to write such a balance equation for each phase:

$$\frac{d(\alpha_g\rho_g.u_g)_i}{dt} = \frac{1}{V_i}\left[(\alpha_g\rho_g Av_g)_{i-\frac{1}{2}}.(u_g+gz)_{i-\frac{1}{2}} - (\alpha_g\rho_g Av_g)_{i+\frac{1}{2}}.(u_g+gz)_{i+\frac{1}{2}}\right]$$

$$+ \frac{A_{s,i}}{V_i}\dot{q}_{gw,i} + \frac{A_{\sigma,i}}{V_i}\dot{q}_{g\sigma,i} + \frac{1}{V_i}\left[(P.A.v_g)_{i-\frac{1}{2}} - (P.A.v_g)_{i+\frac{1}{2}}\right] - P_i\frac{d\alpha_g}{dt} + \frac{E_{g,loss}}{V_i} + \Gamma_g h_g \tag{3}$$

$$\frac{d(\alpha_f\rho_f.u_f)_i}{dt} = \frac{1}{V_i}\left[(\alpha_f\rho_f Av_f)_{i-\frac{1}{2}}.(u_f+gz)_{i-\frac{1}{2}} - (\alpha_f\rho_f Av_f)_{i+\frac{1}{2}}.(u_f+gz)_{i+\frac{1}{2}}\right]$$

$$+ \frac{A_{s,i}}{V_i}\dot{q}_{fw,i} + \frac{A_{\sigma,i}}{V_i}\dot{q}_{f\sigma,i} + \frac{1}{V_i}\left[(P.A.v_f)_{i-\frac{1}{2}} - (P.A.v_f)_{i+\frac{1}{2}}\right] - P_i\frac{d\alpha_f}{dt} + \frac{E_{f,loss}}{V_i} - \Gamma_g h_f \tag{4}$$

## 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):

$$Y_i = f(P_i, X_i) \tag{5}$$

## 1.5    Wall friction, $P_\tau$

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:

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

$$\Delta P_{\tau,i+1} = \frac{1}{4} f_{i+1} \rho_{i+1} \frac{L_{i+1}}{D_{H,i+1}} v_{i+1}^2$$

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.

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

## 1.6    Junction pressure loss, $\Delta P_{loss}$

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

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

# 2 Phasic difference equations

The phasic difference equations arise from equating the relevant phasic mass- and momentum exchange equations. Such equations arise because of the additional condition of balance relative to the interface.

## 2.1 Phasic mass difference

The vapor phase mass conservation becomes:

$$\frac{d(\alpha_g \rho_g)}{dt} - \frac{1}{V} \int_S \alpha_g \rho_g.(\vec{v_g} \cdot \hat{n}).dA = \Gamma_g$$

And the liquid phase mass conservation becomes:

$$\frac{d(\alpha_f \rho_f)}{dt} - \frac{1}{V} \int_S \alpha_f \rho_f.(\vec{v_f} \cdot \hat{n}).dA = -\Gamma_g$$

Subtracting these two equations and applying it to the control volume we get:

$$
\begin{aligned}
\left(\frac{d(\alpha_g \rho_g - \alpha_f \rho_f)}{dt}\right)_i &- \frac{1}{V_i}\left[(\alpha_g \rho_g.A.v_g)_{i-\frac{1}{2}} - (\alpha_g \rho_g.A.v_g)_{i+\frac{1}{2}}\right] \\
&+ \frac{1}{V_i}\left[(\alpha_f \rho_f.A.v_f)_{i-\frac{1}{2}} - (\alpha_f \rho_f.A.v_f)_{i+\frac{1}{2}}\right] \\
&= 2\Gamma_g
\end{aligned}
\tag{6}
$$

## 2.2 Phasic momentum difference

The momentum conservation for each phase is described relative to the interface velocity, $v_\sigma$, and the interface drag force, $F_\sigma$. The vapor phase momentum conservation becomes:

$$
\begin{aligned}
\frac{d(m_g v_g)}{dt} &= \int_S \alpha_g \rho_g.(\vec{v_g}^2 \cdot \hat{n}).dA + m_g g_i - F_{g,\tau} \\
&+ \int_S \alpha_g P \cdot \hat{n}.dA - \gamma_g(v_g - v_\sigma) - F_\sigma - \Delta P_{loss,g}.A_{loss}
\end{aligned}
$$

And the liquid phase momentum conservation becomes:

$$
\begin{aligned}
\frac{d(m_f v_f)}{dt} &= \int_S \alpha_f \rho_f.(\vec{v_f}^2 \cdot \hat{n}).dA + m_f g_i - F_{f,\tau} \\
&+ \int_S \alpha_f P \cdot \hat{n}.dA + \gamma_g(v_f - v_\sigma) + F_\sigma - \Delta P_{loss,f}.A_{loss}
\end{aligned}
$$

Subtracting these two equations we get:

$$\frac{d(m_g v_g)}{dt} - \frac{d(m_f v_f)}{dt} = \int_S \alpha_g \rho_g .(\vec{v_g}^2 \cdot \hat{n}).dA + m_g g_i - F_{g,\tau}$$

$$- \int_S \alpha_f \rho_f .(\vec{v_f}^2 \cdot \hat{n}).dA - m_f g_i + F_{f,\tau}$$

$$+ \int_S (\alpha_g - \alpha_f) P \cdot \hat{n}.dA - \Delta P^*_{loss}.A_{loss}$$

$$- \gamma_g(v_g - v_\sigma) - \gamma_g(v_f - v_\sigma) - 2F_\sigma$$

In this equation the starred quantities (*) denote the difference of the phasic losses instead of the summation. Applying this to a junction we get:

$$\frac{d(\alpha_g \rho_g v_g)_{i+\frac{1}{2}}}{dt} - \frac{d(\alpha_f \rho_f v_f)_{i+\frac{1}{2}}}{dt} = \frac{1}{2}\alpha_g \rho_{g,i+\frac{1}{2}} \cdot \frac{d_{g,i}.(v_{g,i})^2 - d_{g,i+1}.(v_{g,i+1})^2}{\Delta x_{i+\frac{1}{2}}}$$

$$- \frac{1}{2}\alpha_f \rho_{f,i+\frac{1}{2}} \cdot \frac{d_{f,i}.(v_{f,i})^2 - d_{f,i+1}.(v_{f,i+1})^2}{\Delta x_{i+\frac{1}{2}}}$$

$$- (\alpha_g - \alpha_f)\frac{P_{i+1} - P_i}{\Delta x_{i+\frac{1}{2}}} + \alpha_g \rho_{g,i+\frac{1}{2}}.g_{i+\frac{1}{2}} - \alpha_f \rho_{f,i+\frac{1}{2}}.g_{i+\frac{1}{2}} \qquad (7)$$

$$- \frac{\Delta P^*_{\tau,i} A_i}{2V_i} - \frac{\Delta P^*_{\tau,i+1} A_{\tau,i+1}}{2V_{i+1}} - \frac{\Delta P^*_{loss,i+\frac{1}{2}} A_{\tau,i+\frac{1}{2}}}{V_{i+1}}$$

$$- \Gamma_g(v_{g,i+\frac{1}{2}} - v_{\sigma,i+\frac{1}{2}}) - \Gamma_g(v_{f,i+\frac{1}{2}} - v_{\sigma,i+\frac{1}{2}}) - 2\frac{\Delta P_\sigma.A_\sigma}{V^*_{i+\frac{1}{2}}}$$

Where:

$\Delta P_\sigma$   = Inter-phase drag associated pressure loss.

# 3 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 $n + 1$.

## 3.1 Conservation of Mass - finite difference formulation

The finite difference formulation is as follows:

$$\frac{(\alpha_g \rho_g + \alpha_f \rho_f)_i^{n+1} - (\alpha_g \rho_g + \alpha_f \rho_f)_i^n}{\Delta t} = \frac{1}{V_i} \left[ (\alpha_g \rho_g . A)_{i-\frac{1}{2}}^n (.v_g)_{i-\frac{1}{2}}^{n+1} - (\alpha_g \rho_g . A)_{i+\frac{1}{2}}^n (v_g)_{i+\frac{1}{2}}^{n+1} \right]$$
$$+ \frac{1}{V_i} \left[ (\alpha_f \rho_f . A)_{i-\frac{1}{2}}^n (v_f)_{i-\frac{1}{2}}^{n+1} - (\alpha_f \rho_f . A)_{i+\frac{1}{2}}^n (v_f)_{i+\frac{1}{2}}^{n+1} \right]$$

The difference of the product term is linearized as follows:

$$(\alpha_g \rho_g)^{n+1} - (\alpha_g \rho_g)^n = \alpha_g^n (\rho_g^{n+1} - \rho_g^n) + \rho_g^n (\alpha_g^{n+1} - \alpha_g^n)$$
$$(\alpha_f \rho_f)^{n+1} - (\alpha_f \rho_f)^n = \alpha_f^n (\rho_f^{n+1} - \rho_f^n) + \rho_f^n (\alpha_f^{n+1} - \alpha_f^n)$$

Therefore the above equation becomes:

$$\alpha_g^n (\rho_g^{n+1} - \rho_g^n) + \rho_g^n (\alpha_g^{n+1} - \alpha_g^n) + \alpha_f^n (\rho_f^{n+1} - \rho_f^n) + \rho_f^n (\alpha_f^{n+1} - \alpha_f^n)$$
$$= \frac{1}{V_i} \left[ (\alpha_g \rho_g . A)_{i-\frac{1}{2}}^n (.v_g)_{i-\frac{1}{2}}^{n+1} - (\alpha_g \rho_g . A)_{i+\frac{1}{2}}^n (v_g)_{i+\frac{1}{2}}^{n+1} \right] \tag{8}$$
$$+ \frac{1}{V_i} \left[ (\alpha_f \rho_f . A)_{i-\frac{1}{2}}^n (v_f)_{i-\frac{1}{2}}^{n+1} - (\alpha_f \rho_f . A)_{i+\frac{1}{2}}^n (v_f)_{i+\frac{1}{2}}^{n+1} \right]$$

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

$$\frac{d(\alpha_g \rho_g v_g)_{i+\frac{1}{2}}}{dt} + \frac{d(\alpha_f \rho_f v_f)_{i+\frac{1}{2}}}{dt} = \frac{1}{2}\alpha_g \rho_{g,i+\frac{1}{2}} \cdot \frac{d_{g,i}.(v_{g,i})^2 - d_{g,i+1}.(v_{g,i+1})^2}{\Delta x_{i+\frac{1}{2}}}$$

$$+ \frac{1}{2}\alpha_f \rho_{f,i+\frac{1}{2}} \cdot \frac{d_{f,i}.(v_{f,i})^2 - d_{f,i+1}.(v_{f,i+1})^2}{\Delta x_{i+\frac{1}{2}}}$$

$$- \frac{P_{i+1} - P_i}{\Delta x_{i+\frac{1}{2}}} + \alpha_g \rho_{g,i+\frac{1}{2}}.g_{i+\frac{1}{2}} + \alpha_f \rho_{f,i+\frac{1}{2}}.g_{i+\frac{1}{2}}$$

$$- \frac{\Delta P_{\tau,i} A_{\tau,i}}{2V_i} - \frac{\Delta P_{\tau,i+1} A_{\tau,i+1}}{2V_{i+1}}$$

$$- \frac{\Delta P_{loss,i+\frac{1}{2}} A_{i+\frac{1}{2}}}{V_{i+1}} - \Gamma_g(v_{g,i+\frac{1}{2}} - v_{f,i+\frac{1}{2}})$$

