

UNENE Graduate Course
Reactor Thermal-Hydraulics Design and
Analysis

McMaster University

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Equation of State

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Outline

- Thermal-hydraulics Properties
- The Iterative Method
- The Rate Method
- H₂O Property Fits

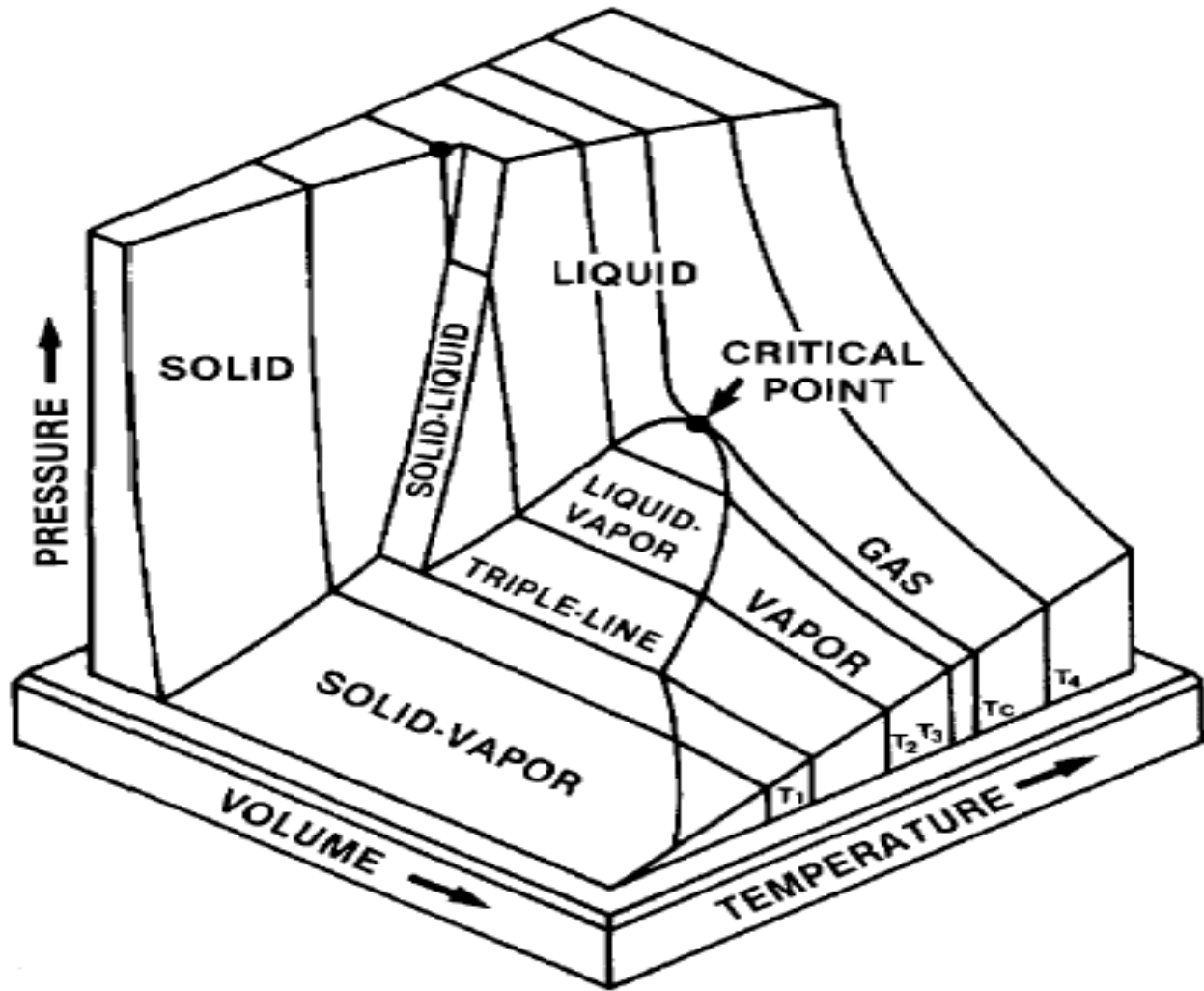
Thermo-Hydraulic Properties

- Equation of state is a relationship between any four thermodynamic properties of a substance

