

## Continuum Description of a Condensation Process in a Flowing System

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### I. Problem Formulation

We have a fluid flowing down a pipe. It's a single component fluid. When the fluid enters the system, it is at a temperature greater than the critical temperature. The pipe is not perfectly insulated. As the fluid flows down the pipe, it loses heat to the surroundings. The temperature drops. As a result, the fluid may partially condense. We want to describe the time and spatial dependence of the system. Specifically, we want the following variables as a function of time and space: the temperature,  $T$ , the pressure,  $p$ , the vapor fraction,  $\phi_V$ , the density of the vapor phase,  $\rho_V$ , and the density of the liquid phase,  $\rho_L$ .

This hand-out assumes that you have already the previous two hand-out in this series. The first hand-out was titled, "Forms of the Microscopic Energy Balance". We will use this as our starting point for our evolution equations. The second hand-out is titled, "Continuum Description of a Condensation Process in a System of Fixed Mass and Fixed Volume". In that hand-out, we examined condensation of a single-component van der Waals gas in a closed system. Now, we have a flowing system. All the other assumptions will be the same.

If we have a single component system and we restrict ourselves to variations in the axial dimension only, then from the previous hand-out titled, "Generalized Evolution Equations for Mass, Momentum and Energy", we know that we will have three balances: one for momentum, one for the axial velocity, and one for the energy.

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}), \quad (1)$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} = -\rho \mathbf{v} \cdot \nabla (\mathbf{v}) - \nabla p - \nabla \cdot \boldsymbol{\tau} - \rho \nabla \hat{\Phi} \quad . \quad (2)$$

$$\rho \frac{\partial \left( \frac{1}{2} v^2 + \hat{H} + \hat{\Phi} \right)}{\partial t} - \frac{\partial p}{\partial t} = -\rho \mathbf{v} \nabla \cdot \left( \frac{1}{2} v^2 + \hat{H} + \hat{\Phi} \right) - \nabla \cdot \mathbf{q} - \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}), \quad (3)$$

We assume the fluid is inviscid and we neglect any potential energy terms. We will have to add a heat loss through the uninsulated walls to the energy balance. Since the problem is one-dimensional, all of the divergences and gradients will become partial derivatives with respect to axial position. We will assume that the thermal conductivity is constant for a given phase, but is not the same for both the liquid and vapor phases. Therefore, we cannot pull the thermal

conductivity out of the divergence. We will obtain the pressure and the enthalpy from an equation of state. In this case, we will use the van der Waals equation of state, because that is the simplest equation of state that one can use and still get vapor-liquid equilibrium (VLE). With all of these changes, the equations become,

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho v}{\partial z}, \quad (4)$$

$$\rho \frac{\partial v}{\partial t} = -\rho v \frac{\partial v}{\partial z} - \frac{\partial p}{\partial z}. \quad (5)$$

$$\rho \frac{\partial \left( \frac{1}{2} v^2 + \hat{H} \right)}{\partial t} - \frac{\partial p}{\partial t} = -\rho v \frac{\partial}{\partial z} \left( \frac{1}{2} v^2 + \hat{H} \right) + \frac{\partial}{\partial z} \left( k_c \frac{\partial T}{\partial z} \right) - \mathbf{Q}, \quad (6)$$

We now remind ourselves of the appropriate variables for describing a two-phase system. Within each infinitesimal volume, we define volume fractions as

$$\phi_L = \frac{V_L}{V} \quad \text{and} \quad \phi_V = \frac{V_V}{V} \quad (7)$$

where

$$1 = \phi_L + \phi_V \quad (8)$$

The volume of this differential element is constant,

$$V = V_L + V_V \quad (9)$$

The mass within this element is composed of liquid and vapor

$$M = M_L + M_V \quad (10)$$

The density of the individual phases within the differential element are

$$\rho_L = \frac{M_L}{V_L} \quad \text{and} \quad \rho_V = \frac{M_V}{V_V} \quad (11)$$

Substituting equation (11) into equation (10) yields

$$M = V\rho = V_L\rho_L + V_V\rho_V \quad (12)$$

Substituting equations (7) and (8) into equation (12) yields

$$\rho = \phi_L \rho_L + \phi_V \rho_V = (1 - \phi_V) \rho_L + \phi_V \rho_V \quad (13)$$

Solving for the vapor fraction yields

$$\phi_V = \frac{\rho - \rho_L}{\rho_V - \rho_L} \quad (14)$$

Therefore, if we know the total density, the liquid density and the vapor density, we can obtain the vapor fraction.