We use the following time notation:

$$\frac{(\alpha_g \rho_g)^n_{i+\frac{1}{2}}(v_g^{n+1} - v_g^n)_{i+\frac{1}{2}}}{\Delta t} + \frac{(\alpha_f \rho_f)^n_{i+\frac{1}{2}}(v_f^{n+1} - v_f^n)_{i+\frac{1}{2}}}{\Delta t}$$

$$= \frac{1}{2}(\alpha_g \rho_g)^n_{i+\frac{1}{2}} \cdot \frac{(d_{g,i}.v_{g,i}^2)^n - (d_{g,i+1}.v_{g,i+1}^2)^n}{\Delta x_{i+\frac{1}{2}}}$$

$$+ \frac{1}{2}(\alpha_f \rho_f)^n_{i+\frac{1}{2}} \cdot \frac{(d_{f,i}.v_{f,i}^2)^n - (d_{f,i+1}.v_{f,i+1}^2)^n}{\Delta x_{i+\frac{1}{2}}} \tag{9}$$

$$- \frac{P_{i+1}^{n+1} - P_i^{n+1}}{\Delta x_{i+\frac{1}{2}}} + (\alpha_g \rho_{g,i+\frac{1}{2}}.g_{i+\frac{1}{2}} + \alpha_f \rho_{f,i+\frac{1}{2}}.g_{i+\frac{1}{2}})^n$$

$$- \frac{\Delta P_{\tau,i}^n A_{\tau,i}}{2V_i} - \frac{\Delta P_{\tau,i+1}^n A_{\tau,i+1}}{2V_{i+1}}$$

$$- \frac{\Delta P_{loss,i+\frac{1}{2}}^n A_{i+\frac{1}{2}}}{V_{i+1}} - \Gamma_g^n(v_{g,i+\frac{1}{2}}^n - v_{f,i+\frac{1}{2}}^n)$$

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

## 3.3 Conservation of Energy - finite difference formulation

We start with the original conservation of energy equation:

$$\frac{d(\alpha_g \rho_g . u_g)_i}{dt} = \frac{1}{V_i}\left[(\alpha_g \rho_g A v_g)_{i-\frac{1}{2}}.(u_g + gz)_{i-\frac{1}{2}} - (\alpha_g \rho_g A v_g)_{i+\frac{1}{2}}.(u_g + gz)_{i+\frac{1}{2}}\right]$$
$$+ \frac{A_{s,i}}{V_i}\dot{q}_{gw,i} + \frac{A_{\sigma,i}}{V_i}\dot{q}_{g\sigma,i} + \frac{1}{V_i}\left[(P.A.v_g)_{i-\frac{1}{2}} - (P.A.v_g)_{i+\frac{1}{2}}\right] - P_i\frac{d\alpha_g}{dt} + \frac{E_{g,loss}}{V_i} + \Gamma_g h_g$$

$$\frac{d(\alpha_f \rho_f . u_f)_i}{dt} = \frac{1}{V_i}\left[(\alpha_f \rho_f A v_f)_{i-\frac{1}{2}}.(u_f + gz)_{i-\frac{1}{2}} - (\alpha_f \rho_f A v_f)_{i+\frac{1}{2}}.(u_f + gz)_{i+\frac{1}{2}}\right]$$
$$+ \frac{A_{s,i}}{V_i}\dot{q}_{fw,i} + \frac{A_{\sigma,i}}{V_i}\dot{q}_{f\sigma,i} + \frac{1}{V_i}\left[(P.A.v_f)_{i-\frac{1}{2}} - (P.A.v_f)_{i+\frac{1}{2}}\right] - P_i\frac{d\alpha_f}{dt} + \frac{E_{f,loss}}{V_i} - \Gamma_g h_f$$

Some special simplification of the vapor generation rate needs to be considered since the interface heat flux is related to this quantity. The total interface heat transfer rate is given by:

$$\frac{A_{\sigma,i}}{V_i}(\dot{q}_{g\sigma} + \dot{q}_{f\sigma}) = \Gamma_g(h_f - h_g)$$

In this equation it is necessary that one understands that the heat transfer to the gas phase is not necessarily the same as that from the liquid phase. An example of such a case is where the liquid phase is at a higher temperature than the vapor phase at which point the system is de-pressurized, at this point heat is being transfered by more evaporation as well at a temperature difference.

Hence we can lump the interface heat transfer rate with the vapor generation rate and thus for the vapor energy conservation we have:

$$\begin{aligned}
\frac{A_{\sigma,i}}{V_i}\dot{q}_{g\sigma} + \Gamma_g h_g &= \frac{A_{\sigma,i}}{V_i}\dot{q}_{g\sigma} + \frac{A_{\sigma,i}}{V_i}\frac{(\dot{q}_{g\sigma} + \dot{q}_{f\sigma})}{(h_f - h_g)}h_g \\
&= \frac{A_{\sigma,i}}{V_i}\left[\dot{q}_{g\sigma} - \frac{(\dot{q}_{g\sigma} + \dot{q}_{f\sigma})}{(h_g - h_f)}h_g\right] \\
&= \frac{A_{\sigma,i}}{V_i}\left[\frac{\dot{q}_{g\sigma}(h_g - h_f) - (\dot{q}_{g\sigma} + \dot{q}_{f\sigma})h_g}{(h_g - h_f)}\right] \\
&= \frac{A_{\sigma,i}}{V_i}\left[\frac{\dot{q}_{g\sigma}h_g - \dot{q}_{g\sigma}h_f - \dot{q}_{g\sigma}h_g - \dot{q}_{f\sigma}h_g}{(h_g - h_f)}\right] \\
&= \frac{A_{\sigma,i}}{V_i}\left[\frac{-\dot{q}_{g\sigma}h_f - \dot{q}_{f\sigma}h_g}{(h_g - h_f)}\right] \\
&= \frac{A_{\sigma,i}}{V_i}\left[\frac{-h_f}{(h_g - h_f)}\right]\dot{q}_{g\sigma} + \frac{A_{\sigma,i}}{V_i}\left[\frac{-h_g}{(h_g - h_f)}\right]\dot{q}_{f\sigma}
\end{aligned}$$

Similarly, for the liquid phase:

$$
\begin{aligned}
\frac{A_{\sigma,i}}{V_i}\dot{q}_{f\sigma} - \Gamma_g h_f &= \frac{A_{\sigma,i}}{V_i}\dot{q}_{f\sigma} - \frac{A_{\sigma,i}}{V_i}\frac{(\dot{q}_{g\sigma} + \dot{q}_{f\sigma})}{(h_f - h_g)}h_f \\
&= \frac{A_{\sigma,i}}{V_i}\left[\dot{q}_{f\sigma} + \frac{(\dot{q}_{g\sigma} + \dot{q}_{f\sigma})}{(h_g - h_f)}h_f\right] \\
&= \frac{A_{\sigma,i}}{V_i}\left[\frac{\dot{q}_{f\sigma}(h_g - h_f) + (\dot{q}_{g\sigma} + \dot{q}_{f\sigma})h_f}{(h_g - h_f)}\right] \\
&= \frac{A_{\sigma,i}}{V_i}\left[\frac{\dot{q}_{f\sigma}h_g - \dot{q}_{f\sigma}h_f + \dot{q}_{g\sigma}h_f + \dot{q}_{f\sigma}h_f}{(h_g - h_f)}\right] \\
&= \frac{A_{\sigma,i}}{V_i}\left[\frac{\dot{q}_{f\sigma}h_g + \dot{q}_{g\sigma}h_f}{(h_g - h_f)}\right] \\
&= \frac{A_{\sigma,i}}{V_i}\left[\frac{h_f}{(h_g - h_f)}\right]\dot{q}_{g\sigma} + \frac{A_{\sigma,i}}{V_i}\left[\frac{h_g}{(h_g - h_f)}\right]\dot{q}_{f\sigma}
\end{aligned}
$$

With these simplifications in hand we can rewrite the energy equations whilst using the following time notation for the vapor phase:

$$
\frac{(\alpha_g \rho_g . u_g)_i^{n+1} - (\alpha_g \rho_g . u_g)_i^{n}}{\Delta t} + P_i^n \left( \frac{\alpha_g^{n+1} - \alpha_g^n}{\Delta t} \right)
$$

$$
= \frac{1}{V_i} \left[ (\alpha_g \rho_g A (u_g + gz))_{i-\frac{1}{2}}^n . (v_g)_{i-\frac{1}{2}}^{n+1} - (\alpha_g \rho_g A (u_g + gz))_{i+\frac{1}{2}}^n . (v_g)_{i+\frac{1}{2}}^{n+1} \right]
$$

$$
+ \frac{A_{s,i}}{V_i} \dot{q}_{gw,i}^n + \frac{1}{V_i} \left[ (P.A)_{i-\frac{1}{2}}^n (v_g)_{i-\frac{1}{2}}^{n+1} - (P.A)_{i+\frac{1}{2}}^n (v_g)_{i+\frac{1}{2}}^{n+1} \right] + \frac{E_{g,loss}^n}{V_i}
$$

$$
+ \frac{A_{\sigma,i}}{V_i} \left[ \frac{-h_f}{(h_g - h_f)} \right] \dot{q}_{g\sigma} + \frac{A_{\sigma,i}}{V_i} \left[ \frac{-h_g}{(h_g - h_f)} \right] \dot{q}_{f\sigma}
$$

And for the liquid phase:

$$
\frac{(\alpha_f \rho_f . u_f)_i^{n+1} - (\alpha_f \rho_f . u_f)_i^{n}}{\Delta t} + P_i^n \left( \frac{\alpha_f^{n+1} - \alpha_f^n}{\Delta t} \right)
$$

$$
= \frac{1}{V_i} \left[ (\alpha_f \rho_f A (u_f + gz))_{i-\frac{1}{2}}^n . (v_f)_{i-\frac{1}{2}}^{n+1} - (\alpha_f \rho_g A (u_f + gz))_{i+\frac{1}{2}}^n . (v_f)_{i+\frac{1}{2}}^{n+1} \right]
$$

$$
+ \frac{A_{s,i}}{V_i} \dot{q}_{fw,i}^n + \frac{1}{V_i} \left[ (P.A)_{i-\frac{1}{2}}^n (v_f)_{i-\frac{1}{2}}^{n+1} - (P.A)_{i+\frac{1}{2}}^n (v_f)_{i+\frac{1}{2}}^{n+1} \right] + \frac{E_{f,loss}^n}{V_i}
$$

$$
+ \frac{A_{\sigma,i}}{V_i} \left[ \frac{h_f}{(h_g - h_f)} \right] \dot{q}_{g\sigma} + \frac{A_{\sigma,i}}{V_i} \left[ \frac{h_g}{(h_g - h_f)} \right] \dot{q}_{f\sigma}
$$

