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# DYNAMIC MODEL OF AN INDUSTRIAL HEAT PUMP USING WATER AS REFRIGERANT

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## ABSTRACT

In order to improve industrial energy efficiency, the development of a high temperature heat pump using water vapor as refrigerant is investigated. Technical problems restraining the feasibility of this industrial heat pump are surmounted by a specifically designed heat pump and the development of a new twin screw compressor. This article presents the development of a new dynamic model of this twin screw compressor and of the heat pump using flash evaporation. This model takes into account the presence and the purging mechanism (purging reservoir) of the non-condensable gases especially during the start-up procedure. A finite-volume (FV) approach is used for the plate heat-exchangers models while a moving boundary (MB) approach between phases is implemented for the purging and the flash evaporation systems models. The models are developed using Modelica as a modeling language without any library involvement and taking into account as many details as possible to closely represent the real system.

## KEYWORDS

Heat pump, high temperature, water, Modelica, transient state, modeling

## NOMENCLATURE

| | | |
|---|---|---|
| $A$ | Cross sectional area | $m^2$ |
| $Coef$ | Smoothing coefficient | - |
| $C_p$ | Specific heat | $Jkg^{-1}K^{-1}$ |
| $C_{scf}$ | Surface enhancement correction factor | - |
| $D$ | Diameter | $m$ |
| $h$ | Specific enthalpy | $Jkg^{-1}$ |
| $K$ | Tuning constant | - |
| $M$ | Mass | $kg$ |
| $\dot{m}$ | Mass flow rate | $kgs^{-1}$ |
| $N_{rpm}$ | Compressor speed | $\min^{-1}$ |
| $P$ | Pressure | $Pa$ |
| $P''$ | Partial pressure | $Pa$ |
| Pr | Prandtl Number | - |
| Re | Reynolds Number | - |
| $t$ | Time | $s$ |
| $T$ | Temperature | $K$ |
| $\Delta T$ | Temperature difference | $K$ |
| $u$ | Specific internal energy | $J(kgK)^{-1}$ |
| $V$ | Volume | $m^3$ |
| $V^i$ | Displacement | $m^3$ |
| $w$ | Velocity | $ms^{-1}$ |
| $\dot{W}$ | Mechanical power | $W$ |
| $x$ | Vapor quality | - |
| $z$ | Axial coordinate along the flow direction | $m$ |

*Greek letters*

| | | |
|---|---|---|
| $\alpha$ | Heat-transfer coefficient | $J(m^2K)^{-1}$ |
| $\eta$ | Efficiency | - |
| $\lambda$ | Thermal conductivity | $W(mK)^{-1}$ |
| $\xi$ | Mass flow coefficient | - |
| $\pi$ | Compression ratio | - |
| $\rho$ | Density | $kgm^{-3}$ |

*Subscripts and superscripts*

| | |
|---|---|
| 1 | Compressor inlet / Flash reservoir vapor outlet |
| 2 | Compressor outlet / Condenser inlet |
| 3 | Condenser outlet / purging system inlet |
| 4 | Purging system outlet / Expansion valve inlet |
| 5 | Expansion valve outlet / Flash reservoir inlet |
| 6 | Flash reservoir liquid outlet |
| 7 | Evaporator outlet / Flash reservoir inlet |
| $v$ | Volumetric |
| $is$ | Isentropic |
| $sat$ | Saturation |
| $cr$ | Critical |
| $r$ | Refrigerant |
| $w$ | Water |
| $p$ | Plate's wall |
| $i$ | $i^{th}$ element |
| $k$ | $k^{th}$ element |
| $c$ | Container |
| $air$ | Dry air |
| $l$ | Liquid |

| | |
|---|---|
| *v* | Water vapor |
| *g* | Gas |
| *f* | Flash |
| *ext* | Exterior |
| *in* | Inlet |
| *out* | Outlet |
| *evap* | Evaporation |
| *cond* | Condensation |

| | |
|---|---|
| HFC | Hydro Fluoro Carbon |
| CFC | Chloro Fluoro Carbon |
| HCFC | Hydro Chloro Fluoro Carbon |
| GPW | Global Warming Potential |
| ODP | Ozone Depletion Potential |
| COP | Coefficient of performance |
| HVAC | Heating Ventilation and Air Conditioning |

# 1. INTRODUCTION

Currently, improving energy efficiency becomes a main challenge for all energy systems due to the sharp increase of fuel prices (FY 2010). This challenge involves a better recovery of heat losses especially at high temperature in several industrial sectors. In addition to energy savings, the environmental context is introduced by further international and local agreements that involve a stronger awareness of environmental concerns especially by emission reduction. Large energy savings and potential environmental benefits are associated with the use of industrial heat recovery systems mainly at high temperature levels.

Several market studies assess a large amount of waste heat in the range 80°C-90°C in different industrial sectors like chemistry, paper drying, cleaning in place, … However, these applications need heat at higher

range of temperature, typically 120°C-130°C (EDF R&D, 2009; Khattar, 2010; Dupont and Sapora, 2009; US DoE, 2003).

A high temperature heat pump concept is technically able to upgrade the waste heat from an evaporation unit to the needed temperature levels at the condensing unit, especially when losses and needs appear simultaneously. Current, heat pumps are limited to heat production at a temperature level of 80°C-90 °C. Therefore the development of a new industrial high temperature heat pump becomes a step to improve industrial energy efficiency which is the goal of the present work.

One of the major problems with the development of this high temperature compression heat pump is the choice of the working fluid and corresponding compressor that can be used for these high ranges of temperatures. Several past studies show that water can be used; nevertheless its use presents lots of technical difficulties. To address this issue, this article presents technical solutions to overcome these problems by designing a special architecture for this heat pump.

The interest of developing a dynamic heat pump model contributes to the validation of this new machine. Hence, a new transient heat pump model is presented using water as refrigerant and taking into account the presence of air that must be removed upon start up phase.

## 2. WATER AS A WORKING FLUID

The choice of the working fluid for this high temperature heat pump should takes into account several considerations like environmental, safety, efficiency, thermodynamic properties.

Calm (2008) brakes history into four refrigerant generations based on defining selection criteria. He discusses the succession of criteria that involved a displacement of earlier working fluids and the renewed interest in natural refrigerants.

The focus on stratospheric ozone depletion involved Vienna convention and resulting Montreal Protocol (1987) that forced the phase out of ozone depletion substances especially CFCs. The primary focus was retained on HCFCs that were adopted as replacements for less ozone damaging out that CFC. But the production of these species was restricted in a first step in 1996 and in a full phase out of consumption by 2030, so HCFCs have been replaced by HFCs.