We can write a balance on the mass of the vapor phase in a differential volume. The accumulation of vapor mass in the element is

$$accumulation = \frac{\partial(\rho_V V_V)}{\partial t} = \Delta V \frac{\partial(\rho_V \phi_V)}{\partial t} \quad (15)$$

The convection of vapor mass is given by

$$\begin{aligned} convection &= (\rho_V V_V \mathbf{v} \cdot \Delta \mathbf{A}')_{in} - (\rho_V V_V \mathbf{v} \cdot \Delta \mathbf{A}')_{out} \\ &= (V \rho_V \phi_V \mathbf{v} \cdot \Delta \mathbf{A}')_{in} - (V \rho_V \phi_V \mathbf{v} \cdot \Delta \mathbf{A}')_{out} \\ &= (\rho_V \phi_V \mathbf{v} \cdot \Delta \mathbf{A})_{in} - (\rho_V \phi_V \mathbf{v} \cdot \Delta \mathbf{A})_{out} \end{aligned} \quad (16)$$

where  $\Delta \mathbf{A}'$  is the dimensionless cross-sectional area of the differential volume normal to the velocity and  $\Delta \mathbf{A} = V \Delta \mathbf{A}'$  is the same with dimensions. The generation of vapor mass is

$$generation = \Delta V r_{vap} \quad (17)$$

Therefore, the vapor mass balance is

$$\Delta V \frac{\partial(\rho_V \phi_V)}{\partial t} = (\rho_V \phi_V \mathbf{v} \cdot \Delta \mathbf{A})_{in} - (\rho_V \phi_V \mathbf{v} \cdot \Delta \mathbf{A})_{out} + \Delta V r_{vap} \quad (18)$$

As always, divide by the volume and take the limit as the differential volume goes to zero.

$$\frac{\partial(\rho_V \phi_V)}{\partial t} = -\nabla \cdot (\rho_V \phi_V \mathbf{v}) + r_{vap} \quad (19)$$

This term has the rate of vaporization in it. We will use this “vapor mass balance” to define the rate of vaporization in terms of known variables later on.

Now we can proceed to further develop the energy balance.

$$\rho \frac{\partial \left( \frac{1}{2} v^2 + \hat{H} \right)}{\partial t} - \frac{\partial p}{\partial t} = -\rho v \frac{\partial}{\partial z} \left( \frac{1}{2} v^2 + \hat{H} \right) + \frac{\partial}{\partial z} \left( k_c \frac{\partial T}{\partial z} \right) - \mathbf{Q}, \quad (6)$$

The specific enthalpy can be expressed as

$$\begin{aligned} \hat{H} &= \frac{N_L m}{Nm} \hat{H}_L + \frac{N_V m}{Nm} \hat{H}_V = \frac{\rho_L V_L \hat{H}_L + \rho_V V_V \hat{H}_V}{\rho_L V_L + \rho_V V_V} \\ &= \frac{\rho_L V_L \hat{H}_L + \rho_V V_V \hat{H}_V}{\rho V} = \frac{\rho_L \phi_L \hat{H}_L + \rho_V \phi_V \hat{H}_V}{\rho} \end{aligned} \quad (20)$$

where  $\hat{H}_L$  and  $\hat{H}_V$  are the specific enthalpies of the liquid and vapor phases. Substituting equation (20) into equation (6) we have

$$\rho v \frac{\partial v}{\partial t} + \rho \frac{\partial \left( \frac{\rho_L \phi_L \hat{H}_L + \rho_V \phi_V \hat{H}_V}{\rho} \right)}{\partial t} - \frac{\partial p}{\partial t} = -\rho v^2 \frac{\partial v}{\partial z} - \rho v \frac{\partial \left( \frac{\rho_L \phi_L \hat{H}_L + \rho_V \phi_V \hat{H}_V}{\rho} \right)}{\partial z} + \frac{\partial}{\partial z} \left( k_c \frac{\partial T}{\partial z} \right) - \mathbf{Q} \quad (21)$$

