

Abstract

This paper aims at assessing the importance of sorption processes in space applications and the necessity of intelligent control systems for sorption processes.

Thermal control and life support systems use extensively sorption processes, taking advantage of their intrinsic stability, their lack of vibrations and their regenerability. ESA's Darwin and Herschel missions' use of sorption cryocoolers is presented. Several life support subsystems employed on ISS are reviewed.

A ground based adsorption chiller developed at Shanghai Jiao Tong University is described along with its nonlinear mathematical model. Based on this, a control system that will provide intelligent switching between the different operation phases of the chiller is designed. A Java software model of the chiller is used as an internal state estimator and as a source of information for a fuzzy inference module.

Key words: *sorption, adsorption, thermal control, life support system, adsorption chiller, control system*

Sorption Processes in Space and Control System for Sorption Process

Ing. Pandele, Constantin Alexandru
email: alexandru.pandele@gmail.com

Supervisors

Ing. Hromcik, Martin, Ph.D,
Czech Technical University in Prague,
Department of Electrical Engineering

Ing. Harlin, Gösta,
Luleå University of Technology:

Prof. Wang, Ruzhu,
Shanghai Jiao Tong University,
Institute of Refrigeration and Cryogenics

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Chapter 1

Review of Sorption Processes in Space

1.1 Sorption - *ab initio*

When we two parted
In silence and tears,
Half broken-hearted
To sever for years,
Pale grew thy cheek and cold,
Colder thy kiss

Lord Byron

Nowadays, it is not unusual to find small sachets of white granules marked "DO NOT EAT!" in shoe boxes or even in food or medicine packages. If one neglects the friendly advice, will most probably experience a dry nose and throat, some coughing and wheezing[1] and a first hand experience of sorption.

The small sachets contain silica gel¹, a substance which has the property of removing moisture from its environment. Even though it was known since XVII-th century, silica gel was merely a scientific curiosity until the XX-th century, when an American chemistry professor patented and used it for the first time in industry as a filter in gas mask canisters[2]. Silica gel is just one example of a sorbent, a solid or liquid substrate onto or into which a substance is sorbed. Sorption is a general term describing either or both of the phenomena of adsorption and absorption. As such it involves the diffusion of liquids or gases into materials of a different state and the adherence to the surface of another molecule. Sorption is usually a reversible process and the reverse process is called desorption.

The main difference between adsorption and absorption resides not in phonetics but in the final location of the sorbed substance. In the case of adsorption, this is the surface of the sorbent (much like magnet attracting iron dust). If we are talking about absorption, the sorbed substance would diffuse in the volume of the sorbent, like water in a sponge.

¹sometimes a mixture of silica gel with more toxic substances

1.1.1 Adsorption

The industrial history of adsorption begins around 3750 BC, when Egyptians and Sumerians use charcoal for reduction of copper, tin and zinc ores for bronze manufacturing. 2000 years later, charcoal is used in medicine to adsorb odorous vapors from putrefactive wounds. Hippocrates and Pliny also recommend it for the treatment of different affections. Adsorption enters the classical era with the experiments of Scheele and Fontana involving different porous materials. Beginning of the XX-th century, adsorption finds its applications in gas masks manufacturing. Nowadays, adsorption research receives a new boost with its use in ecological refrigeration.[3]

These utilizations take advantage of two main properties for adsorption. First, adsorption involves the separation of a substance from one phase accompanied by its accumulation or concentration at the surface of another. Along with a very good energy efficiency, this makes it a good alternative to distillation for performing separation and purification.

Secondly, adsorption is an exothermic process. The molecules that adhere to the surface of the adsorbent release their energy as heat. The amount of heat released by adsorption is 30% - 100% higher than the condensation heat of the same adsorbate. Since, in general, adsorption is stronger than condensation, an adsorbate in liquid form will migrate as vapor to the solid adsorbent in a closed vessel. The liquid will cool down, while the adsorbent will heat up. This allows for the development of refrigeration cycles using heat sources[4].

There are two types of adsorption. When the result of the process is the formation of a new chemical compound, the process is termed chemical adsorption or chemisorption. Physisorption, or physical adsorption occurs when Van der Waals forces bind the adsorbed molecule to the adsorbent surface. Chemical adsorption binding forces are greater than the ones active in physisorption and, thus, it releases more heat. Nonetheless, physical adsorption is preferred for refrigeration cycles since it is easily reversible[4].

Theoretical development

Even though the history of industrial adsorption starts 6000 years ago, its theoretical study is relatively recent. At the end of the XIX-th century, Freundlich and Küster published the first mathematical fit of an adsorption isotherm. It was a purely empirical formula and the "empirical" attribute of adsorption models didn't disappear until now. It was tempered down with a "pseudo-" prefix, most notably by Irving Langmuir and, later, by Stephan Brunauer, Paul Emmett and Edward Teller.

Langmuir assumed that the adsorption site is energetically homogeneous and that only one layer of adsorbate will form on the adsorbent surface. The monolayer theory of Langmuir was generalized by Brunauer, Emmett and Teller. They developed the BET equation, describing adsorption as occurring in a multi-monolayer pattern. Dubinin and Radushkevich contributed the adsorption research with the theory of the volume filling of micropores (TVFM), a theory that explains the mechanism of adsorption on adsorbents with narrow pores proportional to the sizes of adsorbed molecules[3].



Figure 1.1: Silica gel *DO NOT EAT!* sachet (www.hama.de)

1.1.2 Absorption

Absorption is present in human history starting with the first rain after the foremost sparks of rationality and consciousness. It was then that humans discovered one of the first physical laws: a body in contact with water gets wet. Even if the first experience of absorption was very close to a nuisance, humans tamed it and employed it for the sake of hygiene and art.

Much later, at the beginning of the XXth century, absorption started to be used in refrigeration processes[5]. Due to the low efficiency, vapor absorption refrigeration cycles were abandoned in favor of the vapor compression cycles. Nonetheless, absorption refrigeration cycles are still used for recovering waste heat.

1.2 Thermal control sorption systems

As stated in the previous section, one of the uses of sorption is in thermal processes. As such, it found a multitude of applications in space industry. There are a few characteristics of sorption that make it particularly praised as an alternative to spacecrafts' and space instruments' thermal control. First, it involves almost no moving parts. That makes one worry less for the spacecraft attitude control since it doesn't apply (almost any) momentum. Second, sorption cycles are most of the times reversible. That gives a better usage of volume and mass, since these will not vary during the mission. Third, sorption cycles are controllable and intrinsically stable, allowing an active and safe thermal control.

Sorption coolers started to be considered as spacecraft thermal control options in the 1980s. They were using helium as refrigerant and charcoal as sorption bed or hydride chemisorption[6]. Lately, they became more and more popular as cooling solutions close to absolute zero.



Figure 1.2: JPL 20 K charcoal –hydrogen sorption compressor of 1983[6]

1.2.1 Darwin

ESA's Darwin mission will use a combination of 6 free-flying 1.5 m telescopes to search for terrestrial planets orbiting other stars. The mission requires for the optical paths between the central hub and the six telescopes to be controlled and stabilized to less than 10 nm. Such precision asks for a zero-vibration of the optical instruments. Under these requirements, a vibration free sorption cooler was considered as a cryocooler of the optical equipment. 6 configurations were taken into account[7]. The chosen configuration is presented in fig. 1.3, a. It includes two small adsorption stages, both using activated carbon as adsorbent. The first stage uses hydrogen as adsorbate to precool the helium used as the adsorbate of the second stage. Since adsorption cooling is a sequential process, to provide continuous cooling it is necessary to have multiple adsorption processes out of phase. The hydrogen stage has 4, while the helium stage has 12 such processes. For that, the adsorption beds are separated in isolated cells, all connected by a valve check system to the cold stage (fig. 1.3, b). The refrigeration loop starts

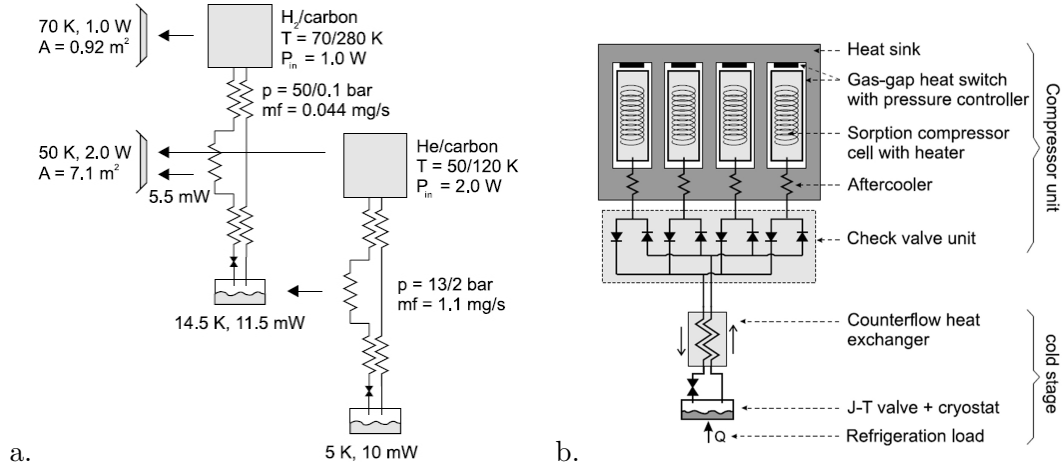


Figure 1.3: a. Chosen configuration of ESA's Darwin mission optical instruments cryocooler [7]; b. schematic of a sorption compressor with a Joule-Thomson cold stage[8]

by applying a thermal load on the cold stage of the cooler. This generates vapor which travels through pipes to a cell in the adsorption phase. After the adsorption process is done, heat is applied on the cell. This increases the pressure in the cell and a controlled, high pressure gas flow is released. Before reaching the cold stage, the gas is precooled by the external radiator[8].

