

# MODELLING APPROACH FOR A LIQUID-INJECTED AMMONIA-WATER SCREW COMPRESSOR

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## ABSTRACT

The present work focuses on a modelling approach for a liquid-injected ammonia-water screw compressor for combined absorption-compression heat pumps (CACHP) at high-temperature operation. The CACHP system combines the technologies of an absorption and vapor compression heat pump with a mixture of ammonia and water as working fluid. The functionality of this process has already been proven in the industrial sector using standard refrigeration components. In recent years, several studies have investigated the CACHP system to identify challenges and opportunities to increase the achievable temperature range and optimize process performance. The compressor was identified as a main critical component for increasing the achievable sink outlet temperature level. For this purpose, this study identifies currently available modelling approaches of liquid-injected screw compressors and investigates their usability in a CACHP system. Based on this, an approach for the modelling of liquid-injected ammonia-water screw compressors is developed.

Keywords: Liquid-Injected Screw Compressor, Combined Absorption-Compression Heat Pump, Ammonia-Water Mixture

## 1. INTRODUCTION

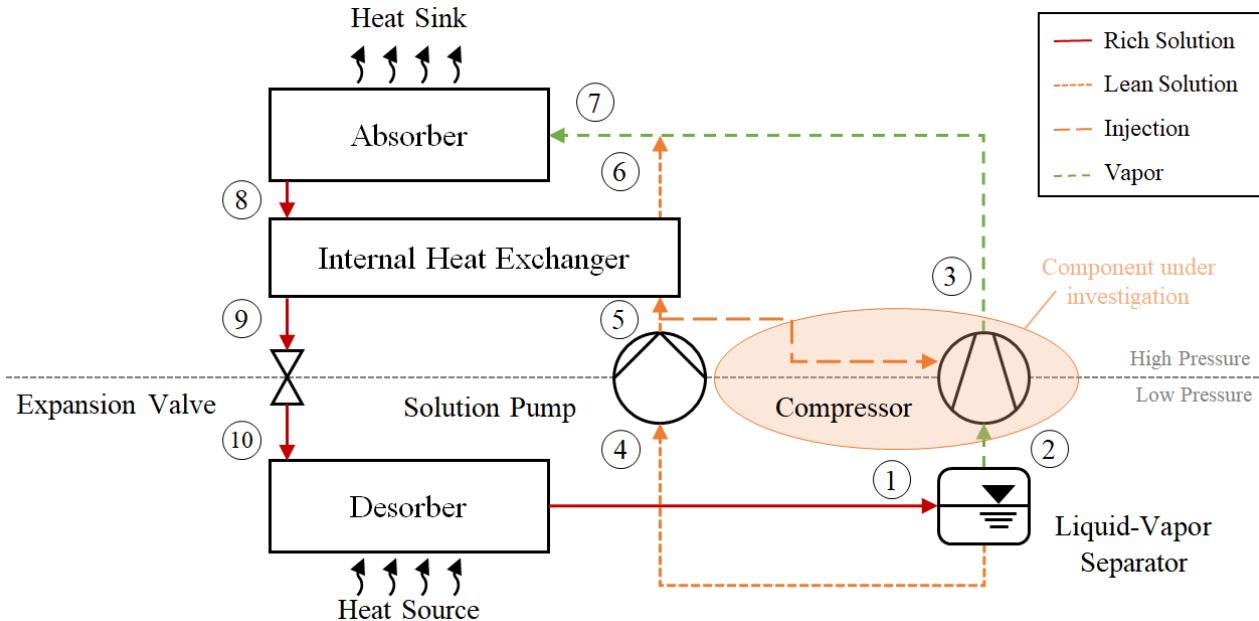
Increasing energy consumption and environmental pollution are of the most important challenges in today's society. According to IEA (2019), energy consumption worldwide grew by 2.3 % in 2018, nearly twice the average rate of growth since 2010. Hence improving the efficiency of energy systems in order to decrease the consumption of resources is of great interest. Using heat pumps with environmentally friendly working fluids such as the natural fluids ammonia and water instead of traditional boilers is an effective measure to reduce energy consumption related to industrial heating applications. Arpagaus et al. (2018) recognized large application potentials, especially in food, paper, metal and chemical industries. In their analysis of the European heat pump market, they found a technical potential of 113 PJ for process heat between 100 °C and 150 °C. A promising approach for industrial high-temperature heat pump applications is provided by combined absorption-compression heat pumps (CACHP) with a zeotropic ammonia-water mixture as working fluid. The working principle of the CACHP system extends a vapor compression heat pump (VCHP) by an additional solution cycle and is based on the Osenbrück cycle (Osenbrück, 1895). This extension offers the typical characteristics of CACHP systems, such as high achievable sink temperatures in combination with large temperature lifts and non-isothermal heat transfers. Nordtvedt et al. (2013) have already demonstrated the functionality of this system in the industrial sector by using standard refrigeration components and achieving sink outlet temperatures of up to 120 °C. In recent years, various authors, such as Jensen (2015) and Nordtvedt (2005), have examined the CACHP system to identify challenges and potentials for the optimization of process parameters. In this context, the compressor was highlighted as a critical component for achieving higher sink outlet temperatures with the associated pressure levels due to the limitation of the compressor discharge temperature. The use of a liquid-injected screw compressor was identified as a promising solution. The focus of this study is the development of a modelling approach of a liquid-injected screw compressor to be utilized in a CACHP system at high-temperature operation. A CACHP test facility is currently being built in a laboratory at the Department of Energy and Process Engineering, NTNU. Among other things, the test facility will be used to examine different compressor arrangements. Using computer modelling to optimize the compressor configuration, and later being able to compare experimental data from the test facility th theoretical data from simulations, is of great value.