Simplification yields

$$\begin{aligned} &\rho v \frac{\partial v}{\partial t} + \frac{\partial (\rho_L \phi_L \hat{H}_L + \rho_V \phi_V \hat{H}_V)}{\partial t} - \frac{\rho_L \phi_L \hat{H}_L + \rho_V \phi_V \hat{H}_V}{\rho} \frac{\partial \rho}{\partial t} - \frac{\partial p}{\partial t} \\ &= -\rho v^2 \frac{\partial v}{\partial z} - v \frac{\partial (\rho_L \phi_L \hat{H}_L + \rho_V \phi_V \hat{H}_V)}{\partial z} + \frac{\rho_L \phi_L \hat{H}_L + \rho_V \phi_V \hat{H}_V}{\rho} v \frac{\partial \rho}{\partial z} + \frac{\partial}{\partial z} \left( k_c \frac{\partial T}{\partial z} \right) - \mathbf{Q} \end{aligned} \quad (22)$$

Eliminate liquid fraction and liquid density,

$$\begin{aligned} &\rho v \frac{\partial v}{\partial t} + \frac{\partial ((\rho - \rho_V \phi_V) \hat{H}_L + \rho_V \phi_V \hat{H}_V)}{\partial t} - \frac{(\rho - \rho_V \phi_V) \hat{H}_L + \rho_V \phi_V \hat{H}_V}{\rho} \frac{\partial \rho}{\partial t} - \frac{\partial p}{\partial t} \\ &= -\rho v^2 \frac{\partial v}{\partial z} - v \frac{\partial ((\rho - \rho_V \phi_V) \hat{H}_L + \rho_V \phi_V \hat{H}_V)}{\partial z} + \frac{(\rho - \rho_V \phi_V) \hat{H}_L + \rho_V \phi_V \hat{H}_V}{\rho} v \frac{\partial \rho}{\partial z} \\ &+ \frac{\partial}{\partial z} \left( k_c \frac{\partial T}{\partial z} \right) - \mathbf{Q} \end{aligned} \quad (23)$$

Simplifying the accumulation terms on the RHS yields

$$\begin{aligned}
& \rho v \frac{\partial v}{\partial t} + \frac{\partial \left( (\rho - \rho_v \phi_v) \hat{H}_L + \rho_v \phi_v \hat{H}_V \right)}{\partial t} - \frac{(\rho - \rho_v \phi_v) \hat{H}_L + \rho_v \phi_v \hat{H}_V}{\rho} \frac{\partial \rho}{\partial t} - \frac{\partial p}{\partial t} \\
&= \rho v \frac{\partial v}{\partial t} + \rho \frac{\partial \hat{H}_L}{\partial t} + \hat{H}_L \frac{\partial \rho}{\partial t} + \rho_v \phi_v \frac{\partial (\hat{H}_V - \hat{H}_L)}{\partial t} + (\hat{H}_V - \hat{H}_L) \frac{\partial \rho_v \phi_v}{\partial t} \\
&\quad - \hat{H}_L \frac{\partial \rho}{\partial t} - \frac{\rho_v \phi_v (\hat{H}_V - \hat{H}_L)}{\rho} \frac{\partial \rho}{\partial t} - \frac{\partial p}{\partial t} \\
&= \rho v \frac{\partial v}{\partial t} + \rho \frac{\partial \hat{H}_L}{\partial t} + \rho_v \phi_v \frac{\partial \Delta \hat{H}_{vap}}{\partial t} + \Delta \hat{H}_{vap} \frac{\partial \rho_v \phi_v}{\partial t} - \frac{\rho_v \phi_v \Delta \hat{H}_{vap}}{\rho} \frac{\partial \rho}{\partial t} - \frac{\partial p}{\partial t}
\end{aligned} \tag{24}$$

Simplifying the convection terms on the LHS of equation (21) yields

$$\begin{aligned}
& -\rho v^2 \frac{\partial v}{\partial z} - v \frac{\partial \left( (\rho - \rho_v \phi_v) \hat{H}_L + \rho_v \phi_v \hat{H}_V \right)}{\partial z} + \frac{(\rho - \rho_v \phi_v) \hat{H}_L + \rho_v \phi_v \hat{H}_V}{\rho} v \frac{\partial \rho}{\partial z} \\
&= -\rho v^2 \frac{\partial v}{\partial z} - v \hat{H}_L \frac{\partial \rho}{\partial z} - \rho v \frac{\partial \hat{H}_L}{\partial z} - v \rho_v \phi_v \frac{\partial \Delta \hat{H}_{vap}}{\partial z} - v \Delta \hat{H}_{vap} \frac{\partial \rho_v \phi_v}{\partial z} + \hat{H}_L v \frac{\partial \rho}{\partial z} + \frac{\rho_v \phi_v \Delta \hat{H}_{vap}}{\rho} v \frac{\partial \rho}{\partial z} \\
&= -\rho v^2 \frac{\partial v}{\partial z} - \rho v \frac{\partial \hat{H}_L}{\partial z} - v \rho_v \phi_v \frac{\partial \Delta \hat{H}_{vap}}{\partial z} - v \Delta \hat{H}_{vap} \frac{\partial \rho_v \phi_v}{\partial z} + \frac{\rho_v \phi_v \Delta \hat{H}_{vap}}{\rho} v \frac{\partial \rho}{\partial z}
\end{aligned} \tag{25}$$