The total power used by this configuration is 7.9W, total area of radiators is 18.6m² and the total mass is 83kg. The system can easily be made redundant since the active parts (i.e. without radiators) are very small and weight less than 4kg. Moreover, using out of phase working cells includes a intrinsic redundancy quality into the system. The control inputs of the system are the heat applied to the cells during desorption and the opening/closing of valves. The control is time based, with 10 minute duration cycles. The system can provide 10mW of refrigeration power at 4.5K[7].

1.2.2 Herschel

Herschel mission is scheduled to be launched in late 2008, becoming the largest (3.5m) infrared space observatory. It will be placed in the second Lagrange point of the Sun-Earth system. Three scientific instruments are going to be aboard the spacecraft: HIFI

— Heterodyne Instrument for the Far Infrared, PACS — Photodetector Array Camera and Spectrometer, and SPIRE — Spectral and Photometric Imaging Receiver[9].



Figure 1.4: ESA's Herschel spacecraft [9]

Both PACS and SPIRE instruments will require sub-Kelvin temperatures for observing previously unexplored wavelengths. Due to the nature of their observations, they also require a vibration-free environment. Two helium sorption coolers developed at the Service des Basses Températures of the Commissariat à l'Energie Atomique (CEA-SBT) will provide the required 300 mK operation environment for both SPIRE and PACS. Both coolers are identical except the mechanical interfaces with the instruments. Nonetheless, they were designed to be interchangeable, reducing the development risks[10].

The Herschel sorption coolers use only an adsorption cycle with helium (He^3) and activated carbon. They comprise an adsorption pump containing the activated carbon, a pumping line, an evaporator holding a porous material (an alumina sponge required to confine the liquid in the evaporator by capillary attraction, in the absence of gravitation) and two heat switches. The two heat switches use the fact that the presence or the absence of a gas between two thermal conductors allows or blocks the heat transfer between the two conductors. The gas handling is achieved with miniature cryogenic adsorption pumps[10].

The sorption cooler cycle involves basically two main phases (fig. 1.5): condensation and low temperature, with an intermediary cooling phase. During condensation, a small amount of heat is applied on the sorption pump, making it release the adsorbed helium. The helium is precooled by the heat sink shunt and condenses into the evaporator. In this phase the evaporator is connected to the heat sink (the heat switch is ON). For the second phase, the sorption pump is connected to the heat sink (heat switch ON), while the evaporator is isolated (heat switch OFF). The helium from the evaporator is adsorbed in the activated carbon, providing the necessary cooling for the instrument's

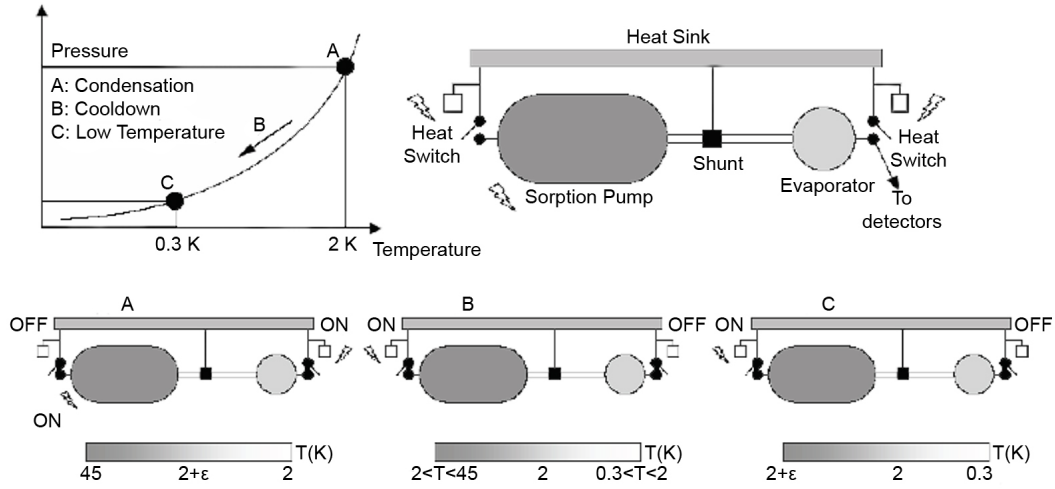


Figure 1.5: Schematic of the Herschel adsorption cooler

detector. The specifications of the coolers give at least 46 hours of $10\mu W$ heat lift at $0.29K$. Since a single adsorption cycle is present, the cooling is not continuous. The condensation and cooling phase can be seen as a recycling phase and, according to specifications, should be less than 2 hours. The volume is $2300cm^3$ and the mass is less than $1.8kg$ (fig. 1.6)[10].

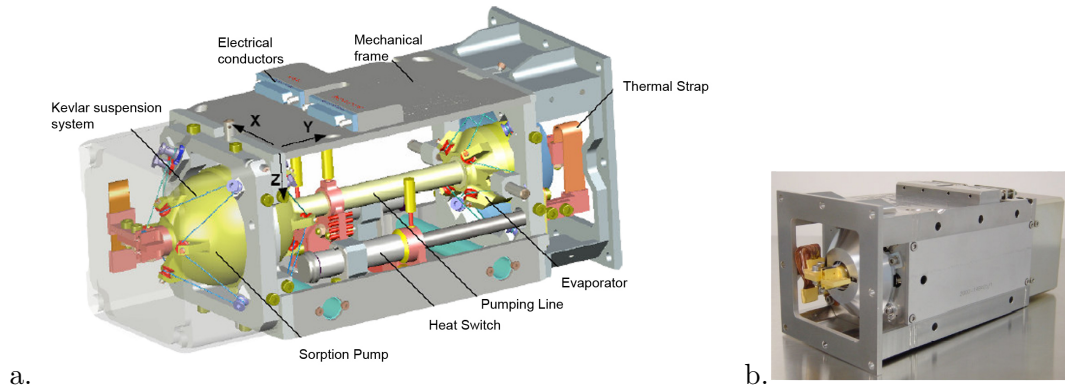


Figure 1.6: a. Overall 3D view of the Herschel cooler [10]; b. SPIRE flight model cooler[10]

1.3 Life support sorption systems

A spacecraft life support system (LSS) is a complex of chemical and physical systems that allows human presence in space. Oxygen, thermal comfort and water can be supplied in an open loop, but a key concept of a long duration mission (space stations, interplanetary flight, Moon or Mars bases) LSS is *recycling*. It includes subsystems for air revitalisation, thermal control and water recovery. LSS is *recycling*. It includes subsystems for air revitalisation, thermal control and water recovery.

An adult requires about $1kg$ of oxygen, $8.5kg$ of water for drinking and hygiene and

0.6kg of dry food[11]. That gives about 10kg of daily consumables. Each kilogram delivered on a low Earth orbit (LEO) costs an average 4240 \$[12]. The daily costs for an astronaut on a LEO orbit would add up to 42400 \$, that doesn't include the storage costs. It would be thus difficult and extremely costly to provide water or air in a non-recyclable way, and it would also be against one of the first lessons Mother Nature teaches us.

Regenerative life support systems started to be tested in USSR in 1960's. Salut-4 was the first space station provided with a water recovery system from humidity condensate (WRS-C). In 1987 Mir was fitted with an improved version of WRS-C and with a carbon dioxide removal system. A water recovery from urine system (WRS-U) was installed on Mir in 1990. The experience accumulated with Mir was employed for the International Space Station life support system (ISS). Many of ISS' LSS present components have been previously thoroughly tested in the Russian space station. Nowadays, closed loop solutions are designed and tested for the ISS and for future missions to Mars or on Moon[11].

