Numerical Simulation of Ammonia-Water Solution Based Heat Absorber

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Abstract: This article provides an insight into the numerical simulation of an ammonia-water solution-based plate heat absorber, which is a crucial part of an absorption chiller. These chillers could be used as part of a stratified chilled-water storage tank configuration for coupling to a small modular reactor. The common approach utilized in the process of designing the chiller is to call the absorber a "black box" without considering the processes inside. It follows that the resulting design must be highly oversized to ensure reliable operation of the system. This article focuses on the obstacles that needs to be overcome in order to simulate the processes inside the absorber, such as stream breakup into separate droplets or absorption of ammonia. Unfortunately, we do not have any experimental data we could use to validate our simulations and thus this article should be looked at as a "proof of concept" and a possible guideline for simulations of similar phenomenon.

Keywords: Absorption, chiller, CFD simulation, fluid flow, ammonia-water solution

1. Introduction

According to the Mittermaier and Ziegler [2], global performance of an absorption chiller is highly influenced by low efficiency of the heat and mass transfer process in the absorber. It follows that the absorber can be considered as one of the most critical components of the absorption chiller and thus further research aimed at increasing the efficiency of the absorber is considered as highly desired [3].

This paper focuses on 3D simulations of the processes occurring inside the absorber, which allows for studying the local phenomena occurring inside and cannot be obtained by experimental or global research [4]. Firstly, we focus on simulations of the inlet region (see Figure 1), in which a break-up of water stream into separate droplets occurs. The distribution of these droplets at the inlet to the middle part of an absorber influences the process of ammonia diffusion and thus the efficiency of the device. Homogenous distribution and smaller size of droplets, i.e. large mass-transfer area, are the main criteria for evaluation of the design of an inlet region. Secondly, the middle part of an absorber is simulated. Given the fact that separate water droplets distributed in gaseous ammonia are entering this region, the interfacial area between these phases is significantly larger in this part of an absorber compared to any other and thus the absorption process must be simulated in this region. Finally, the rich solution is accumulated in the outlet region. This part of an absorber has not been simulated so far and thus is not presented in this article.

2. Description of Absorber

Conceptually, an absorber consists of a series of parallel plates that are placed

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one above the other to allow the formation of a series of channels for fluid flow between them. It follows that the design of an absorber resembles the design of a plate heat exchanger in which the hot fluid is assumed to be ammonia-water solution and the cold one, i.e. the coolant, is supposed to be water. However, there is significant difference in the design of an inlet area belonging to the channels in which an absorption occurs because there are two different phases entering these channels that needs to be mixed.
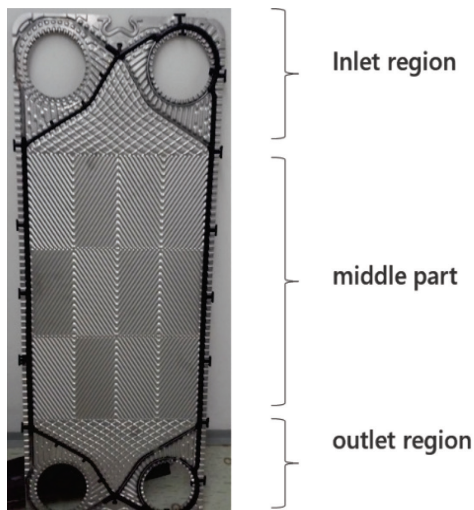

Figure 1: Absorber regions.

The vaporous ammonia is brought together with the ammonia-poor aqueous solution and it results in dissolution of ammonia into the poor solution. The aqueous solution increases its ammonia concentration and during this process, heat is released. With the increasing temperature of the solution, the capability of ammonia to dissolve decreases significantly and therefore it is needed to remove the heat and maintain low temperature of the aqueous solution.

Albeit it might segue from the current discourse it would not be altogether irrelevant to adduce here the fact that the dissolution of ammonia represents the main advantage of absorption chillers over the conventional reciprocating ones. The pressure of incompressible rich-ammonia solution is increased with the use of a pump and thus the power requirements for such process are only a fraction of those for a comparable compressor needed to increase the pressure in conventional chillers.