Later on, new findings and political debates on global warming potential become daily events with the global climate change. In 1997, the Kyoto protocol set binding targets for greenhouse gas emissions especially for HFCs. These restrictions are forcing shifts to a new generation of refrigerants which respect environmental issue.

In addition, for the aimed application, chosen refrigerant should be non-toxic, non-flammable, chemically inert, present reasonable working pressures and suitable thermodynamic properties for high temperature levels.

Beyond its environmental behavior, the working fluid of the heat pump should produce the maximum cooling capacity for the minimum input power, it should lead to high performance refrigeration cycles.

In general, synthetic refrigerants dominate in vapor compression refrigeration systems. Nowadays, research tries to investigate with attention the use of natural refrigerants with reduced environmental impact.Several studies (Chamoun et al. 2011; EDF R&D, 2009) selected water to be the refrigerant for this high temperature heat pump.

Water is an abundant constituent of earth's biosphere. In refrigeration applications, the use of water has been limited to absorption systems around a binary fluid. This natural fluid is a very attractive refrigerant, lots of studies compared water to other refrigerants from different point of views (Chamoun et al, 2011; Kilicarslan and Muller, 2005). Others made investigations and discussed the feasibility of a refrigerating machine using water vapor as refrigerant (Van Orshoven, 1993; Lachner et al. 2007; Wight, 2000).

Water vapor is an environmental friendly refrigerant with no Ozone Depletion Potential (ODP) and a Global Warming Potential ($GWP_{100yr}$) less than 1. It is non-toxic, non-flammable, and chemically inert at high temperature and needs low compressing pressures. Water has a high critical temperature therefore its thermodynamic properties suites high temperature ranges. Otherwise, it is easily available with low costs. Water has high theoretical coefficient of performance (COP) due to its high latent heat of vaporization compared to other traditional refrigerants. Hence, the use of water as refrigerant in this high temperature heat pump offer several potentially significant advantages but involves technical and feasibility difficulties.

Several problems limit the feasibility of an industrial heat pump working with water at high temperature levels of 80°C to 90 °C on evaporation unit and 120°C to 130°C on condensing unit:

### 2.1. Compressors technical problems

EDF R&D (2009) shows that currently, water vapor compression at high level of temperature can be performed by a several industrial compressors:

- Blowers allow compression of a high mass flow rate but under low compression ratios (corresponding 5 to 7 K).
- Multi-stages blowers allow an increase of $\Delta T$ to 10 to 12 K.
- Lobe compressors are adapted to low flow rates but with higher $\Delta T$ to 20 K. These compressors have a poor isentropic efficiency.
- Classical centrifugal compressors (mechanical bearings) cannot be used for such high temperature levels (T>100°C) because of an imperfect sealing which involves water leakage to lubricating oil.

Therefore, the largest obstacle is associated with the compressor. Adapted compressor should simultaneously satisfy different requirements at high temperature levels like:

- High compression ratio corresponding to 40 K
- High volumetric flow capacity
- High efficiency

To overcome this compression problem, PACO Project launched the development of a new twin screw compressor manufactured by SRM (Svenska Rotor Maskiner). An adaptation of such air compressor to water vapor could satisfy this heat pump demand after some modifications (water injection, sealing, …). This type of compressor presents high compression ratio (corresponding to 40 - 50 K), sufficient isentropic and high volumetric efficiency.

### 2.2. Evaporation below atmospheric pressure

In this industrial heat pump system a substantial amount of air will have to be removed upon start up. Indeed, evaporating at a pressure below atmospheric pressure recommends leak tightness at low pressure part of the heat pump but the sealing cannot be assured perfectly especially in compression phase. A leakage rate of non-condensable gases penetrates from the low pressure side to the system. The presence of significant amounts of air in the system will degrade the heat transfer capability of the condenser and reduce the capacity of the compressor. To overcome this issue, a special purging system must be implemented to eliminate these gases and increase the performance of the cycle.

Another effect of this evaporation pressure is that water vapor presents a high specific volume at the compressor suction. Hence the heat exchangers should be large enough to allow phase change. This issue is overcome by designing special liquid-liquid heat exchangers coupled to a flash evaporation system with a re-circulating flow through the heat exchanger.

In addition, the twin screw compressor allows a high volumetric flow rate compliant with water high specific volume due to its high rotational speed and high volumetric efficiency.

### 2.3. High superheat at the compressor outlet

In the compression process, discharge superheat is high and could reach up 204K without water injection which can damage the compressor screws and the condenser unit. This risk can be reduced by designing a specific saturated liquid injection to obtain a saturated state vapor at the outlet of the compressor.

The remaining step before manufacturing this heat pump is the validation of the design of the different components and of the overall architecture. In addition, the problem of start-up procedure should be overcome especially that the system is saturated by a substantial amount of air that will have to be removed upon start up phase.

The development of a heat pump model is a solution to gain an improved understanding of the characteristics of the cycle and to predict the evolution of the system.

# 3. MODELLING APPROACHES

Browne and Bansal (1998) distinguished the two main modeling approaches available in the literature, namely the steady state and transient approaches.

In this work, the transient approach is adopted to model the water vapor heat pump. Many benefits could be expected from such dynamic model like:

- Large reduction in time and costs spent on design and tests (design of heat exchangers, implementation of the heat pump in industrial processes) to achieve an optimal performance through the evaluation of different configurations.
- Identification of significant opportunities for development by easily changing component configurations and parameters through a computer simulation.
- Better control of the purging of non-condensable gases from the system as evaporation pressure is below atmospheric pressure.
- Investigating and solving the problem of start-up when some air is initially present in the system.
- Improvement of energy efficiency by choosing the best control strategies.

Therefore, the interest is related to transient modeling strategies. An overview of adopted strategies and approaches associated to dynamical modeling of HVAC and liquid chillers equipments is presented below.

## 3.1. State-of-the-art on dynamic models

The literature distinguishes different transient modeling strategies for air-to-air and liquid chillers models.

Bendapudi and Braun (2002) reviewed dynamic modeling of vapor compression equipments and distinguished in the literature two predominant approaches for the modeling of heat exchangers, the moving-boundary (MB) and finite-volume (FV) methods.

In the moving-boundary method, the heat exchanger is divided into control volumes that have moving boundaries with the evolution of the system related to the refrigerant transitions between single and two phase flow. With the finite volume method, the heat exchanger is divided into a number of fixed and equal-sized control volumes.

Dhar and Soedel (1979) presented one of the first models of a complete vapor compression refrigeration system. This model of a window air conditioner was built from first principles using a moving boundary approach in the heat exchangers.

MacArthur (1984) presented one of the earliest models based on the finite-volume method. The presented model was simplified by decoupling the thermal response of the heat exchanger from the pressure response, which results in less accurate predictions for the mass distribution in the heat exchanger. By combining the mass and energy balance equations, MacArthur and Grald (1987) resolved this issue and allowed to dedicate the pressure response. Rassmussen et al. (1987) improved this refined model by including the compressor's prime mover, namely an engine.

