# ThermoCycle Moving Boundary Model

Adriano Desideri

Thermodynamics Laboratory University of Liège Liège, Belgium adesideri@ulg.ac.be Jorrit Wronski

Department of Mechanical Engineering Technical University of Denmark Kgs. Lyngby, Denmark jowr@mek.dtu.dk

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#### Abstract

The authors present a new moving boundary model that was integrated into the ThermoCycle package written in the Modelica language. Focusing on a seamless integration with existing components, this new component allows to calculate dynamic heat transfer in an efficient and robust way covering the full range of possible operating points in the liquid, two-phase, gas and supercritical domain. A basic validation performed with heat transfer data from two different experiments with evaporators shows that the model is able to reliably predict heat exchanger performance. The flexible implementation allows to compare different heat transfer correlations, which are made freely available as part of the ThermoCycle library.

### 1 Introduction and Motivation

Moving boundary (MB) models are established tools to calculate heat exchanger performance in both steady-state and dynamic operation. A fictitious heat transfer channel is split up into different sections and with each section accounting for a different fluid state. In the case of an evaporator the maximum number of sections N is 3 for a) subcooled, b) two-phase and c) superheated state. At higher pressures, the fluid might enter the supercritical state. Hence, there are four different sections out of which a maximum of three can occur simultaneously. The name moving boundary is derived from the fact that the interfaces between these sections do not have a fixed spatial position but merely a fixed thermodynamic location depending on the presence of liquid and gaseous fluid, respectively. The actual existence of a certain section and its length are determined based on the fluid state resulting in variable sectioning. A fixed total length superimposes the required boundary condition to calculate the length of each section.

Moving boundary formulations are a good compromise between computational efficiency, robustness and accuracy[2].

## 2 Formulation

### 2.1 Assumptions

- i. The tube is cylindrical with a constant cross sectional area
- ii. The velocity of the fluid is uniform on the cross sectional area
- iii. The enthalpy of the fluid is linear in each region of the tube (sub-cooled, two-phase, super-heated)
- iv. Pressure is considered constant (at least for now)
- v. The secondary fluid is treated as a constant heat capacity fluid

### 2.2 Equations

Thermodynamic properties are calculated using Coolprop [1]. The state variable selected are p and  $\bar{h}$ . The heat transfer coefficients on primary side  $(U_{\rm pf,1}, U_{\rm pf,2}, U_{\rm pf,3})$  and secondary side  $(U_{\rm sf,1}, U_{\rm sf,2}, U_{\rm sf,3})$  are calculated using appropriate heat transfer models. Different model of void fraction  $\bar{\alpha}$  have been also implemented.

### 2.2.1 Mass Balance: derivation process

The mass balance in the differential form can be written as:

$$\frac{\partial A \cdot \rho}{\partial t} + \frac{\partial \dot{m}}{\partial z} = 0 \tag{1}$$

To get the mass balance over a certain region (e.g. the sub-cooled region from 0 to  $L_1$ ), we need to integrate over z equation 1:

$$\int_0^{L_1} \frac{\partial A \cdot \rho_1}{\partial t} dz + \int_0^{L_1} \frac{\partial \dot{m}}{\partial z} dz = 0$$
 (2)

Applying Leibniz rule for the first term and solving the integral for the second term of equation 2, results:

$$A \cdot \left[ \frac{d}{dt} \cdot \int_0^{L_1} \rho_1 dz - \rho_1(L_1) \cdot \frac{dL_1}{dt} \right] = \dot{m}_{\rm in} - \dot{m}_{12}$$
 (3)

Solving the first term of equation 3 results in:

$$\frac{d}{dt} \cdot \int_0^{L_1} \rho_1 dz = \frac{d}{dt} \cdot (\overline{\rho}_1 \cdot L_1) = \overline{\rho}_1 \cdot \frac{dL_1}{dt} + L_1 \cdot \frac{d\overline{\rho}_1}{dt}$$
 (4)

The bar over the density indicates that a mean value of the zone is considered. Substituting equation 4 in equation 3 results in:

$$A \cdot \left[ L_1 \cdot \frac{d\overline{\rho}_1}{dt} + (\overline{\rho}_1 - \rho_1) \cdot \frac{dL_1}{dt} \right] = \dot{m}_{\rm in} - \dot{m}_{12}$$
 (5)

which represents the mass balance for the first zone of the heat exchanger. The same procedure can be applied to develop the mass balance for the second and the third zone of the heat exchanger.