3. Inlet region

3.1. Description of inlet region geometry

As previously mentioned, the inlet area (depicted in Figure 2) is considered as an area where both the gaseous ammonia and ammonia-poor aqueous solution (water) enters channels of the absorber. The aqueous solution flows in the inner pipe and through several small connecting circular channels (channels A) enters the outer space filled with gaseous ammonia. These channels create several continuous aqueous jets that break up once they hit walls. Arising droplets and gaseous ammonia then move together through the bigger hexagonal channels B towards the body of the exchanger where the dissolution of ammonia occurs.
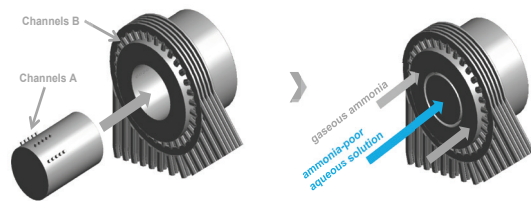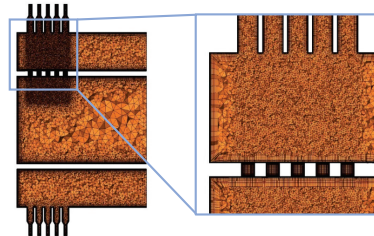

Figure 2: Inlet area with highlighted channels.

Figure 3: Detail of computational mesh.

3.2. Computational mesh of inlet region

To simulate the fluid flow in the inlet region, ANSYS CFX was used mainly due to our previous experience with this particular software. The computational mesh (see Figure 3) was unstructured, conformal and composed of tetrahedrons. Regarding the sizing of the elements, the smallest elements (with the size of approx. d/20, where d is the diameter of channels A) were in the region in which stream break-up was expected. It is worth mentioning that the size of the largest elements does not exceed 2d, where d is the diameter of channels A. The inflation layer was modelled using 15 layers and the global value of Y+ parameter was significantly lower than 1. The total number of elements in the computational mesh reaches 28 mil.

3.3. Simulation setup of simulation of inlet region

Concerning the simulation setup, the SST k-ω turbulence model was used for the multiphase flow simulation. Bear in mind that no mass transfer between the phases is modeled in this region. Gaseous ammonia inflows through the annular inlet at a rate of 0.05181 kg/s. Liquid water ammonia solution inflows through the inner pipe inlet at a rate of 1.3976 kg/s. At the outlet, an absolute pressure of 2.62 bar was defined. Surface tension of 0.0722 N/m and wall contact angle of 72° were used. Last but not least, gravity of 9.81 m s^{-2} was applied and all walls were assumed as hydraulically smooth with no slip boundary condition applied.

At first, we intended to run a steady-state simulation so that the results at the outlet of the inlet region could be applied as an inlet boundary condition for the middle region. This would allow us to divide the simulation of entire absorber into several parts, saving the time for debugging and furthermore would allow to decrease computational demands. Unfortunately, the first few simulations proved that the stream break-up and resulting multiphase fluid flow inside the inlet region is highly time-dependent and thus we were unable to achieve a reasonable convergence for steady-state simulation. It follows that all presented simulations are transient and even though they are presented as separate simulations, in the end it is intended to combine all of them in order to simulate the entire absorber channel.

3.4. Results of fluid flow in inlet region

In Figure 4, there are depicted contours of volume fraction for the simulated inlet region in selected time. Red color denotes 100% of liquid water, whereas blue color means 100% of gaseous ammonia. It can be observed that selected computational model does not allow for precise simulation of interface between gas and liquid phase and thus the size of droplets cannot be evaluated with the current setup. Nevertheless, the results give us the distribution of both phases in each of the channels connecting the middle region. To achieve a homogeneous distribution over the channel outlets is one of the important criteria for evaluation of the inlet region design. No particular conclusions are discussed in this article as that would be beyond the intention of this article. Out of curiosity, the simulation on a regular PC with 32 cores and 512 GB of RAM took around 2 days.
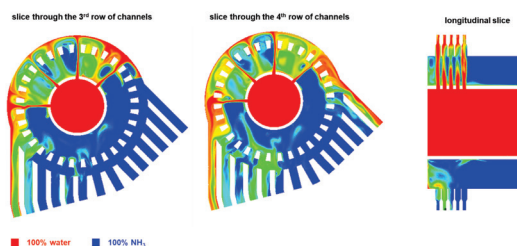

Figure 4: Results of simulation of inlet region.