## 2. THE COMBINED ABSORPTION-COMPRESSION HEAT PUMP

This section deals with the presentation of the combined heat pump cycle with ammonia-water mixture as working fluid as well as the characteristics and requirements for compressors used in the CACHP system.

### 2.1. Combined Heat Pump Cycle with Ammonia-Water Mixture as Working Fluid

The most basic type of CACHP is the Osenbrück cycle, named after its inventor (Osenbrück, 1895). The Osenbrück cycle is illustrated in Figure 1. In what follows, the working principle of this cycle is explained, based on theory presented by Nordtvedt (2005) and Jensen et al. (2014).



**Figure 1: Simplified schematic of a combined absorption-compression heat pump cycle**

In the CACHP, the evaporator and condenser are replaced by the desorber and absorber. The rich solution at low pressure (10) enters the desorber where heat from the source is transferred. This causes the temperature to rise and the solubility of the ammonia-water mixture to decrease. Hence vapor is generated, and a two-phase mixture leaves the desorber (1). The low-pressure vapor and lean solution are separated before they are drawn towards the compressor (2) and pump (4) respectively. The compressor increases the pressure and temperature of the vapor (2 to 3), while the pump elevates the pressure of the lean solution correspondingly (4 to 5). The temperature rise over the pump is minor. Therefore, to improve the performance of the cycle, an internal heat exchanger (IHX) is added to the solution sub-cycle. Heat is exchanged between the lean and rich solutions, causing a temperature rise in the lean solution (5 to 6) and a temperature drop in the rich solution (8 to 9). The high-pressure lean solution (6) is mixed with the high-pressure vapor (3) at the entrance of the absorber (7). In the absorber, vapor is absorbed into the liquid phase rejecting heat to the heat sink fluid. The ammonia concentration in the liquid phase gradually increases, so that the absorption process leads to a saturated liquid at the absorber outlet. The rich solution eventually passes through the solution heat exchanger before being throttled to desorber pressure (8 to 9 to 10), thus completing the cycle.

Nordtvedt (2005) and Jensen et al. (2014) point out several advantages with utilization of CACHP. Compared to a VCHP using a single working fluid, the working fluid pair in a CACHP offers much more design flexibility. By altering the composition of the working pair, i.e., the refrigerant-to-absorbent ratio, the properties of the working fluid can be adapted to the heat source and heat sink properties, as well as properties of each heat pump component, to obtain optimal working conditions. Industrial heat supply and recovery of surplus heat requires large heat source and heat sink temperature glides. Contrary to the isothermal processes of evaporation and condensation in a VCHP, the absorption and desorption processes in a CACHP are non-isothermal processes. By

matching the temperature glides of the working fluid with the temperature glides of the heat source and heat sink fluids, the thermal losses are reduced, resulting in a higher COP. This makes the CACHP suitable for many industrial applications. Another suitable feature of the CACHP is that using a zeotropic mixture reduces the required high-pressure level. The sink temperature from a conventional VCHP is limited because the condenser pressure becomes too high, whereas a CACHP can achieve much higher sink temperatures due to the reduced high-pressure level.