$$\pi (P, V, T, M) = 0 \quad \pi (P, v, T) = 0$$

- Why do we need the equation of state?
 - 4 dependent variables (density, temperature, pressure and velocity); 3 conservation equations (mass, momentum and energy)
- For given values of pressure and temperature, the calculation of other properties is relatively straightforward
- Determination of pressure from known values of other thermodynamic properties requires iteration (characteristic of the equation of state)
- Conservation equations are all cast as rate equations, whereas the equation of state is typically written as an algebraic equation

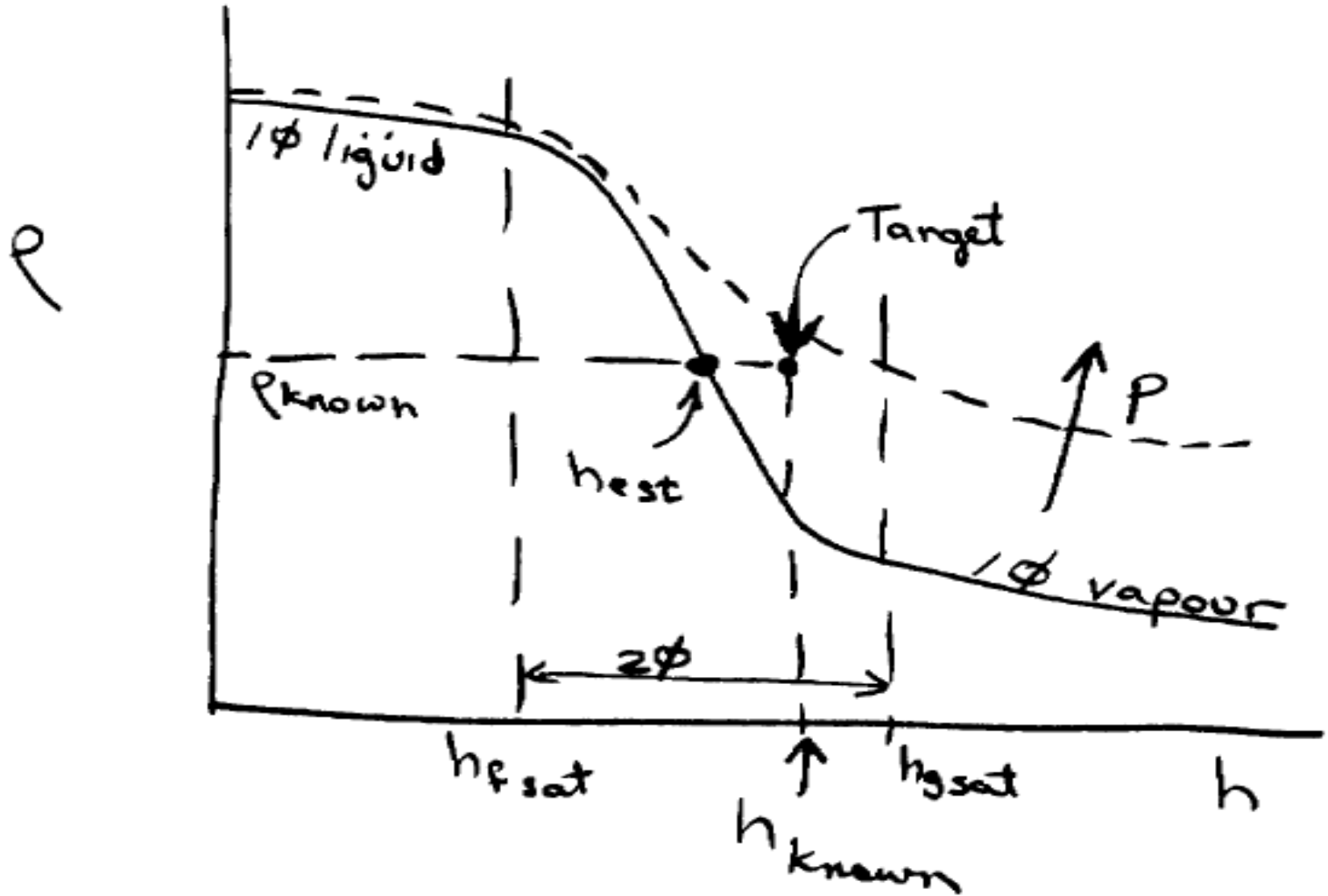
P-v-T surface of Water



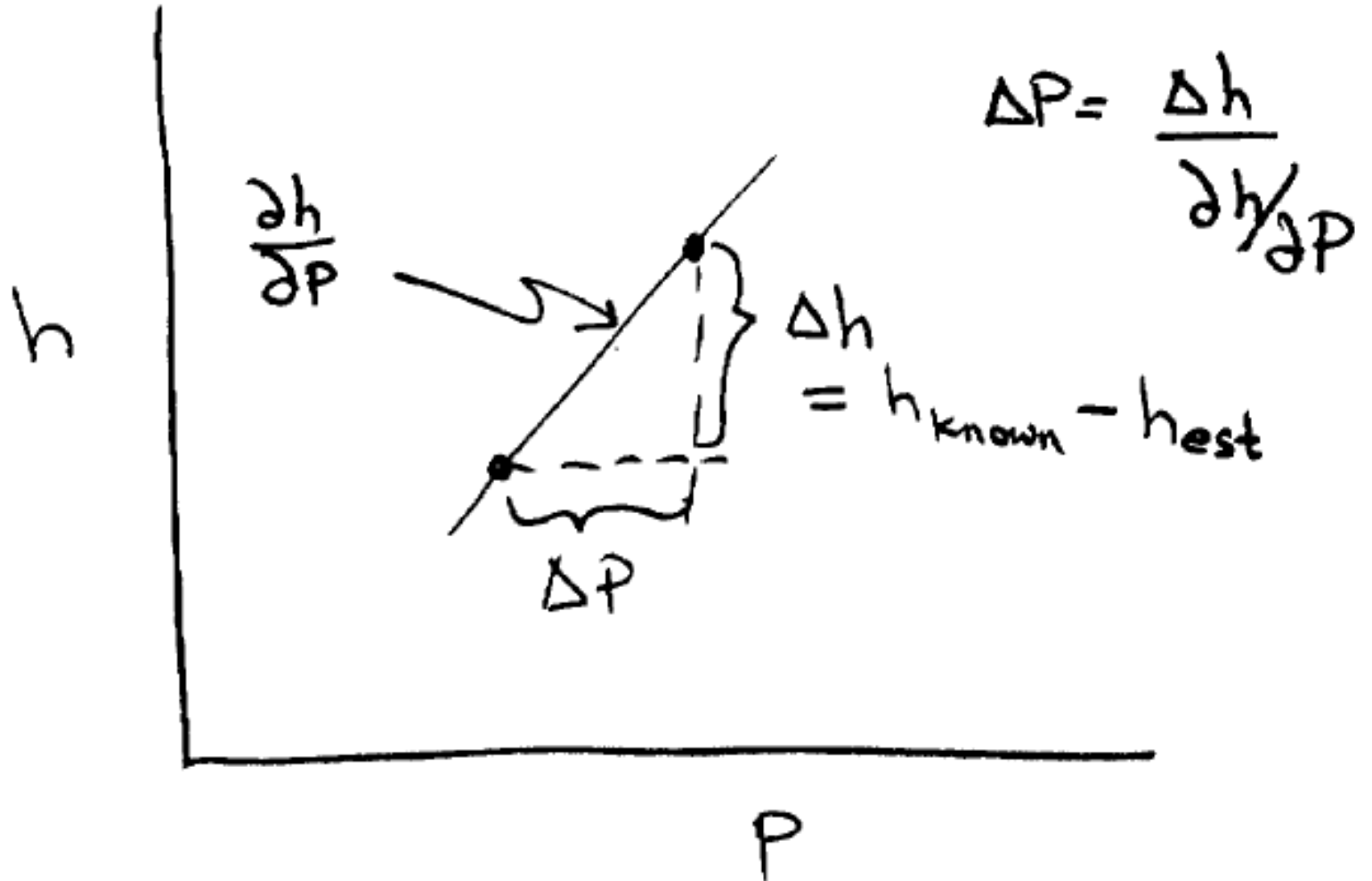
The Iterative Method

- Given the density and enthalpy of a volume of water, the task at hand is to find the associated values of pressure and temperature
- The iteration process
 - Guess the pressure (pressure at previous time step)
 - Calculate h_{fsat} and h_{gsat} (saturation enthalpies for gas and liquid)
 - If $h > h_{gsat}$ the fluid is single-phase steam
 - If $h < h_{fsat}$ the fluid is single-phase water
 - Otherwise, the fluid is two-phase mixture

Numerical Search for P Given ρ and h