Browne and Bansal (1998) presented the philosophy and challenges behind developing simulation models of liquid chillers. They also presented steady and transient modeling approaches of the different elements of the machine. Later on, Browne and Bansal (2002) presented a liquid chiller model using twin screw compressor which was considered as a steady state device with an assumed isentropic compression. The refrigerant in the heat exchangers was modeled quasi-statically.

Khoury et al. (2001) presented numerical predictions from transient and steady state models. The transient model was based on the finite volume method for the heat exchangers using void fraction to determine the slip ratio of the two phases.

More recently, Haberschill et al. (2003) presented a dynamic model using the discretised approach based on MacArthur and Grald (1987) and Machado (1996) for the heat exchangers and a steady state compressor model developed by Gay (1999). On the same base, Guitari (2005) and Haberschill et al. (2007) modeled dynamically a heat pump using $CO_2$ as refrigerant and validated this model experimentally. Schalbart (2006) developped a dynamic model of refrigeration system equipped with a centrifugal compressor.

Pfafferott et al. (2004) presented a heat pump model based on thermo fluid library using the modeling language Modelica. He used the finite volume method as discretization schema. Similarly, a Modelica-based dynamic simulation model was developed for a chilled-water cooling coil based on Dymola™ and the Air Conditioning Library (Li et al. 2010).

Bendapudi et al. (2005) developed a centrifugal chiller model using finite volume method for shell and tube heat exchangers. They discussed different aspects like mesh dependence, integration order and step size. Their model was validated using data from R-134a centrifugal chiller. Later Bendapudi et al. (2008) developed and compared FV and MB formulations for transients in centrifugal chillers. They concluded that FV formulations are slightly more accurate but MB formulations are much faster. Besides, it is found that FV formulations are much robust through start-up and all load-change transients.

McKinley and Alleyne (2008) described an advanced, non-linear, moving boundary heat exchanger model for vapor compression cycles. Based on this work, Li and Alleyne (2010) presented a complete dynamic vapor compression cycle model that is able to describe several transient behaviors in heat exchangers and to maintain some stability under compressor shut-down and start-up.

Dynamic performance of vapor compression systems has been of interest for well over 30 years from Dhar and Soedel (1979) and through to Li and Alleyne (2010). As can be seen from the history of work on the topic, interest appears to be growing in recent years on development of better and more detailed dynamic models to predict an evolution of the system that closely match the real evolution of the actual system.

In earlier years, air to air systems were preponderant, opposed to actual growing interest in chiller systems, specifically liquid chillers. A listing of liquid chillers appears in this last scope of the literature (Bendapudi et al., 2005; Browne and Bansal, 2002; Haberschill et al., 2003; Li et al., 2010).

In the present article, we focus on liquid chiller systems based on screw compressors. Examining these models, a single dynamic heat pump model using a screw compressor that include detailed heat exchangers and which could adequately model large and small scale transients is not available. Browne and Bansal (2002) developed and compared a dynamic model with a dynamic neural model of a screw chiller system treating quasi-statically the refrigerant in the heat-exchangers.

In addition, a chiller system using water as refrigerant and taking into account the presence of non-condensable gases is not available. Even the mechanism of purging of these gases out of the system especially in start-up phase should be taken into account. Finally, no model for the flash evaporation system used in the real system is available in literature.

As conclusion one can state that a large volume of literature related to dynamic modeling of vapor compression equipments was reviewed. It was found that no model exists that could predict the complete dynamic performance of the high temperature heat pump described above. Therefore, a new dynamic heat pump model using water as refrigerant is developed using Modelica as a modeling language without any library involvement and taking into account as many details as possible to closely represent the real system.

# 4. MODEL DESCRIPTION

## 4.1. Modelica

Modelica is a hierarchical object-oriented physical modeling language to model complex and heterogeneous physical systems which is developed through an international effort (Fritzon, 2003; Modelica, 2010). The models in Modelica are mathematically described by differential, algebraic and discrete equations.

The most important reasons to adopt Modelica for the modeling task are the following:

- Modelica is based on equations instead of assignment statements, which permits acausal modeling without need to consider calculation order (design components by fixing operating conditions, predict response of the system by fixing component specifications, …).
- Modelica has a multi-domain modeling capability (combining mechanical engineering, control engineering, thermodynamics, hydraulics etc.).
- Modelica is an object-oriented language (which grants the possibility to re-use a component in another group assembled to form another model).

A Modelica translator is needed to transform a Modelica model into a Differential Algebraic Equation (DAE) system with fixed causality. Therefore, transformation algorithms have to be applied to transform equations into a form which can be integrated with standard methods. These transformation algorithms and solvers are available in two commercial simulation environments, Dymola™ and MathModelica™. In the present case, Dymola™ is adopted as a simulation environment which includes a graphical user interface (GUI) for model editing and browsing, Modelica translator, simulation engine, visualization of results, interface with Matlab/SIMULINK™ and ability of hardware-in-the-loop simulation. DASSL (Petzold, 1982) is used as integrator which is designed to solve DAEs. The numerical solution with DASSL is very reliable and efficient due to symbolic pre-processing (Otter, 2009).

In addition, Modelica provides a set of industrial formulations for the thermodynamic properties of water and steam based on IAPWS/IF97 formulations (Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam). These industrial standards present a trade-off between accuracy and calculation speed. Wagner et al. (2000) presented details related to these formulations dividing the states of water and steam

into five different regions. These functions to calculate thermodynamic properties of water and steam in different states based on the pressure and specific enthalpy as principle variable.

### 4.2. Heat pump architecture

The overall model of the heat pump using water as a refrigerant is based on one stage simple vapor compression refrigeration cycle consisting of a screw compressor, a condenser, a non-condensable purging system, a thermostatic expansion valve, a two phase flash separator, an evaporator (Fig. 1).

In this refrigerating cycle, the gas mixture enters into the suction side of the compressor (state 1) to be compressed and discharged at state 2. Then, it enters the condenser at high pressure and condenses by releasing heat to external cooling water. The fluid leaves the condenser at state 3 to enter the purging system where non condensable gases are eliminated. Then, the liquid phase of the refrigerant (state 4) enters into the expansion valve (throttling expansion device) and reaches the inlet of the flash reservoir (state 5). A re-circulating mass flow rate of liquid phase (state 6) leaves the tank to absorb heat through the evaporator and re-enters the tank at state 7. Another mass flow rate at state 6 leaves this tank to be injected into the compressor. The vapor in this reservoir is created by flash evaporation to assure a sufficient mass flow rate at the inlet of the compressor. For the development of the overall heat pump model, the initial mass of air is present only in the two reservoirs volumes at the start-up phase.