## 2.2. Characteristics and Requirements for Compressors Used in the CACHP System

Based on the results of a previous investigation of available compressors for use in an ammonia-water CACHP system, the following characteristics and requirements for the compressor are listed (Ahrens et al., 2019):

### Material compatibility

Ammonia can cause corrosion in contact with materials such as copper, copper-based alloys and zinc. It is of high importance to choose ammonia-compatible materials in all parts of the compressor that are in contact with the working fluid. Stainless steel and aluminium are fully compatible with ammonia, and therefore among the most widely used materials in CACHP systems.

### Discharge temperature

Due to the relatively low density and specific heat capacity of ammonia, high temperatures can arise during compression. Jensen (2015) identified the discharge temperature as the dominating constraint in an ammonia-water CACHP. Excessive temperatures can cause decomposition of the working fluid, breakdown of seals and compressor failure. It is therefore crucial to select a compressor capable of handling or curtailing high discharge temperatures.

### Liquid resistance

Due to the design of the CACHP system and the properties of the ammonia-water mixture, it is possible that the suction vapor will contain droplets of water. Hence, it is important that the compressor is resistant to liquid carry-over. Choosing a liquid-resistant compressor also gives much more operational flexibility, e.g., the possibility of operating closer to the two-phase region and using liquid injection.

### Oil-free operation

It is desirable to have a compressor capable of oil-free operation, since oil has been proven to diminish the performance of the rest of the CACHP system (Zaytsev and Infante Ferreira, 2002; Nordtvedt, 2005). Additionally, costs related to oil separation are avoided.

A screw compressor with injection of liquid ammonia-water should be capable of meeting all the above-mentioned characteristics and requirements. According to investigations of Zaytsev and Ferreira (2002) and other authors, liquid injection has a generally positive influence on the volumetric and isentropic efficiency of the compressor and can serve various functions, such as lubrication, sealing and decreasing of the discharge temperature through the compression process. However, the complexity of the processes involved in injection and compression also leads to various challenges. On the one hand, the optimal location for an effective injection must be determined. Then, the quantity and type of injection must be determined with respect to the effects on the compression process and performance. The use of the zeotropic ammonia-water mixture in a two-phase process represents a special challenge due to its thermodynamic properties.

As such a liquid-injected screw compressor is not yet commercially available, there is great uncertainty regarding the design and operation of the compressor. The analysis of the compressor with the help of thermodynamical and mathematical models can provide a better understanding and a reduction of the uncertainties. In the following, the developed modelling approach is presented accordingly.

### **3. IDENTIFICATION OF EXISTING MODELLING APPROACHES**

The aim of the development of a modelling approach is the investigation of compressor behavior as well as a better understanding of the ongoing processes and associated phenomena. A computer model of the liquid-injected screw compressor can help to determine the required injection mass flows based on the fulfillment of the given requirements, such as the maximum discharge temperature. Additionally, the number and position of the inlet ports can be adjusted to optimize their placement for the intended operation. The CACHP test facility is capable of testing different compressor arrangements, as described previously. This involves varying the streams used for liquid injection. Specifically, both the lean solution downstream of the solution pump, e.g. upstream of the IHX (see Figure 1), and the strong solution upstream of the expansion valve can be used. As a result, the mass fraction of ammonia and water of the injected liquid varies depending on the stream used and the effects on compressor performance can be investigated. Subsequently an optimization can be carried out. Another important function of the computer model is the planning and preparation of experimental tests and the subsequent evaluation and validation of the results. Since the design of experiments and evaluation is also desirable for the entire CACHP system, the screw compressor model should be integrable into bigger system models. Further on, approaches available in the literature are presented and examined regarding their usability.