Error Correction Scheme



The Iterative Method – Two-phase Equilibrium

- Given the density and enthalpy of a volume of water, the task at hand is to find the associated values of pressure and temperature

$$v = \frac{1}{\rho} = v_f(P) + x_{\text{est}} v_{fg}(P)$$

$$h_{\text{est}} = \bar{h}_f(P) + x_{\text{est}} h_{fg}(P)$$

- The pressure iteration continues until the pressure converges with some tolerance

$$\Delta P = \frac{\Delta h}{(\partial h / \partial P)_\rho} \quad P = P + \Delta P$$

The Iterative Method – Single-phase

- For single-phase fluid

$$\rho = \rho(P, T) \quad \text{and} \quad h = h(P, T)$$

- For guessed pressure and temperature, density and enthalpy can be found directly from property tables; Taylor's series expansion is used:

$$\rho = \rho_{\text{est}} + \left. \frac{\partial \rho}{\partial T} \right|_P \Delta T + \left. \frac{\partial \rho}{\partial P} \right|_T \Delta P \quad h = h_{\text{est}} + \left. \frac{\partial h}{\partial T} \right|_P \Delta T + \left. \frac{\partial h}{\partial P} \right|_T \Delta P$$

- Using a guess for the increment of density and enthalpy, the increments for pressure and temperature can be found