We now substitute equation (24) and (25) into equation (23).

$$\begin{aligned}
& \rho v \frac{\partial v}{\partial t} + \rho \frac{\partial \hat{H}_L}{\partial t} + \rho_v \phi_v \frac{\partial \Delta \hat{H}_{vap}}{\partial t} + \Delta \hat{H}_{vap} \frac{\partial \rho_v \phi_v}{\partial t} - \frac{\rho_v \phi_v \Delta \hat{H}_{vap}}{\rho} \frac{\partial \rho}{\partial t} - \frac{\partial p}{\partial t} \\
&= -\rho v^2 \frac{\partial v}{\partial z} - \rho v \frac{\partial \hat{H}_L}{\partial z} - v \rho_v \phi_v \frac{\partial \Delta \hat{H}_{vap}}{\partial z} - v \Delta \hat{H}_{vap} \frac{\partial \rho_v \phi_v}{\partial z} + \frac{\rho_v \phi_v \Delta \hat{H}_{vap}}{\rho} v \frac{\partial \rho}{\partial z} + \frac{\partial}{\partial z} \left( k_c \frac{\partial T}{\partial z} \right) - \mathbf{Q}
\end{aligned} \tag{26}$$

Also, we are going to rearrange equation (19) for  $r_{vap}$

$$r_{vap} = \frac{\partial (\rho_v \phi_v)}{\partial t} + \frac{\partial (\rho_v \phi_v v)}{\partial z} = \frac{\partial (\rho_v \phi_v)}{\partial t} + v \frac{\partial (\rho_v \phi_v)}{\partial z} + \rho_v \phi_v \frac{\partial v}{\partial z} \tag{27}$$

and substitute that into equation (26)

$$\begin{aligned}
\rho v \frac{\partial v}{\partial t} + \rho \frac{\partial \hat{H}_L}{\partial t} + \rho_V \phi_V \frac{\partial \Delta \hat{H}_{vap}}{\partial t} - \frac{\rho_V \phi_V \Delta \hat{H}_{vap}}{\rho} \frac{\partial \rho}{\partial t} - \frac{\partial p}{\partial t} = -\rho v^2 \frac{\partial v}{\partial z} - \rho v \frac{\partial \hat{H}_L}{\partial z} \\
- v \rho_V \phi_V \frac{\partial \Delta \hat{H}_{vap}}{\partial z} + \frac{\rho_V \phi_V \Delta \hat{H}_{vap}}{\rho} v \frac{\partial \rho}{\partial z} - \Delta \hat{H}_{vap} r_{vap} + \Delta \hat{H}_{vap} \rho_V \phi_V \frac{\partial v}{\partial z} + \frac{\partial}{\partial z} \left( k_c \frac{\partial T}{\partial z} \right) \cdot \mathbf{Q}
\end{aligned} \tag{28}$$

Collecting like terms, we have

$$\begin{aligned}
\rho v \frac{\partial v}{\partial t} + \rho \frac{\partial \hat{H}_L}{\partial t} + \rho_V \phi_V \frac{\partial \Delta \hat{H}_{vap}}{\partial t} - \frac{\rho_V \phi_V \Delta \hat{H}_{vap}}{\rho} \frac{\partial \rho}{\partial t} - \frac{\partial p}{\partial t} = \left( \Delta \hat{H}_{vap} \rho_V \phi_V - \rho v^2 \right) \frac{\partial v}{\partial z} \\
- \rho v \frac{\partial \hat{H}_L}{\partial z} - v \rho_V \phi_V \frac{\partial \Delta \hat{H}_{vap}}{\partial z} + \frac{\rho_V \phi_V \Delta \hat{H}_{vap}}{\rho} v \frac{\partial \rho}{\partial z} - \Delta \hat{H}_{vap} r_{vap} + \frac{\partial}{\partial z} \left( k_c \frac{\partial T}{\partial z} \right) \cdot \mathbf{Q}
\end{aligned} \tag{29}$$

The PDE only has derivatives (either temporal or spatial) of the density and velocity, as well as the enthalpy and pressure. The enthalpy and pressure will be related to the density and temperature via an equation of state. Notably, there are no time derivatives of vapor fractions in the equation.