### 2.2.2 Energy Balance: derivation process

The energy balance for a zone of the heat exchanger can be written as:

$$A \cdot \frac{\partial(\rho_1 \cdot h_1 - p)}{\partial t} + \frac{\partial(h_1 \cdot \dot{m})}{\partial z} = \dot{Q}$$
 (6)

Integrating over length results in:

$$A \cdot \int_{0}^{L_{1}} \frac{\partial (\rho_{1} \cdot h_{1})}{\partial t} dz - A \cdot L_{1} \cdot \frac{dp}{dt} + \int_{0}^{L_{1}} \frac{\partial (h_{1} \cdot \dot{m})}{\partial z} dz = \dot{Q}$$
 (7)

where the pressure term is not integrated because is considered constant all over the length. Applying Leibniz rule for the first term of equation 7 results in:

$$A \cdot \left[ \frac{d}{dt} \int_{0}^{L_{1}} (\rho_{1} \cdot h_{1}) dz - (\rho \cdot h)_{L_{1}} \cdot \frac{dL_{1}}{dt} \right] - A \cdot L_{1} \cdot \frac{dp}{dt} = \dot{m}_{\rm in} \cdot h_{\rm in} - \dot{m}_{12} \cdot h_{12} + \dot{Q}$$
 (8)

Solving the integral for the first term of equation results in

$$\frac{d}{dt} \int_0^{L_1} (\rho_1 \cdot h_1) dz = \frac{d}{dt} (\overline{\rho}_1 \cdot \overline{h}_1 \cdot L_1) = \overline{\rho}_1 \overline{h}_1 \frac{dL_1}{dt} + \overline{h}_1 L_1 \frac{d\overline{\rho}_1}{dt} + \overline{\rho}_1 L_1 \frac{d\overline{h}_1}{dt}$$
(9)

Substituting equation 9 into equation 8 and arranging the terms results in:

$$AL_1 \cdot \left[ \bar{\rho}_1 \cdot \frac{d\bar{h}_1}{dt} + \bar{h}_1 \cdot \frac{d\bar{\rho}_1}{dt} - \frac{dp}{dt} \right] + A(\bar{\rho}_1 \bar{h}_1 - \rho_1 h_1) \frac{dL_1}{dt} = \dot{m}_{\rm in} \cdot h_{\rm in} - \dot{m}_{12} \cdot h_{12} + \dot{Q} \quad (10)$$

which represents the energy balance for the first zone of the heat exchanger. The same procedure can be applied to develop the energy balance for the second and the third zone of the heat exchanger.

### SUB-COOLED ZONE

## Primary fluid

Conservation equations

Mass balance

$$A\left[L_1 \cdot \frac{d\bar{\rho}_1}{dt} + (\bar{\rho}_1 - \rho_1) \cdot \frac{dL_1}{dt}\right] = \dot{m}_{\rm in} - \dot{m}_{12} \tag{11}$$

Energy balance

$$AL_{1}\left[\bar{\rho}_{1}\cdot\frac{d\bar{h}_{1}}{dt}+\bar{h}_{1}\cdot\frac{d\bar{\rho}_{1}}{dt}-\frac{dp_{1}}{dt}\right]+A\left(\bar{\rho}_{1}\bar{h}_{1}-\rho_{1}h_{1}\right)\frac{dL_{1}}{dt}=\dot{m}_{\mathrm{in}}\dot{h}_{\mathrm{in}}-\dot{m}_{\mathrm{A}}\dot{h}_{\mathrm{A}}+\dot{Q}_{\mathrm{r}1}$$
(12)

$$\frac{d\bar{\rho}_1}{dt} = \left[\frac{\partial\bar{\rho}_1}{\partial p_1} + \frac{1}{2} \cdot \frac{\partial\bar{\rho}_1}{\partial\bar{h}_1} \cdot \frac{\partial h_1}{\partial p_1}\right] \frac{dp_1}{dt} + \frac{1}{2} \cdot \frac{\partial\bar{\rho}_1}{\partial\bar{h}_1} \cdot \frac{dh_{\rm in}}{dt}$$
(13)

$$\frac{d\bar{h}_1}{dt} = \frac{1}{2} \cdot \left[ \frac{\partial \bar{h}_1}{\partial p_1} \cdot \frac{dp_1}{dt} + \frac{dh_{\rm in}}{dt} \right]$$
 (14)

