A MATHEMATICAL MODEL FOR THE SIMULATION OF TWO-PHASE COMPRESSION IN THERMAL NON-EQUILIBRIUM

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Abstract. When a pure refrigerant in a two-phase state undergoes a reduction of volume, the volume of the vapour phase is going to follow closely the total reduction of volume, while the liquid phase volume variation is negligible in comparison to this total reduction. This variation of vapour volume induces a rise in temperature, creating a thermal disequilibrium between the two phases, whereas the mechanical equilibrium is maintained. Heat transfer, condensation and evaporation are thereby going to occur between the two phases, leading to variations in pressure that are difficult to predict. In this paper, a mathematical model for simulating a two-phase compression (or expansion) assuming a thermal non-equilibrium is proposed. This model is intended to be used as a core model for the simulation of displacement compressors using deterministic modelling. The model is applied to a piston-cylinder setup simulating a simple variation of volume over time, as well as a resting phase allowing to reach a final state in both thermal and mechanical equilibrium. External heat transfers and leakages are considered in the equations but will be set at zero in the simulation. The simulated fluid is the refrigerant R1233zd(E). The results of this application are discussed in terms of work consumption and isentropic efficiency, showing that irreversibilities are unavoidable when working in thermal non-equilibrium.

Keywords. Two-phase compression, Thermal non-equilibrium, Mathematical model, Deterministic model.

Nomenclature

Q	Vapour quality (mass fraction) (-)
V	Volume (m³)
T	Temperature (K)
p	Pressure (Pa)
v	Specific volume (m³/kg)
u	Specific internal energy (J/kg)
h	Specific enthalpy (J/kg)
m	Mass (kg)
$\dot{Q}$	Heat transfer rate (W)
$\dot{m}$	Mass transfer rate (kg/s)
A	Area (m²)
U	Internal energy (J) / heat transfer coefficient (W/(m²K))

Special characters

θ	Angle (rad)
ω	Rotational speed (rad/s)
ε_{is}	Isentropic efficiency (-)
ρ	Density (kg/m³)
$\dot{\Phi}$	Energy transfer rate (W)
α	Vapour volume fraction or void fraction (-)

Subscripts and superscripts

g	Vapour phase
l	Liquid phase
ϕ	Any phase
cv	Control volume
σ	At saturation
$cond$	Condensation

1 Introduction

The deterministic modelling of compression and expansion processes is widely used to help understanding the behaviour of displacement machines. Such modelling technique is able to predict variation of temperature and pressure induced by the reduction/expansion of volume. Along with the prediction of internal leakages, heat transfer and mechanical losses, the performance of displacement machines can be accurately predicted with a limited number of empirical parameters.

Two-phase compression modelling can be used for several purposes:

- In oil-flooded compression/expansion considering the heat exchange between the liquid phase (mainly oil) and the vapour phase (refrigerant), in screw and scroll compressors [1], [2]
- In compression-resorption heat pumps using wet compression to improve the coefficient of performance, using twin-screw compressors [3], [4]
- In the modelling of liquid slugging, useful to predict the behaviour of compressors under the presence of liquid during cold start-up [5], [6], [7]

- In the compression/expansion of pure-refrigerant or oil-refrigerant mixture with low superheat, used, for instance, in the trilateral flash cycle using Lysholm turbine, single-screw expanders or in the regen-by-two cycle, using scroll compressors and expanders [1], [8], [9].

Amongst the cited authors, several assume a thermal equilibrium between the two phases for simplicity reasons ([2], [4], [5], [6], [8]). In [6], the two phases are modelled separately, but the evaporation rate is analytically determined to always reach the thermal equilibrium. As a pure fluid (R290) is being used, no concentration equation is applied. The thermodynamic variables used are the density and the temperature, but no information is provided regarding the equation of state. The authors of [2], [4] model a two-phase compression using mixtures (oil-refrigerant or ammonia-water), inducing the use of a concentration equation. Moreover, in both papers, the use of pressure, temperature and concentration as independent thermodynamic variables allows the calculation of the remaining properties. Finally, in [5], [8], an homogeneous phase is modelled using a pure fluid. The authors of [5] provide an analytical formula for the calculation of the variation rate of vapour quality with the shaft angle ($\mathrm{d}Q/\mathrm{d}\theta$). Thereby, it seems that the vapour quality and the temperature are used as thermodynamic variables to determine the state of the fluid. In [8], the two-phase density and a uniform temperature are used to determine the state of the fluid in a two-phase scroll compressor deterministic model.

On the other hand, several authors ([1], [3]) propose a thermal non-equilibrium modelling. A deterministic model applied to an oil refrigerant-mixture expansion using a single-screw expander is developed in [1]. This model uses a concentration equation for the oil content and uses the density and the temperature as independent thermodynamic variables for both liquid and vapour phases. Although it does not show how the condensation/evaporation effect of the refrigerant can be figured out, it constitutes a base for the mathematical developments shown in this article. In [3], the author developed a two-phase compression model for a twin-screw compressor used in compression-resorption heat pumps, using the pressure, temperature and sorbent concentration as independent thermodynamic variables with the Ziegler-Trepp equation of state (EoS).