These two equations present some difficulty with the non-linear term $(\alpha \rho . u)_i^{n+1}$ and hence we can linearize this as follows:

$$
(\alpha \rho . u)_i^{n+1} - (\alpha \rho . u)_i^{n} = (\alpha \rho)^n (u^{n+1} - u^n) + (\alpha u)^n (\rho^{n+1} - \rho^n) + (\rho u)^n (\alpha^{n+1} - \alpha^n)
$$

Therefore the equations above become:

For the vapor phase:

$$
\frac{(\alpha_g\rho_g)_i^n(u_g^{n+1}-u_g^n)_i + (\alpha_g u_g)_i^n(\rho_g^{n+1}-\rho_g^n)_i + (\rho_g u_g)_i^n(\alpha_g^{n+1}-\alpha_g^n)_i}{\Delta t} + P_i^n\left(\frac{\alpha_g^{n+1}-\alpha_g^n}{\Delta t}\right)
$$

$$
= \frac{1}{V_i}\left[(\alpha_g\rho_g A(u_g+gz))_{i-\frac{1}{2}}^n.(v_g)_{i-\frac{1}{2}}^{n+1} - (\alpha_g\rho_g A(u_g+gz))_{i+\frac{1}{2}}^n.(v_g)_{i+\frac{1}{2}}^{n+1}\right]
$$

$$
+ \frac{A_{s,i}}{V_i}\dot{q}_{gw,i}^n + \frac{1}{V_i}\left[(P.A)_{i-\frac{1}{2}}^n(v_g)_{i-\frac{1}{2}}^{n+1} - (P.A)_{i+\frac{1}{2}}^n(v_g)_{i+\frac{1}{2}}^{n+1}\right] + \frac{E_{g,loss}^n}{V_i}
$$

$$
+ \frac{A_{\sigma,i}}{V_i}\left[\frac{-h_f}{(h_g-h_f)}\right]\dot{q}_{g\sigma} + \frac{A_{\sigma,i}}{V_i}\left[\frac{-h_g}{(h_g-h_f)}\right]\dot{q}_{f\sigma}
$$

(10)

And for the liquid phase:

$$
\frac{(\alpha_f\rho_f)_i^n(u_f^{n+1}-u_f^n)_i + (\alpha_f u_f)_i^n(\rho_f^{n+1}-\rho_f^n)_i + (\rho_f u_f)_i^n(\alpha_f^{n+1}-\alpha_f^n)_i}{\Delta t} + P_i^n\left(\frac{\alpha_f^{n+1}-\alpha_f^n}{\Delta t}\right)
$$

$$
= \frac{1}{V_i}\left[(\alpha_f\rho_f A(u_f+gz))_{i-\frac{1}{2}}^n.(v_f)_{i-\frac{1}{2}}^{n+1} - (\alpha_f\rho_g A(u_f+gz))_{i+\frac{1}{2}}^n.(v_f)_{i+\frac{1}{2}}^{n+1}\right]
$$

$$
+ \frac{A_{s,i}}{V_i}\dot{q}_{fw,i}^n + \frac{1}{V_i}\left[(P.A)_{i-\frac{1}{2}}^n(v_f)_{i-\frac{1}{2}}^{n+1} - (P.A)_{i+\frac{1}{2}}^n(v_f)_{i+\frac{1}{2}}^{n+1}\right] + \frac{E_{f,loss}^n}{V_i}
$$

$$
+ \frac{A_{\sigma,i}}{V_i}\left[\frac{h_f}{(h_g-h_f)}\right]\dot{q}_{g\sigma} + \frac{A_{\sigma,i}}{V_i}\left[\frac{h_g}{(h_g-h_f)}\right]\dot{q}_{f\sigma}
$$

(11)

## 3.4 Phasic mass difference

We start with the base equation:

$$\left(\frac{d(\alpha_g\rho_g - \alpha_f\rho_f)}{dt}\right)_i - \frac{1}{V_i}\left[(\alpha_g\rho_g.A.v_g)_{i-\frac{1}{2}} - (\alpha_g\rho_g.A.v_g)_{i+\frac{1}{2}}\right]$$
$$+ \frac{1}{V_i}\left[(\alpha_f\rho_f.A.v_f)_{i-\frac{1}{2}} - (\alpha_f\rho_f.A.v_f)_{i+\frac{1}{2}}\right]$$
$$= 2\Gamma_g$$

And we apply the following time discretization:

$$\left(\frac{(\alpha_g\rho_g - \alpha_f\rho_f)^{n+1} - (\alpha_g\rho_g - \alpha_f\rho_f)^n}{\Delta t}\right)_i - \frac{1}{V_i}\left[(\alpha_g\rho_g.A)_{i-\frac{1}{2}}^n(.v_g)_{i-\frac{1}{2}}^{n+1} - (\alpha_g\rho_g.A)_{i+\frac{1}{2}}^n(v_g)_{i+\frac{1}{2}}^{n+1}\right]$$
$$+ \frac{1}{V_i}\left[(\alpha_f\rho_f.A)_{i-\frac{1}{2}}^n(v_f)_{i-\frac{1}{2}}^{n+1} - (\alpha_f\rho_f.A)_{i+\frac{1}{2}}^n(v_f)_{i+\frac{1}{2}}^{n+1}\right]$$
$$= 2(\Gamma_g)_j^{n+1}$$

Again we can apply the linearization:

$$(\alpha_g\rho_g)^{n+1} - (\alpha_g\rho_g)^n = \alpha_g^n(\rho_g^{n+1} - \rho_g^n) + \rho_g^n(\alpha_g^{n+1} - \alpha_g^n)$$
$$(\alpha_f\rho_f)^{n+1} - (\alpha_f\rho_f)^n = \alpha_f^n(\rho_f^{n+1} - \rho_f^n) + \rho_f^n(\alpha_f^{n+1} - \alpha_f^n)$$

And hence we get:

$$\alpha_g^n(\rho_g^{n+1} - \rho_g^n) + \rho_g^n(\alpha_g^{n+1} - \alpha_g^n) - \alpha_f^n(\rho_f^{n+1} - \rho_f^n) + \rho_f^n(\alpha_f^{n+1} - \alpha_f^n)$$
$$- \frac{1}{V_i}\left[(\alpha_g\rho_g.A)_{i-\frac{1}{2}}^n(.v_g)_{i-\frac{1}{2}}^{n+1} - (\alpha_g\rho_g.A)_{i+\frac{1}{2}}^n(v_g)_{i+\frac{1}{2}}^{n+1}\right]$$
$$+ \frac{1}{V_i}\left[(\alpha_f\rho_f.A)_{i-\frac{1}{2}}^n(v_f)_{i-\frac{1}{2}}^{n+1} - (\alpha_f\rho_f.A)_{i+\frac{1}{2}}^n(v_f)_{i+\frac{1}{2}}^{n+1}\right]$$
$$= 2(\Gamma_g)_j^{n+1}$$

(12)

## 3.5 Phasic momentum difference

We start with the previously derived equation:

$$
\frac{d(\alpha_g \rho_g v_g)_{i+\frac{1}{2}}}{dt} - \frac{d(\alpha_f \rho_f v_f)_{i+\frac{1}{2}}}{dt} = \frac{1}{2} \alpha_g \rho_{g,i+\frac{1}{2}} \cdot \frac{d_{g,i} \cdot (v_{g,i})^2 - d_{g,i+1} \cdot (v_{g,i+1})^2}{\Delta x_{i+\frac{1}{2}}}
$$

$$
- \frac{1}{2} \alpha_f \rho_{f,i+\frac{1}{2}} \cdot \frac{d_{f,i} \cdot (v_{f,i})^2 - d_{f,i+1} \cdot (v_{f,i+1})^2}{\Delta x_{i+\frac{1}{2}}}
$$

$$
- (\alpha_g - \alpha_f) \frac{P_{i+1} - P_i}{\Delta x_{i+\frac{1}{2}}} + \alpha_g \rho_{g,i+\frac{1}{2}} \cdot g_{i+\frac{1}{2}} - \alpha_f \rho_{f,i+\frac{1}{2}} \cdot g_{i+\frac{1}{2}}
$$

$$
- \frac{\Delta P^*_{\tau,i} A_i}{2V_i} - \frac{\Delta P^*_{\tau,i+1} A_{\tau,i+1}}{2V_{i+1}} - \frac{\Delta P^*_{loss,i+\frac{1}{2}} A_{\tau,i+\frac{1}{2}}}{V_{i+1}}
$$

$$
- \Gamma_g (v_{g,i+\frac{1}{2}} - v_{\sigma,i+\frac{1}{2}}) - \Gamma_g (v_{f,i+\frac{1}{2}} - v_{\sigma,i+\frac{1}{2}}) - 2 \frac{\Delta P_\sigma . A_\sigma}{V^*_{i+\frac{1}{2}}}
$$

And we apply the following time discretization:

$$
\frac{(\alpha_g \rho_g)^n_{i+\frac{1}{2}} (v_g^{n+1} - v_g^{n+1})}{\Delta t} - \frac{(\alpha_f \rho_f)^n_{i+\frac{1}{2}} (v_f^{n+1} - v_f^{n+1})}{\Delta t}
$$

$$
= \frac{1}{2} (\alpha_g \rho_g)^n_{i+\frac{1}{2}} \cdot \frac{d_{g,i}^n \cdot (v_{g,i}^n)^2 - d_{g,i+1}^n \cdot (v_{g,i+1}^n)^2}{\Delta x_{i+\frac{1}{2}}}
$$

$$
- \frac{1}{2} (\alpha_f \rho_f)^n_{i+\frac{1}{2}} \cdot \frac{d_{f,i}^n \cdot (v_{f,i}^n)^2 - d_{f,i+1}^n \cdot (v_{f,i+1}^n)^2}{\Delta x_{i+\frac{1}{2}}}
$$

$$
- (\alpha_g - \alpha_f)^n_{i+\frac{1}{2}} \frac{P_{i+1}^{n+1} - P_i^{n+1}}{\Delta x_{i+\frac{1}{2}}} + (\alpha_g \rho_g . g)^n_{i+\frac{1}{2}} - (\alpha_f \rho_f . g)^n_{i+\frac{1}{2}}
$$

$$
- \left( \frac{\Delta P^*_{\tau,i} A_i}{2V_i} - \frac{\Delta P^*_{\tau,i+1} A_{\tau,i+1}}{2V_{i+1}} \right)^n - \left( \frac{\Delta P^*_{loss,i+\frac{1}{2}} A_{\tau,i+\frac{1}{2}}}{V_{i+1}} \right)^n
$$

$$
- \Gamma_g^n (v_{g,i+\frac{1}{2}}^{n+1} - v_{\sigma,i+\frac{1}{2}}^n) - \Gamma_g^n (v_{f,i+\frac{1}{2}}^{n+1} - v_{\sigma,i+\frac{1}{2}}^n) - 2 \frac{\Delta P_\sigma^n . A_\sigma}{V^*_{i+\frac{1}{2}}}
$$