#### **Liquid-Injected Screw Compressor Models in the Literature**

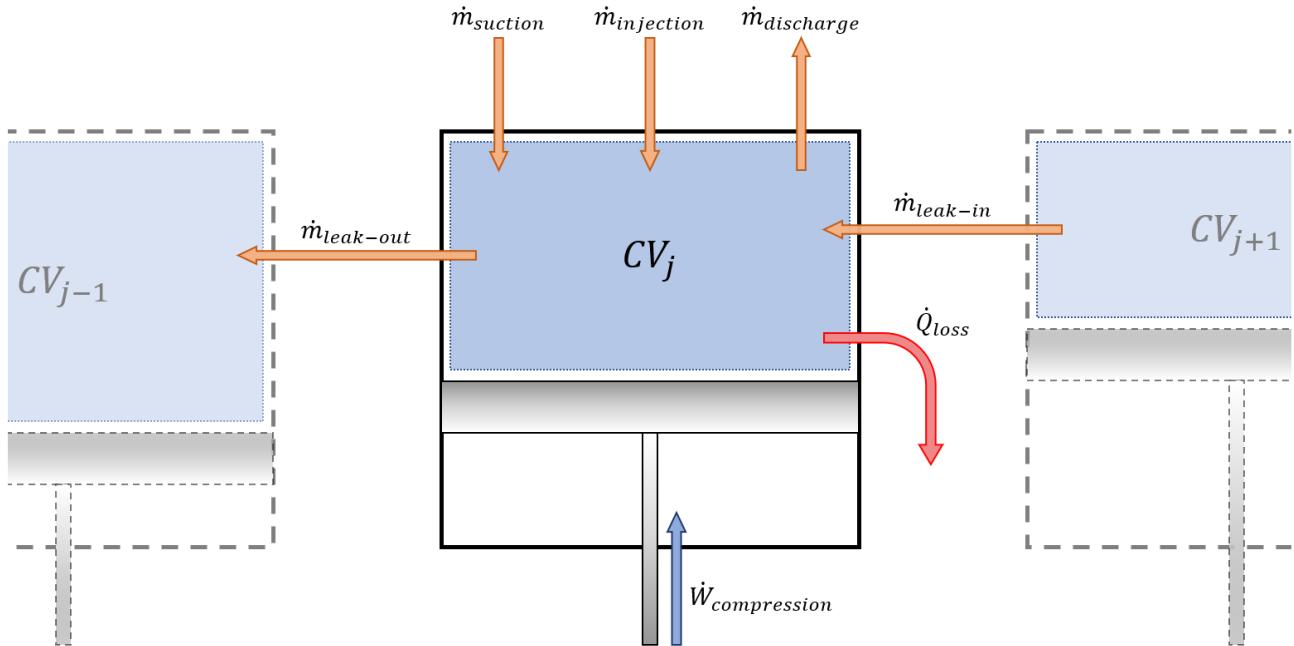
A large number of models of varying complexity and scope are described in the literature. Three main types of modelling techniques are the most common when dealing with computer modelling of screw compressors, namely empirical, analytical and numerical methods. Empirical models are based on curve fitting or statistical analysis of test data. As very little test data is available for the type of compressor under investigation here, an empirical approach is considered unsuitable. Analytical models are based on pressure-volume diagrams developed from simple analytical curves, e.g., polytropic curves, or test data. Since ammonia-water is a zeotropic mixture with intricate thermophysical properties using an analytical approach may involve uncertainties and challenges. However, employing analytical curves to a certain extent can be an effective means to simplify complex thermodynamic problems. In the two-phase compression model discussed below, polytropic relations are employed to simplify calculations regarding compression work. In cases where test data and/or analytical relations are not sufficient, numerical models must be developed. Numerical screw compressor models can be either quasi-one-dimensional or three-dimensional, depending on its field of application. Quasi-one-dimensional models are based on mass and energy conservation equations applied to a relatively small number of chambers. In three-dimensional models on the other hand, the compressor is divided into countless finite-sized elements and conservation of momentum is applied in addition to conservation of mass and energy. Three-dimensional modelling, more commonly known as CFD analysis, involves heavy calculations and time-consuming developing procedures. For the model under development here it is desirable to be able to investigate multiple compressor configurations, e.g., injection port locations, in an efficient manner, and three-dimensional modelling is thus considered to be unsuitable. The focus is set on quasi-one-dimensional numerical models.