In this paper, a model similar to the expansion model of [1] is developed. The equations are solved to calculate the specific volume and temperature variation rates of both phases with the shaft angle of the displacement machine. The model takes into account the non-equilibrium between the two phases, considering the mass and heat exchanges between them. The interactions between the two phases are thoroughly described, in the case of the compression as well as an expansion. The equations are applied to a simple piston-cylinder setup filled with a saturated liquid-vapour R1233zd(E) mixture. The volume contained in the piston-cylinder setup is decreased at a fixed rate, until reaching a constant value where the system can rest until the thermal equilibrium is re-established. The evolution of pressure inside the cylinder is tracked, as well as the temperatures and masses of the liquid and vapour phases. The external heat transfer and leakages are taken into account in the equations; however, they will be neglected in the piston-cylinder application. The model developed in the paper constitute a base for a scroll compressor deterministic model, intended to be validated by the authors using experimental data from [10].

2 Mathematical model

The mathematical model is split into 3 parts: the interface interactions, the mass conservations equations and the energy conservation equations. The objective is to obtain the variation of pressure, under a variation of volume in which the two-phase fluid is initially at rest, in thermal and mechanical equilibrium. For the sake of simplicity, since the model is intended for use as a compressor deterministic model, the derivatives will be expressed in terms of shaft angle variation (θ), and the speed of the compressor is given by the variable ω (in rad/s). As already stated, the two independent thermodynamic variables used to define the properties of both phases are the temperature and the density. Those variables are used along with the Helmhotz equation of state to determine other thermophysical properties such as the pressure, enthalpy and entropy. The variation of volume of the liquid phase with regards to the pressure being negligible, the pressure of the control volume is going to be set based on the vapour phase properties. To decrease the computational time of the model, the abstract state module of CoolProp has been used to compute the thermophysical properties.

A representation of the studied control volume can be found in Figure 1. The control volume is subject to a volume variation rate $\mathrm{dV_{CV}}/\mathrm{d}\theta$ distributed into volume variations of the vapour and liquid phases, $\mathrm{dV_g}/\mathrm{d}\theta$ and $\mathrm{dV_l}/\mathrm{d}\theta$, respectively. The computations of the temperature and specific volume of both phases along the variation of volume with the shaft angle are computed using the backward Euler method, where the specific volume is converted into the density for the equation of state afterward:

$$T_\phi^k(\theta) = T_\phi^{k-1}(\theta) + \frac{\mathrm{d}T_\phi}{\mathrm{d}\theta}\mathrm{d}\theta \tag{1}$$

$$v_\phi^k(\theta) = v_\phi^{k-1}(\theta) + \frac{\mathrm{d}v_\phi}{\mathrm{d}\theta}\mathrm{d}\theta \tag{2}$$

Where ϕ stands for the liquid or vapour phase and $\mathrm{d}\theta$ is the shaft angle step used. The mass and energy conservation equations will thereby help in determining $\mathrm{d}T_\phi/\mathrm{d}\theta$ and $\mathrm{d}v_\phi/\mathrm{d}\theta$, for both phases.

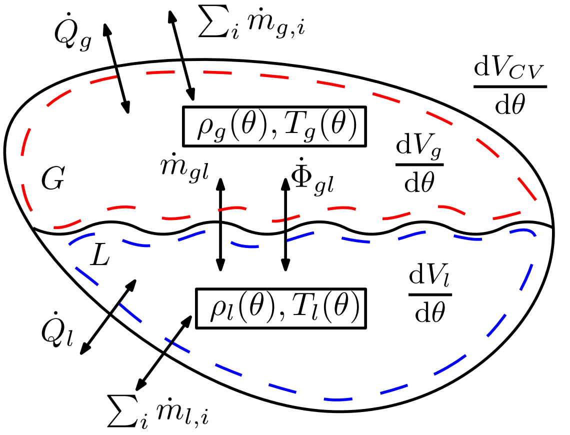

Figure 1: Definition of the control volume and the interactions with its environment.

2.1 *Interface interactions*

A pure fluid in a two-phase state, respecting thermal and mechanical equilibrium, can be seen as an heterogeneous mixture of a saturated vapour and saturated liquid, in given proportion, quantified by a mass fraction called the vapour quality, defined as:

$$\mathrm{Q} = m_g/(m_l + m_g) \tag{3}$$

Where g stands for the vapour phase and l for the liquid phase.

When such a fluid in two-phase state undergoes a decrease of volume, with neither external and internal heat transfer nor mass transfer, the density of the vapour phase is going to increase as well as its temperature, inducing a rise in pressure. Regarding the liquid phase, its change in temperature and in volume is negligible under the effect of the pressure only, creating a thermal non-equilibrium between the two phases, while the mechanical equilibrium is maintained all along the compression. The liquid phase therefore becomes a subcooled liquid phase, due to the rise of pressure at constant temperature. Depending on the shape of the vapour saturation curve, increasing the pressure of the saturated vapour phase may or may not create condensation. Most refrigerants used being dry fluids, the rise of pressure of the saturated vapour phase is going to create a new liquid phase, at the vapour phase temperature, as illustrated in Figure 3. If the mass and heat transfer are considered between the two phases, the new liquid phase is going to mix with the original liquid phase, thereby increasing its temperature. The difference in temperature between the vapour and liquid phase is also resulting in condensation/evaporation between the two phases, thereby inducing a mass transfer. These two effects have a role in the change of volume and mass of both liquid and vapour phases, having a significant impact on the resulting pressure. The difficulties encountered in the modelling of those effects have been described in [9], where the two-phase expansion of pure refrigerant R134a in a Lysholm turbine is investigated. Several authors have modelled the interaction between the two phases in thermal non-equilibrium under some assumptions. In both [7], [11], the energy transfer rate from the liquid phase to the vapour phase (either by heat transfer or mass transfer) $\dot{\Phi}_{\mathrm{lg}}$ and from the vapour phase to the liquid phase $\dot{\Phi}_{\mathrm{gl}}$ are defined as:

$$\dot{\Phi}_{gl} = \dot{Q}_{gl} + \dot{m}_{gl} h_g \tag{4}$$

$$\dot{\Phi}_{lg} = \dot{Q}_{lg} + \dot{m}_{lg} h_l \tag{5}$$

Where $\dot{\mathrm{Q}}_{\mathrm{lg}}$, $\dot{Q}_{gl}$ are the heat transfer rates and $\dot{m}_{gl}$, $\dot{\mathrm{m}}_{\mathrm{lg}}$, the mass transfer rates. The interface between the vapour phase (G) and the liquid phase (L) can thereby be defined and the interactions are represented in Figure 2. This interface can be seen as an infinitely thin boundary between the two extended control volumes represented by the vapour and liquid phases. Therefore, the gradient of temperature that can appear between the two phase is not embedded inside the interface but in the extended control volumes boundaries, allowing to respect the temperature continuity though the control volumes boundaries and the interface.

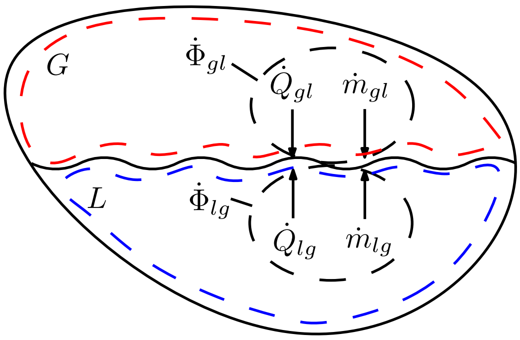

Figure 2: Interface interactions.

From the mass and energy conservation at the interface, the following equalities can be deduced:

$$\dot{m}_{gl} + \dot{m}_{lg} = 0 \tag{6}$$

$$\dot{\Phi}_{gl} + \dot{\Phi}_{lg} = 0 \tag{7}$$

The heat transfer rates toward the interface can be defined considering an interface at the saturation temperature from the pressure p, they can be written as[1]:

$$\dot{Q}_{gl} = AU_l\left(T_g - T^{\sigma}(p)\right) \tag{8}$$

$$\dot{Q}_{lg} = AU_g\left(T_l - T^{\sigma}(p)\right) \tag{9}$$

Where $\mathrm{AU_l}$, $\mathrm{AU_g}$ are the heat transfer coefficients from the interface to the liquid phase and vapour phase, respectively. Isolating the mass flow rate from the vapour phase to the liquid phase $\dot{m}_{gl}$ from equations (4), (5), (6) and (7) gives:

$$\dot{m}_{gl} = \frac{-(\dot{Q}_{gl} + \dot{Q}_{lg})}{(h_g - h_l)} = \frac{-(\dot{Q}_{gl} + \dot{Q}_{lg})}{\Delta h^{SH} + \Delta h^{\sigma} + \Delta h^{SC}} \tag{10}$$

Where Δh^{SH} is the sensible heat of superheating (from the saturated vapour state reference), Δh^{SC} is the sensible heat of subcooling and Δh^{σ} is the latent heat. The problem identified with this definition is the fact that it does not take into account the partial evaporation (also called flash)/partial condensation coming from the compression of the saturated vapour phase/expansion of the saturated liquid phase as illustrated in the Figure 3. As previously explained, the compression of the saturated vapour present in the two-phase mixture results in the creation of a liquid phase at the temperature of the vapour phase, which is going to mix with the liquid phase and thereby change its temperature, resulting in a change of volume of the liquid phase. Depending on the initial vapour quality of the compression, this effect can be negligible, especially for low vapour qualities where the amount of liquid coming from the saturated vapour compression would be too small to affect significantly the liquid phase temperature. The same effect is observed during the expansion of a saturated liquid phase, which creates a vapour phase at the liquid phase temperature (see blue transformation in Figure 3). This partial evaporation is also called flashing.

Eventually, the mass transfer from the vapour phase to the liquid phase $\mathrm{m}^{\sigma}_{\mathrm{gl}}$ and the mass transfer from the liquid phase to the vapour phase $\mathrm{m}^{\sigma}_{\mathrm{lg}}$ can simply be defined as follows:

$$m^{\sigma}_{gl} = m_g \cdot \max\left(0, \frac{v^{\sigma}_g(p) - v_g}{v^{\sigma}_g(p) - v^{\sigma}_l(p)}\right) \tag{11}$$

$$m^{\sigma}_{\mathrm{lg}} = m_l \cdot \max\left(0, \frac{v_l - v^{\sigma}_l(p)}{v^{\sigma}_g(p) - v^{\sigma}_l(p)}\right) \tag{12}$$

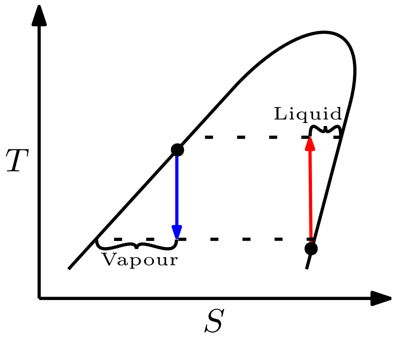

Figure 3: Saturated vapour compression in red, saturated liquid expansion in blue.