Spacecraft life support systems extensively employ sorption processes in most of its subsystems[11, 13, 14, 15]. A simplified schematic of the current ISS water and air loop is presented in fig. 1.7. This shows how several parallel processes that are responsible for cabin atmosphere quality control and water recovery include sorption stages.

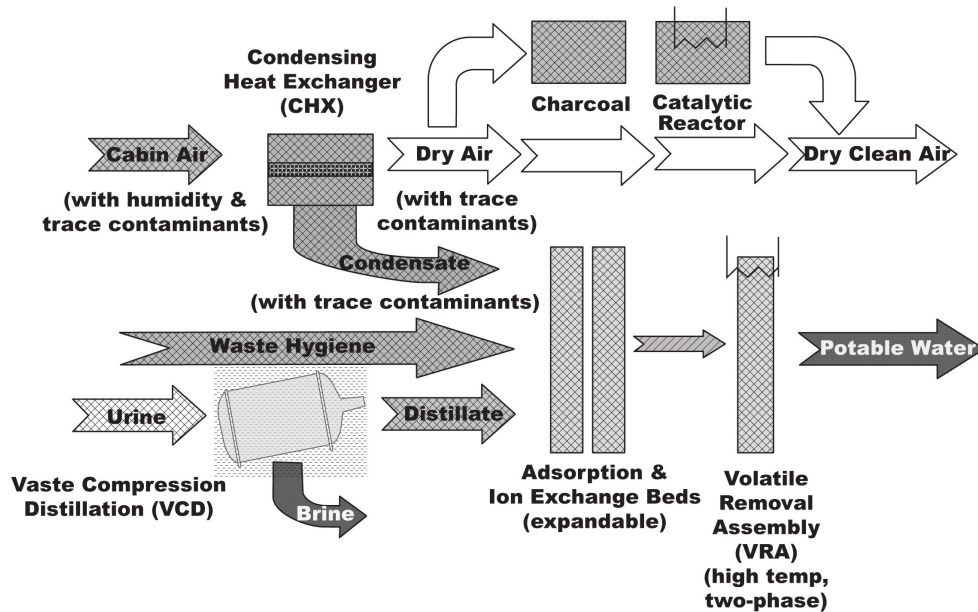


Figure 1.7: ISS air quality control and water recovery architecture[15]

Air revitalisation (AR) systems provide the basic purification and replenishment functions required to maintain breathing quality air within the space settlements[16]. For that they produce oxygen and nitrogen, and remove carbon dioxide and trace organics. Thermal control (TC) systems are sometimes seen as integrant part of the AR[14] and are responsible for temperature and humidity control.

Carbon dioxide can be removed from the cabin air using different types of sorption processes. Zeolites can be used as a selective adsorbent for CO_2 . However, water vapor is preferentially adsorbed by zeolites and it has to be removed before the air reaches the

sorption bed. The zeolite sorption beds can be easily regenerated by applying heat or vacuum or a combination of both. The resulting CO_2 has a high purity and can be used in CO_2 reduction processes for oxygen recovery[14].

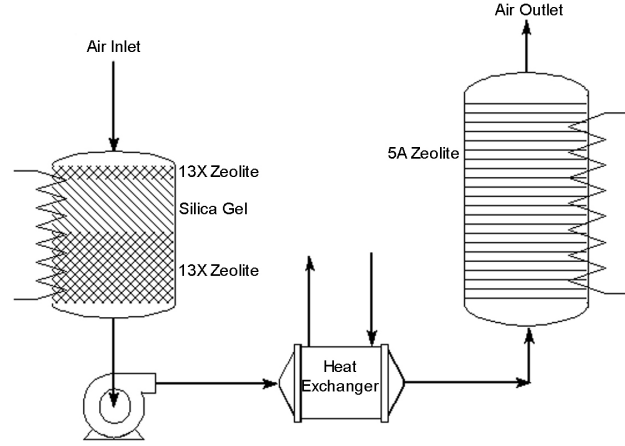


Figure 1.8: ISS CDRA basic scheme [16]

The US module of the International Space Station has a carbon dioxide removal assembly (CDRA) based on this technology (fig. 1.8)[17]. It includes four sorption beds: two for water removal and two for CO_2 removal. First the air is pumped through a dessicant bed of zeolites and silica gel and then released through a zeolite sorption bed. When one dessicant bed and one CO_2 bed are in sorption, the other two are in desorption/regeneration phase. Currently the CO_2 is released into space, but it is possible to use it in a Sabatier reactor for oxygen recovery[17].

Chemical absorption can also be used for CO_2 removal. The best and most used alternatives are lithium hydroxide ($LiOH$), silver oxide (Ag_2O) and solid phase amines. Chemical absorption takes place in the presence of water. A system that uses this technology will remove humidity along with CO_2 . Lithium hydroxide has a long history of use in space applications due both to its high capacity and simplicity of operation. However, $LiOH$ is not recyclable[14].

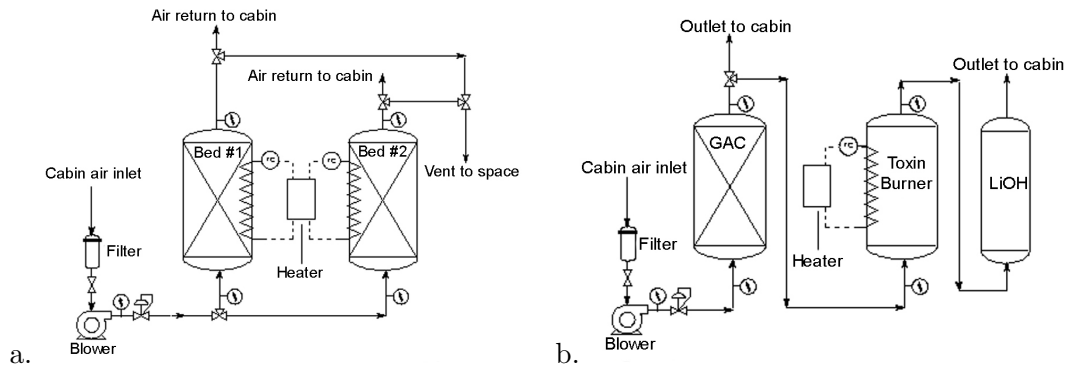


Figure 1.9: a. Russian trace contaminant control system; b. US trace contaminant control system[16]

Trace contaminants appear in the cabin environment due to human and animal presence, experiments, leakage and off-gassing of hardware. They come in very small

quantities but, due to the closed environment of the cabin, their concentration can reach hazardous levels[14]. Two different solutions for trace contaminants removal are present on the ISS in the Russian and the US module respectively (fig.1.9).

The Russian version uses two adsorption beds working out of phase. Activated carbon is used as adsorber. The beds can be regenerated using a small flow of non-oxidizing purge gas or under vacuum conditions. The American version uses an expendable, phosphoric acid impregnated, activated carbon bed. This facilitates ammonia gas removal. Some of the resulting air is returned in the cabin and some is further routed to a catalytic toxin burner. The acid gases resulting from the toxin burner are removed by the $LiOH$ sorption bed.

The primary (portable) life support system (PLSS) is the system that permits astronauts to have extravehicular activities. Activated charbon is used as odors adsorbent and $LiOH$ as carbon dioxide remover. A much lighter and more efficient version could be realised if the non-regenerative $LiOH$ sorption bed would be replaced by a regenerative sorbent[18].

1.4 Conclusions

Sorption processes are essential for life support systems in space and become more and more attractive as thermal control solutions for space instruments. Due to the intrinsic stability, most² of the reviewed sorption processes use very basic control solutions, i.e. fixed operation times. Nonetheless, intelligent control based on input properties could increase sorption processes' efficiency. Also, sorption process modelling could be used for fault detection. The next chapters will present a ground based sorption system and a control solution based on the its internal parameter estimation by means of a software model.

²*most* is used here because this information was not available for all the systems. On the other hand, no information was found on other types of sorption process control

Chapter 2

Silica Gel - Water Adsorption Chiller

An adsorption chiller is a machine capable of transforming heat into cooling power by using one or more adsorption processes. A very basic human discovery is the fact that cooling is required when too much heat is present. Thus, developing an adsorption chiller that could transform the uncomfortable solar heat excess into pleasant, noiseless, environmentally friendly and cheap cooling is the purpose of many research groups around the world[19].

2.1 Process Description

There are many adsorption chiller prototypes in the world, some of them making it to the commercial and mass production phase[19]. This chapter will focus on the one developed at the Institute of Refrigeration and Cryogenics, Shanghai Jiao Tong University, China, and described in [20] and [21]. It uses silica gel as adsorbent and water as adsorbate. Even though they might use a different working pair than silica gel and water, most of the adsorption chiller prototypes and commercial versions have a similar structure and working sequence.