Zaytsev (2003) developed a numerical wet screw compressor model. He defined the control volume as the volume of one rotor cavity, and established equations for conservation of mass and energy within each control volume. Equations for both homogeneous and heterogeneous conditions were developed, but only the homogeneous model was implemented due to lack of sub-models for mass and heat transfer required in the heterogeneous model. Infante Ferreira et al. (2006) further developed the homogenous model and utilized it in theoretical investigations on the ideal injection port location. Zaytsev's equations are exclusively fitted for step-by-step calculation of changes in pressure and temperature of the ammonia-water mixture throughout the compression process, and thus the equations are rather complex and challenging to interpret. This makes the model hard to modify or further develop and unsuited for implementation into bigger system models. Chamoun et al. (2013) presented a different numerical approach to screw compressor modelling. Their model was developed and solved using the Modelica language [Modelica Association] and Dymola [Dassault Systemes, France]. Compared to Zaytsev, the approach developed by Chamoun et al. offers less complexity and higher flexibility with respect to implementation into bigger system models. However, the model is based on compression of pure water, and the liquid injection port is rigidly placed at the suction end. The Modelica model structure is considered to be a good starting point, but substantial adaptations must be made to the model in order to utilize it for investigations on ammonia-water screw compressors with optional injection port locations.

#### 4. MODELLING APPROACH OF A LIQUID-INJECTED SCREW COMPRESSOR

A screw compressor simulation model is developed using the Modelica language, based on knowledge obtained from existing compressor models in the literature. The model takes into account the effect of leakage flows, heat losses and liquid injection, and it can be used for both steady-state and transient analysis of such phenomena. The model is aimed at efficient investigations on different compressor arrangements and operating conditions, as well as effortless implementation into bigger system models.

It is a quasi-one-dimensional numerical model with multiple control volumes, where each control volume is defined as the volume of one rotor cavity. Basic equations for conservation of mass and energy is applied to each control volume. The thermodynamic properties of ammonia-water are continuously calculated through utilization of the TILMedia library [TLK-Thermo GmbH, Germany] in Modelica, under the assumption that conditions within each control volume are homogeneous.



**Figure 2: Schematic showing the mass and energy flows associated with each control volume**

The size of the control volumes varies with time based on the rotational speed and the geometrical properties of the compressor. The volume increases when a control volume is in the suction phase, while it decreases during the compression and discharge phases. The volume variation is identical for all the control volumes, but there is a time delay between each one, e.g., control volume  $j$  can undergo a volume decrease simultaneously as control volume  $j-1$  undergoes a volume increase. This results in different pressure, temperature, mass and internal energy in each control volume at each point in time. The flow of mass and energy due to leakage gaps in the compressor is taken into account by interconnecting the control volumes as illustrated in Figure 2. Leakage mass flow rates are calculated from