Now, in a one-phase region, we have two degrees of freedom and the enthalpy and pressure are functions of both the density and temperature.

$$H = H(\rho, T) \tag{30.a}$$

$$p = p(\rho, T) \tag{30.b}$$

Therefore, the time derivative is going to be written as

$$\frac{\partial H}{\partial t} = \left( \frac{\partial H}{\partial T} \right)_\rho \frac{\partial T}{\partial t} + \left( \frac{\partial H}{\partial \rho} \right)_T \frac{\partial \rho}{\partial t} \tag{31}$$

The presence of the time derivative of the temperature is acceptable. We will use the energy balance to solve for the temperature as a function of time. The presence of the time derivative of the density is also not a problem, since we have an expression for the evolution of the density from the continuity equation. If we directly substitute the continuity equation into equation (31), we have

$$\frac{\partial H}{\partial t} = \left( \frac{\partial H}{\partial T} \right)_\rho \frac{\partial T}{\partial t} - \left( \frac{\partial H}{\partial \rho} \right)_T \nabla \cdot (\rho \mathbf{v}) \quad \text{for one phase} \tag{32}$$

Now when we have two phases, we have one degree of freedom and the enthalpies and the pressure are a function of temperature only

$$H_L = H_L(\rho_L(T), T) \quad \text{and} \quad H_V = H_V(\rho_V(T), T) \quad (33.a)$$

$$p = p(T) \quad (33.b)$$

Therefore, the time derivative is going to be written as

$$\begin{aligned} \frac{\partial H_L}{\partial t} &= \left( \frac{\partial H_L}{\partial T} \right)_{sat} \frac{\partial T}{\partial t} + \left( \frac{\partial H_L}{\partial \rho_L} \right)_{sat} \frac{\partial \rho_L}{\partial t} \\ &= \left( \frac{\partial H_L}{\partial T} \right)_{sat} \frac{\partial T}{\partial t} + \left( \frac{\partial H_L}{\partial \rho_L} \right)_{sat} \left( \frac{\partial \rho_L}{\partial T} \right)_{sat} \frac{\partial T}{\partial t} \quad \text{for two phases} \\ &= \left[ \left( \frac{\partial H_L}{\partial T} \right)_{sat} + \left( \frac{\partial H_L}{\partial \rho_L} \right)_{sat} \left( \frac{\partial \rho_L}{\partial T} \right)_{sat} \right] \frac{\partial T}{\partial t} \end{aligned} \quad (34)$$

So, in order to solve this problem, we will need the thermodynamic partial derivatives that appear in equations (32) and (34). In order to proceed any farther, we have to identify a specific equation of state.

It is true that the rate of vaporization does appear in the energy balance, but this we know because

$$r_{vap} = \rho_V \frac{\partial \phi_V}{\partial t} + \phi_V \frac{\partial \rho_V}{\partial t} + \nu \rho_V \frac{\partial \phi_V}{\partial z} + \nu \phi_V \frac{\partial \rho_V}{\partial z} + \rho_V \phi_V \frac{\partial \nu}{\partial z} \quad (35)$$

where  $\rho_V$  will come from the thermodynamic analysis and where the temporal and spatial derivatives can be related to the temperature via

$$\frac{\partial \rho_V}{\partial t} = \left( \frac{\partial \rho_V}{\partial T} \right)_{sat} \frac{\partial T}{\partial t} \quad (36)$$

and

$$\frac{\partial \rho_V}{\partial z} = \left( \frac{\partial \rho_V}{\partial T} \right)_{sat} \frac{\partial T}{\partial z} \quad (37)$$

where the partial derivative  $\left( \frac{\partial \rho_V}{\partial T} \right)_{sat}$  comes from the thermodynamic equation of state. Also we know that

$$\phi_V = \frac{\rho - \rho_L}{\rho_V - \rho_L} \quad (14)$$

so that the time derivative is

$$\frac{\partial \phi_V}{\partial t} = \frac{1}{\rho_V - \rho_L} \left( \frac{\partial \rho}{\partial t} - \frac{\partial \rho_L}{\partial t} \right) - \frac{\rho - \rho_L}{(\rho_V - \rho_L)^2} \left( \frac{\partial \rho_V}{\partial t} - \frac{\partial \rho_L}{\partial t} \right) \quad (36)$$