 $Constitutive\ equations$ 

$$\bar{h}_1 = \frac{1}{2}(h_{\rm in} + h_{\rm l})$$
 (15)

$$subcool = setState\_ph(p_1, \bar{h}_1)$$
 (16)

$$sat = setSat\_p(p_2) \tag{17}$$

$$\rho_{l} = bubbleDensity(sat) \tag{18}$$

$$h_1 = bubbleEnthalpy(sat) (19)$$

$$\frac{\partial \bar{h}_{l}}{\partial p_{1}} = dBubbleEnthalpy\_dPressure(sat) \tag{20}$$

$$\frac{\partial \bar{\rho}_1}{\partial \bar{h}_1} = density\_derh\_p(subcool)$$
 (21)

$$\frac{\partial \bar{\rho}_1}{\partial p_1} = density\_derp\_h(subcool)$$
 (22)

$$\bar{T}_1 = temperature(subcool)$$
 (23)

$$\dot{Q}_{\rm r,1} = \pi D L_1 U_{\rm pf,1} (T_{\rm w,1} - \bar{T}_1)$$
(24)

### Metal wall

## $Conservation\ equations$

Energy balance:

$$C_{\rm w}(M_{\rm tot} \cdot \frac{L_1}{L}) \cdot \frac{dT_{\rm w,1}}{dt} + \frac{M_{\rm tot}}{L} (T_{\rm w,1} - T_{\rm w,12}) \frac{dL_1}{dt} = \dot{Q}_{\rm sf,1} - \dot{Q}_{\rm r,1}$$
 (25)

Constitutive equation

$$T_{w,12} = \frac{T_{w,1}L_2 + T_{w,2}L_1}{L_1 + L_2}$$
 (26)

$$C_{\rm w} = const.$$
 (27)

$$M_{\text{tot}} = const.$$
 (28)

$$L = const. (29)$$

#### TWO-PHASE ZONE

### Primary fluid

Conservation equations

Mass balance:

$$A \left[ L_2 \cdot \frac{d\bar{\rho}_2}{dt} + (\bar{\rho}_2 - \rho_{\rm v}) \cdot \frac{dL_2}{dt} + (\rho_{\rm l} - \rho_{\rm v}) \cdot \frac{dL_1}{dt} \right] = \dot{m}_{\rm A} - \dot{m}_{23}$$
 (30)

Energy balance:

$$A\left[L_{2} \cdot \frac{d\bar{\rho}_{2}\bar{h}_{2}}{dt} + (\bar{\rho}_{2}\bar{h}_{2} - \rho_{v}h_{v}) \cdot \frac{dL_{2}}{dt} + (\rho_{l}h_{l} - \rho_{v}h_{v}) \cdot \frac{dL_{1}}{dt} - L_{2} \cdot \frac{dp_{2}}{dt}\right] = \dot{m}_{A}\dot{h}_{A} - \dot{m}_{23}\dot{h}_{23} + \dot{Q}_{r,2}$$
(31)

$$\frac{d\bar{\rho}_{2}}{dt} = \left(\frac{\partial\rho_{v}}{\partial p_{2}} \cdot \bar{\alpha} + \frac{\partial\rho_{l}}{\partial p_{2}} \cdot (1 - \bar{\alpha})\right) \cdot \frac{dp_{2}}{dt} + \left(\rho_{v} - \rho_{l}\right) \cdot \left[\frac{\partial\bar{\alpha}}{\partial p_{2}} \cdot \frac{dp_{2}}{dt} + \frac{\partial\bar{\alpha}}{\partial h_{\text{OUT,alpha}}} \cdot \frac{dh_{\text{OUT,alpha}}}{dt}\right]$$
(32)