$$\dot{m} = A_{eff} \sqrt{2\rho\Delta p} \quad \text{Eq. (1)}$$

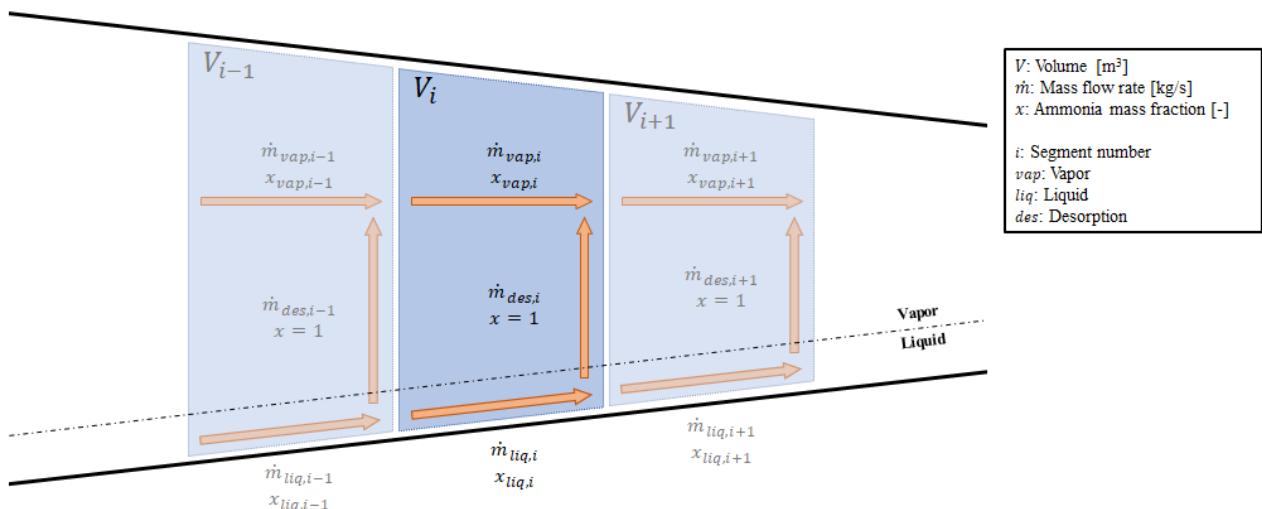
where  $A_{eff}$  is the effective flow area of the leakage gap,  $\rho$  is the density of the working fluid upstream of the flow, and  $\Delta p$  is the pressure difference across the gap. Mass flow rates related to suction, injection and discharge are also calculated using Equation 1. For instance, in calculations of suction mass flow rates  $A_{eff}$  represents the effective flow area of the suction port,  $\rho$  represents the density of the fluid in the suction line, and  $\Delta p$  represent the pressure difference between the suction line and the control volume. Here  $A_{eff}$  varies with time as the control volume goes through the suction phase, while it is set to zero during the compression and discharge phases.

The model is implemented and solved using the Dymola modelling environment. Compared to screw compressor models found in the literature the developed model has low complexity, making it easier to interpret and to modify in accordance with special analysis requirements. Regardless of the relatively low complexity the model can be used to produce detailed data for numerous compressor configurations without the need of experimental data.

## Two-Phase Compression Model

The previous described Modelica model can give detailed insight into the process that takes place within a screw compressor during operation. However, the model has some analysis limitations. In each compression chamber the working fluid is treated as a single unit with homogeneous properties. This forces certain constraints on the state of the fluid, e.g., liquid and superheated vapor cannot be present simultaneously in one chamber. In reality, a thin film of liquid can be present along the inner surface of a compression chamber even though the vapor inside the chamber is in a superheated state. As a matter of fact, a portion of the working fluid always being in a liquid state is essential for safe and efficient operation of oil-free screw compressors. In addition, TILMedia library used for ammonia-water property calculations in the Modelica model is based on a vapor-liquid equilibrium assumption. With this modelling approach it is not possible to investigate the potential consequences of non-equilibrium during high-speed operation.

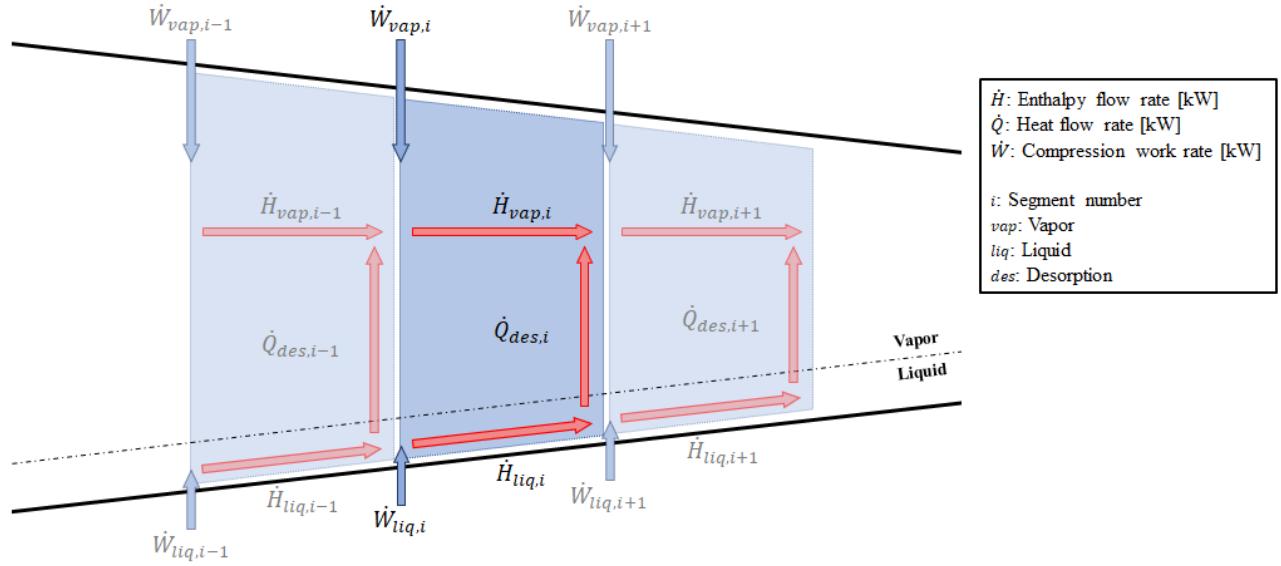
To compensate for any inaccuracies the Modelica model may have, a secondary calculation model is developed using the Engineering Equation Solver (EES) [F-Chart Software, USA]. This model is to be used for detailed thermodynamic analysis of the two-phase process that takes place during the compression phase. Contrary to the Modelica model, the EES model disregards the suction and discharge phases. Polytropic relations are employed to simplify calculations regarding compression work. The aim is to get a better understanding of the intercorrelation between liquid and vapor during two-phase compression, and thereby being able to carry out comprehensive investigations on the impact of liquid injection. Figures 3 and 4 illustrate the schematic representation of the mass and energy flows associated with each segment.