which can be written as

$$\frac{\partial \phi_V}{\partial t} = \frac{1}{\rho_V - \rho_L} \frac{\partial \rho}{\partial t} - \left[ \frac{1}{\rho_V - \rho_L} \left( \frac{\partial \rho_L}{\partial T} \right) \Big|_{sat} + \frac{\rho - \rho_L}{(\rho_V - \rho_L)^2} \left( \left( \frac{\partial \rho_V}{\partial T} \right) \Big|_{sat} - \left( \frac{\partial \rho_L}{\partial T} \right) \Big|_{sat} \right) \right] \frac{\partial T}{\partial t} \quad (37)$$

and the spatial derivative is

$$\frac{\partial \phi_V}{\partial z} = \frac{1}{\rho_V - \rho_L} \frac{\partial \rho}{\partial z} - \left[ \frac{1}{\rho_V - \rho_L} \left( \frac{\partial \rho_L}{\partial T} \right) \Big|_{sat} + \frac{\rho - \rho_L}{(\rho_V - \rho_L)^2} \left( \left( \frac{\partial \rho_V}{\partial T} \right) \Big|_{sat} - \left( \frac{\partial \rho_L}{\partial T} \right) \Big|_{sat} \right) \right] \frac{\partial T}{\partial z} \quad (38)$$

Therefore, we have all the information we need to solve the problem.

If we are only interested in the steady state behavior of the system, the energy balance of equation (29) becomes

$$0 = \left( \Delta \hat{H}_{vap} \rho_V \phi_V - \rho v^2 \right) \frac{\partial v}{\partial z} - \rho v \frac{\partial \hat{H}_L}{\partial z} - v \rho_V \phi_V \frac{\partial \Delta \hat{H}_{vap}}{\partial z} + \frac{\rho_V \phi_V \Delta \hat{H}_{vap}}{\rho} v \frac{\partial \rho}{\partial z} - \Delta \hat{H}_{vap} r_{vap} + \frac{\partial}{\partial z} \left( k_c \frac{\partial T}{\partial z} \right) - \mathbf{Q} \quad (39)$$

If we have no flow in the system (and thus no spatial derivatives), the energy balance becomes,

$$\rho \frac{\partial \hat{H}_L}{\partial t} + \rho_V \phi_V \frac{\partial \Delta \hat{H}_{vap}}{\partial t} - \frac{\rho_V \phi_V \Delta \hat{H}_{vap}}{\rho} \frac{\partial \rho}{\partial t} - \frac{\partial p}{\partial t} = -\Delta \hat{H}_{vap} r_{vap} - \mathbf{Q} \quad (40)$$

In order to compare with our previous lecture package, if we make the additional assumption that the volume of the container is fixed, we have constant total density

$$\rho \frac{\partial \hat{H}_L}{\partial t} + \rho_V \phi_V \frac{\partial \Delta \hat{H}_{vap}}{\partial t} - \frac{\partial p}{\partial t} = -\Delta \hat{H}_{vap} r_{vap} - \mathbf{Q} \quad (41)$$

This is equivalent to our energy balance from the non-flowing case, except that here we have written it in terms of the enthalpy, rather than the internal energy.



## II. Derivation for van der Waals Equation of State

At this point we need an equation of state. We will proceed with the van der Waals (vdW) equation of state (EOS), since it is the simplest EOS that allows for vapor liquid equilibrium (VLE).

The pressure for the vdW EOS is given by

$$p = \frac{RT}{V_m - b} - \frac{a}{V_m^2} \quad (33)$$

where  $V_m$  is a molar volume, related to our density via

$$V_m = \frac{m}{\rho} \quad (34)$$

The specific enthalpy of the vdW fluid is

$$H = \frac{RT}{m} \left( \frac{3}{2} - 2 \frac{a\rho}{mRT} + \frac{m}{m - \rho b} \right) \quad (35)$$

We will need the following derivatives

$$\left( \frac{\partial H}{\partial T} \right)_p = \frac{R}{m} \left[ \frac{3}{2} + \frac{m}{m - \rho b} \right] \quad (36)$$

$$\left( \frac{\partial H}{\partial \rho} \right)_T = \frac{RT}{m} \left( -2 \frac{a}{mRT} + \frac{bm}{(m - \rho b)^2} \right) \quad (37)$$