### 4.3. Compressor

In general, a compressor may be modeled either from basic engineering principles or from known (manufacturers) maps of its performance.

First principles approach is more expensive computationally and must be used if no performance maps are available (Bendapudi and Braun, 2002). However, using maps keeps the model more stable and close to known performance. It also makes it easier to keep track of uncertainly. In our case of study, a lack of information on design shapes of rotors leads to adopt performance maps provided by the manufacturer for the compressor model.

Since the compressor operates at high speeds, the compressor transients associated with changes in boundary conditions are small in relation to those of the heat-exchangers. Therefore, the compressor could be modeled as if under steady-state, assuming that it reaches its operating speed instantaneously.

The present compressor model is similar to that developed by Browne and Bansal (2002) which was validated for single and double screw. This model takes as inputs the suction pressure and enthalpy and the discharge pressure. It calculates as output the mass flow rate, the enthalpy at discharge port and the power required for the compression. The mass flow rate of the refrigerant is calculated as:

$$\dot{m} = \eta_v \rho_1 V^i \frac{N_{rpm}}{60} \tag{1}$$

The input work to the refrigeration cycle is expressed as:

$$\dot{W} = \dot{m} \frac{h_{2is} - h_1}{\eta_{is}} \tag{2}$$

The total electrical work input was calculated from Eq. (2) with constant (assumed) motor efficiency (95%). The isentropic and volumetric efficiencies were provided by the manufacturer of the compressor and were expressed as biquadratic and quadratic functions respectively of refrigerant flow rate and system pressure ratio using regressions on experimental data.

As mentioned before, due to the high superheat of steam induced by the compression process, saturated liquid is injected in order to obtain a saturated vapor state at the outlet of the compressor.

### 4.4. Heat-exchangers

The condenser and the evaporator are both gasketed plate heat-exchangers. The developed model follows a generic approach suitable for either. The fluids flow a counter-flow configuration along these heat-exchangers.

In term of modeling approach, the finite volume formulation was adopted. The transient conservation equations are applied to a number of fixed and equal-sized control volumes, which results in a system of ordinary differential equations.

***Simplifying assumptions***

The following simplifying assumptions are made in the development of this model:

- One dimensional flow,

Truly, refrigerant flow is three dimensional. However, a dominant flow direction is clear between refrigerant inlet and outlet. As a result, one dimensional refrigerant flow is a reasonable assumption.

- Negligible pressure drop,

Since water properties are a very weak function of pressure, pressure drops have a little impact on heat transfer on the water side. On the refrigerant side, the path between inlet and outlet is short and flow areas available between plates are large. This results in small pressure drops that can be neglected. In addition, manufacturing specifications estimate a negligible pressure loss in order of few mbar.

- Negligible viscous dissipation,

The viscous dissipation is smaller than the dominant energy transfer between the heat exchanger walls and the refrigerant from first side and liquid water from other. Therefore this viscous dissipation could safely be ignored.

- Negligible axial conduction,

Refrigerant state, water and wall temperature vary along the length of the plates. These temperatures gradients can induce heat diffusion in the axial direction. However, the high flow rates and the high Péclet number (which quantifies the relative effects of convection and diffusion modes of heat transfer) allow neglecting this axial conduction.

- Negligible plate material resistance.

The conductivity and surface area of the plates are high and there is little resistance to transversal heat transfer. However, capacitance is more significant and is accounted for.

***<u>Finite volume formulations</u>***

The application of these assumptions results in eliminating the momentum equation from consideration, and in adopting these forms of the conservation of mass and energy:

*Mass balance for refrigerant*

$$\frac{\partial \rho_r}{\partial t} + \frac{\partial (\rho w)_r}{\partial z} = 0 \qquad (3)$$

*Energy balance for refrigerant*

$$\frac{\partial(\rho u)_r}{\partial t}+\frac{\partial(\rho uw+Pw)_r}{\partial z}+\frac{\partial(\alpha_r(T_r-T_p))}{\partial z}=0 \tag{4}$$

*Energy balance for plate's wall*

$$(C_p\rho A)_p\frac{\partial T_p}{\partial t}+\frac{\partial(\alpha_w(T_p-T_w))}{\partial z}-\frac{\partial(\alpha_r(T_r-T_p))}{\partial z}=0 \tag{5}$$

*Energy balance for water*

$$(\rho A)_w\frac{\partial h_w}{\partial t}-(\rho Aw)_w\frac{\partial h_w}{\partial z}-\frac{\partial(\alpha_w(T_p-T_w))}{\partial z}=0 \tag{6}$$

Pressure and enthalpy are the main variables in each control volume. Based on the finite-volume formulations, the heat exchanger is divided into N equal control volumes along the length of each plate. The above equations are discretized and linearized for i sub volumes limited by k and k+1 boundary at time t using the discretization technique presented in figure 2, which yields for the $i^{th}$ control volume:

*Mass balance for refrigerant*

$$a_i\frac{dP_{r,i}}{dt}+b_i\frac{dh_{r,i}}{dt}=\dot{m}_{r,k}-\dot{m}_{k+1} \tag{7}$$

*Energy balance for refrigerant*

$$c_i\frac{dP_{r,i}}{dt}+d_i\frac{dh_{r,i}}{dt}=\dot{m}_{r,k}h_{r,k}-\dot{m}_{r,k+1}h_{r,k+1}+\alpha_{r,i}S_i(T_{p,i}-T_{r,i}) \tag{8}$$

*Energy balance for plate's wall*

$$e_i\frac{dT_{p,i}}{dt}=\alpha_{r,i}S_i(T_{r,i}-T_{p,i})-\alpha_{w,i}S_i(T_{p,i}-T_{w,i}) \tag{9}$$

*Energy balance for water*

$$f_i\frac{d(h_{w,i})}{dt}=\dot{m}_{w,k+1}h_{w,k+1}-\dot{m}_{w,k}h_{w,k}+\alpha_{w,i}S_i(T_{w,i}-T_{p,i}) \tag{10}$$

Where the coefficients $a_i, b_i, c_i, d_i, e_i$ and $f_i$ are defined as:

$$a_i=V_{r,i}(\frac{\partial\rho_{r,i}}{\partial P_{r,i}})_{h_{r,i}} \qquad b_i=V_{r,i}*(\frac{\partial\rho_{r,i}}{\partial h_{r,i}})_{P_{r,i}}$$

$$c_{r,i} = V_{r,i}(h_{r,i} * (\frac{\partial \rho_{r,i}}{\partial P_{r,i}})_{h_{r,i}} - 1) \qquad d_i = V_{d,i}(h_{r,i} * (\frac{\partial \rho_{r,i}}{\partial h_{r,i}})_{P_{r,i}} + \rho_{r,i})$$

$$e_i = (MC_p)_{p,i} \qquad f_i = (V_{w,i} * \rho_{w,i})$$

In this work, a linear enthalpy and mass flow rate profile assumption is made in all elementary control volumes:

$$h_i = \frac{h_k + h_{k+1}}{2} \quad \text{and} \quad \dot{m}_i = \frac{\dot{m}_k + \dot{m}_{k+1}}{2}$$