$$\frac{d\bar{\rho}_{2}\bar{h}_{2}}{dt} = \left[\bar{\alpha}\cdot\left(\frac{\partial\rho_{v}}{\partial p_{2}}\cdot h_{v} + \frac{\partial h_{v}}{\partial p_{2}}\cdot\rho_{v}\right) + (1-\bar{\alpha})\cdot\left(\frac{\partial\rho_{l}}{\partial p_{2}}\cdot h_{l} + \frac{\partial h_{l}}{\partial p_{2}}\cdot\rho_{l}\right)\right]\cdot\frac{dp_{2}}{dt} + \left(\rho_{v}h_{v} - \rho_{l}h_{l}\right)\cdot\left[\frac{\partial\bar{\alpha}}{\partial p_{2}}\cdot\frac{dp_{2}}{dt} + \frac{\partial\bar{\alpha}}{\partial h_{OUT,alpha}}\cdot\frac{dh_{OUT,alpha}}{dt}\right]$$
(33)

Constitutive equations

$$\bar{\rho}_2 = \rho_{\rm v}\bar{\alpha} + \rho_{\rm l} \cdot (1 - \bar{\alpha}) \tag{34}$$

$$\bar{\rho}_2 \bar{h}_2 = \rho_{\rm v} h_{\rm v} \bar{\alpha} + \rho_{\rm l} h_{\rm l} \cdot (1 - \bar{\alpha}) \tag{35}$$

$$\rho_{\rm v} = dew Density(sat) \tag{36}$$

$$h_{\rm v} = dewEnthalpy(sat)$$
 (37)

$$\frac{\partial \bar{h}_{v}}{\partial p_{2}} = dDewEnthalpy\_dPressure(sat)$$
 (38)

$$\bar{T}_2 = temperature(sat)$$
 (39)

$$\dot{Q}_{\rm r,2} = \pi D L_2 U_{\rm pf,2} (T_{\rm w,2} - \bar{T}_2) \tag{40}$$

Metal Wall

Conservation equation

Energy balance:

$$C_{\mathbf{w}} \cdot \frac{M_{\text{tot}}}{L} \cdot \left[L_{2} \cdot \frac{d\mathbf{T}_{\mathbf{w},2}}{dt} + (\mathbf{T}_{\mathbf{w},12} - \mathbf{T}_{\mathbf{w},23}) \frac{dL_{1}}{dt} + (\bar{\mathbf{T}}_{\mathbf{w},2} - \mathbf{T}_{\mathbf{w},23}) \frac{dL_{2}}{dt}\right] = \dot{Q}_{\text{sf},2} - \dot{Q}_{\mathbf{r},2} \quad (41)$$

## SUPER-HEATED ZONE

### Primary fluid

 $Conservation\ equations$ 

Mass balance:

$$A[L_3 \cdot \frac{d\bar{\rho}_3}{dt} + (\rho_v - \bar{\rho}_3) \cdot (\frac{dL_1}{dt} + \frac{dL_2}{dt})] = \dot{m}_{23} - \dot{m}_{out}$$
 (42)

Energy balance:

$$AL_{3}[\bar{\rho}_{3} \cdot \frac{d\bar{h}_{3}}{dt} + \bar{h}_{3} \cdot \frac{d\bar{\rho}_{3}}{dt} - \frac{dp_{3}}{dt}] + A(\rho_{v}h_{v} - \bar{\rho}_{3}\bar{h}_{3}) \cdot (\frac{dL_{1}}{dt} + \frac{dL_{2}}{dt}) = \dot{m}_{23}\dot{h}_{v} - \dot{m}_{out}\dot{h}_{out} + \dot{Q}_{r,3}$$
(43)

$$\frac{d\bar{\rho}_3}{dt} = \left[\frac{\partial\bar{\rho}_3}{\partial p_3} + \frac{1}{2} \cdot \frac{\partial\bar{\rho}_3}{\partial\bar{h}_3} \cdot \frac{\partial\bar{h}_v}{\partial p_3}\right] \frac{dp_3}{dt} + \frac{1}{2} \cdot \frac{\partial\bar{\rho}_3}{\partial\bar{h}_3} \cdot \frac{dh_{\text{out}}}{dt}$$
(44)

$$\frac{d\bar{h}_3}{dt} = \frac{1}{2} \cdot \left[ \frac{\partial \bar{h}_v}{\partial p_3} \cdot \frac{dp_3}{dt} + \frac{dh_{\text{out}}}{dt} \right] \tag{45}$$