Figure 2.1 shows the structure of the silica gel – water adsorption chiller. It has three vacuum chambers and an 11-valve system. Chambers A and B are two basically identical adsorption/desorption chambers working out of phase. Each of them have a condenser, an adsorber or adsorption bed and an isolator or water evaporator (WE). Chamber C is a methanol gravitational heat pipe or methanol evaporator (ME). In order to improve performance, a vacuum valve is installed between chamber A and chamber B. At the end of the adsorption/desorption phase this valve will open and hot vapor from the desorbing chamber will flow into the adsorbing chamber.

2.1.1 Working principle

The chiller cycle has six phases. One such cycle can be:

1. Chamber A in desorption and chamber B in adsorption

In this phase all the valves are closed, except 2, 3, 6 and 7. That makes the hot water to flow in the chamber A adsorber and the cooling water to flow first in the chamber B condenser, then in the chamber A condenser and then in the chamber B adsorber. The

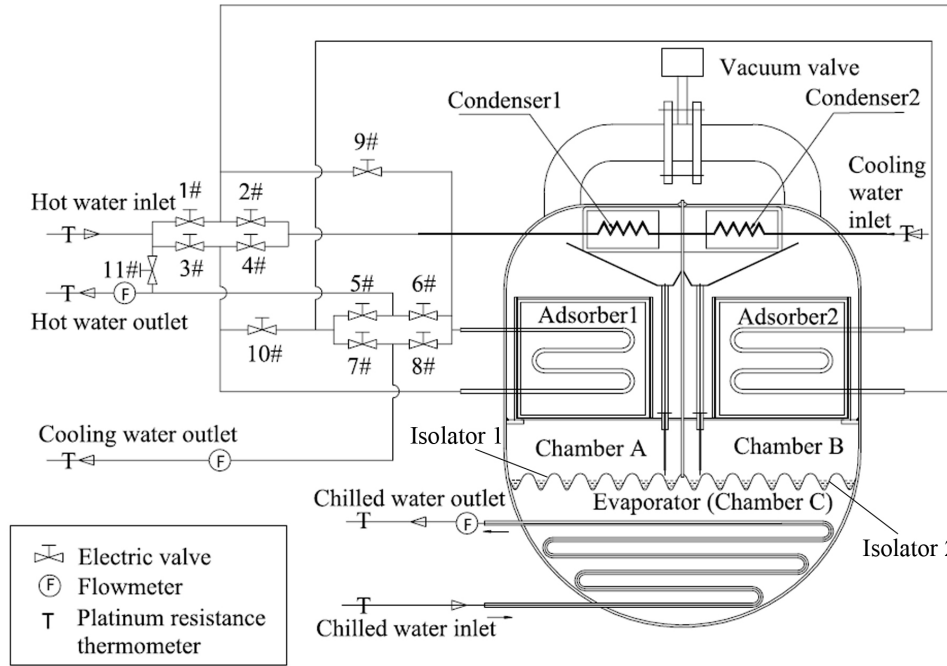


Figure 2.1: Schematic diagram of the SJTU adsorption chiller[20]

water to be chilled flows only inside the evaporator. Adsorber 1 is heated and begins to desorb. The vapor condenses first on the isolator 1. This increases the temperature of the isolator until it becomes higher than the condenser's. At this point, vapor condenses on the condenser and will continue to collect on the isolator. Adsorber 2 is cooled and starts adsorption. Water in the isolator 2 is transported as vapor to the adsorber, which decreases the isolator's temperature. When the isolator temperature becomes lower than the saturation temperature of methanol in chamber C, the heat pipe starts to work. The methanol evaporates from the lower, warmer, part of the chamber, lowering the temperature of the water to be chilled. It condensates in the upper, colder, part of the chamber and collects due to gravity in the lower part (fig. 2.2). In this phase, the temperature of the WE1 is the highest and that of the WE2 is the lowest between WE1, WE2 and ME. Heat only transfers from ME to WE2. During this phase the condenser in chamber B has almost no influence over the process.

2. Mass recovery from chamber A to chamber B

When adsorption/desorption finishes, the vacuum valve opens. The high temperature, high pressure vapor from chamber A flows into chamber B with high speed. Adsorber 1 continues to desorb and adsorber 2 to adsorb. At the end of this phase the pressure in both chambers is the same. During this phase, the isolator 1 temperature decreases and the isolator 2 temperature increases.

3. Heat recovery from chamber A to chamber B

The purpose of this phase is to recover the hot water used to heat adsorber 1 instead of wasting it when the adsorber switches from desorption to adsorption. Valve 11 is

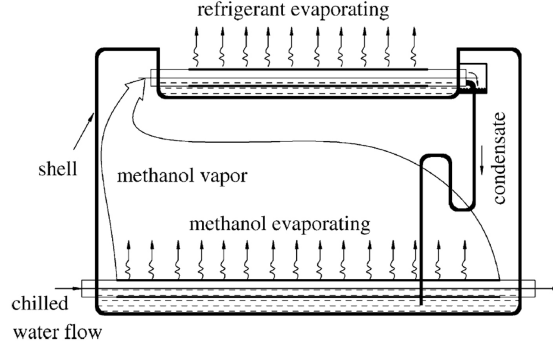


Figure 2.2: Schematic diagram of the methanol gravitational heat pipe[20]

opened and hot water will stop flowing inside the chiller. Valves 2, 3 and 6 are closed while valves 4 and 9 are opened. This will make the cooling water (passing first through the condensers) to push the hot water residing in adsorber 1 into adsorber 2. The duration of this phase is determined by the flowrate of the cooling water.

4. Chamber B in desorption and chamber A in adsorption

Valve 8 is opened while valves 7 and 9 are closed. Then valves 1, 5 are opened and 11 closed. Adsorber 1 adsorbs and Adsorber 2 desorbs. Condenser 2 starts to work when isolator 2 reaches a temperature higher than its own. Isolator 1 works both as a water evaporator and methanol condenser. The process is similar to the one in the first phase.

5. Mass recovery from chamber B to chamber A

This phase is similar to the second phase. The vapor flows from chamber B to chamber A and WE1 heats up while WE2 cools down.

6. Heat recovery from chamber B to chamber C

This phase is similar to third phase. Valve 11 is opened, valves 1, 4 are closed. Then valve 2 and 10 are opened, valve 5 is closed. After this phase, the cycle begins again.

In fig. 2.3 is presented the pressure –temperature diagram of the process cycle. The ideal cycle is given by $A \rightarrow B \rightarrow C \rightarrow D \rightarrow E \rightarrow F \rightarrow A$. $A \rightarrow B$ and $D \rightarrow E$ are heat recovery phases, $B \rightarrow C$ and $E \rightarrow F$ are heating/desorption and cooling/adsorption phases, $C \rightarrow D$ and $F \rightarrow G$ are mass recovery phases. The practical cycle is $A \rightarrow B \rightarrow n \rightarrow C \rightarrow q \rightarrow D \rightarrow E \rightarrow m \rightarrow F \rightarrow p \rightarrow A$.

2.2 Mathematical Model

The mathematical model is built upon a lumped parameter model described in [20] and [22]. The parameters used in the model are listed in Table 2.1. The main simplifying assumptions are:

1. the temperature and pressure are uniform throughout the whole adsorber;
2. the water is adsorbed uniformly and is liquid in the adsorbent;

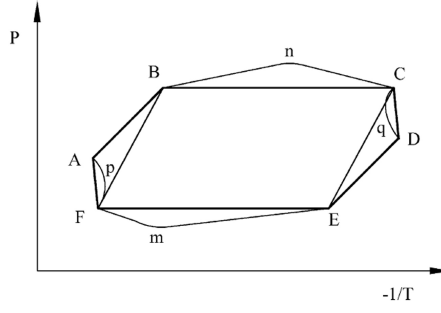


Figure 2.3: Pressure - Temperature diagram for the adsorption chiller cycle[20]

3. the pressure difference between the adsorber and condenser is neglected;
4. the vapor inside the chambers is saturated vapor
5. the heat conduction of the shell connecting the adsorber to the condenser and the evaporator is neglected;
6. there is no heat exchange between the two isolators;
7. the system has no heat losses to the environment.

To describe the adsorption chiller it is necessary to write the equation for adsorption rate and the energy and mass balances for each of its components.