***<u>Heat-transfer coefficients</u>***

The heat transfer coefficient of the refrigerant condensing side is determined based on the relation provided by Shah (1979):

$$\alpha = C_{scf,c} \frac{\lambda_l}{D} 0.023 \mathrm{Re}_l^{0.8} \mathrm{Pr}_l^{0.4} \left[ (1-x)^{0.8} \frac{3.8x^{0.76}(1-x)^{0.04}}{(P_{sat}/P_{cr})^{0.38}} \right] \tag{11}$$

For the liquid phase heat transfer coefficient, the Dittus-Boelter correlation is used:

$$\alpha = C_{scf,w} \frac{\lambda_l}{D} 0.023 \mathrm{Re}_l^{0.8} \mathrm{Pr}_l^{0.4} \tag{12}$$

The heat transfer coefficients were tuned using scaling factors $C_{scf}$ to account for the surface extension of the plates.

***<u>Solution</u>***

These equations are applied to the N control volumes and result in a system of 2N coupled, first-order, linearized, ordinary differential equations with 2N unknowns:

- Pressure $\qquad P_r = P_{r,i}$ for $1 \xrightarrow{i} N$
- Enthalpies $\qquad h_{r,i}$ for $1 \xrightarrow{i} N$
- Mass flow rate $\qquad \dot{m}_k$ for $2 \xrightarrow{k} N$

To solve these 2N equations and determine these 2N unknowns, the initial conditions consist of the refrigerant and water states and the temperature of the wall. The boundary conditions are:

- Mass flow rate of refrigerant entering and leaving the heat exchanger

- Mass flow rate of the water entering the heat exchanger

- Enthalpy of refrigerant entering the heat exchanger

- Enthalpy of water entering the heat exchanger

### 4.5. Tri phases separators

This part presents the model of two different elements in this refrigeration system:

- Non-condensable purging system
- Two phases flash separator with air

These both elements are cylindrical tanks of known dimensions containing a gas and a liquid phase., The gas phase is a mixture of air and water vapor. The presence of air is due to the initial conditions where all the installation is filled by air.

Although these two elements play different roles, with different inlets and outlets, the same general principle can be used with some specific adaptations.

This model is based on the equations derived from the mass and energy balances on the system and necessary equations for properties calculations. At the inlet of the separator, the refrigerant flow is split into two phases. Following the conservation of mass and energy for these phases, enthalpy and pressure evolution of the system are integrated to calculate the other properties of each phase.

***Assumptions***

The following assumptions are made for the study of the separator:

- The system is in thermodynamic equilibrium,

- The dry air in the separator is considered as perfect gas,

- The mixture of dry air and water vapor is homogeneous,

- Liquid density is supposed constant,

- The container's thermal resistance is ignored,

- The flash evaporation is assumed adiabatic (isenthalpic).

***Formulations***

The equations of conservation of mass and energy for each phase can be discretized and linearized at each time t using the discretization technique presented below.

The discretization method is based on the choice of two different control volumes (Fig. 3), namely one for the mass balance and the other for the energy balance where the gas phases are coupled in the same control volume. The fact of supposing a homogenous mixture means a unique temperature $T_g$ for the whole gas phase (a coupled energy equation) and a total pressure equal to the sum of air and water vapor partial pressures as follow

$$T_g = T_v(P_v, h_v) = T_{air}(P_{air}, h_{air})$$

$$P_g = P''_{air} + P''_v$$

$P''_{air}$ and $P''_v$ are the partial pressures calculated for the total gas volume $V_g$ which is the sum of the dry air phase and water vapor volumes. The separator's total volume is constant. As a result, the sum of volumes of gas and liquid is constant and equal to the total volume of the container:

$$V_c = V_g + V_l$$

For this container, three inlet mass flow rates and three outlet mass flow rates are presented to model all possible flows into and out of the system.

The resulting balance equations for this container are as follow:

*Mass balance for liquid phase*

$$a_l \frac{d(V_l)}{dt} = \dot{m}_{l,in} - \dot{m}_{l,out} + \dot{m}_{cond} - \dot{m}_{evap} \tag{13}$$

*Energy balance for liquid phase*

$$\begin{aligned} b_l \frac{dP_l}{dt} + c_l \frac{dh_l}{dt} + d_l \frac{dV_l}{dt} &= \dot{m}_{l,in} h_{l,in} - \dot{m}_{l,out} h_{l,out} + \dot{m}_{cond} h_{l,sat} - \dot{m}_{evap} * h_{v,sat} \\ &+ \alpha_{gl} S_{gl}(T_g - T_l) - \alpha_{lc} S_{lc}(T_l - T_c) \end{aligned} \tag{14}$$

*Mass balance for vapor phase*

$$a_v \frac{dP''_v}{dt} + b_v \frac{dh_v}{dt} + c_v \frac{dV_g}{dt} = \dot{m}_{v,in} - \dot{m}_{v,out} - \dot{m}_{cond} + \dot{m}_{evap} \tag{15}$$

*Mass balance for dry air phase*

$$a_{air}\frac{dP''_{air}}{dt}+b_{air}\frac{dh_{air}}{dt}+c_{air}\frac{dV_g}{dt}=\dot{m}_{air,in}-\dot{m}_{air,out} \tag{16}$$

*Energy balance for gas phases*

$$\begin{aligned}\frac{dU_g}{dt}&=d_{air}\frac{dP''_{air}}{dt}+e_{air}\frac{dh_{air}}{dt}+d_v\frac{dP''_v}{dt}+e_v\frac{dh_v}{dt}+(f_{air}+f_v)\frac{dV_g}{dt}\\ \frac{dU_g}{dt}&=\dot{m}_{v,in}h_{v,in}-\dot{m}_{v,out}h_{v,out}+\dot{m}_{air,in}h_{air,in}-\dot{m}_{air,out}h_{air,out}-\dot{m}_{cond}h_{l,sat}+\dot{m}_{évap}*h_{v,sat}\\ &-\alpha_{gl}S_{gl}(T_g-T_l)-\alpha_{gc}S_{gc}(T_g-T_c)\end{aligned} \tag{17}$$