Where v is the specific volume and σ stands for the saturation properties. Finally, the corresponding energy transfer from one phase to the other can be defined as follows, where the enthalpy of vaporisation is considered inherently of the compression/expansion of the saturated phase.

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[1] The notations AU_l and AU_g, to the authors perspective, could be switched in both equations. However, the adopted notation appears in this form in the literature.

$$\Phi_{\mathrm{gl}}^{\sigma} = \mathrm{m}_{\mathrm{gl}}^{\sigma} \cdot \mathrm{h}_{\mathrm{l}}^{\sigma}(\mathrm{p}) \tag{13}$$

$$\Phi_{\mathrm{lg}}^{\sigma} = \mathrm{m}_{\mathrm{lg}}^{\sigma} \cdot \mathrm{h}_{\mathrm{g}}^{\sigma}(\mathrm{p}) \tag{14}$$

2.2 *Mass conservation equations*

The total mass transfer rate condensed from the vapour phase to the liquid phase is defined as:

$$\frac{\mathrm{d}m_{cond}}{\mathrm{d}\theta} = \frac{1}{\omega}\dot{m}_{gl} + \frac{1}{\mathrm{d}\theta}\left(m_{gl}^{\sigma} - m_{lg}^{\sigma}\right) \tag{15}$$

The mass conservation equations can simply be written considering the mass flow rates entering/leaving both phases and the interaction between them (condensation rate) that is represented by Equation (15):

$$\frac{\mathrm{dm_g}}{\mathrm{d\theta}} = \frac{1}{\omega}\left(\sum_{\mathrm{i}} \dot{\mathrm{m}}_{\mathrm{g,i}} - \frac{\mathrm{dm_{cond}}}{\mathrm{d\theta}}\right) \tag{16}$$

$$\frac{\mathrm{d}m_{\mathrm{l}}}{\mathrm{d\theta}} = \frac{1}{\omega}\left(\sum_{i} \dot{m}_{\mathrm{l},i} + \frac{\mathrm{d}m_{cond}}{\mathrm{d\theta}}\right) \tag{17}$$

The specific volume variation rates can then be defined with the following definition:

$$\frac{\mathrm{d}v_{\phi}}{\mathrm{d\theta}} = \frac{1}{\mathrm{m}_{\phi}}\frac{\mathrm{d}V_{\phi}}{\mathrm{d\theta}} - \frac{\mathrm{V}_{\phi}}{\mathrm{m}_{\phi}^{2}}\frac{\mathrm{d}m_{\phi}}{\mathrm{d\theta}} \tag{18}$$

Where the volume variation rates of both phases can be linked together with the control volume variation rate:

$$\frac{\mathrm{d}V_g}{\mathrm{d\theta}} = \frac{\mathrm{d}V_{CV}}{\mathrm{d\theta}} - \frac{\mathrm{d}V_l}{\mathrm{d\theta}} \tag{19}$$

Finally, the derivative of the liquid volume $\mathrm{dV_l}/\mathrm{d\theta}$ can be conveniently expanded to explicit the dependency from the liquid phase temperature T_l, while neglecting the effect of pressure:

$$\frac{\mathrm{d}V_l}{\mathrm{d\theta}} = v_l\frac{\mathrm{d}m_l}{\mathrm{d\theta}} + m_l\frac{\mathrm{d}v_l}{\mathrm{d\theta}} \tag{20}$$

$$= v_l\frac{\mathrm{d}m_l}{\mathrm{d}\theta} + m_l\left(\frac{\partial v_l}{\partial T}\right)_p\frac{\mathrm{d}T_l}{\mathrm{d}\theta}$$

The whole system of equations is therefore dependant on the variation rate of the liquid phase temperature, that is going to be computed from the energy conservation equations.

2.3 *Energy conservation equations*

The conservation of energy is applied in the same way for both phases, with derivatives expressed relative to time first:

$$\frac{\mathrm{dU_{\phi}}}{\mathrm{dt}} = \sum_{\mathrm{i}} \dot{\mathrm{m}}_{\phi,\mathrm{i}}\,\mathrm{h}_{\phi,\mathrm{i}} + \dot{\mathrm{W}}_{\phi} + \dot{\mathrm{Q}}_{\phi} \pm \dot{\Phi}_{\mathrm{cond}} \tag{21}$$

Where U_{ϕ} is the internal energy of the phase represented by ϕ. The boundary work rate exchanged with the corresponding phase can be rewritten as:

$$\dot{W}_{\phi} = -\mathrm{p}\frac{\mathrm{dV_{\phi}}}{\mathrm{dt}} \tag{22}$$

Regarding the condensation energy transferred rate, it comes from interface interactions and can be defined as:

$$\dot{\Phi}_{cond} = \dot{\Phi}_{gl} + \frac{\omega}{\mathrm{d\theta}}\left[\mathrm{m}_{\mathrm{gl}}^{\sigma} \cdot \mathrm{h}_{\mathrm{l}}^{\sigma}(\mathrm{T_l}) - \mathrm{m}_{\mathrm{lg}}^{\sigma} \cdot \mathrm{h}_{\mathrm{g}}^{\sigma}(\mathrm{T_g})\right] \tag{23}$$