4. Middle region

4.1. Description of middle region geometry and mesh

The computational domain of our middle region represents the volume between two corrugated plates of the absorber. In order to speed up the simulations, it was decided to use only a part of the middle region, as can be seen in Figure 6. Please bear in mind that publishing of the plates dimensions is forbidden due to signed non-disclosure agreement.

Concerning the computational mesh, a polyhedral mesh with approx. 26 mil. cells was prepared. The size of the elements is approx. t/5, where t is the smallest gap between two corrugated plates.
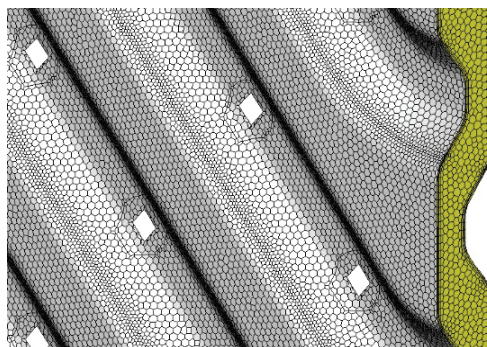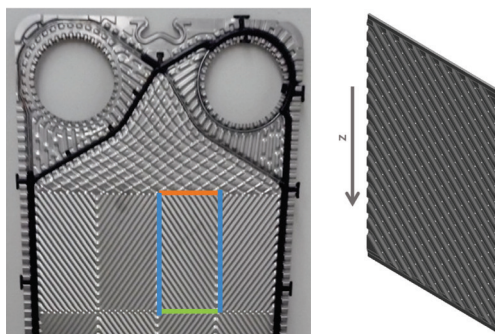

Figure 5: Computational mesh of middle section.

Figure 6: Geometry of middle section.

4.2. Theory of absorption process

The theoretical description of ammonia absorption into the liquid water is well known and widely described in various sources, for instance [5] or [6]. In short, the absorption is considered to be a two-stage process which starts by dissolving of gaseous ammonia into liquid water. Then, in the second stage, the chemical reaction in liquid phase between ammonia and water follows, namely the ionization:

$$NH_3 + H_2O = NH^{4+} + OH^-$$
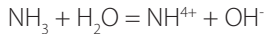
From the aforementioned follows that there are also two approaches for modeling the absorption phenomenon. The first one takes only the dissolution into account, meaning that at the outlet of the computational domain, there will be two separate species (ammonia and water) and both will be in liquid state. To simulate this first stage of absorption process, an equilibrium must be defined for example by Henry Law, Raoult's law or with a real measured equilibrium curve. To simulate the second phase, it is necessary to define the reaction rate, for example with the use of Arrhenius equation. It should be also pointed out, that in this case, there will be a mixture of water and ammonia (ammonium hydroxide) at the outlet of the computational domain.

The drawbacks of absorption simulation lie mainly in the variety of methods how to proceed with the simulation. Real equilibrium line is not always known and thus an approximation is applied which in this case can significantly decreases the accuracy of the simulation, for example Henry's law is a linear function, whereas real equilibrium line is not linear. Then, to use the Arrhenius equation for reaction rate, one must know activation energy and pre-exponential factor. Furthermore, properties such as diffusivity, viscosity, thermal conductivity etc. for the species and the resulting mixture are necessary in order to model the absorption. Here lies another problem, since it is very difficult to obtain these data (for example REFPROP does not provide diffusivity or thermal conductivity of ammonium hydroxide).

4.3. Simulation setup of absorption process

For this transient simulation, ANSYS Fluent was chosen over the CFX in previous simulations, mainly because of its various advanced options for multiphase flow modeling. In the following simulation, the absorption process was simulated only by its first stage, meaning the ionization is not accounted for and thus there will be two separate species at the outlet.

For the simulation of the mixture flow, the *Eulerian – Eulerian* model was used, which should provide reasonable results in cases where phases interaction must be accounted for [7]. Moreover, the implicit *Multi-Fluid VOF model* for *Eulerian-Eulerian model* was used, the interface between phases was modeled as a sharp one and the turbulence was modeled with widely used *SST k-ω* turbulence model.