$$\Delta \rho = \rho - \rho_{\text{est}} \quad \Delta h = h - h_{\text{est}}$$

The Iterative Method – Single-phase

$$\Delta P = \frac{\left(\frac{\partial h}{\partial T}\right)_P \Delta \rho - \left(\frac{\partial \rho}{\partial T}\right)_P \Delta h}{\left(\frac{\partial \rho}{\partial P}\right)_T \left(\frac{dh}{dT}\right)_P - \left(\frac{\partial \rho}{\partial T}\right)_P \left(\frac{\partial h}{\partial P}\right)_T} \quad \Delta T = \frac{\left(\frac{\partial h}{\partial P}\right)_T \Delta \rho - \left(\frac{\partial \rho}{\partial T}\right)_T \Delta h}{\left(\frac{\partial \rho}{\partial T}\right)_P \left(\frac{dh}{dP}\right)_T - \left(\frac{\partial \rho}{\partial P}\right)_T \left(\frac{\partial h}{\partial T}\right)_P}$$

$$\Delta P = G_{1P} \Delta \rho + G_{2P} \Delta h$$

$$\Delta T = G_{1T} \Delta \rho + G_{2T} \Delta h$$

$$P = P + \Delta P \quad \text{and} \quad T = T + \Delta T$$

- The iteration is repeated until until pressure and temperature converge with some tolerance

The Rate Method

- The rate method eliminates the need for iteration with no loss of accuracy
- The rate method is consistent with the conservation equation form
- The current form of the rate equation consistent with the Porsching Method