2.2.1 Adsorption equation

In [23], Saha et al. express the adsorption rate starting from a modified Freundlich equation. The adsorption rate can be written as:

$$\frac{dx}{dt} = \frac{15 \cdot D_{s0}}{Rp^2} \cdot \exp\left(\frac{-E_a}{R \cdot T_{bed}}\right) \cdot \left\{ A(T_{bed}) \cdot \left[\frac{P_v(T_{wv})}{P_v(T_{bed})} \right]^{B(T_{bed})} - x \right\} \quad (2.1)$$

where T_{bed} is the temperature of the adsorption bed; T_{wv} is the saturation temperature of the water vapor inside the chamber; $P_v(T)$ is the saturation pressure corresponding to temperature T and is computed according to (2.2); $A(T)$ and $B(T)$ are empirical expressions characterizing the silica bed[23] and can be calculated with (2.3).

$$P_v(T) = 0.0000888 \cdot T^3 - 0.0013802 \cdot T^2 + 0.0857427 \cdot T + 0.4709375 \quad (2.2)$$

$$\begin{aligned} A(T) &= A_0 + A_1 \cdot T + A_2 \cdot T^2 + A_3 \cdot T^3 \\ B(T) &= B_0 + A_1 \cdot T + B_2 \cdot T^2 + B_3 \cdot T^3 \end{aligned} \quad (2.3)$$

2.2.2 Energy balance equations

The energy balance for the adsorption beds can be written as:

$$\begin{aligned} \frac{d}{dt} [(C_s \cdot M_a + C_w \cdot M_a \cdot x + M_{ab} \cdot C_{cu} + M_{fin} \cdot C_{al}) \cdot T_{bed}] \\ = C_w \cdot \dot{m}_w (T_{bed,in} - T_{bed,out}) + M_a \cdot q_{st} \cdot \frac{dx}{dt} + \delta \cdot C_{wv} \cdot M_a \cdot (T_{wv} - T_{bed}) \cdot \frac{dx}{dt} \end{aligned} \quad (2.4)$$

Symbol	Value	Units	Property name
C_w	4180	$J \cdot kg^{-1} \cdot K^{-1}$	water specific heat
C_{wv}	1850	$J \cdot kg^{-1} \cdot K^{-1}$	water vapor specific heat
C_s	924	$J \cdot kg^{-1} \cdot K^{-1}$	silica gel specific heat
C_{cu}	336	$J \cdot kg^{-1} \cdot K^{-1}$	copper specific heat
C_{al}	905	$J \cdot kg^{-1} \cdot K^{-1}$	aluminium specific heat
C_{me}	2335	$J \cdot kg^{-1} \cdot K^{-1}$	methanol specific heat
L_w	$2.257 \cdot 10^6$	$J \cdot kg^{-1} \cdot K^{-1}$	latent heat of water
L_{me}	$1.101 \cdot 10^6$	$J \cdot kg^{-1} \cdot K^{-1}$	latent heat of methanol
KA_{ab}	24585	$W \cdot K^{-1}$	coef. of ads. bed heat exchange
$KA_{c_{in}}$	8408.64	$W \cdot K^{-1}$	coef. of condenser heat input
$KA_{c_{out}}$	26146.6	$W \cdot K^{-1}$	coef. of condenser heat output
$KA_{i_{in}}$	19292	$W \cdot K^{-1}$	coef. of isolator heat input
$KA_{i_{out}}$	13338	$W \cdot K^{-1}$	coef. of isolator heat output
$KA_{e_{in}}$	10050	$W \cdot K^{-1}$	coef. of evaporator heat input
$KA_{e_{out}}$	4995	$W \cdot K^{-1}$	coef. of evaporator heat output
R	8.31	$J \cdot mol^{-1} \cdot K^{-1}$	ideal gas constant
D_{s0}	$2.54 \cdot 10^{-4}$	$m^2 s^{-1}$	diffusion coefficient
E_a	$4.2 \cdot 10^4$	$J \cdot mol^{-1}$	activation energy
R_p	$3.57 \cdot 10^{-4}$	m	average radius of adsorbent particles
q_{st}	$2.8 \cdot 10^6$	$J \cdot kg^{-1}$	isosteric heat of adsorption
x_0	0.346	$kg \cdot kg^{-1}$	characteristic parameter of adsorption
M_a	52	kg	silica gel (adsorbent) mass
M_{ab}	100	kg	mass of ads. bed copper components
M_{fin}	20	kg	mass of ads. bed aluminium fins
M_c	15.2	kg	mass of condenser copper components
M_i	120	kg	mass of isolator copper components
M_w	20	kg	mass of water inside the chamber
M_e	65.1	kg	mass of evaporator copper components
M_{me}	20	kg	mass of methanol in the evaporator
\dot{m}_h	1	$kg \cdot s^{-1}$	hot water mass flow
\dot{m}_c	1.35	$kg \cdot s^{-1}$	cool water mass flow
\dot{m}_{ch}	0.5	$kg \cdot s^{-1}$	chilled water mass flow
A_0	31.198	NA	empiric coef.
A_1	-0.26650	K^{-1}	empiric coef.
A_2	$769 \cdot 10^{-6}$	K^{-2}	empiric coef.
A_3	$73898 \cdot 10^{-11}$	K^{-3}	empiric coef.
B_0	41.581	NA	empiric coef.
B_1	-0.35435	K^{-1}	empiric coef.
B_2	$10199 \cdot 10^{-7}$	K^{-2}	empiric coef.
B_3	$-97034 \cdot 10^{-11}$	K^{-3}	empiric coef.

Table 2.1: Parameters and constants used in the adsorption chiller mathematical model

$$T_{bed,out} = T_{bed} + (T_{bed,in} - T_{bed}) \cdot \exp\left(-\frac{KA_{ab}}{C_w \cdot \dot{m}_w}\right) \quad (2.5)$$

where δ is 0 for desorption and 1 for adsorption; $T_{bed,in}$ and $T_{bed,out}$ are the temperatures of the cooling/heating water before and after passing through the adsorption bed; \dot{m}_w is the water mass flow through the bed.

During desorption and the following mass recovery phase, heating water passes through the adsorption bed. During adsorption and the following mass recovery phase, cooling water passes through the adsorber. In heat recovery phase, the cooling water pushes the hot water from the desorbing bed to the adsorbing bed. Thus, the flow of water is \dot{m}_c . During heat recovery, $T_{bed,in}$ can be approximated as an average between the temperature of the water coming out from the desorption bed and the temperature of the water coming out from the adsorption bed at the end of the previous phase.

For the condensers, the energy balance is given by:

$$\begin{aligned} \frac{d}{dt} \cdot C_{cu} \cdot M_c \cdot T_{con} &= C_w \cdot \dot{m}_c \cdot (T_{con,in} - T_{con,out}) \\ &\quad - \delta \cdot \left[L_w \cdot M_a \cdot \frac{dx}{dt} + C_{wv} \cdot M_a \cdot (T_{con} - T_{bed}) \right] \end{aligned} \quad (2.6)$$

$$T_{con,out} = T_{con} + (T_{con,in} - T_{con}) \cdot \exp\left(-\frac{KA_{c_{in}}}{C_w \cdot \dot{m}_c}\right) \quad (2.7)$$

where T_{con} is the temperature of the condenser; $T_{con,in}$ and $T_{con,out}$ are the temperatures of the cooling water before and after entering the condenser. δ is 1 when desorption happens ($dx/dt < 0$) and the condenser is colder than the isolator; is 0 otherwise, including during mass recovery.

Each isolator has the following energy balance:

$$\begin{aligned} \frac{d}{dt} [(C_{cu} \cdot M_i + C_w \cdot M_w) \cdot T_{iso}] &= \delta_1 \cdot KA_{i_{out}} \cdot (T_{me,v} - T_{iso}) \\ &\quad - \delta_2 \cdot L \cdot M_a \cdot \frac{dx}{dt} \\ &\quad - (1 - \delta_2) \cdot \left[\delta_3 \cdot L \cdot M_a \cdot \frac{dx}{dt} + (1 - \delta_3) \cdot C_w \cdot M_a \cdot \frac{dx}{dt} \cdot (T_{iso} - T_{con}) \right] \end{aligned} \quad (2.8)$$

where T_{iso} is the temperature of the isolator; $T_{me,v}$ is the saturation temperature of the methanol vapor inside the evaporator; δ_1 is 1 for $T_{me,v} > T_{iso}$ and 0 otherwise; δ_2 is 0 for desorption and heat recovery after adsorption, and is 1 for adsorption and heat recovery after desorption; δ_3 is 0 for $T_{iso} > T_{con}$ and 1 otherwise. During mass recovery though, a different equation describes the energy balance inside the isolator:

$$\begin{aligned} \frac{d}{dt} [(C_{cu} \cdot M_i + C_w \cdot M_w) \cdot T_{iso}] &= \delta_1 \cdot KA_{i_{out}} \cdot (T_{me,v} - T_{iso}) \\ &\quad + (2 \cdot \delta_2 - 1) \cdot L \cdot \left(\dot{m}_{rec} - M_a \cdot \left| \frac{dx}{dt} \right| \right) \end{aligned} \quad (2.9)$$

where \dot{m}_{rec} is the vapor flow rate from desorption chamber to adsorption chamber and is given by (2.10).