(13)

## 3.6 Equation of state numerical implementation

The equation of state refers to the lookup of thermo-physical properties of a fluid given certain parameters of which the most prominent are pressure, $P$, and internal energy, $u$. For the simulation of non-condensible fluids (i.e. air), as is done in the RELAP5 code [2], one can add the contribution of non-condensible mass fraction, $X_n$, however such a capability will be added later. For the current capability a linearization of the following function calls are needed:

$$\rho_g = \rho_g(P, u_g)$$
$$\rho_f = \rho_f(P, u_f)$$

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

$$\left(\frac{d\rho}{du}\right)_i^n = \frac{\rho_{EOS}(P_i^n, T_i^n + \Delta T) - \rho_{EOS}(P_i^n, T_i^n - \Delta T)}{u_{EOS}(P_i^n, T_i^n + \Delta T) - u_{EOS}(P_i^n, T_i^n - \Delta T)}$$

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

For the vapor phase:

$$(\rho_g^{n+1} - \rho_g^n)_i = \left(\frac{d\rho_g}{du_g}\right)_i^n \cdot (u_g^{n+1} - u_g^n)_i \tag{14}$$

And the liquid phase:

$$(\rho_f^{n+1} - \rho_f^n)_i = \left(\frac{d\rho_f}{du_f}\right)_i^n \cdot (u_f^{n+1} - u_f^n)_i \tag{15}$$

## 3.7 Semi-implicit approach

From the set of equations 8 to 15 we can develop a system of unknowns. Before we depict how this is done, let us repeat these equations all together:

**(eq. 8) Mixture Mass:**

$$\alpha_g^n(\rho_g^{n+1} - \rho_g^n) + \rho_g^n(\alpha_g^{n+1} - \alpha_g^n) + \alpha_f^n(\rho_f^{n+1} - \rho_f^n) + \rho_f^n(\alpha_f^{n+1} - \alpha_f^n)$$

$$= \frac{1}{V_i}\left[(\alpha_g\rho_g.A)_{i-\frac{1}{2}}^n(.v_g)_{i-\frac{1}{2}}^{n+1} - (\alpha_g\rho_g.A)_{i+\frac{1}{2}}^n(v_g)_{i+\frac{1}{2}}^{n+1}\right]$$

$$+ \frac{1}{V_i}\left[(\alpha_f\rho_f.A)_{i-\frac{1}{2}}^n(v_f)_{i-\frac{1}{2}}^{n+1} - (\alpha_f\rho_f.A)_{i+\frac{1}{2}}^n(v_f)_{i+\frac{1}{2}}^{n+1}\right]$$

**(eq. 12) Phasic mass difference:**

$$\alpha_g^n(\rho_g^{n+1} - \rho_g^n) + \rho_g^n(\alpha_g^{n+1} - \alpha_g^n) - \alpha_f^n(\rho_f^{n+1} - \rho_f^n) + \rho_f^n(\alpha_f^{n+1} - \alpha_f^n)$$

$$- \frac{1}{V_i}\left[(\alpha_g\rho_g.A)_{i-\frac{1}{2}}^n(.v_g)_{i-\frac{1}{2}}^{n+1} - (\alpha_g\rho_g.A)_{i+\frac{1}{2}}^n(v_g)_{i+\frac{1}{2}}^{n+1}\right]$$

$$+ \frac{1}{V_i}\left[(\alpha_f\rho_f.A)_{i-\frac{1}{2}}^n(v_f)_{i-\frac{1}{2}}^{n+1} - (\alpha_f\rho_f.A)_{i+\frac{1}{2}}^n(v_f)_{i+\frac{1}{2}}^{n+1}\right] = 2(\Gamma_g)_j^{n+1}$$

**(eq. 9$^+$) Momentum summation:**

$$\frac{(\alpha_g\rho_g)_{i+\frac{1}{2}}^n(v_g^{n+1} - v_g^n)_{i+\frac{1}{2}}}{\Delta t} + \frac{(\alpha_f\rho_f)_{i+\frac{1}{2}}^n(v_f^{n+1} - v_f^n)_{i+\frac{1}{2}}}{\Delta t}$$

$$= \frac{1}{2}(\alpha_g\rho_g)_{i+\frac{1}{2}}^n \cdot \frac{(d_{g,i}.v_{g,i}^2)^n - (d_{g,i+1}.v_{g,i+1}^2)^n}{\Delta x_{i+\frac{1}{2}}} + \frac{1}{2}(\alpha_f\rho_f)_{i+\frac{1}{2}}^n \cdot \frac{(d_{f,i}.v_{f,i}^2)^n - (d_{f,i+1}.v_{f,i+1}^2)^n}{\Delta x_{i+\frac{1}{2}}}$$

$$- \frac{P_{i+1}^{n+1} - P_i^{n+1}}{\Delta x_{i+\frac{1}{2}}} + (\alpha_g\rho_{g,i+\frac{1}{2}}.g_{i+\frac{1}{2}} + \alpha_f\rho_{f,i+\frac{1}{2}}.g_{i+\frac{1}{2}})^n$$

$$- \frac{\Delta P_{\tau,i}^n A_{\tau,i}}{2V_i} - \frac{\Delta P_{\tau,i+1}^n A_{\tau,i+1}}{2V_{i+1}} - \frac{\Delta P_{loss,i+\frac{1}{2}}^n A_{i+\frac{1}{2}}}{V_{i+\frac{1}{2}}} - \Gamma_g^n(v_{g,i+\frac{1}{2}}^n - v_{f,i+\frac{1}{2}}^n)$$

**(eq. 9⁻) Momentum summation:**

$$\frac{(\alpha_g \rho_g)^n_{i-\frac{1}{2}}(v_g^{n+1}-v_g^n)_{i-\frac{1}{2}}}{\Delta t} + \frac{(\alpha_f \rho_f)^n_{i-\frac{1}{2}}(v_f^{n+1}-v_f^n)_{i-\frac{1}{2}}}{\Delta t}$$

$$= \frac{1}{2}(\alpha_g \rho_g)^n_{i-\frac{1}{2}} \cdot \frac{(d_{g,i-1}\cdot v^2_{g,i-1})^n - (d_{g,i}\cdot v^2_{g,i})^n}{\Delta x_{i-\frac{1}{2}}} + \frac{1}{2}(\alpha_f \rho_f)^n_{i-\frac{1}{2}} \cdot \frac{(d_{f,i-1}\cdot v^2_{f,i-1})^n - (d_{f,i}\cdot v^2_{f,i})^n}{\Delta x_{i-\frac{1}{2}}}$$

$$- \frac{P_i^{n+1}-P_{i-1}^{n+1}}{\Delta x_{i-\frac{1}{2}}} + (\alpha_g \rho_{g,i-\frac{1}{2}}\cdot g_{i-\frac{1}{2}} + \alpha_f \rho_{f,i-\frac{1}{2}}\cdot g_{i-\frac{1}{2}})^n$$

$$- \frac{\Delta P^n_{\tau,i-1}A_{\tau,i-1}}{2V_{i-1}} - \frac{\Delta P^n_{\tau,i}A_{\tau,i}}{2V_i} - \frac{\Delta P^n_{loss,i+\frac{1}{2}}A_{i+\frac{1}{2}}}{V_{i-\frac{1}{2}}} - \Gamma_g^n(v^n_{g,i-\frac{1}{2}} - v^n_{f,i-\frac{1}{2}})$$

**(eq. 13⁺) Momentum difference:**

$$\frac{(\alpha_g \rho_g)^n_{i+\frac{1}{2}}(v_g^{n+1}-v_g^{n+1})_{i+\frac{1}{2}}}{\Delta t} - \frac{(\alpha_f \rho_f)^n_{i+\frac{1}{2}}(v_f^{n+1}-v_f^{n+1})_{i+\frac{1}{2}}}{\Delta t}$$

$$= \frac{1}{2}(\alpha_g \rho_g)^n_{i+\frac{1}{2}} \cdot \frac{d^n_{g,i}\cdot (v^n_{g,i})^2 - d^n_{g,i+1}\cdot (v^n_{g,i+1})^2}{\Delta x_{i+\frac{1}{2}}} - \frac{1}{2}(\alpha_f \rho_f)^n_{i+\frac{1}{2}} \cdot \frac{d^n_{f,i}\cdot (v^n_{f,i})^2 - d^n_{f,i+1}\cdot (v^n_{f,i+1})^2}{\Delta x_{i+\frac{1}{2}}}$$

$$- (\alpha_g - \alpha_f)^n_{i+\frac{1}{2}}\frac{P_{i+1}^{n+1}-P_i^{n+1}}{\Delta x_{i+\frac{1}{2}}} + (\alpha_g \rho_g \cdot g)^n_{i+\frac{1}{2}} - (\alpha_f \rho_f \cdot g)^n_{i+\frac{1}{2}} - \left(\frac{\Delta P^*_{\tau,i}A_i}{2V_i} - \frac{\Delta P^*_{\tau,i+1}A_{\tau,i+1}}{2V_{i+1}}\right)^n - \left(\frac{\Delta P^*_{loss,i+\frac{1}{2}}A_{\tau,i+\frac{1}{2}}}{V_{i+\frac{1}{2}}}\right)^n$$

$$- \Gamma_g^n(v^{n+1}_{g,i+\frac{1}{2}} - v^n_{\sigma,i+\frac{1}{2}}) - \Gamma_g^n(v^{n+1}_{f,i+\frac{1}{2}} - v^n_{\sigma,i+\frac{1}{2}}) - 2\frac{\Delta P^n_\sigma \cdot A_\sigma}{V^*_{i+\frac{1}{2}}}$$

**(eq. 13⁻) Momentum difference:**

$$\frac{(\alpha_g\rho_g)^n_{i-\frac{1}{2}}(v_g^{n+1}-v_g^{n+1})_{i-\frac{1}{2}}}{\Delta t} - \frac{(\alpha_f\rho_f)^n_{i-\frac{1}{2}}(v_f^{n+1}-v_f^{n+1})_{i-\frac{1}{2}}}{\Delta t}$$

$$= \frac{1}{2}(\alpha_g\rho_g)^n_{i-\frac{1}{2}}\cdot\frac{d^n_{g,i-1}\cdot(v^n_{g,i-1})^2 - d^n_{g,i}\cdot(v^n_{g,i})^2}{\Delta x_{i-\frac{1}{2}}} - \frac{1}{2}(\alpha_f\rho_f)^n_{i-\frac{1}{2}}\cdot\frac{d^n_{f,i-1}\cdot(v^n_{f,i-1})^2 - d^n_{f,i}\cdot(v^n_{f,i})^2}{\Delta x_{i-\frac{1}{2}}}$$

$$- (\alpha_g-\alpha_f)^n_{i-\frac{1}{2}}\frac{P_i^{n+1}-P_{i-1}^{n+1}}{\Delta x_{i-\frac{1}{2}}} + (\alpha_g\rho_g.g)^n_{i-\frac{1}{2}} - (\alpha_f\rho_f.g)^n_{i-\frac{1}{2}} - \left(\frac{\Delta P^*_{\tau,i-1}A_{i-1}}{2V_{i-1}} - \frac{\Delta P^*_{\tau,i}A_{\tau,i}}{2V_i}\right)^n - \left(\frac{\Delta P^*_{loss,i-\frac{1}{2}}A_{\tau,i-\frac{1}{2}}}{V_{i-\frac{1}{2}}}\right)^n$$

$$- \Gamma_g^n(v_{g,i-\frac{1}{2}}^{n+1} - v^n_{\sigma,i-\frac{1}{2}}) - \Gamma_g^n(v_{f,i-\frac{1}{2}}^{n+1} - v^n_{\sigma,i-\frac{1}{2}}) - 2\frac{\Delta P_\sigma^n.A_\sigma}{V^*_{i-\frac{1}{2}}}$$