*Energy balance for container's wall*

$$(MC_p)_c\frac{dT_c}{dt}=\alpha_{gc}S_{gc}(T_g-T_c)+\alpha_{lc}S_{lc}(T_l-T_c)-\alpha_{cext}S_{cext}(T_c-T_{ext}) \tag{18}$$

Where the coefficients $a_i, b_i, c_i, d_i, e_i$ and $f_i$ are defined as:

$$a_l=\rho_l \qquad b_l=-V_l \qquad c_l=V_l\rho_l \qquad d_l=h_l\rho_l$$

$$a_v=V_g\left(\frac{\partial\rho_v}{\partial P''_v}\right)_{h_v} \qquad d_v=V_g\left(h_v\left(\frac{\partial\rho_v}{\partial P''_v}\right)_{h_v}-1\right)$$

$$b_v=V_g\left(\frac{\partial\rho_v}{\partial h_v}\right)_{P''_v} \qquad e_v=V_g\left(\rho_v+h_v\left(\frac{\partial\rho_v}{\partial h_v}\right)_{P''_v}\right)$$

$$c_v=\rho_v \qquad f_v=h_v\rho_v$$

$$a_{air}=V_g\left(\frac{\partial\rho_{air}}{\partial P''_{air}}\right)_{h_{air}} \qquad d_{air}=V_g\left(h_{air}\left(\frac{\partial\rho_{air}}{\partial P''_{air}}\right)_{h_{air}}-1\right)$$

$$b_{air}=V_g\left(\frac{\partial\rho_{air}}{\partial h_{air}}\right)_{P''_{air}} \qquad e_{air}=V_g\left(\rho_{air}+h_{air}\left(\frac{\partial\rho_{air}}{\partial h_{air}}\right)_{P''_{air}}\right)$$

$$c_{air}=\rho_{air} \qquad f_{air}=h_{air}\rho_{air}$$

***<u>Solution</u>***

Equations 13 to 18 are applied to the container's control volumes and result in a system of 8 coupled, first-order, linearized, ordinary differential equations with 8 unknowns $P_l, P''_{air}, P''_v, h_l, h_{air}, h_v, V_l, V_g$.

To solve these 8 equations and determine these 8 unknowns, the initial conditions are supposed for a fixed initial volume of liquid with saturated moist air, the whole system (walls, liquid, gas) being at 20°C.

***Non-condensable purging system***

In such system a substantial amount of air will have to be removed upon start up. Another issue associated with the evaporation pressure of water which is below atmospheric pressure is that non-condensable gases will flow from the compressor to the system. The presence of significant amounts of air in the system will degrade the heat transfer capability of the condenser and reduce the capacity of the compressor.

A specific design of a purging system is necessary to eliminate theses gases and to increase the performance of the cycle. Unfortunately, this air purging system will also remove some water vapor along with air. This water must be made up somewhere in the system and in our case it will be added to the flash reservoir. The purging system is located between the condenser and the expansion device in the high pressure branch of the system.

The condensing vapor leaves the condenser to enter this purging reservoir with an amount of air coming from the low pressure branch. Two outlets exist for this reservoir, the gases outlet to the exterior of the system through an expansion valve built in on the top of the reservoir and the water outlet to the expansion valve and then to the low pressure branch.

***Two phases flash Separator with air***

As mentioned before, the flash evaporation will be used to create vapor at the suction of the compressor. Therefore, a flash evaporation vessel model is coupled to the evaporator model in order to exchange heat with external sources and to flash after a pressure reduction in a throttling device.

As presented in the Figure 4, the refrigerant leaves the expansion valve to enter the vessel. A re-circulating mass flow rate leaves the tank to exchange heat in the heat exchanger and to re-enter the vessel. A part of this flow immediately flashes into vapor at lower pressure and the other part is cooled to the saturation temperature at the reduced pressure.

In our model, the evaporated mass flow rate is calculated from a heat balance on liquid bulk in the flash evaporation chamber. Moreover, the kinetics of flash evaporation and the slight evolution of the throttling

device walls' temperature during it, make us think that energy supplied by walls during flashing is negligible when compared to the other terms of the equation balance (Saury et al., 2002). Thus, the energy released by the sudden temperature drop is completely used to vaporize a quantity $\dot{m}_{v,f}$ of the re-circulating flow rate of distilled water $\dot{m}_f$ calculated using:

$$\dot{m}_{v,f} = \dot{m}_f \frac{h_f - h_{l,f}}{h_{v,f} - h_{l,f}} \tag{19}$$

### 4.6. Valves

The primary purpose of the expansion valve is to expand refrigerant from the purging system at high pressure to the flash separator at lower pressure. The behavior of the expansion valve is described by an orifice model. This model is steady state (Cleland, 1983) and is based on the following assumptions (Dhar and Soedel, 1979; MacArthur, 1984; Outtagarts, 1994; Shalbart, 2006):

- Isenthalpic expansion,
- Negligible heat losses (No heat exchanges between the refrigerant and the valve),
- No mass accumulation (Reduced size),
- Negligible thermal inertia of the valve,
- Negligible mechanical inertia of the refrigerant.

The mass flow rate through the valve is determined as:

$$\dot{m} = \xi A \sqrt{2\rho_{in}(P_{in} - P_{out})} \tag{20}$$

Since the expansion is assumed isenthalpic:

$$h_{in} = h_{out} \tag{21}$$

The same valve model is used for the purging valve; its opening depends on the concentration of air present in the reservoir. The control of the valve is done using a smoothing coefficient $Coef$ to eliminate the simulation problems of the model using:

$$\xi = K(1 - \exp((-\frac{P''_{air}}{Coef})^2)) \tag{22}$$

## 5. RESULTS OF SIMULATIONS

In this section, simulation results concerning the start-up of this heat pump are presented. This allows to investigatethe purging procedure of the substantial amount of air present initially in the system. In addition, the time evolution of the main parametersare presented in order to follow and understand the behaviour of the system.

For this set of results, the heat exchangers are supposed at hot start in equilibrium with the external sources. The start-up of the circulating pump induces a mass flow rate at the inlet of the evaporator which exchanges heat in the evaporator with the external source to be flashed in the flash reservoir at a lower range of pressure. This flash evaporation cycle increases gradually the temperature of the flash reservoir components (Fig. 5).

At initial conditions, the flash reservoir is saturated by a 100% relative humidity moist air at 27°C with a water vapor partial pressure of 3500 Pa.

The main mass flow rate is simulated by imposing a compressor rotational speed from zero to 4700 rpm using a step time for start-up of 1500 s. This increase of the mass flow rate at the compressor suction (Fig. 6) leads to a decrease in the mass of the gaseous phase (water vapor and air) present in the flash reservoir.