The Rate Method – Two-Phase Equil Fluid

- We wish to relate the rate of change of pressure to rates of change in density and enthalpy:

$$dP = G_1 d\rho + G_2 dh \quad \frac{dP}{dt} = G_1 \frac{d\rho}{dt} + G_2 \frac{dh}{dt}$$

- For two-phase homogeneous mixture, and differentiating the equations below:

$$v = v_f + xv_{fg} \quad v_{fg} \equiv v_g - v_f \text{ and } h_{fg} \equiv h_g - h_f$$

$$h = h_f + xh_{fg}$$

$$\frac{dh}{dt} = \left(\frac{\partial h}{\partial P} \right)_\rho \frac{dP}{dt} = \left[\frac{\partial h_f}{\partial P} + h_{fg} \frac{\partial x}{\partial P} + x \frac{\partial h_{fg}}{\partial P} \right] \frac{dP}{dt}$$

$$\frac{dx}{dP} = \frac{\partial \left(\frac{v - v_f}{v_{fg}} \right)}{\partial P} = -\frac{1}{v_{fg}} \left[\frac{\partial v_f}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right] \quad \text{for density constant}$$

The Rate Method – Two-Phase Equil Fluid

$$\frac{dh}{dt} = \left\{ \frac{\partial h_f}{\partial P} + x \frac{\partial h_{fg}}{\partial P} - \frac{h_{fg}}{v_{fg}} \left[\frac{\partial v_f}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right] \right\} \frac{dP}{dt}$$

$$\begin{aligned} \frac{dP}{dt} &= \frac{v_{fg}}{\left\{ v_{fg} \left[\frac{\partial h_f}{\partial P} + x \frac{\partial h_{fg}}{\partial P} \right] - h_{fg} \left[\frac{\partial v_f}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right] \right\}} \frac{dh}{dt} \\ &= \frac{v_{fg}}{\{\text{DENOMINATOR}\}} \frac{dh}{dt} = G_2 \frac{dh}{dt} . \end{aligned}$$

$$\frac{dP}{dt} = \frac{-h_{fg}}{\{\text{DENOMINATOR}\}} \frac{dv}{dt} = \frac{h_{fg} v^2}{\{\text{DENOMINATOR}\}} \frac{d\rho}{dt} = G_1 \frac{d\rho}{dt} .$$

$$\frac{dP}{dt} = G_1 (P, x) \frac{d\rho}{dt} + G_2 (P, x) \frac{dh}{dt} .$$

The Rate Method – Two-Phase Equil Fluid

$$\rho = M/V \text{ and } h = H/M,$$

$$\frac{d\rho}{dt} = \frac{1}{V} \frac{dM}{dt} - \frac{M}{V^2} \frac{dV}{dt}$$

$$\frac{dh}{dt} = \frac{1}{M} \frac{dH}{dt} - \frac{H}{M^2} \frac{dM}{dt}.$$

$$\frac{dP}{dt} = \left(\frac{G_1}{V} - \frac{G_2 H}{M^2} \right) \frac{dM}{dt} + \frac{G_2}{M} \frac{dH}{dt} - \frac{G_1 M}{V^2} \frac{dV}{dt}.$$

$$\frac{dP}{dt} = \frac{F_1 \frac{dM}{dt} + F_2 \frac{dH}{dt} + F_3 \frac{dV}{dt}}{M_g F_4 + M_f F_5}$$

The Rate Method – Two-Phase Equil Fluid

$$F_1 = h_g v_f - h_f v_g$$

$$F_2 = v_g - v_f$$

$$F_3 = h_f - h_g$$

$$F_4 = \frac{\partial h_g}{\partial P} (v_g - v_f) - \frac{\partial v_g}{\partial P} (h_g - h_f)$$

$$F_5 = \frac{\partial h_f}{\partial P} (v_g - v_f) - \frac{\partial v_f}{\partial P} (h_g - h_f)$$

$$M_g \equiv x M$$

$$M_f \equiv (1 - x) M.$$

The Rate Method – Single-Phase Fluid

- We wish to relate the rate of change of pressure to rates of change in density and enthalpy:

$$\frac{dP}{dt} = G_{1P} \frac{d\rho}{dt} + G_{2P} \frac{dh}{dt} \quad \frac{dT}{dt} = G_{1T} \frac{d\rho}{dt} + G_{2T} \frac{dh}{dt} .$$