**(eq. 10) Vapor energy:**

$$\frac{(\alpha_g\rho_g)^n_i(u_g^{n+1}-u_g^n)_i + (\alpha_g u_g)^n_i(\rho_g^{n+1}-\rho_g^n)_i + (\rho_g u_g)^n_i(\alpha_g^{n+1}-\alpha_g^n)_i}{\Delta t} + P_i^n\left(\frac{\alpha_g^{n+1}-\alpha_g^n}{\Delta t}\right)$$

$$= \frac{1}{V_i}\left[(\alpha_g\rho_g A(u_g+gz))^n_{i-\frac{1}{2}}\cdot(v_g)^{n+1}_{i-\frac{1}{2}} - (\alpha_g\rho_g A(u_g+gz))^n_{i+\frac{1}{2}}\cdot(v_g)^{n+1}_{i+\frac{1}{2}}\right]$$

$$+ \frac{A_{s,i}}{V_i}\dot{q}^n_{gw,i} + \frac{1}{V_i}\left[(P.A)^n_{i-\frac{1}{2}}(v_g)^{n+1}_{i-\frac{1}{2}} - (P.A)^n_{i+\frac{1}{2}}(v_g)^{n+1}_{i+\frac{1}{2}}\right] + \frac{E^n_{g,loss}}{V_i} + \frac{A_{\sigma,i}}{V_i}\left[\frac{-h_f}{(h_g-h_f)}\right]\dot{q}_{g\sigma} + \frac{A_{\sigma,i}}{V_i}\left[\frac{-h_g}{(h_g-h_f)}\right]\dot{q}_{f\sigma}$$

**(eq. 11) Liquid energy:**

$$\frac{(\alpha_f\rho_f)^n_i(u_f^{n+1}-u_f^n)_i + (\alpha_f u_f)^n_i(\rho_f^{n+1}-\rho_f^n)_i + (\rho_f u_f)^n_i(\alpha_f^{n+1}-\alpha_f^n)_i}{\Delta t} + P_i^n\left(\frac{\alpha_f^{n+1}-\alpha_f^n}{\Delta t}\right)$$

$$= \frac{1}{V_i}\left[(\alpha_f\rho_f A(u_f+gz))^n_{i-\frac{1}{2}}\cdot(v_f)^{n+1}_{i-\frac{1}{2}} - (\alpha_f\rho_g A(u_f+gz))^n_{i+\frac{1}{2}}\cdot(v_f)^{n+1}_{i+\frac{1}{2}}\right]$$

$$+ \frac{A_{s,i}}{V_i}\dot{q}^n_{fw,i} + \frac{1}{V_i}\left[(P.A)^n_{i-\frac{1}{2}}(v_f)^{n+1}_{i-\frac{1}{2}} - (P.A)^n_{i+\frac{1}{2}}(v_f)^{n+1}_{i+\frac{1}{2}}\right] + \frac{E^n_{f,loss}}{V_i} + \frac{A_{\sigma,i}}{V_i}\left[\frac{h_f}{(h_g-h_f)}\right]\dot{q}_{g\sigma} + \frac{A_{\sigma,i}}{V_i}\left[\frac{h_g}{(h_g-h_f)}\right]\dot{q}_{f\sigma}$$

**(eq. 14) Vapor equation of state:**

$$(\rho_g^{n+1} - \rho_g^n)_i = \left(\frac{d\rho_g}{du_g}\right)_i^n \cdot (u_g^{n+1} - u_g^n)_i$$

**(eq. 15) Liquid equation of state:**

$$(\rho_f^{n+1} - \rho_f^n)_i = \left(\frac{d\rho_f}{du_f}\right)_i^n \cdot (u_f^{n+1} - u_f^n)_i$$

Each of these equations can be written in terms of the unknowns at the new time, $n+1$ (remembering that $\alpha_f = 1 - \alpha_g$) as follows:

$$A(\rho_g)_i + B(\rho_f)_i + C(u_g)_i + D(u_f)_i + E(v_g)_{i-\frac{1}{2}} + F(v_g)_{i+\frac{1}{2}} + G(v_f)_{i-\frac{1}{2}} + H(v_f)_{i+\frac{1}{2}} + I(\alpha_g)_i + J(P)_{i-1} + K(P)_i + L(P)_{i+1} = M$$

So now we have:

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Eq.8 | A8 | B8 | – | – | E8 | F8 | G8 | H8 | I8 | – | – | – |
| Eq.12 | A12 | B12 | – | – | E12 | F12 | G12 | H12 | I12 | – | – | – |
| Eq.9a | – | – | – | – | – | F9a | – | H9a | – | – | K9a | L9a |
| Eq.9b | – | – | – | – | E9b | – | G9b | – | – | J9b | K9b | – |
| Eq.13a | – | – | – | – | – | F13a | – | H13a | – | – | K13a | L13a |
| Eq.13b | – | – | – | – | E13b | – | G13b | – | – | J13b | K13b | – |
| Eq.10 | A10 | – | C10 | – | E10 | F10 | – | – | I10 | – | – | – |
| Eq.11 | – | B11 | – | D11 | – | – | G11 | H11 | I11 | – | – | – |
| Eq.14 | A14 | – | C14 | – | – | – | – | – | – | – | – | – |
| Eq.15 | – | B15 | – | D15 | – | – | – | – | – | – | – | – |

with unknown vector:

$$\begin{bmatrix} (\rho_g)_i \\ (\rho_f)_i \\ (u_g)_i \\ (u_f)_i \\ (v_g)_{i-\frac{1}{2}} \\ (v_g)_{i+\frac{1}{2}} \\ (v_f)_{i-\frac{1}{2}} \\ (v_f)_{i+\frac{1}{2}} \\ (\alpha_g)_i \\ (P)_{i-1} \\ (P)_i \\ (P)_{i+1} \end{bmatrix}$$

equals:

$$\begin{bmatrix} M8 \\ M12 \\ M9a \\ M9b \\ M13a \\ M13b \\ M10 \\ M11 \\ M14 \end{bmatrix}$$

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

...

$$eq.6, \quad \frac{\rho_{i+\frac{1}{2}}^n . v_{i+\frac{1}{2}}^{n+1} - \rho_{i+\frac{1}{2}}^n . v_{i+\frac{1}{2}}^n}{\Delta t} = \rho_{i+\frac{1}{2}}^n \cdot \frac{d_i.(v_i^n)^2 - d_{i+1}.(v_{i+1}^n)^2}{\Delta x_{i+\frac{1}{2}}}$$

$$- \frac{P_{i+1}^{n+1} - P_i^{n+1}}{\Delta x_{i+\frac{1}{2}}} + \rho_{i+\frac{1}{2}}^n . g_{i+\frac{1}{2}}$$

$$- \frac{\Delta P_{\tau,i}^n}{2\Delta x_{i+\frac{1}{2}}} - \frac{\Delta P_{\tau,i+1}^n}{2\Delta x_{i+\frac{1}{2}}} - \frac{\Delta P_{loss,i+\frac{1}{2}}^n}{\Delta x_{i+\frac{1}{2}}}$$

...

$$eq.7, \quad \frac{\rho_{i-\frac{1}{2}}^n . v_{i-\frac{1}{2}}^{n+1} - \rho_{i-\frac{1}{2}}^n . v_{i-\frac{1}{2}}^n}{\Delta t} = \rho_{i-\frac{1}{2}}^n \cdot \frac{d_{i-1}.(v_{i-1}^n)^2 + d_i.(v_i^n)^2}{\Delta x_{i-\frac{1}{2}}}$$

$$- \frac{P_i^{n+1} - P_{i-1}^{n+1}}{\Delta x_{i-\frac{1}{2}}} + \rho_{i-\frac{1}{2}}^n . g_{i-\frac{1}{2}}$$

$$- \frac{\Delta P_{\tau,i-1}^n}{2\Delta x_{i-\frac{1}{2}}} - \frac{\Delta P_{\tau,i}^n}{2\Delta x_{i-\frac{1}{2}}} - \frac{\Delta P_{loss,i-\frac{1}{2}}^n}{\Delta x_{i-\frac{1}{2}}}$$

...

$$eq.8, \quad \frac{(\rho_i^{n+1}.u_i^{n+1} - \rho_i^n.u_i^n)}{\Delta t} = \frac{1}{V_i} \left[ (\rho A u)_{i-\frac{1}{2}}^n . v_{i-\frac{1}{2}}^{n+1} - (\rho A u)_{i+\frac{1}{2}}^n . v_{i+\frac{1}{2}}^{n+1} \right]$$

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

$$+ \frac{A_{s,i}}{V_i} \dot{q}_i^n + \frac{1}{V_i} \left[ (P.A)_{i-\frac{1}{2}}^n . v_{i-\frac{1}{2}}^{n+1} - (P.A)_{i+\frac{1}{2}}^n . v_{i+\frac{1}{2}}^{n+1} \right]$$

$$- \frac{E_{loss,i}^n}{V_i}$$

...