At the beginning, the sucked mass flow rate is composed mainly by air, which leads to a decrease of the partial pressure of dry air in the flash reservoir and therefore to a decrease of the total pressure in the reservoir. This reduction of the total pressure increases the flash rate, which increases the partial pressure of the vapor phase (Fig. 7).

After a while, air is removed from the low pressure side to the high pressure side and accumulated in the purging system to be eliminated gradually owing to the non-condensable controlled valve.

The mass flow rate imposed by the compressor condenses in the condenser and releases heat to the environment (cooling water) at high pressure level and leaves the condenser to the purging reservoir.

As mentioned above, initially, air is the major constituent of this mass flow rate. Hence, the partial pressure of air increases while the purging system is removing a mixture of air and water vapor simultaneously. The concentration of air decreases in the main mass flow rate which increases the concentration of water vapor. Hence, the partial pressure of water vapor increases which increases of the condensing overall pressure (Fig. 8).

It is noticed that in these conditions at 30 min after start-up beginning, air existing in the installation is only present at high pressure side in the purging system with a mass percentage of gaseous phase of 0.7%.

## 6. CONCLUSION

In order to develop a new heat pump at high temperature ranges, water was chosen as the refrigerant since that fluid respect environmental issues, safety and performance criteria. Several technical problems limit the feasibility of this industrial heat pump. In order to overcome these problems, the development of a new twin screw compressor with high volumetric and adiabatic efficiencies and able to compress water vapor for temperature lifts of 40K has started. A special design of the whole heat pump is undertaken and presented. This design is due to the particular properties of water vapor (very low density, high superheated vapor) and the presence of non-condensable gases in the heat pump.

A transient model of this heat pump was developed using Modelica in order to understand the interactions between its different components, especially during start-up operation. This model presents the evolution of the system which is initially saturated by air that will be gradually removed by a special purging system to reach higher efficiency of the heat pump.

An improved understanding of the characteristics of the cycle and a prediction of the evolution of the system are provided. In addition, this model aims the validation of the design of the different components and the overall architecture and could help for the implementation of the heat pump in industrial processes.