$$\dot{m}_{rec} = \sqrt{\frac{2 \cdot A^2 [P_v(T_{wv,des}) - P_v(T_{wv,ads})]}{v_{wv}}} \quad (2.10)$$

v_{wv} is the specific volume of the water vapor (m^3/kg). This is calculated using eq. (2.11), which was obtained by fitting experimental data to an exponential sum. In eq. (2.10), the average value of the specific water vapor volume in each chamber is used.

$$v_{wv}(T_{wv}) = 6.858 \cdot 10^{11} \cdot \exp(-0.08161 \cdot T_{wv}) + 1.706 \cdot 10^6 \cdot \exp(-0.03737 \cdot T_{wv}) \quad (2.11)$$

The evaporator energy balance is given by:

$$\frac{d}{dt} [(C_{cu} \cdot M_e + C_{me} \cdot M_{me}) \cdot T_{eva}] \quad (2.12)$$

$$= C_w \cdot \dot{m}_{ch} \cdot (T_{chill,in} - T_{chill,out}) - \delta \cdot K A_{i_{in}} \cdot (T_{me,v} - T_{iso})$$

$$T_{chill,out} = T_{eva} + (T_{chill,in} - T_{eva}) \cdot \exp\left(-\frac{K A_{e_{in}}}{C_w \cdot \dot{m}_{ch}}\right) \quad (2.13)$$

In eq. (2.12), δ is 1 whenever one of the isolators has the temperature lower than the evaporator, and 0 otherwise. When δ is 1, T_{iso} is the temperature of the cooler isolator.

2.2.3 Mass balance equations

An essential internal variable of each chamber is the vapor saturation temperature. This can be calculated from the mass balance inside the chambers. Thus, the saturation temperature of the methanol vapor inside the evaporator can be determined from the following equation:

$$K A_{e_{out}} \cdot (T_{eva} - T_{me,v}) = \delta \cdot K A_{i_{in}} \cdot (T_{iso} - T_{me,v}) \quad (2.14)$$

where T_{iso} and δ are like above. If none of the isolators has a temperature lower than the temperature of the evaporator, the saturation temperature of the methanol vapor is given by the evaporator temperature.

For the water vapor saturation temperature inside the adsorption/desorption chambers, several equations have to be used depending on the phase and on components' temperature. Thus, for the adsorption chamber, the mass balance is given by:

$$M_a \cdot \frac{dx}{dt} = \frac{K A_{i_{out}} \cdot (T_{iso} - T_{wv})}{L_w} \quad (2.15)$$

For desorption, eq. (2.15) is used while the temperature of the condenser is higher than the temperature of the isolator. When the condenser becomes cooler than the isolator, the water vapor will condense on it and the mass balance reflects this change:

$$M_a \cdot \frac{dx}{dt} = \frac{K A_{c_{out}} \cdot (T_{con} - T_{wv})}{L_w} \quad (2.16)$$

In mass recovery, the things become even more complicated, since the recovery mass flow \dot{m}_{rec} has to be taken into account. For the adsorbing chamber, the mass balance in this case is:

$$M_a \cdot \frac{dx}{dt} = \dot{m}_{rec} - \frac{K A_{i_{out}} \cdot (T_{wv} - T_{iso})}{L_w} \quad (2.17)$$

while for the desorption chamber:

$$-M_a \cdot \frac{dx}{dt} = \dot{m}_{rec} - \frac{K A_{i_{out}} \cdot (T_{iso} - T_{wv})}{L_w} \quad (2.18)$$

Equations (2.17) and (2.18) are an approximation of the actual mass balance, in the sense that some small oscillations might occur at the end of the mass recovery phase (before the pressure in the two chambers becomes homogenous). These oscillations can be neglected by considering that no mass exchange happens between the two chambers once \dot{m}_{rec} reaches for the first time 0. In this case, the final vapor saturation temperature can be approximated as the average between the saturation temperatures in each chamber at the beginning of mass recovery.

2.3 Performance criteria

There are four parameters required for evaluating the chiller performance[20, 21].

The refrigerating capacity is given by:

$$Q_{ref} = \text{frac} \int_0^{t_{cycle}} C_w \cdot \dot{m}_{ch} \cdot (T_{chill,in} - T_{chill,out}) dt_{cycle} \quad (2.19)$$

The sorption coefficient of performance (SCP) is given by:

$$SCP = \frac{Q_{ref}}{M_a} \quad (2.20)$$

The heating power used by the chiller is:

$$Q_h = \text{frac} \int_0^{t_{cycle}} C_w \cdot \dot{m}_h \cdot (T_{heat,in} - T_{heat,out}) dt_{cycle} \quad (2.21)$$

The overall coefficient of performance(COP) is:

$$COP = \frac{Q_{ref}}{Q_h} \quad (2.22)$$

Chapter 3

Adsorption control system

Ἄνθρωπος μέτρον

Man, the measure (of all things)

Protagoras

The sorption processes in general and the adsorption chiller in particular offer some difficult challenges for the control engineer:

- the sorption process mathematical model strongly nonlinear;
- the process is going through several quite different phases, and even phases can be divided in subphases (i.e. in desorption, first water vapor condenses on the isolator, and then on the condenser);
- there is not much information regarding the internal variables, since they are difficult or expensive to measure;
- some sorption processes present inputs that variate on a large range (the adsorption chiller presented in the previous chapter is one of these with the hot water input ranging between 60°C and 95°C);
- in the case of the adsorption chiller¹, there are no means to control the input flow.

In the next sections, a basic control solution that tries to address these challenges is presented for the adsorption chiller.

3.1 Structure of the control system

As stated before, there is almost no information regarding the internal process variables. In the following, only the input and output temperature of the water flows will be considered as measurable.

The structure of the control system is presented in fig. 3.1. P is the adsorption chiller, M is a software model of the chiller acting as a internal state estimator and I is a fuzzy inference module. The three inputs of the adsorption chiller (heating, cooling and chilling water temperature) are measured and supplied to the software model. The model provides a complete set of the internal variables. The most important ones are the

¹but not only - see for example the ISS LSS: a constant air flow passes through the sorption stages, otherwise the quality of air will suffer

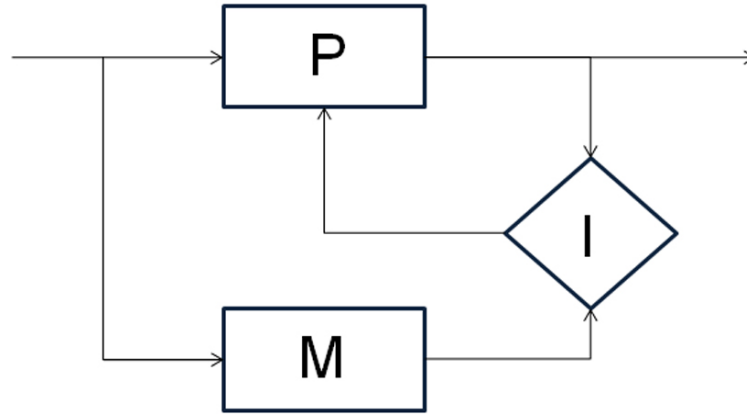


Figure 3.1: Control structure for the adsorption chiller

adsorption rate, the adsorption capacity and the mass recovery flow. The fuzzy inference module compares the output of the system with the output of the model and, based on this comparison a trust degree is given to the estimated internal variables. Based on the internal variables provided by the model and the trust degree the model has, the inference module decides if the process should switch to the next phase.

3.2 Adsorption chiller software model

The model was developed in Java based on the mathematical model presented in the previous chapter. An object oriented programming language is suitable for simulating the behaviour of each component. The class structure is shown in fig. 3.2 The abstract class

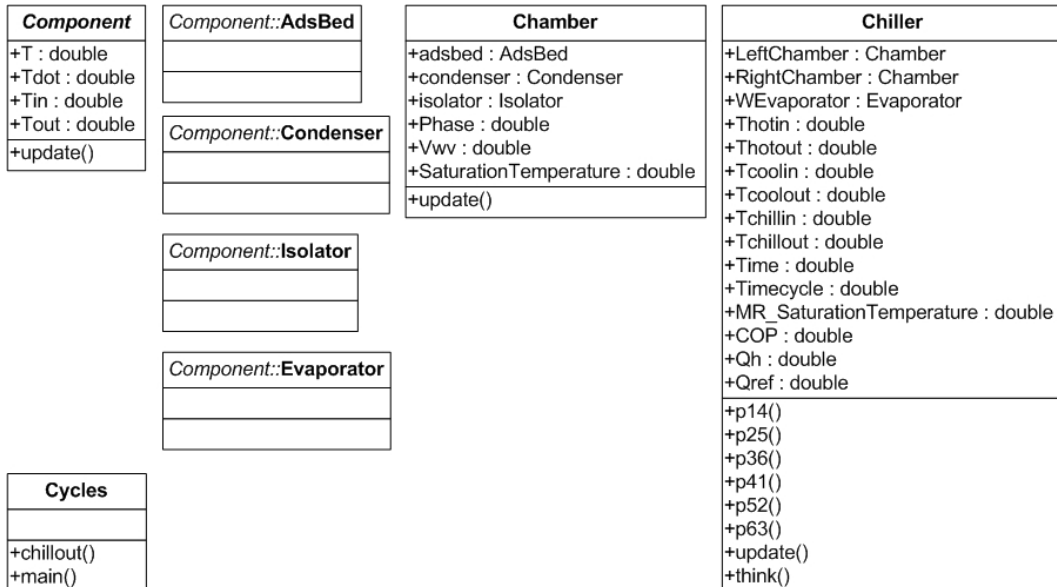


Figure 3.2: Class structure of the Java adsorption chiller model

Component defines the structure for the adsorption bed, condenser, isolator and evaporator classes. The Chamber class objects include one AdsBed object, one Condenser object and one Isolator object. A Chiller class object includes two Chamber objects.