**Figure 3: Schematic representation of the mass flows associated with each segment**

The total volume of the compressor is divided into a variable definable number of segments. Mass and energy flows, as shown in the Figures 3 and 4, flow through the individual segments with their respective pressure, temperature and ammonia mass fraction for the gas and liquid phase. This is a different approach compared to the Modelica model, where the mass and energy flows are kept within the changing control volumes. The liquid injection is performed in single segments, which can be variably selected and varied. During evaporation of the liquid with heat extraction of the superheated vapor caused by the compression process, it is expected that ammonia desorption ( $x=1$ ) from the liquid will occur due to the thermodynamic properties of the ammonia-water mixture. Generated backflows as well as temperature-related condensation and/or absorption processes are

considered and represented with negative sign (contrary to the arrows shown). For the investigation of potential consequences, a non-equilibrium factor between vapor and liquid phase is implemented for each segment.



**Figure 4: Schematic representation of the energy flows associated with each segment**

The implemented functions in the two-phase compression model thus enable the detailed thermodynamic analysis originally described and provide a supporting approach to the Modelica model.

## 5. CONCLUSIONS

Within the scope of this study, a modelling approach for a liquid-injected ammonia-water screw compressor was developed, to be utilized in a CACHP system at high-temperature operation. At the beginning, the general functionality and advantages of the CACHP system were presented, followed by a discussion of the characteristics and requirements for the compressor to be used. Subsequently, the objectives for the development of the modelling approach were specified and, based on this, existing models in the literature were identified and examined with regard to their usability in a CACHP system. Based on this, a modelling approach for liquid-injected ammonia-water screw compressors was developed.

The developed screw compressor model was implemented and solved using the Modelica language with the modelling environment Dymola. The model takes into account the effect of leakage flows, heat losses and liquid injection, and it can be used for both steady-state and transient analysis of such phenomena. Compared to other screw compressor models in the literature, the developed model has a low complexity, which makes it easier to interpret and modify in accordance with the specific analysis requirements. Despite the relatively low complexity, the model can be used to generate detailed data for numerous compressor configurations without the need of experimental test data. An additional calculation model was developed to compensate for any inaccuracies the Modelica model may have. This model is intended to be used for a detailed thermodynamic analysis of the two-phase compression process and provides the possibility to vary the injection ports as well as the equilibrium factor to represent the vapor-liquid phase in non-equilibrium.

As defined in the requirements, the developed modelling approach aims at efficient investigations of different compressor arrangements and operating conditions as well as at an easy implementation into larger system models. In the further course of the project the model will be extensively tested, evaluated and verified. Subsequently, the simulation results will support the planning and preparation of different compressor arrangements as well as the experimental evaluation.

## ACKNOWLEDGEMENTS

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