## 7. ACKNOWLEDGEMENTS

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## 9. FIGURES

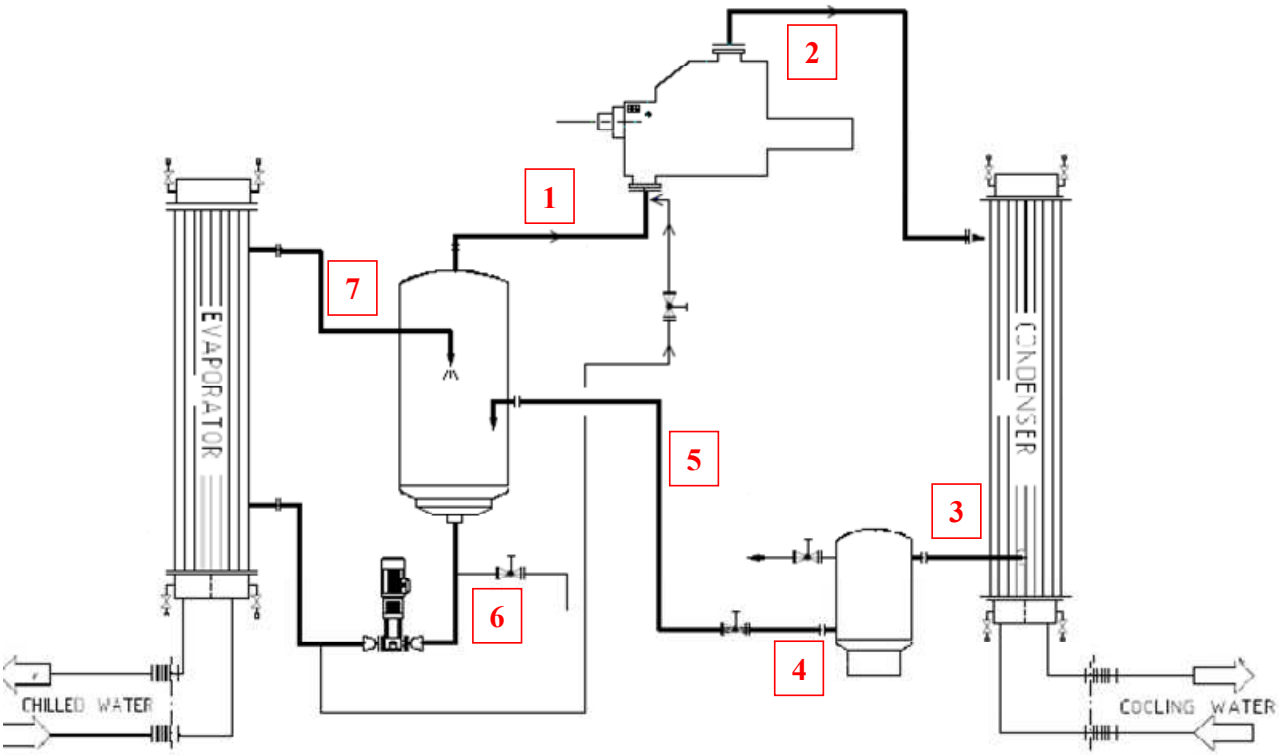


**Figure 1. Schematic representation of the model**

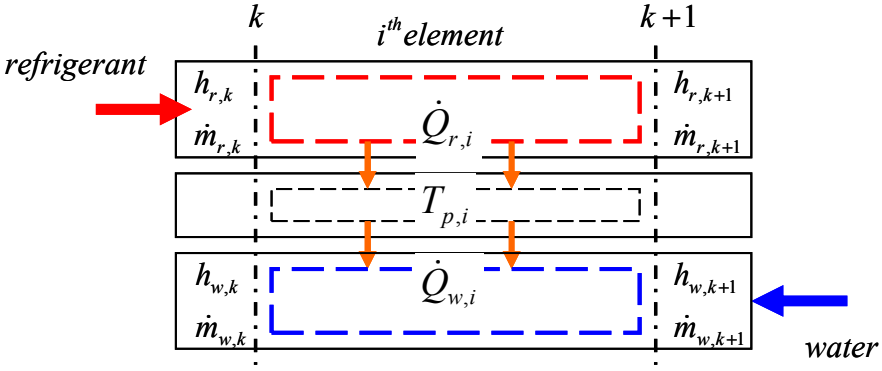


**Figure 2. Heat-exchangers discretization model**

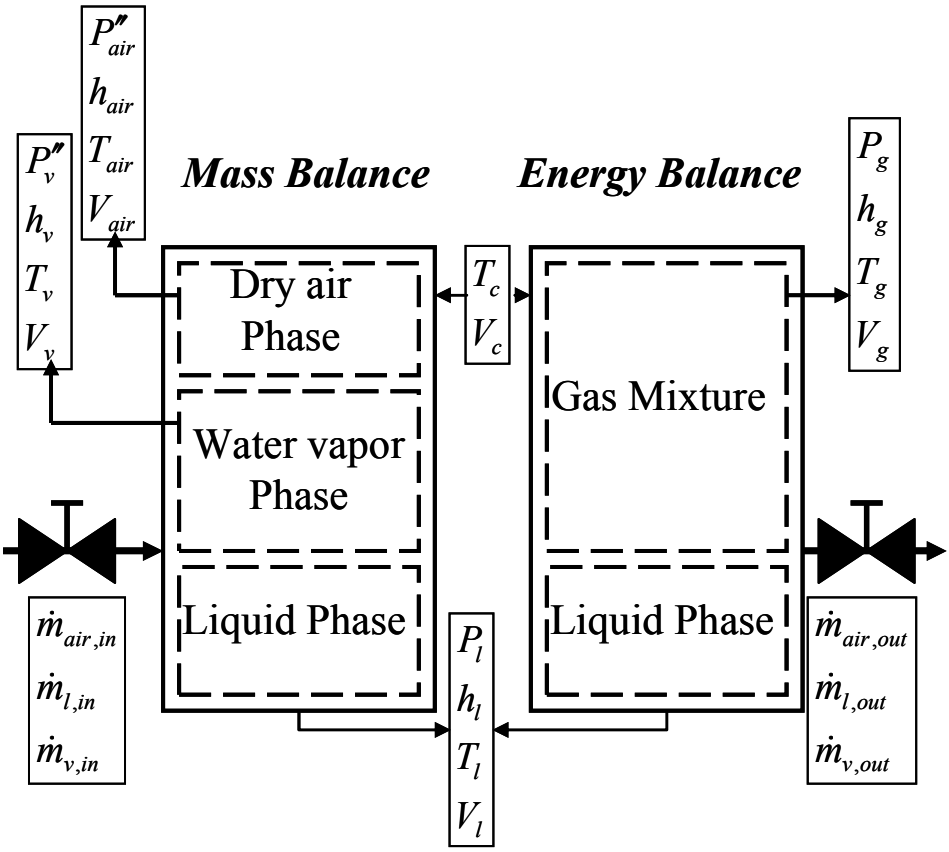


**Figure 3. Mass and energy control volumes of the reservoir model**

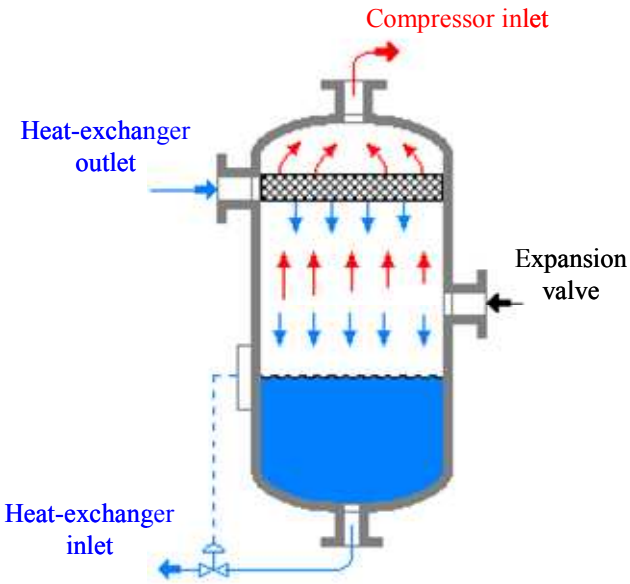


**Figure 4. Flash reservoir model**

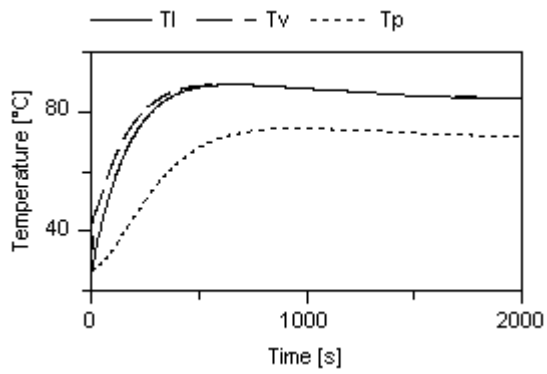


**Figure 5. Temperature of the flash reservoir components vs. time**

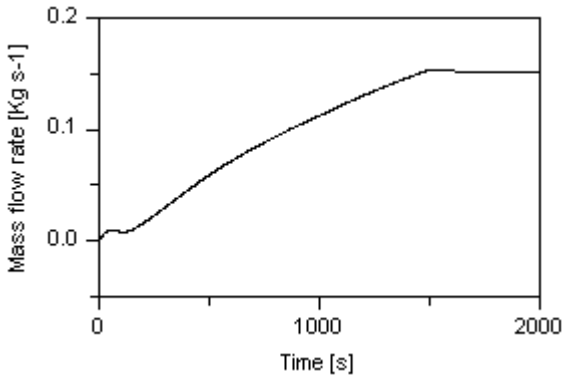


**Figure 6. Compressor mass flow rate vs. time**

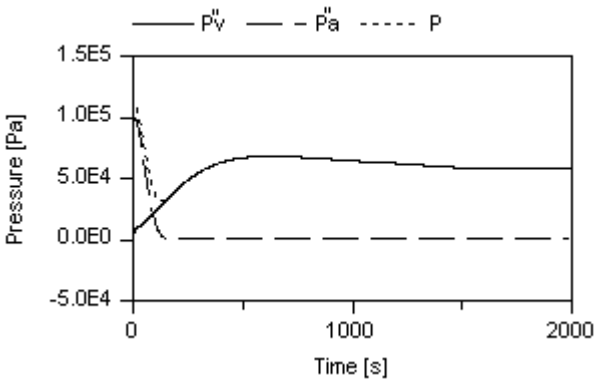


**Figure 7. Low pressures vs. time**

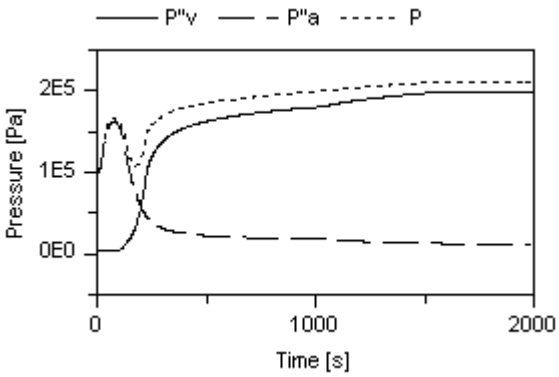


**Figure 8. High pressures vs. time**