Table 1: Boundary conditions for absorption simulation.

Inlet		
Materials	*Parameters*	*Value*
Mixture	Initial Gauge Pressure	0 Pa (reference value 1 atm)
Vapor	Mass flow rate Total temperature Species Mass Fractions H_2O	0.0026 kg/s 294.65 K 0.003
Liquid	Mass flow rate Total temperature Species Mass Fractions H_2O	0.0699 kg/s 312.65 K 0.634
Outlet		
Materials	*Parameters*	*Value*
Mixture	Initial Gauge Pressure	0 Pa (reference value 1 atm)
Vapor	Total temperature Species Mass Fractions H_2O	294.65 K 0.003
Liquid	Total temperature Species Mass Fractions H_2O	312.65 K 0.63

Two mixtures were created for simulation of gas-liquid flow - gas and liquid mixture. The former represents the gaseous ammonia and water vapor, whereas the latter denotes the ammonia and water liquid. The gas mixture was chosen as the main phase.

Heat transfer between the phases was simulated using the heat transfer coefficient modeled with a dimensionless Nusselt Number of value 3.8. To simulate mass transfer between phases, an equilibrium was defined with Henry's Law and Van't Hoff correlation (reference Henry's constant = 0.0169; temperature dependence = 4200).

It is worth mentioning that ANSYS uses REFPROP data for refrigerant properties which database does not have any standard enthalpy for liquid ammonia, therefore this value must be added manually. Furthermore, the default molar mass of liquid ammonia must be changed to 17 g/mol, since the molar mass from REFROP database is 28 g/mol which is incorrect. Surprisingly, molar mass for vapor ammonia is correct in REFPROP database with value of 17 g/mol.

4.4. Results of absorption simulation

In Figure 7 there are depicted volume and mass fraction contours of the simulation results in selected time. The volume fraction contours show the distribution of liquid mixture (liquid ammonia and liquid water) and gas mixture (gaseous ammonia and water vapor). It can be seen that in the lower part of the domain, the volume of liquid mixture is increasing, meaning the gaseous ammonia is dissolving into the liquid poor solution. This absorption process can be more clearly seen when taking a look at the mass fraction contours of liquid NH3.
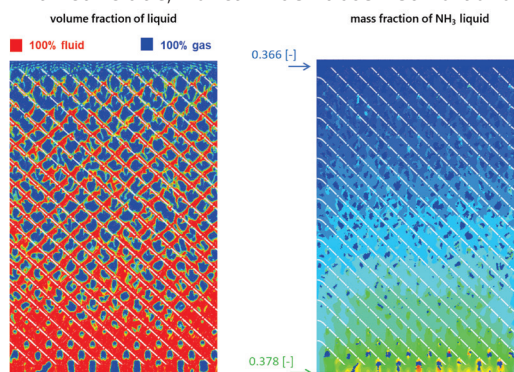
To conclude, it can be observed that the

Figure 7: Results of absorption simulation.

simulation of absorption process works as expected, the simulation converged very well but unfortunately, we do not possess any relevant experimental data that could validate our results. Out of curiosity, the simulation for this small part of middle region took more or less one day on a regular PC with 32 cores and 512 GB of RAM.

5. Conclusion

The aim of this article was to provide an overview of the simulation of an ammonia-water solution-based heat absorber. The CFD simulations should help to optimize the design of this crucial part of an absorption chiller and thus avoid the need for oversizing the absorber. In the article, we discussed simulations of the inlet region and middle part of an absorber, we outlined the difficulties in performing these simulations and we briefly discussed the results. The main drawback of our simulations clearly lies in the fact that we do not possess any experimental data for validation of the results.

This work was done as part of a larger European project for the German producers of absorption chillers AGO AG, and thus evaluating practical usability of these CFD simulations is necessary. From this point of view, it is fair to admit that the computational time (remember 2 days for inlet region, 1 day for section of middle part) for the absorber would surely exceed reasonable value. It follows that for our future research activity, we aim to focus on further simplifications of the problem, mainly switching to 1D dimension and using 3D simulations only for analysis of selected regions in the absorber, instead of focusing on 3D simulations of the entire absorber.

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