- For single-phase fluid we do not need to account for the sorting out between the phases, thus the derivation is more direct and less complex

$$P = \pi(\rho, h)$$

$$\rho = \rho(P, T)$$

$$\frac{dP}{dt} = \left. \frac{\partial P}{\partial \rho} \right|_h \frac{d\rho}{dt} + \left. \frac{\partial P}{\partial h} \right|_\rho \frac{dh}{dt}$$

$$h = h(P, T)$$

The Rate Method – Single-Phase Fluid

$$\frac{d\rho}{dt} = \left. \frac{\partial \rho}{\partial P} \right|_T \frac{dP}{dt} + \left. \frac{\partial \rho}{\partial T} \right|_P \frac{dT}{dt}$$

$$\frac{dh}{dt} = \left. \frac{\partial h}{\partial P} \right|_T \frac{dP}{dt} + \left. \frac{\partial h}{\partial T} \right|_P \frac{dT}{dt} .$$

- Solving for dP/dt and dT/dt we get:

$$\frac{dP}{dt} = \frac{\left. \frac{\partial h}{\partial T} \right|_P \frac{d\rho}{dt} - \left. \frac{\partial \rho}{\partial T} \right|_P \frac{dh}{dt}}{\left. \frac{\partial \rho}{\partial P} \right|_T \left. \frac{\partial h}{\partial T} \right|_P - \left. \frac{\partial \rho}{\partial T} \right|_P \left. \frac{\partial h}{\partial P} \right|_T} \quad \frac{dT}{dt} = \frac{\left. \frac{\partial h}{\partial P} \right|_T \frac{d\rho}{dt} - \left. \frac{\partial \rho}{\partial T} \right|_T \frac{dh}{dt}}{\left. \frac{\partial \rho}{\partial T} \right|_P \left. \frac{\partial h}{\partial P} \right|_T - \left. \frac{\partial \rho}{\partial P} \right|_T \left. \frac{\partial h}{\partial T} \right|_P}$$

The Rate Method – Single-Phase Fluid

- The extensive form of the equations is also easily obtained

$$\frac{dP}{dt} = \frac{F_{1P} \frac{dM}{dt} + F_{2P} \frac{dH}{dt} + F_{3P} \frac{dV}{dt}}{M_v F_{4P} + M_l F_{5P}}$$

$$\frac{dT}{dt} = \frac{F_{1T} \frac{dM}{dt} + F_{2T} \frac{dH}{dt} + F_{3T} \frac{dV}{dt}}{M_v F_{4T} + M_l F_{5T}}$$

The Rate Method – Single-Phase Fluid

$$F_{1P} = \rho \left(\frac{\partial h}{\partial T} \right)_P + h \left(\frac{\partial \rho}{\partial T} \right)_P$$

$$F_{2P} = - \left(\frac{\partial \rho}{\partial t} \right)_P$$

$$F_{3P} = - \rho^2 \left(\frac{\partial \rho}{\partial T} \right)_P$$

$$F_{4P} = 0 \text{ for subcooled, } = \left(\frac{d\rho}{dP} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{dh}{dP} \right)_T \text{ for superheated}$$

$$F_{5P} = \left(\frac{d\rho}{dP} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{dh}{dP} \right)_T \text{ for subcooled } = 0 \text{ for superheated}$$

$$F_{1T} = \rho \left(\frac{\partial h}{\partial T} \right)_P + h \left(\frac{\partial \rho}{\partial T} \right)_P$$

$$F_{2T} = - \left(\frac{\partial \rho}{\partial t} \right)_T$$

$$F_{3T} = - \rho \left(\frac{\partial h}{\partial T} \right)_T$$

$$F_{4T} = - F_{4P}$$

$$F_{5T} = - F_{5P}$$

M_v = mass of vapour phase = 0 for subcooled, = M for superheated

M_l = mass of liquid phase = M for subcooled = 0 for superheated

The Rate Method – Two-Phase Non-Eq Fluid

- The rate form for the two-phase non-equilibrium case is a simple extension of the single-phase non-equilibrium case