Constitutive equations

$$vap = setState(p_3, \bar{h}_3) \tag{46}$$

$$\bar{h}_3 = \frac{1}{2}(h_{\rm v} - h_{\rm out})$$
 (47)

$$\frac{\partial \bar{\rho}_3}{\partial \bar{h}_3} = density\_derh\_p(vap) \tag{48}$$

$$\frac{\partial \bar{\rho}_3}{\partial p_3} = density\_derp\_h(vap) \tag{49}$$

$$\bar{T}_3 = temperature(vap)$$
 (50)

$$\dot{Q}_{\rm r,3} = \pi D L_3 U_{\rm pf,3} (T_{\rm w,3} - \bar{T}_3)$$
 (51)

Metal wall

 $Conservation\ equations$ 

Energy balance:

$$C_{\rm w} \frac{M_{\rm tot}}{L} \cdot [L_3 \cdot \frac{dT_{\rm w,3}}{dt} + (T_{\rm w,23} - T_{\rm w,3})(\frac{dL_1}{dt} + \frac{dL_2}{dt})] = \dot{Q}_{\rm sf,3} - \dot{Q}_{\rm r,3}$$
 (52)

Constitutive equations

$$T_{w,23} = \frac{T_{w,3}L_2 + T_{w,2}L_3}{L_2 + L_3}$$
 (53)

### 2.3 Heat Transfer

Based on Nusselt number (Nu) from Reynolds number (Re) and Prandtl number (Pr) for a characteristic length L. Angles are usually calculated in radians or  $\pi$ .

# 2.4 Pressure Drop

# 3 Results and Discussion

Compared to [3], the model ....

[4]

[5]

# 4 Conclusion

# 4.1 Secondary fluid

The secondary fluid is treated as a constant heat capacity fluid. Two different method to solve the heat exchanger are developed. Newton law of cooling and epsilon-NTU.

# 5 Modelling

#### 5.1 Modelica Characteristics

- Enthalpy controls switching
- Only length gets defined, no zones get disabled. Their respective length might be set to  $10^{-10}$  though.
- Solid wall with constant properties is included in the cell of the primary fluid.
- Should length L be treated as input, output or as a variable in the connectors?
- Implementation of heat transfer and void fractions models starting with [3] and Sylvain's EES file.

# 6 Old secondary fluid formulation

## Secondary fluid: sub-cooled zone

Conservation equation

Energy balance:

$$\rho_{\rm sf} A_{\rm sf} \left[ L_1 \cdot \frac{dh_{\rm sf,1}}{dt} + (h_{\rm sf,1} - h_{\rm sf,12}) \frac{dL_1}{dt} \right] = \dot{m}_{\rm sf} (h_{\rm sf,in} - h_{\rm sf,12}) + \dot{Q}_{\rm sf,1}$$
 (54)

Constitutive equations

$$h_{\rm sf,12} = \frac{h_{\rm sf,1}L_2 + h_{\rm sf,2}L_1}{L_1 + L_2} \tag{55}$$

$$Q_{\text{sf},1} == \pi D L_1 U_{\text{sf},1} (T_{\text{w},1} - \bar{T}_{\text{sf},1})$$
(56)

$$sfzone1 = setState(p1, h_{sf,1})$$
(57)

$$T_{\rm sf,1} = temperature(sfzone1)$$
 (58)

### Secondary fluid

Conservation equation

Energy balance:

$$\rho_{\rm sf} A_{\rm sf} \left[ L_2 \cdot \frac{dh_{\rm sf,2}}{dt} + (h_{\rm sf,12} - h_{\rm sf,23}) \frac{dL_1}{dt} (h_{\rm sf,2} - h_{\rm sf,23}) \frac{dL_2}{dt} \right] = \dot{m}_{\rm sf} (h_{\rm sf,12} - h_{\rm sf,23}) + \dot{Q}_{\rm sf,1}$$
(59)

Constitutive equations

$$Q_{\rm sf,2} == \pi D L_2 U_{\rm sf,2} (T_{\rm w,2} - \bar{T}_{\rm sf,2}) \tag{60}$$

$$sfzone2 = setState(p2, h_{sf,2})$$
(61)

$$\bar{T}_{sf,2} = temperature(sfzone2)$$
 (62)