The Cycles class includes the *main()* method where a Chiller object is instantiated, and a *chillout()* method that outputs the simulation results to text files.

Two critical aspects of the model implementation proved to be the initialization of the state variables and the update procedure. To reflect the reality as close as possible, all internal temperatures are initialized to 25°C. The adsorption capacity for each of the two beds is initialized with 0.2 kg kg^{-1} . The adsorption rate is considered initially 0. The model requires a few cycles (4-5 cycles usually) to produce the expected outputs. This is why, a setup procedure of 10 complete cycles is run before all simulations.

The component update procedure has some small differences for each phase. This is why the Chiller class provides 6 methods (*p13()* ... *p61()*) that offer a proper update sequence in each phase. The detailed update sequences are presented in fig. 3.6. The model is updated every 0.1s.

Figure 3.3 shows the simulation results for 900s adsorption/desorption time, 180s mass recovery time and 30s heat recovery time, with the inputs set at 80.

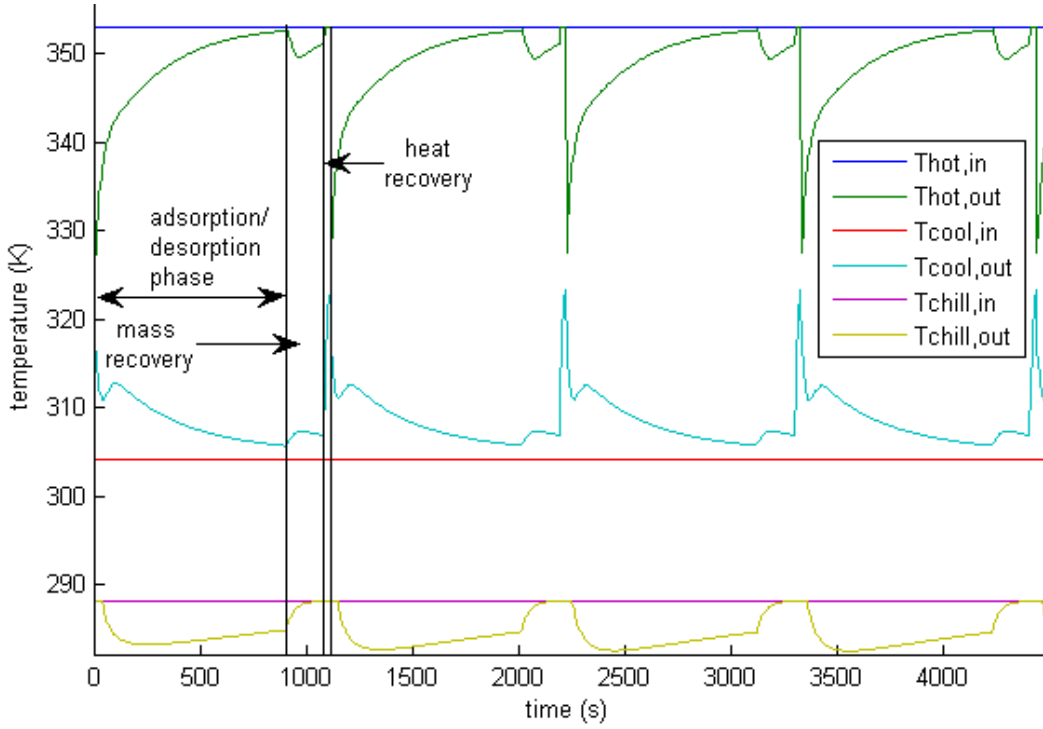


Figure 3.3: Constant inputs simulation results

For model validation, experimental data was collected and compared with the model simulation results. The water flows differ in this case. \dot{m}_h is 0.5 kg/s , \dot{m}_c is 1.15 kg/s and \dot{m}_{ch} is 0.45 kg/s . The results are presented in fig. 3.4. For most of the experiment, the model can be considered accurate. The output of hot water is not well modeled for the first adsorption/desorption phase, but that is because of the setup sequence which is done at constant input temperatures. Figure 3.5 shows the evolution of some internal variables as estimated by the model. The average COP is 0.4.