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

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

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

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

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

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

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

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:

$$\frac{d\rho_{i+\frac{1}{2}}}{dt} = -v_{i+\frac{1}{2}} \cdot \frac{d\rho}{dx} \quad and \quad \frac{du_{i+\frac{1}{2}}}{dt} = -v_{i+\frac{1}{2}} \cdot \frac{du}{dx}$$

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

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

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 $\rho_i^{n+1}$ from the conservation of mass equation and finally $u_i^{n+1}$ from the equation of state interpolation.
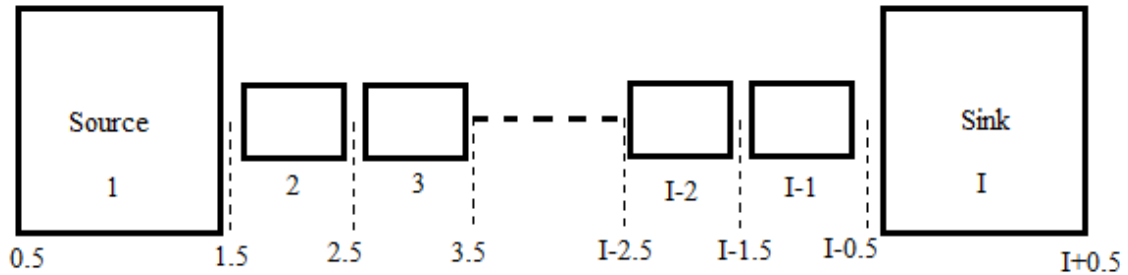


**Figure 2:** Simple layout of multiple control volumes.

## 3.8 Solution algorithm

**Step 1 - Preliminaries**

Load all control volumes. Input parameters:

- Area, $A$

- Length, $L$

- Pressure, $P$

- Temperature, $T$

- Elevation change, $\Delta z$

- Wall roughness, $\epsilon$

- 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, $\rho_i$, from:

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

Internal energy, $u_i$, from:

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

Dynamic viscosity, $\mu_i$, from:

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

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

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

**Step 4**

Determine all junction and control volume $z$ values using control volume $\Delta z$ 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 $\rho^n_{i+\frac{1}{2}}$ as follows:

$$\rho^n_{i+\frac{1}{2}} = \rho^{n-1}_{i+\frac{1}{2}} - v^n_{i+\frac{1}{2}} \cdot \frac{\Delta t}{\Delta x_{i+\frac{1}{2}}} \cdot (\rho^n_{i+1} - \rho^n_i)$$

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

$$u^n_{i+\frac{1}{2}} = u^{n-1}_{i+\frac{1}{2}} - v^n_{i+\frac{1}{2}} \cdot \frac{\Delta t}{\Delta x_{i+\frac{1}{2}}} \cdot (u^n_{i+1} - u^n_i)$$

### Step 6

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

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

Dynamic viscosity, $\mu_i$, from:

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

Reynolds number, $Re_i$, from:

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

Friction pressure drop, $\Delta P_\tau$, from:

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

With:

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

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:

$$\rho_i^{n+1} = \rho_i^n + B_5.v_{i-\frac{1}{2}}^{n+1} - C_5.v_{i+\frac{1}{2}}^{n+1} \tag{16}$$

**Step 8**

Determine the elements of equation 6:

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

$$- \frac{P^{n+1}_{i+1} - P^{n+1}_i}{\Delta x_{i+\frac{1}{2}}} + \rho^n_{i+\frac{1}{2}} \cdot g_{i+\frac{1}{2}}$$

$$- \frac{\Delta P^n_{\tau,i}}{2\Delta x_{i+\frac{1}{2}}} - \frac{\Delta P^n_{\tau,i+1}}{2\Delta x_{i+\frac{1}{2}}} - \frac{\Delta P^n_{loss,i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}}$$

Where the elements are:

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

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

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

$$F_6 = \frac{\Delta t \Delta P^n_{\tau,i}}{2\Delta x_{i+\frac{1}{2}}}, \quad G_6 = \frac{\Delta t \Delta P^n_{\tau,i+1}}{2\Delta x_{i+\frac{1}{2}}} + \frac{\Delta t \Delta P^n_{loss,i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}}$$

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

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:

$$v^{n+1}_{i+\frac{1}{2}} = H_6 - I_6.P^{n+1}_{i+1} + I_6.P^{n+1}_i \tag{17}$$

**Step 9**

Determine the elements of equation 7:

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

$$- \frac{P^{n+1}_i - P^{n+1}_{i-1}}{\Delta x_{i-\frac{1}{2}}} + \rho^n_{i-\frac{1}{2}}.g_{i-\frac{1}{2}}$$

$$- \frac{\Delta P^n_{\tau,i-1}}{2\Delta x_{i-\frac{1}{2}}} - \frac{\Delta P^n_{\tau,i}}{2\Delta x_{i-\frac{1}{2}}} - \frac{\Delta P^n_{loss,i-\frac{1}{2}}}{\Delta x_{i-\frac{1}{2}}}$$

Where the elements are:

$$B_7 = \rho^n_{i-\frac{1}{2}}.v^n_{i-\frac{1}{2}}$$

$$C_7 = \Delta t \rho^n_{i-\frac{1}{2}} \cdot \frac{d_{i-1}.(v^n_{i-1})^2 - d_i.(v^n_i)^2}{\Delta x_{i-\frac{1}{2}}}$$

$$D_7 = \frac{\Delta t}{\Delta x_{i-\frac{1}{2}}}, \quad E_7 = \Delta t \rho^n_{i-\frac{1}{2}}.g_{i-\frac{1}{2}}$$

$$F_7 = \frac{\Delta t \Delta P^n_{\tau,i-1}}{2\Delta x_{i-\frac{1}{2}}}, \quad G_7 = \frac{\Delta t \Delta P^n_{\tau,i}}{2\Delta x_{i-\frac{1}{2}}} + \frac{\Delta t \Delta P^n_{loss,i-\frac{1}{2}}}{\Delta x_{i-\frac{1}{2}}}$$

$$H_7 = \frac{B_7 + C_7 + E_7 - F_7 - G_7}{\rho^n_{i-\frac{1}{2}}}, \quad I_7 = \frac{D7}{\rho^n_{i-\frac{1}{2}}}$$

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:

$$v^{n+1}_{i-\frac{1}{2}} = H_7 - I_7.P^{n+1}_i + I_7.P^{n+1}_{i-1} \tag{18}$$

**Step 10**

Determine the elements of equation 8:

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

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

$$+ \frac{A_{s,i}}{V_i}\dot{q}_i^n + \frac{1}{V_i}\left[(P.A)_{i-\frac{1}{2}}^n.v_{i-\frac{1}{2}}^{n+1} - (P.A)_{i+\frac{1}{2}}^n.v_{i+\frac{1}{2}}^{n+1}\right]$$

$$- \frac{E_{loss,i}^n}{V_i}$$

Where the elements are:

$$C_8 = \frac{\Delta t(\rho A u)_{i-\frac{1}{2}}^n}{V_i}, \quad D_8 = \frac{\Delta t(\rho A u)_{i+\frac{1}{2}}^n}{V_i}$$

$$E_8 = \frac{\Delta t(\rho A g z)_{i-\frac{1}{2}}^n}{V_i}, \quad F_8 = \frac{\Delta t(\rho A g z)_{i+\frac{1}{2}}^n}{V_i}$$

$$G_8 = \frac{\Delta t A_{s,i}}{V_i}\dot{q}_i^n$$

$$H_8 = \frac{\Delta t(P.A)_{i-\frac{1}{2}}^n}{V_i}, \quad I_8 = \frac{\Delta t(P.A)_{i+\frac{1}{2}}^n}{V_i}$$

$$J_8 = \frac{\Delta t E_{loss,i}^n}{V_i}$$

$$K_8 = G_8 - J_8$$

$$L_8 = C_8 + E_8 + H_8$$

$$M_8 = D_8 + F_8 + I_8$$

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:

$$\rho_i^{n+1}.u_i^{n+1} - \rho_i^n.u_i^n = K_8 + L_8.v_{i-\frac{1}{2}}^{n+1} - M_8.v_{i+\frac{1}{2}}^{n+1} \tag{19}$$

**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:

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

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

To get:

$$\rho_i^{n+1} u_i^{n+1} - \rho_i^n u_i^n = B_9.\rho_i^{n+1} - C_9 \tag{20}$$

**Step 12**

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

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

$$eq\ 11, \quad v_{i+\frac{1}{2}}^{n+1} = H_6 - I_6.P_{i+1}^{n+1} + I_6.P_i^{n+1}$$

$$eq\ 12, \quad v_{i-\frac{1}{2}}^{n+1} = H_7 - I_7.P_i^{n+1} + I_7.P_{i-1}^{n+1}$$

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

$$eq\ 14, \quad \rho_i^{n+1}u_i^{n+1} - \rho_i^n u_i^n = B_9.\rho_i^{n+1} - C_9$$

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:

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

$$= \rho_i^n + B_5 H_7 - B_5 I_7.P_i^{n+1} + B_5 I_7.P_{i-1}^{n+1} - C_5 H_6 + C_5 I_6.P_{i+1}^{n+1} - C_5 I_6.P_i^{n+1}$$

$$= \rho_i^n + B_5 H_7 - C_5 H_6 + B_5 I_7.P_{i-1}^{n+1} - B_5 I_7.P_i^{n+1} - C_5 I_6.P_i^{n+1} + C_5 I_6.P_{i+1}^{n+1}$$

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

More simplistically we define:

$$B_{10} = \rho_i^n + B_5 H_7 - C_5 H_6$$

$$C_{10} = B_5 I_7$$

$$D_{10} = B_5 I_7 + C_5 I_6$$

$$E_{10} = C_5 I_6$$

To arrive at:

$$\rho_i^{n+1} = B_{10} + C_{10}.P_{i-1}^{n+1} - D_{10}.P_i^{n+1} + E_{10}.P_{i+1}^{n+1} \tag{21}$$

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

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

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:

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

We need to also insert equations 11 and 12:

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

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:

$$\rho_i^{n+1} = E_{14} + F_{14}.P_{i-1}^{n+1} - G_{14}.P_i^{n+1} + H_{14}.P_{i+1}^{n+1} \tag{22}$$

Now all thats left is to equate equation 15 and 16:

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

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

We now have a single equation for each control volume:

$$\left(C_{10} - F_{14}\right)P_{i-1}^{n+1} + \left(G_{14} - D_{10}\right)P_i^{n+1} + \left(E_{10} - H_{14}\right)P_{i+1}^{n+1} = E_{14} - B_{10} \tag{23}$$

**Step 13**

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

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

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:

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

**Step 17**

Advance the time values.

# 4  Flow regimes

In order to visualize the different fluid flow regimes (see Figure 3) let us consider a relatively fast flowing liquid, initially in the **sub-cooled convection regime**, with a heat flux applied to the walls such that, in combination with the convection heat transfer coefficient, the wall's surface temperature is just above the saturation temperature of the liquid. In this case nucleate boiling will occur (hence the **nucleate boiling regime**) and the formed bubbles will be swept away into the bulk of the flow, some of which coalesce into bigger bubbles whilst others transfer heat to the surrounding liquid phase (via sophisticated mechanisms) and collapse, leading to an increase in the liquid temperature. The increased liquid temperature downstream of this point, assuming the heat flux remains constant elevates the surface temperature even higher and the amount of tiny bubbles created increases further. A bubbly flow regime is created that is very turbulent and has an increasingly significant vapor void fraction (increased $\alpha_g$). This regime is aptly named the **bubbly flow regime** (observe the upper sections of the top left schematic in Figure 3).