$$\frac{dP_k}{dt} = G_{1P}^k \frac{d\rho_k}{dt} + G_{2P}^k \frac{dh_k}{dt}$$

$$\frac{dT_k}{dt} = G_{1T}^k \frac{d\rho_k}{dt} + G_{2T}^k \frac{dh_k}{dt}$$

Where k represents either water or steam

- The derivatives of density and enthalpy are available in the rate form of the equation of state

The Rate Method - Summary of the F Functions

Table 4.1 Summary of the F functions for the rate form of the equation of state

Case	F_1	F_2	F_3	F_4	F_5
2 ϕ equilibrium (all derivatives along saturation line)	$h_g v_f - h_f v_g$	v_{fg}	h_{fg}	$\frac{\partial h_g}{\partial P} v_{fg} - \frac{\partial v_g}{\partial P} h_{fg}$	$\frac{\partial h_f}{\partial P} v_{fg} - \frac{\partial v_f}{\partial P} h_{fg}$
1 ϕ non- equilibrium pressure	$\rho \left(\frac{\partial h}{\partial T} \right)_P + h \left(\frac{\partial \rho}{\partial T} \right)_P$	$-\left(\frac{\partial \rho}{\partial T} \right)_P$	$-\rho^2 \left(\frac{\partial h}{\partial T} \right)_P$	$\left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{\partial h}{\partial P} \right)_T$	$\left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{\partial h}{\partial P} \right)_T$ subcooled 0 superheated
1 ϕ non- equilibrium temperature	$\rho \left(\frac{\partial h}{\partial P} \right)_T + h \left(\frac{\partial \rho}{\partial P} \right)_T$	$-\left(\frac{\partial \rho}{\partial P} \right)_T$	$-\rho^2 \left(\frac{\partial h}{\partial P} \right)_T$	$-F_{4P}$	$-F_{5P}$

The Rate Method - Summary of the G Functions

Table 4.2 Summary of the G functions for the rate form of the equation of state

Case	G_1	G_2
2 ϕ equilibrium (all derivatives along saturation line)	$\frac{h_{fg} v^2}{\left\{ v_{fg} \left[\frac{\partial h_f}{\partial P} + x \frac{\partial h_{fg}}{\partial P} \right] - h_{fg} \left[\frac{\partial v_f}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right] \right\}}$	$\frac{v_{fg}}{\left\{ v_{fg} \left[\frac{\partial h_f}{\partial P} + x \frac{\partial h_{fg}}{\partial P} \right] - h_{fg} \left[\frac{\partial v_f}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right] \right\}}$
1 ϕ non-equilibrium pressure	$\frac{\left(\frac{\partial h}{\partial T} \right)_P}{\left[\left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{\partial h}{\partial P} \right)_T \right]}$	$\frac{-\left(\frac{\partial \rho}{\partial T} \right)_P}{\left[\left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{\partial h}{\partial P} \right)_T \right]}$
1 ϕ non-equilibrium temperature	$\frac{\left(\frac{\partial h}{\partial P} \right)_T}{\left[\left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{\partial h}{\partial P} \right)_T - \left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P \right]}$	$\frac{-\left(\frac{\partial \rho}{\partial P} \right)_T}{\left[\left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{\partial h}{\partial P} \right)_T - \left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P \right]}$

H2O Property Fits

- Steam-water properties are calculated using standard routines
 - CATHENA has built in and stand-alone property tables
 - TH codes use different forms of property tables – need to make sure understand differences in property tables that can create some differences in results
- The overall approach is based on careful attention to the fitting around the saturation line which separates single-phase from two-phase applications
 - Most codes operate near saturation line

H2O Property Fits

- Density, enthalpy and other properties vary more strongly with temperature than with pressure

$$\rho(P,T) = \rho_{\text{sat}}(T) + \left. \frac{\partial \rho}{\partial P} \right|_T (P - P_{\text{sat}}(T))$$