This term is taken with a negative sign for the vapour phase and with a positive sign for the liquid phase, in the energy conservation equation. Equation (21) can be rewritten with derivatives relative to the shaft angle θ:

$$\frac{\mathrm{d}U_{\phi}}{\mathrm{d\theta}} = \frac{1}{\omega}\sum_{i} \dot{m}_{\phi,i}\,h_{\phi,i} - \mathrm{p}\frac{\mathrm{dV_{\phi}}}{\mathrm{d\theta}} + \frac{1}{\omega}\dot{Q}_{\phi} \pm \frac{1}{\omega}\dot{\Phi}_{cond} \tag{24}$$

The left-hand term of Equation (24) can be reformulated using the mass and the specific internal energy of the corresponding phase:

$$\frac{\mathrm{d}U_{\phi}}{\mathrm{d\theta}} = \frac{\mathrm{d}\left(m_{\phi}u_{\phi}\right)}{\mathrm{d\theta}} = u_{\phi}\frac{\mathrm{d}m_{\phi}}{\mathrm{d\theta}} + m_{\phi}\frac{\mathrm{d}u_{\phi}}{\mathrm{d\theta}} \tag{25}$$

Moreover, knowing that, derived from the Maxwell equations:

$$\left(\frac{\partial u_{\phi}}{\partial \mathrm{v}}\right)_{\mathrm{T}} = \left[\mathrm{T}_{\phi}\left(\frac{\partial \mathrm{p}}{\partial \mathrm{T}}\right)_{\mathrm{v}} - \mathrm{p}\right] \tag{26}$$

The derivative $\mathrm{d}u_{\phi}/\mathrm{d\theta}$ of Equation (25) can be expressed as follows:

$$\frac{\mathrm{d}u_{\phi}}{\mathrm{d\theta}} = \left[\left(\frac{\partial u_{\phi}}{\partial \mathrm{T}}\right)_{v}\frac{\mathrm{d}T_{\phi}}{\mathrm{d\theta}} + \left[T_{\phi}\left(\frac{\partial \mathrm{p}}{\partial \mathrm{T}}\right)_{v} - p\right]\frac{\mathrm{d}v_{\phi}}{\mathrm{d\theta}}\right] \tag{27}$$

By substituting the expression of $\mathrm{d}v_{\phi}/\mathrm{d\theta}$ from Equation (18), $\mathrm{d}U_{\phi}/\mathrm{d\theta}$ can be developed as follows:

$$\frac{\mathrm{d}U_\phi}{\mathrm{d}\theta} = u_\phi \frac{\mathrm{d}m_\phi}{\mathrm{d}\theta} + m_\phi \left(\frac{\partial u_\phi}{\partial \mathrm{T}}\right)_v \frac{\mathrm{d}T_\phi}{\mathrm{d}\theta} \tag{28}$$

$$+T_\phi \left(\frac{\partial p}{\partial T}\right)_v \frac{\mathrm{d}V_\phi}{\mathrm{d}\theta} - T_\phi \left(\frac{\partial p}{\partial T}\right)_v v_\phi \frac{\mathrm{d}m_\phi}{\mathrm{d}\theta}$$

$$-p \frac{\mathrm{d}V_\phi}{\mathrm{d}\theta} + p v_\phi \frac{\mathrm{d}m_\phi}{\mathrm{d}\theta}$$

Given the fact that $u_\phi + \mathrm{p} v_\phi = h_\phi$ and simplifying the term $-\mathrm{p}\mathrm{d}V_\phi/\mathrm{d}\theta$ is both Equation (24) and (28), the term in $\mathrm{d}T_\phi/\mathrm{d}\theta$ can be isolated, giving:

$$m_\phi \left(\frac{\partial u_\phi}{\partial T}\right)_v \frac{\mathrm{d}T_\phi}{\mathrm{d}\theta} = \frac{1}{\omega} \sum_i \dot{m}_{\phi,i}\, h_{\phi,i} + \frac{1}{\omega} \dot{Q}_\phi \tag{29}$$

$$\pm \frac{1}{\omega} \dot{\Phi}_{cond} - h_\phi \frac{\mathrm{d}m_\phi}{\mathrm{d}\theta}$$

$$-T_\phi \left(\frac{\partial \mathrm{p}}{\partial \mathrm{T}}\right)_v \left(\frac{\mathrm{d}V_\phi}{\mathrm{d}\theta} - v_\phi \frac{\mathrm{d}m_\phi}{\mathrm{d}\theta}\right)$$