Of course as the amount of bubbles in the flow increases the tiny bubbles start to coalesce so fast and in such great volumes that one can no longer say that the flow is bubbly and the bubbles now become fairly large in comparison to the effective flow area. The bigger bubbles then become slug-like and hence this regime is named the **slug flow regime**. Multiple slugs can also coalesce to form bigger slugs. These slugs can then disrupt local heat transfer when it moves over a section that was normally liquid cooled and therefore, in the presence of a constant heat flux, leads to a considerably higher wall surface temperature. At the point that this slug then leaves this location the dry (vapor, not liquid) surface is quenched with cooler more effective liquid behind the slug. Unfortunately, this effect in itself leads to big bubble formation from nucleate boiling and hence the bubbles and resulting slugs become ever bigger as the flow progresses downstream. When the liquid to bubbles ratio become such that one cannot distinguish vapor bubbles from other one transitions into the **annular mist flow regime** where eventually the vapor fraction is so large that liquid exists only in the form of a film and a dispersed mist of droplets.

Eventually the flow becomes so heated and so energetic that it becomes nearly impossible for liquid droplets to remain present and hence the flow becomes very dry to the point where one can name the flow regime the **dispersed flow regime**. Beyond this point the flow is so dry that *superheating* of the vapor occurs.

With higher heat fluxes the rate of evaporation at the surface will be so high that the layer can now longer sustain a liquid layer and hence a vapor layer starts to form. At this point, with a lower density fluid now in contact with the surface the effective heat transfer is reduced causing the surface temperature to rise higher. This situation is then a break away unstable situation and the heat flux, at which this occurs, is called the **Critical Heat Flux (CHF)**. The dynamic situation (see Figure 4) then ultimately leads to **inverted annular flow** which is the same as annular flow but with the central annular region now filled with liquid instead of vapor. At the point where this column breaks apart the **inverted slug flow** regime dominates. Lastly, the slugs heat up and reduce in size until when is left with just **dispersed**
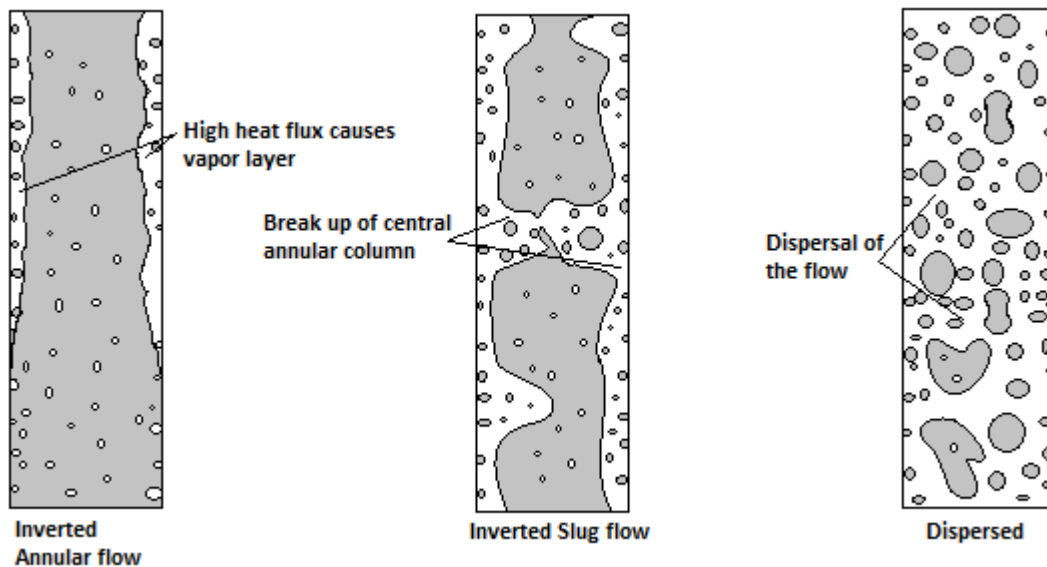
**flow**.

For all the sections that follow, the discussion is limited to **macro-channels** with $D_h > 3\ mm$ as recommended and adopted by *Cheng et. al* [1]. Channels sizes below these values are classified as mini- or micro-channels and cannot be regarded as equivalent to macro-channels.
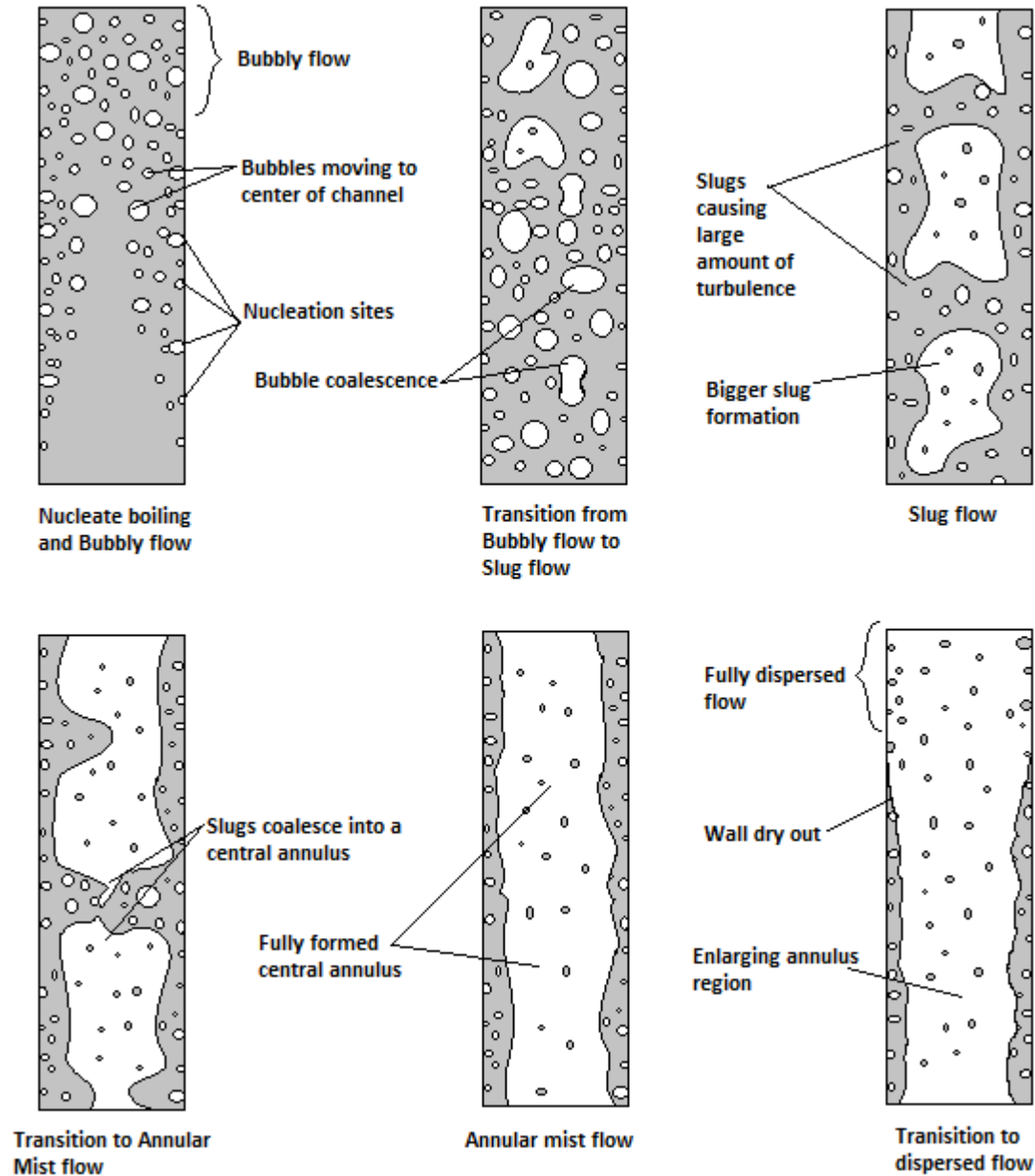
**Figure 3:** Schematic showing different flow regimes for heat transfer below the critical heat flux (CHF).

**Figure 4:** Schematic showing different flow regimes for heat transfer above the critical heat flux (CHF).

## 4.1 Horizontal- versus Vertical flow

For vertical flow the movement of bubbles is normally away from the wall (due to the liquid surface tension) symmetrically along the axis of flow because that is the direction towards which gravity is aligned. Horizontal flow has the complication that bubbles and hence the majority of the void tends to move to the upper sections of the flow channels due to buoyancy. Both these effects lead to the phenomena of **stratification**. Stratification is the process during which a multi-component fluid is segregated into its different components in such a way that the fluid no longer behaves equivalent to its fully homogenized multi-component form. Even though the study of stratification is vast, and complicated, we can use this visualization to understand that flow regimes are highly dependent on the **geometry of the flow and its orientation relative to gravity** (i.e. azimuthal angle).

# 5 Test cases

In order to test various aspects of the thermal-hydraulic code it is necessary to construct a collection of test cases. These are:

1. Simple horizontal flow. No heat transfer, no junction form loss.

2. Simple horizontal flow with junction form loss.

3. Horizontal flow with heat transfer.

4. Vertical flow without heat transfer.

5. Vertical flow with heat transfer.

For all these cases, let us use the following geometry:
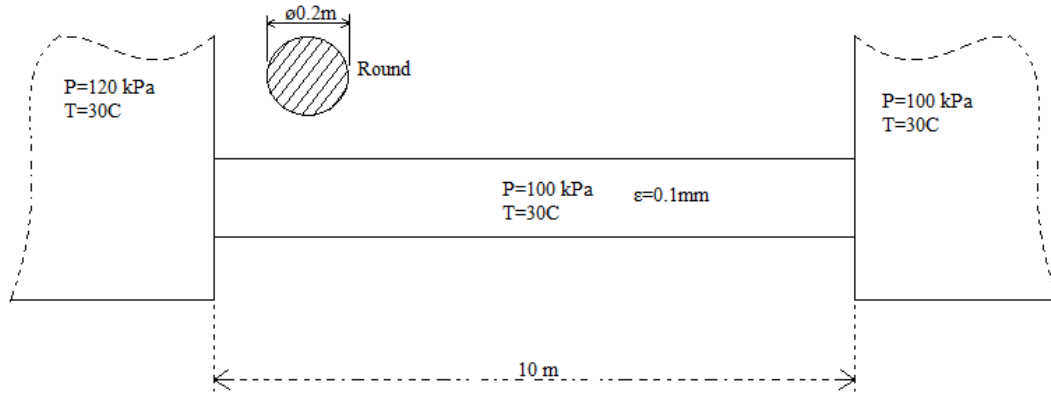


**Figure 5:** Test case geometry.

# 6 Heat block submodel

## 6.1 The heat conduction equation

The generalized heat conduction equation takes the following form:

$$\frac{dT}{dt} = \alpha \nabla^2 T + \frac{1}{\rho C_p} \dot{e}_{gen} \tag{24}$$

In slab geometry this equation takes the form:

$$\frac{dT}{dt} = \frac{1}{\rho C_p} \frac{d}{dx}\left(k\frac{dT}{dx}\right) + \frac{1}{\rho C_p} \dot{e}_{gen} \tag{25}$$