- Both the properties and their derivatives must be free of discontinuities to establish numerical stability
- Discontinuities in properties can arise especially due to flow regime changes
 - Therefore, carefully chosen smoothing techniques must be used to avoid sudden changes in properties due to flow regime changes

Density vs Pressure Diagram

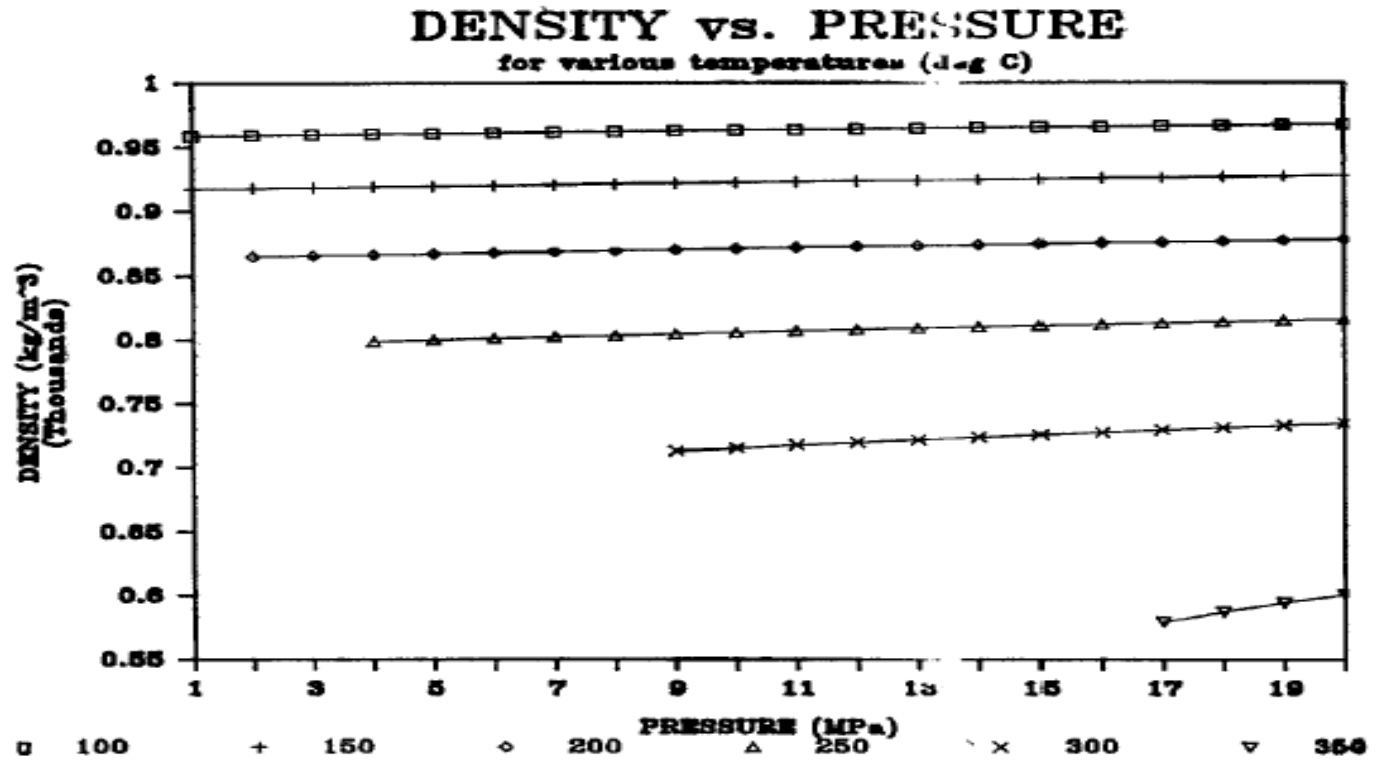


Figure 4.4 Density vs. pressure at various temperatures in subcooled water.

Questions?