For the liquid phase, the derivative of the volume can be substituted from Equation (20), isolating the term in $\mathrm{d}T_\mathrm{l}/\mathrm{d}\theta$ therefore gives:

$$m_l \frac{\mathrm{d}T_l}{\mathrm{d}\theta} \left[\left(\frac{\partial u_l}{\partial \mathrm{T}}\right)_v + T_l \left(\frac{\partial \mathrm{p}}{\partial T}\right)_v \left(\frac{\partial v_l}{\partial \mathrm{T}}\right)_\mathrm{p}\right] = \tag{30}$$

$$\frac{1}{\omega} \sum_i \dot{m}_{l,i}\, h_{\mathrm{l},i} + \frac{1}{\omega} \dot{Q}_l + \frac{1}{\omega} \dot{\Phi}_{cond} - h_l \frac{\mathrm{d}m_l}{\mathrm{d}\theta}$$

The derivative of the liquid phase temperature $\mathrm{d}T_l/\mathrm{d}\theta$ can therefore be calculated only based on the interface interactions, the external heat transfer and mass flow rates, and does not depend on the total volume reduction. The last term of Equation (30) takes into account the fact that if some liquid is added/removed at the same enthalpy as the liquid phase, its temperature is not going to change.

The vapour phase volume variation rate $\mathrm{d}V_g/\mathrm{d}\theta$ can now be computed from Equation (19). Isolating the term in $\mathrm{d}T_g/\mathrm{d}\theta$ gives, for the vapour phase:

$$\mathrm{m_g} \frac{\mathrm{dT_g}}{\mathrm{d}\theta} \left(\frac{\partial \mathrm{u_g}}{\partial \mathrm{T}}\right)_\mathrm{v} = \frac{1}{\omega} \sum_i \dot{m}_{\mathrm{g},i}\, h_{\mathrm{g},i} + \frac{1}{\omega} \dot{Q}_\mathrm{g} \tag{31}$$

$$-\frac{1}{\omega} \dot{\Phi}_{cond} - h_g \frac{\mathrm{d}m_g}{\mathrm{d}\theta}$$

$$-T_\mathrm{g} \left(\frac{\partial \mathrm{p}}{\partial \mathrm{T}}\right)_v \left(\frac{\mathrm{d}V_\mathrm{g}}{\mathrm{d}\theta} - v_\mathrm{g} \frac{\mathrm{d}m_\mathrm{g}}{\mathrm{d}\theta}\right)$$

Thus, the variation of the vapour phase temperature depends on the mass and heat transfers as well as the variation of its volume. Once again, the fourth left-hand term takes into account the mass exchange with the same enthalpy as the vapour phase, which would not change the temperature. The last term takes into account the variation of internal energy due to the change in specific volume, at a constant pressure.

Equations (30) and (31) requires the calculation of several derivatives, for instance, the derivative $\left(\partial \mathrm{u}_\phi / \partial \mathrm{T}\right)_\mathrm{v}$ can not always be replaced by the specific heat at constant volume, as sometimes, two-phase conditions can occur in one of the phase, leading to more internal energy balancing the phase change. These derivatives are therefore going to be directly calculated when those two-phase conditions are met, using a backward difference method for the vapour phase and a forward difference method for the liquid phase, to ensure the no-crossing of the saturation curves:

$$\left(\frac{\partial \mathrm{u_g}}{\partial \mathrm{T}}\right)_\mathrm{v} = \frac{\mathrm{u}\left(\mathrm{v_g}, \mathrm{T_g}\right) - \mathrm{u}\left(\mathrm{v_g}, \mathrm{T_g} - \mathrm{dT}\right)}{\mathrm{dT}} \tag{32}$$

$$\left(\frac{\partial \mathrm{u}_l}{\partial \mathrm{T}}\right)_\mathrm{v} = \frac{\mathrm{u}(\mathrm{v}_l, \mathrm{T}_l + \mathrm{dT}) - \mathrm{u}(\mathrm{v}_l, \mathrm{T}_l)}{\mathrm{dT}} \tag{33}$$

Regarding the term $(\partial v_l / \partial \mathrm{T})_\mathrm{p}$, it must be computed as a function of the pressure and the temperature, i.e., subcooled conditions close to saturation must be ensured. To avoid property calculation error, a temperature shift $\Delta T = 1$ [K] is introduced, which does not significantly change the results of the derivative. The derivative is thereby calculated as:

$$\left(\frac{\partial v_l}{\partial \mathrm{T}}\right)_\mathrm{p} = \frac{\mathrm{v}(p, \mathrm{T_l} - \Delta T + \mathrm{dT}) - \mathrm{v}(\mathrm{p}, \mathrm{T_l} - \Delta T - \mathrm{dT})}{2\mathrm{dT}} \tag{34}$$

Finally, the derivative $(\partial \mathrm{p} / \partial \mathrm{T})_v$ is calculated similarly for a subcooled and superheated state, where a shift is introduced to ensure being in the single-phase region:

$$\left(\frac{\partial p}{\partial \mathrm{T}}\right)_\mathrm{v} = \frac{\mathrm{p}\left(\rho_\phi, \mathrm{T}_\phi + \Delta T + \mathrm{dT}\right) - \mathrm{p}\left(\rho_\phi, \mathrm{T}_\phi + \Delta T - \mathrm{dT}\right)}{2\mathrm{dT}} \tag{35}$$

The remaining derivative to be calculated is $(\partial \mathrm{p} / \partial \mathrm{T})_v$ in the two-phase region, which can be done using the Clapeyron equation:

$$\left(\frac{\partial \mathrm{p}}{\partial \mathrm{T}}\right)_\mathrm{v} = \frac{h_g^\sigma(p) - h_l^\sigma(p)}{T_\phi \left(v_g^\sigma(p) - v_l^\sigma(p)\right)} \tag{36}$$