In the one phase region, we substitute equations (36) and (37) into equation (30)

$$\frac{\partial H}{\partial t} = \frac{R}{m} \left[ \frac{3}{2} + \frac{m}{m - \rho b} \right] \frac{\partial T}{\partial t} - \frac{RT}{m} \left( -2 \frac{a}{mRT} + \frac{bm}{(m - \rho b)^2} \right) \nabla \cdot (\rho \mathbf{v}) \quad (38)$$

In a two phase system, we can write equation (35) for each phase.

$$H_L = \frac{RT}{m} \left( \frac{3}{2} - 2 \frac{a\rho_L}{mRT} + \frac{m}{m - \rho_L b} \right) \quad \text{and} \quad H_V = \frac{RT}{m} \left( \frac{3}{2} - 2 \frac{a\rho_V}{mRT} + \frac{m}{m - \rho_V b} \right) \quad (39)$$

In the two-phase system, there is only one degree of freedom, which we choose as the temperature, therefore, our energy balance changed to that of equation (32) and as a result, we not only need the derivatives in equation (36) and (37) but we also need the change in density

with respect to temperature along the saturation line. We have previously derived this result in the hand-out for the closed system. Here we simply restate it,

$$\left. \frac{\partial V_m^V}{\partial T} \right|_{sat} = \frac{\frac{k_B}{V_m^L - b} - \frac{k_B}{V_m^V - b} + k_B \left[ \ln \left( \frac{V_m^L - b}{V_m^V - b} \right) + \frac{b}{V_m^V - b} - \frac{b}{V_m^L - b} \right]}{\left( \frac{k_B T}{(V_m^L - b)^2} - 2 \frac{a}{V_m^{L^3}} \right) - \left( \frac{k_B T}{V_m^L - b} + \frac{k_B T b}{(V_m^L - b)^2} - \frac{2a}{V_m^{L^2}} \right)} - \frac{\left( \frac{k_B T}{V_m^V - b} + \frac{k_B T b}{(V_m^V - b)^2} - \frac{2a}{V_m^{V^2}} \right) - \left( \frac{k_B T}{(V_m^V - b)^2} - 2 \frac{a}{V_m^{V^3}} \right)}{\left( \frac{k_B T}{V_m^L - b} + \frac{k_B T b}{(V_m^L - b)^2} - \frac{2a}{V_m^{L^2}} \right) - \left( \frac{k_B T}{(V_m^L - b)^2} - 2 \frac{a}{V_m^{L^3}} \right)} \quad (40)$$

$$\left. \frac{\partial V_m^L}{\partial T} \right|_{sat} = \frac{\frac{k_B}{V_m^L - b} - \frac{k_B}{V_m^V - b} + \left( \frac{k_B T}{(V_m^V - b)^2} - 2 \frac{a}{V_m^{V^3}} \right) \left. \frac{\partial V_m^V}{\partial T} \right|_{sat}}{\left( \frac{k_B T}{(V_m^L - b)^2} - 2 \frac{a}{V_m^{L^3}} \right)} \quad (41)$$

Differentiating equation (34), we have

$$\frac{\partial \rho}{\partial T} = -\frac{\rho^2}{m} \frac{\partial V_m}{\partial T} \quad (42)$$

so we have the derivatives of the density that we require in the energy balance.

### III. The Solution Algorithm

The big picture is that we have three nonlinear partial differential equations that we wish to solve, namely the mass, momentum, and energy balance. We have three unknowns,  $\rho(t, \mathbf{r})$ ,  $\mathbf{v}(t, \mathbf{r})$ ,  $T(t, \mathbf{r})$ . At each point in time and space, we will require a number of other quantities, which will be determined not through the integration of an evolution equation but rather from a thermodynamic constraint. These quantities include

- (i) the number of phases,
- (ii) the density of the hypothetical one phase system,  $\rho(t, \mathbf{r})$ ,
- (iii) the pressure of the hypothetical one phase system,
- (iv) the density of the hypothetical liquid of the two phase system,
- (v) the density of the hypothetical vapor of the two phase system,
- (vi) the pressure (vapor pressure) of the two phase system, and
- (vii) the volume fraction of the vapor phase.

The algorithm goes as follows. At any point in time and space, we know the current temperature. If this temperature is above the critical temperature, we have a one phase system. If this temperature is below the critical temperature, then we must determine the number of phases. This determination is made by first iteratively calculating the vapor pressure and liquid and vapor densities of the two phase system. If the density of the one phase system falls between the densities of the two phase system, then the one phase system lies within the two-phase envelope and will separate into two phases. At this point, we use equation (14) to calculate the vapor fraction and we have everything we need to evaluate all of the terms on the RHS of the mass, momentum, and energy balances.