And in cylindrical geometry this equation takes the form:

$$\frac{dT}{dt} = \frac{1}{\rho C_p} \frac{1}{r} \frac{d}{dr}\left(k.r.\frac{dT}{dr}\right) + \frac{1}{\rho C_p} \dot{e}_{gen} \tag{26}$$

Typical boundary conditions for such second order differential equations are the symmetry or insulated boundary condition:

$$\left.\frac{dT}{dx}\right|_L = 0 \quad or \quad \left.\frac{dT}{dr}\right|_R = 0$$
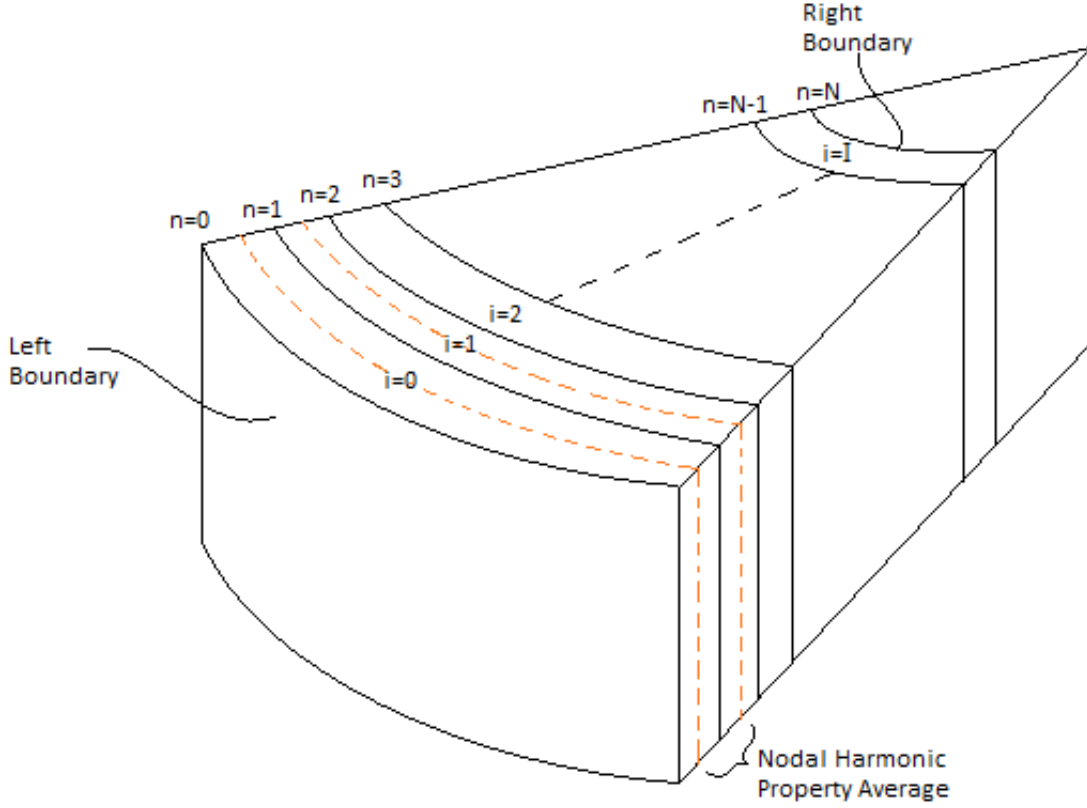
The constant temperature boundary condition:

$$\left.\frac{dT}{dt}\right|_L = 0 \quad or \quad \left.\frac{dT}{dt}\right|_R = 0$$

And the surface convection boundary condition:

$$k\frac{dT}{dx}\bigg|_L^{+,-} = h(T_L - T_{\inf})$$

$$or$$

$$k\frac{dT}{dr}\bigg|_R^{+,-} = h(T_R - T_{\inf})$$

## 6.2   Numerical form of the heat conduction equation

Consider the nodalization as shown in Figure 6 below.



**Figure 6:** Heat block nodalization.

We can linearize the derivatives of equation 20 as follows:

$$\frac{T_n^{t+1} - T_n^t}{\Delta t} = \frac{1}{\rho_n C_{p,n}} \frac{1}{r_n \Delta r_n} \left( k_i^t . r_i . \frac{T_{n+1}^{t+1} - T_n^{t+1}}{\Delta r_i} - k_{i-1}^t . r_{i-1} \frac{T_n^{t+1} - T_{n-1}^{t+1}}{\Delta r_{i-1}} \right) + \frac{1}{\rho_n C_{p,n}} \dot{e}_{gen,n}^t \quad (27)$$

In this formulation the nodal points $r_1, r_2, \ldots, r_N$ are defined by the user. $\Delta r_i$ is defined only on intervals. The value of $r_i$ is the halfway point between the nodes on either side of the interval. The values of $\rho_n$, $C_{p,n}$ and $\dot{e}_{gen,n}$ are calculated from the arithmetic average of the adjoining intervals as follows:

$$\rho_n = \frac{(r_n + \frac{1}{2}\Delta r_n)^2 - (r_n)^2}{r_{i=n-1}^2 - r_{i=n}^2} \cdot \rho_{i=n-1} + \frac{(r_n)^2 - (r_n - \frac{1}{2}\Delta r_n)^2}{r_{i=n-1}^2 - r_{i=n}^2} \cdot \rho_{i=n}$$

$$C_{p,n} = \frac{(r_n + \frac{1}{2}\Delta r_n)^2 - (r_n)^2}{r_{i=n-1}^2 - r_{i=n}^2} \cdot C_{p,i=n-1} + \frac{(r_n)^2 - (r_n - \frac{1}{2}\Delta r_n)^2}{r_{i=n-1}^2 - r_{i=n}^2} \cdot C_{p,i=n}$$

$$\dot{e}_{gen,n} = \frac{(r_n + \frac{1}{2}\Delta r_n)^2 - (r_n)^2}{r_{i=n-1}^2 - r_{i=n}^2} \cdot \dot{e}_{gen,i=n-1} + \frac{(r_n)^2 - (r_n - \frac{1}{2}\Delta r_n)^2}{r_{i=n-1}^2 - r_{i=n}^2} \cdot \dot{e}_{gen,i=n}$$

## 6.3  Solution algorithm

**Step 1**

Load all heat block:

- Load mesh points, $r_n$, and initial temperatures, $T_n^t$

- Calculate $\Delta r_n$ and $\Delta r_i$

- Calculate intervals, $r_i$

- Load thermal properties, $k_i$, $C_{p,i}$ and $\rho_i$

- Load initial temperature, $T_n$

- Set boundary conditions, *Convection*, *Symmetry* or *Temperature*

- Set interval heat generation, $\dot{e}_{gen,n}$

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

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

**Step 2**

Set thermal conditions:

- Set boundary conditions, $Convection(h, T_{\inf})$, $Symmetry$ or $Temperature(T)$

- Set interval heat generation, $\dot{e}_{gen,n}$

**Step 3a - Inner mesh points**

Determine the elements of equation 21:

$$\frac{T_n^{t+1} - T_n^t}{\Delta t} = \frac{1}{\rho_n C_{p,n}} \frac{1}{r_n \Delta r_n} \left( k_i^t . r_i . \frac{T_{n+1}^{t+1} - T_n^{t+1}}{\Delta r_i} - k_{i-1}^t . r_{i-1} \frac{T_n^{t+1} - T_{n-1}^{t+1}}{\Delta r_{i-1}} \right) + \frac{1}{\rho_n C_{p,n}} \dot{e}_{gen,n}^t$$

Where the elements are:

$$B_{21} = \frac{\Delta t}{\rho_n C_{p,n}} \cdot \frac{k_i^t . r_i}{r_n . \Delta r_n . \Delta r_i} \quad and \quad C_{21} = \frac{\Delta t}{\rho_n C_{p,n}} \cdot \frac{k_i^t . r_i}{r_n . \Delta r_n . \Delta r_i}$$

$$D_{21} = \frac{\Delta t}{\rho_n C_{p,n}} \cdot \frac{k_{i-1}^t . r_{i-1}}{r_n . \Delta r_n . \Delta r_{i-1}} \quad and \quad E_{21} = \frac{\Delta t}{\rho_n C_{p,n}} \cdot \frac{k_{i-1}^t . r_{i-1}}{r_n . \Delta r_n . \Delta r_{i-1}}$$

$$F_{21} = \frac{\Delta t}{\rho_n C_{p,n}} \dot{e}_{gen,n}^t$$

To get:

$$\therefore T_n^{t+1} - T_n^t = B_{21}.T_{n+1}^{t+1} - C_{21}.T_n^{t+1} - D_{21}.T_n^{t+1} + E_{21}.T_{n-1}^{t+1} + F_{21}$$

With further simplification we can write this as:

$$-E_{21}.T_{n-1}^{t+1} + T_n^{t+1} + C_{21}.T_n^{t+1} + D_{21}.T_n^{t+1} - B_{21}.T_{n+1}^{t+1} = F_{21} + T_n^t$$

And finally:

$$\left(-E_{21}\right)T_{n-1}^{t+1} + \left(1 + C_{21} + D_{21}\right)T_n^{t+1} + \left(-B_{21}\right)T_{n+1}^{t+1} = \left(F_{21} + T_n^t\right) \tag{28}$$

**Step 3b - Left convection boundary condition**

This is the same as **step 3a** but with a change. For a convection boundary condition the following applies:

$$k_{i-1}^t.r_{i-1}\frac{T_n^{t+1} - T_{n-1}^{t+1}}{\Delta r_{i-1}} \quad \rightarrow \quad h_n^t.r_n(T_n^{t+1} - T_{\text{inf},n})$$

Therefore, $E_{21}$ is zero and $D_{21}$ becomes:

$$D_{21} = \frac{\Delta t}{\rho_n C_{p,n}} \cdot \frac{h_n^t}{\Delta r_n}$$

Also $F_{21}$ now receives the known contribution from $T_{inf,n}$ and becomes:

$$F_{21} = \frac{\Delta t}{\rho_n C_{p,n}}\dot{e}_{gen,n}^t + D_{21}.T_{\text{inf},n}$$

**Step 3c - Right symmetry boundary condition**

This is the same as **step 3a** but with a change. For a symmetry boundary condition the following applies:

$$k_i^t.r_i.\frac{T_{n+1}^{t+1} - T_n^{t+1}}{\Delta r_i} \quad \rightarrow \quad 0$$

Therefore, $B_{21}$ and $C_{21}$ is zero with no changes to $F_{21}$.

**Step 4**

Using equation 22, in the form $\quad a_i.T_{n-1}^{t+1} + b_i.T_n^{t+1} + c_i.T_{n+1}^{t+1} = d_i \quad$ we can construct a linear system $Ax = b$ as follows:

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

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

# References

[1] *Two-Phase Flow Patterns and Flow-Pattern Maps: Fundamentals and Applications*, ASME, Applied Mechanics Reviews, 2008.

[2] Shieh, A.S., Ransom, V.H., Krishnamurthy, R., *RELAP5/MOD3 Code Manual Volume 6: Validation of numerical techniques in RELAP5/MOD3*, NUREG/CR-5535/Rev 1.