2.4 Summary

Eventually, the system of equation can be solved step by step to obtain the four derivates required to obtain the updated state after an angle step. As a reminder, those four derivatives are $\mathrm{d}v_g/\mathrm{d}\theta$, $\mathrm{d}v_l/\mathrm{d}\theta$, $\mathrm{d}T_g/\mathrm{d}\theta$ and $\mathrm{d}T_l/\mathrm{d}\theta$. First, the derivatives from Equations (32), (33), (34), (35) and (36) should be calculated using the previous state of temperature and density. The interface interactions should then be defined, using the heat transfer coefficients from the interface to the liquid phase U_l and to the vapour phase U_g in order to obtain the condensation mass flow rate $\mathrm{d}m_{cond}/\mathrm{d}\theta$ and condensation energy transfer rate $\dot{\Phi}_{cond}$, from Equations (15) and (23). Then, the mass derivatives of both phases can be calculated using the mass conservation Equations (16) and (17). Afterwards, using the mass flow rate and heat transfer rate of the liquid phase (as the pressure effect is neglected), $\mathrm{d}T_l/\mathrm{d}\theta$ can be calculated, using Equation (30). The latter term allows to define the variation of volume of the vapour phase $\mathrm{d}V_g/\mathrm{d}\theta$ via Equations (20) and (19) and, therefore, the derivatives $\mathrm{d}v_g/\mathrm{d}\theta$, $\mathrm{d}v_l/\mathrm{d}\theta$ using Equation (18). Finally, Equation (31) can be used to obtain $\mathrm{d}T_g/\mathrm{d}\theta$ and the backward Euler method of Equations (1) and (2) can be used to obtain the next temperature and specific volume of both phases.

Table 1: Initial state before the compression.

V_i[cm³]	Q_i[-]	α_i[-]	P_i[Pa]	T_i[K]
80	0.4	0.9889	$1.5 \cdot 10^5$	302.2

3 Results and discussion

In this section, the two-phase compression model is going to be applied to a simple piston-cylinder setup represented in Figure 4.

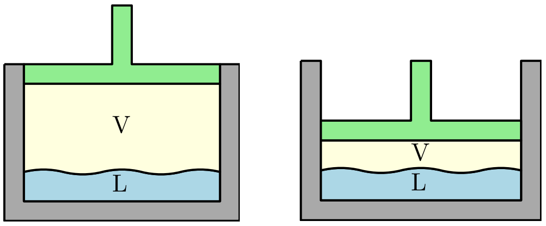

Figure 4: Piston-cylinder setup to simulate a two-phase compression, initial state on left and final state on right.

The two-phase compression with given initial conditions is going to be thoroughly analysed using pressure-enthalpy and temperature-entropy diagram. Then, the energy consumption of the compression is going to be calculated and an isentropic efficiency defined. In this application, pure refrigerant R1233zd(E) in a two-phase state is going to be compressed, and the state evolution of the two phases analysed along the compression. The volume defined by the piston-cylinder setup is going to be decreased linearly with a rate similar to what can be observed in a scroll compressor running at a speed of 2000 RPM, with a volume ratio of 5 reached after approximately 0.01 second. Then the system is going to be left at rest until the thermal equilibrium is reached again. The initial state can be found in Table 1, where Q_i stands for the initial vapour quality in mass fraction while α_i is the volume fraction or so-called void fraction.

In this simulation, heat transfer coefficients from the phases to the interface U_ϕ have been randomly fixed at 70000 W/(m²K) and the area A is simply taken as being the cylinder cross-section area.

The variation of the temperatures of both phases as well as the pressure ratio over time can be found in Figure 5. Point 1 corresponds to the initial state, point 2 to the state right after volume reduction and point $2''$ after the resting period, after which the thermal equilibrium is reached again.

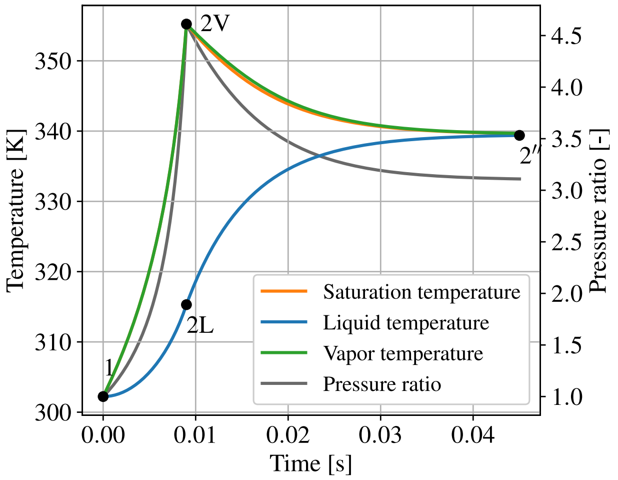

Figure 5: Evolution of the temperatures of both phases and evolution of the pressure ratio with time.

The pressure ratio reaches its maximum just after the reduction of volume and the same holds for the vapour phase temperature. Regarding the liquid phase temperature, due to the high heat transfer coefficients used, it follows closely the vapour phase temperature, allowing to re-establish the equilibrium after a resting period of less than 0.05 second. During the resting period, the pressure decreases due to condensation decreasing the vapour phase density, generating an expansion with an increasing volume but a decreasing mass, inducing a reduction in the vapour phase density.