# Secondary fluid-SuperHeated zone

 $Conservation\ equations$ 

Energy balance:

$$\rho_{\rm sf} A_{\rm sf} [L_3 \cdot \frac{d\bar{h}_{\rm sf,3}}{dt} + (h_{\rm sf,23} - h_{\rm sf,3}) (\frac{dL_1}{dt} + \frac{dL_2}{dt})] = \dot{m}_{\rm sf} (h_{\rm sf,23} - h_{\rm sf,OUT}) + \dot{Q}_{\rm sf,3}$$
(63)

 $Constitutive\ equations$ 

$$h_{\rm sf,23} = \frac{h_{\rm sf,3}L_2 + h_{\rm sf,2}L_3}{L_2 + L_3} \tag{64}$$

$$Q_{\rm sf,3} = \pi D L_3 U_{\rm sf,3} (T_{\rm w,3} - \bar{T}_{\rm sf,3})$$
 (65)

$$sfzone3 = setState(p3, h_{sf,3})$$

$$(66)$$

$$\bar{T}_{\mathrm{sf,3}} = temperature(sfzone3)$$
 (67)

# References

- [1] Ian H. Bell, Sylvain Quoillin, Jorrit Wronski, and Vincent Lemort. Coolprop: An open-source reference-quality thermophysical property library. In *submitted abstract to ASME-ORC 2013 2nd International Seminar on ORC Power Systems*, 2013.
- [2] Satyam Bendapudi, James E. Braun, and Eckhard A. Groll. A comparison of moving-boundary and finite-volume formulations for transients in centrifugal chillers. *International Journal of Refrigeration*, 31(8):1437–1452, 2008.
- [3] Martin Ryhl Kærn. Analysis of Flow Maldistribution in Fin-and-tube Evaporators for Residential Air-conditioning Systems. Phd thesis, Technical University of Denmark, 2011.
- [4] Wei-Jiang Zhang and Chun-Lu Zhang. A generalized moving-boundary model for transient simulation of dry-expansion evaporators under larger disturbances. *International Journal of Refrigeration*, 29(7):1119–1127, November 2006.
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# Glossary

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A Area (m<sup>2</sup>).
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L Length (m).

N Number of sections.

Q Heat (J).

T Temperature (K).

U Heat transfer coefficient (W m<sup>-2</sup> K<sup>-1</sup>).

 $\bar{T}$  Average temperature (K).

 $\bar{h}$  Average specific enthalpy (J kg<sup>-1</sup>).

 $\dot{Q}$  Heat flow (W).

 $\dot{m}$  Mass flow (kg s<sup>-1</sup>).

c Specific heat capacity  $(J kg^{-1} K^{-1})$ .

h Specific enthalpy (J kg<sup>-1</sup>).

p Pressure (Pa).

t Time (s).

v Velocity (m s<sup>-1</sup>).

#### Acronyms

MB moving boundary.

## **Dimensionless Numbers**

Nu Nusselt number:  $\frac{\text{convection}}{\text{conduction}} = \frac{UL}{\lambda}$ .

Pr Prandtl number:  $\frac{\text{viscous diffusion}}{\text{thermal diffusion}} = \frac{c_p \mu}{\lambda}$ .

Re Reynolds number:  $\frac{\text{inertia}}{\text{viscosity}} = \frac{\rho \, v \, L}{\mu}$ .

# Greek Symbols

- $\bar{\alpha}$  Average void fraction (ND).
- $\lambda$  Thermal conductivity (W m<sup>-1</sup> K<sup>-1</sup>).
- $\mu$  Dynamic viscosity (Pas).
- $\pi$  ratio of circumference of circle to its diameter.
- $\bar{\rho}$  Average density (kg m<sup>-3</sup>).
- $\rho$  Density of a material or medium (kg m<sup>-3</sup>).

# Subscripts

- 12 at the interface of zone 1 and 2.
- 1 in zone 1.
- 23 at the interface of zone 2 and 3.
- 2 in zone 2.
- 3 in zone 3.

in at the inlet.

1 saturated liquid.

out at the outlet.

**pf** primary fluid.

sf secondary fluid.

 ${f v}$  saturated vapour.

p at constant pressure.