#### IV. Transport properties for a two-phase system.

At this point, we have the thermodynamic properties of the material. However, we need the transport properties, specifically the thermal conductivity. The simplest level of approximation is to provide a constant value or a simple function for the thermal conductivity of the liquid and the thermal conductivity of the vapor phase, then create a rule for the thermal conductivity of the two-phase mixture. Here we provide such an example.

For a monatomic, ideal gas from kinetic theory, we know that the thermal conductivity is given by equation (9.3-12) of BSL2

$$k_c^V = \frac{2}{3\pi} \frac{\sqrt{\pi m k_B T}}{\pi d^2} \hat{C}_v^V \quad (43)$$

For a monatomic liquid, the thermal conductivity can be approximated via Bridgman's equation (9.4-2) and (9.4-4) of BSL2

$$k_c^L = 3k_B \left( \frac{\rho^L}{m} \right)^{\frac{2}{3}} v_s = 3k_B \left( \frac{\rho^L}{m} \right)^{\frac{2}{3}} \sqrt{\frac{C_p}{C_v} \left( \frac{\partial p}{\partial \rho^L} \right)_T} \quad (44)$$

Now, in a region with two phases, the conductivity of the mixture depends upon the orientation of the two phases. We begin the analysis with Fourier's law for a system with variation in one-dimension

$$q = -k_c \frac{dT}{dz} \quad (45)$$

where  $q$  is the conductive heat flux. For the case of heat transfer in parallel (where we imagine that the liquid and vapor form layers parallel to the flow direction), we know that the driving force,  $\frac{dT}{dz}$ , is the same at steady state in each region since they connect to the same initial and

final boundaries. If we write equation (45) for each of the two phases as well as for the total system (T), and equate the gradients across the vapor and liquid phases, we have

$$\left. \frac{dT}{dz} \right|^T = \left. \frac{dT}{dz} \right|^L = \left. \frac{dT}{dz} \right|^V \quad (46)$$

We also acknowledge that the total rate of transport is the sum of the rate of transport in each of the three regions,

$$A_z^T q^T = A_z^L q^L + A_z^V q^V \quad (47)$$

where  $A_z^J$  is the cross-sectional area of phase  $J$ . In the assumption of parallel phases, one might simply equate the ratio of areas to the phase volume fractions  $A_z^J / A_z^T = \phi^J$ . Combining equations (45), (46) and (47) and this assumption lead to an expression for the total thermal conductivity parallel to the flow direction,

$$k_{c\parallel}^T = \phi^L k_c^L + \phi^V k_c^V \quad (48)$$

For the case of mass transport in series (where the liquid and vapor phases form layers perpendicular to the flow direction), we acknowledge that at steady state the flux in equation (45) is the same for each region and for the system total. Furthermore, the cross-sectional area of each region relevant to transport perpendicular to the flow is constant. Therefore, we have

$$q^T = q^L = q^V \quad (49)$$

Furthermore, we acknowledge that the total driving force is the sum of the driving forces across each region,

$$\left. \frac{dT}{dz} \right|^T = \left. \frac{dT}{dz} \right|^L + \left. \frac{dT}{dz} \right|^V \quad (50)$$

Combining equations (45), (49) and (50) lead to an expression for the total diffusivity perpendicular to the interface,

$$\frac{1}{k_{c\perp}^T} = \frac{1}{k_c^L} + \frac{1}{k_c^V} \quad (51)$$

In reality, it is unlikely that a two phase system are distributed in parallel or perpendicular slabs, but rather some complicated geometry that delivers a mean thermal conductivity somewhere between these two limits. Moreover, this geometry is surely a function of volume fraction of the two phases. Imagine a phase that is mostly vapor. It has small droplets of liquid in it. This can be modeled as a system that has a purely vapor phase in parallel with a vapor/liquid phase in series. Thus substituting equation (51) into (48), we have

$$k_c^T = \left( \phi^L + (1-\varepsilon)\phi^V \right) \left( \frac{1}{k_c^L} + \frac{1}{k_c^V} \right)^{-1} + \varepsilon\phi^V k_c^V \quad (52)$$

where  $\varepsilon$  is bound between 0 and 1 and is 0 to retrieve the limit in which the phases are just in series. It increases as the degree of parallel resistance increases. The quantitative value of  $\varepsilon$  and its dependence on the other variables in the system would have to be determined by fitting to experiment or theory. An analogous expression could be generated for the case where we have mostly liquid phase with a few vapor bubbles.