The pressure-enthalpy and temperature-entropy diagrams of the transformation can be found in Figure 6 and Figure 7.

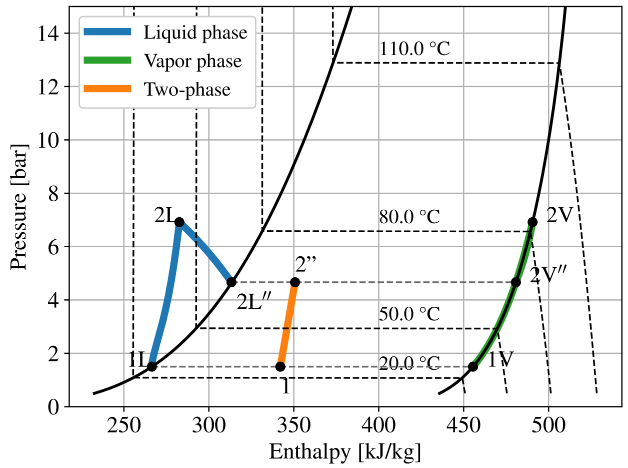

Figure 6: Pressure-enthalpy diagram of the two-phase compression.

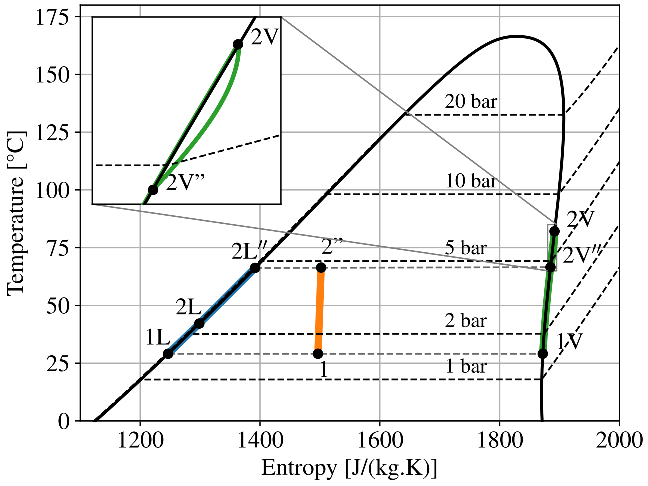

Figure 7: Temperature-entropy diagram of the two-phase compression.

The observation of those two diagrams allows a deep understanding of what is occurring along the compression in both phases. The first observation that can be made is the fact that the vapour phase follows the vapour saturation line during the compression, while the liquid phase becomes subcooled due to the rise of pressure. During the resting period, the saturated vapour becomes superheated due to the expansion (decrease in density) generated by the condensation between the two phases. Therefore, a pseudo-state, where a superheated phase is mixed with a subcooled phase is met during the resting phase, until the equilibrium is re-established, allowing to reach back two saturated phases at the same temperature.

The energy consumption of the compression can be calculated in two different ways, calculating both terms of the energy conservation equation applied to the studied case (no heat exchange considered):

$$\Delta U = W_{cp} \tag{37}$$

Calculating the results from both side of the equation allows checking the consistency of the model. The right-hand side of the equation gives:

$$\Delta U = \frac{m_g}{m_{cv}} u_g(\rho_g, T_g) + \frac{m_l}{m_{cv}} u_l(\rho_l, T_l) \tag{38}$$

$$- m_{cv} u(Q_i, T_i) = 18.66 \ [J]$$

While the left-hand side can be calculated as:

$$W_{cp} = -\int_{V_i}^{V_f} p dV = 18.82 \ [J] \tag{39}$$

The difference between the two values can be explained by the numerical errors introduced by the Euler backward method.

Finally, the isentropic efficiency of the process can be calculated, using the definition hereunder. The definition is only valid when the thermal equilibrium is reached (same temperature for both phases), which is respected in this case.

$$\varepsilon_{is} = \frac{m_{cv} \Delta u_{is}}{\Delta U} = 86.45 \ [\%] \tag{40}$$

Which means that, even without external heat transfer, nor leakage, nor friction introduced, a two-phase compression creates irreversibilities due to the heat transfer between the two phases. If the heat transfer coefficients U_ϕ were higher, the difference between the phases temperatures would be lower, resulting in a higher isentropic efficiency. A complete analysis of the evolution of this isentropic efficiency under various conditions will be part future works from the authors.

4 Conclusions

In this work, a two-phase compression (and expansion) mathematical model with thermal non-equilibrium has been introduced. The model takes as inputs heat transfer, mass transfer and the control volume evolution with a fictitious shaft angle and gives as outputs the thermodynamic properties evolutions of the two phases. The interface interaction along the control volume reduction allows to determine the evolution rate of the specific volumes as well as the temperatures of both phases a by applying mass and energy balance equations.

Moreover, the simulation of a simple piston-cylinder setup is analysed, showing how, under specific initial conditions and heat transfer coefficients at the interface, the temperature of both phases evolve as well as the pressure, even when the system is left at rest. Finally, an isentropic efficiency is introduced, showing that irreversibilities are unavoidable when compressing two-phase fluid.

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