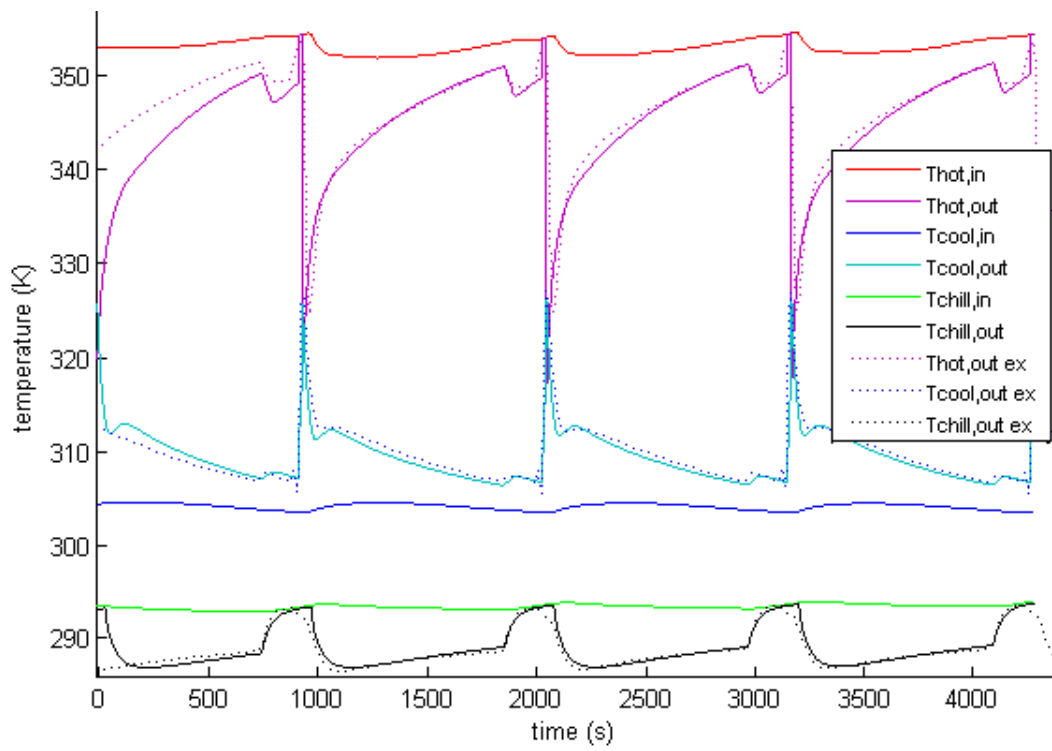


Figure 3.4: Software model validation

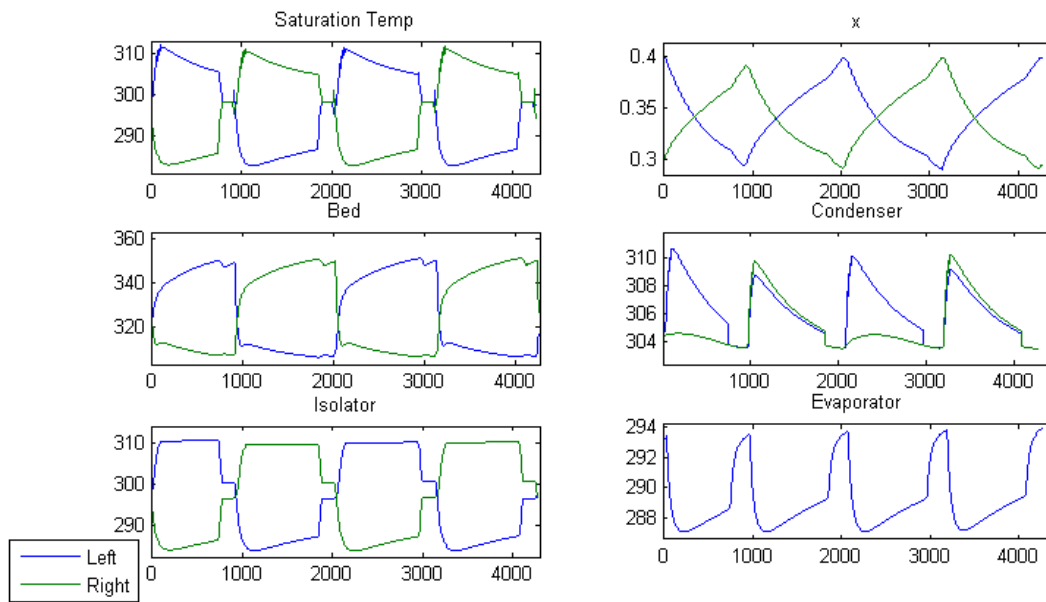


Figure 3.5: Estimated internal variables

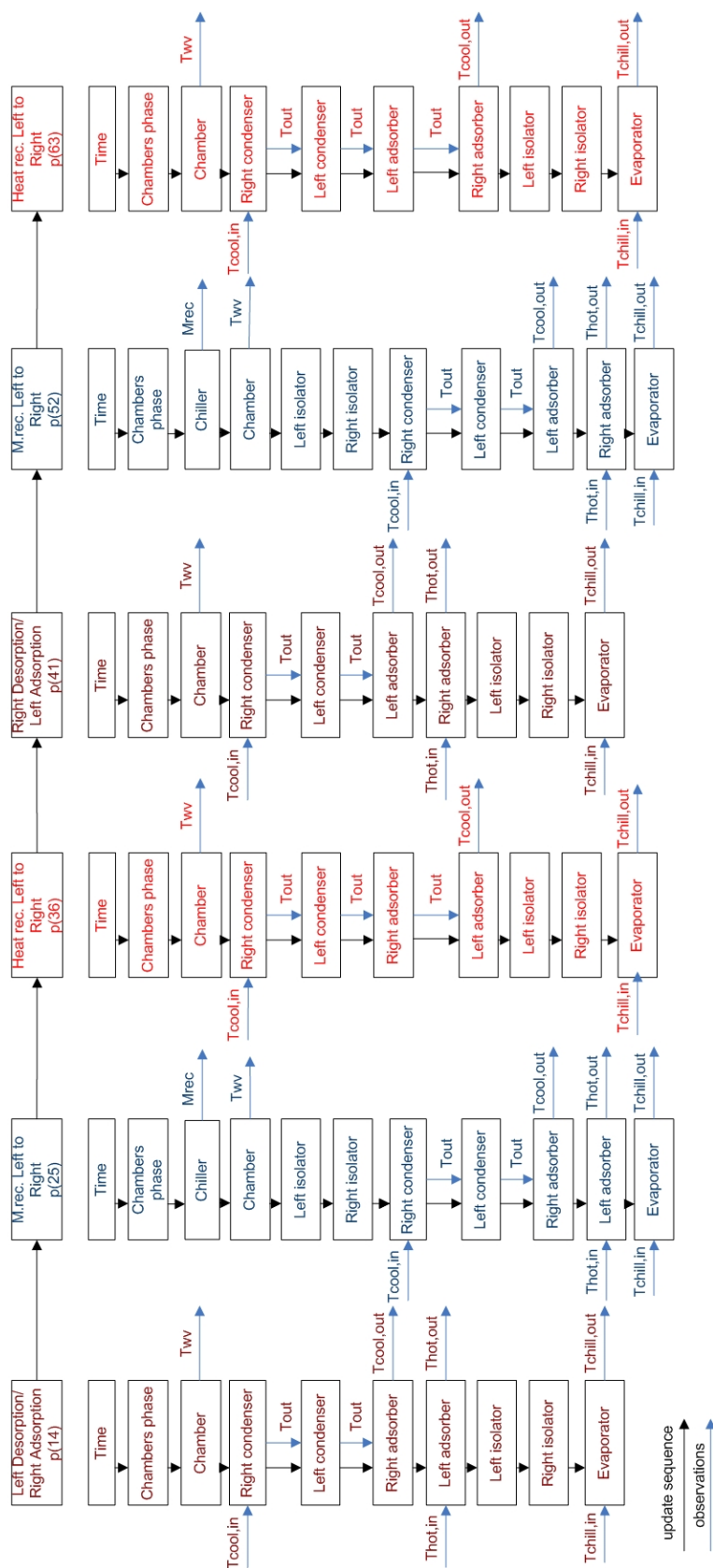


Figure 3.6: Update sequence for each phase of the chiller model

3.3 Basic inference module

The purpose of the inference module is to determine whether the chiller needs to switch to the next phase in order to maximize performance. For that it tries to make effective use of the available expert knowledge and of the estimated internal states. A fuzzy controller allows expert knowledge integration and was chosen as the core of the inference module.

The first step was to provide a basic set of rules that define the moment the chiller has to switch from adsorption/desorption phase to mass recovery. Since a good estimation of internal variables is expected from the software chiller model, this basic set was built around the adsorption rate parameter. The Mamdani-type fuzzy rules are:

```

if Adsorption Rate is High then Wait
if Adsorption Rate is Low  then Switch
if Desorption Rate is High then Wait
if Desorption Rate is Low  then Switch

```

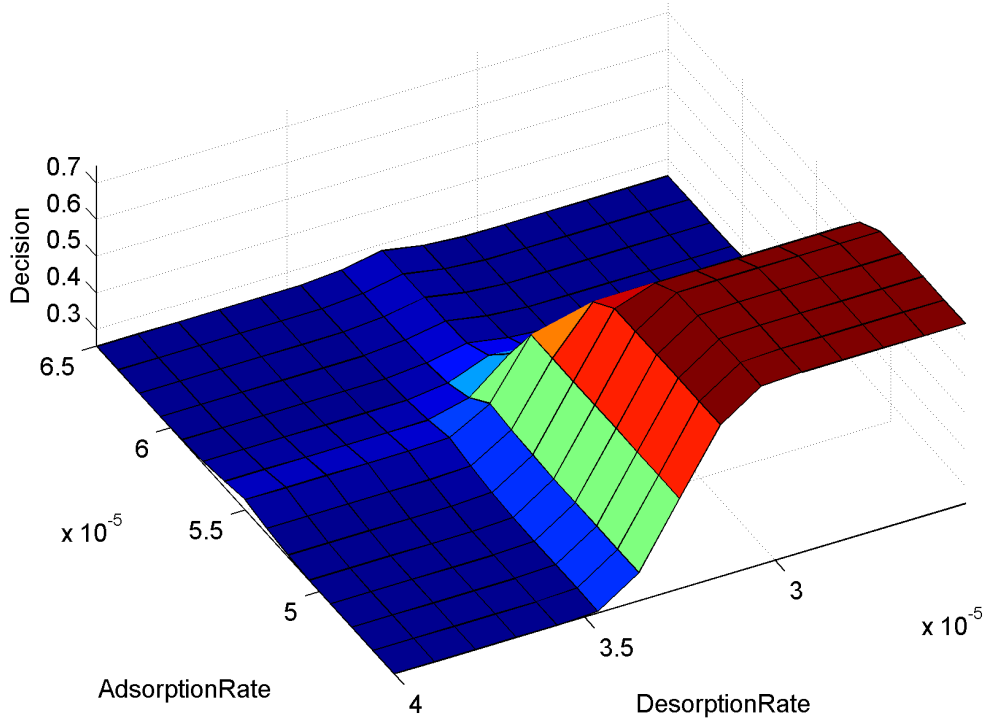


Figure 3.7: Basic inference set of rules

It is more difficult to decide when to switch from mass recovery to heat recovery phase, especially based on estimated internal variables. In [21] is noted that mass recovery phase is important for low heating flow temperatures, but it doesn't have a big influence regarding the overall performance of the system in the case of high heating flow temperatures. Moreover, extended mass recovery times reduce the COP as in this periods the chiller doesn't provide refrigeration. Thus, at this stage, the inference module will consider the mass recovery phase finished 10 seconds after the water vapor saturation temperature becomes homogenous in the two chambers.

Unlike the previous situations, switching from heat recovery to adsorption/desorption phase doesn't require too much computational power. It is necessary to know the cold

fluid flow rate and the length of the internal pipe system to determine an optimal switch time for this phase. The optimal heat recovery time is 30 seconds.

The inference module is tested for the same set of inputs that was used for the software model validation. The result is presented in fig. 3.8. The average COP obtained for this simulation is 0.5. This is better than the one obtained in model validation.

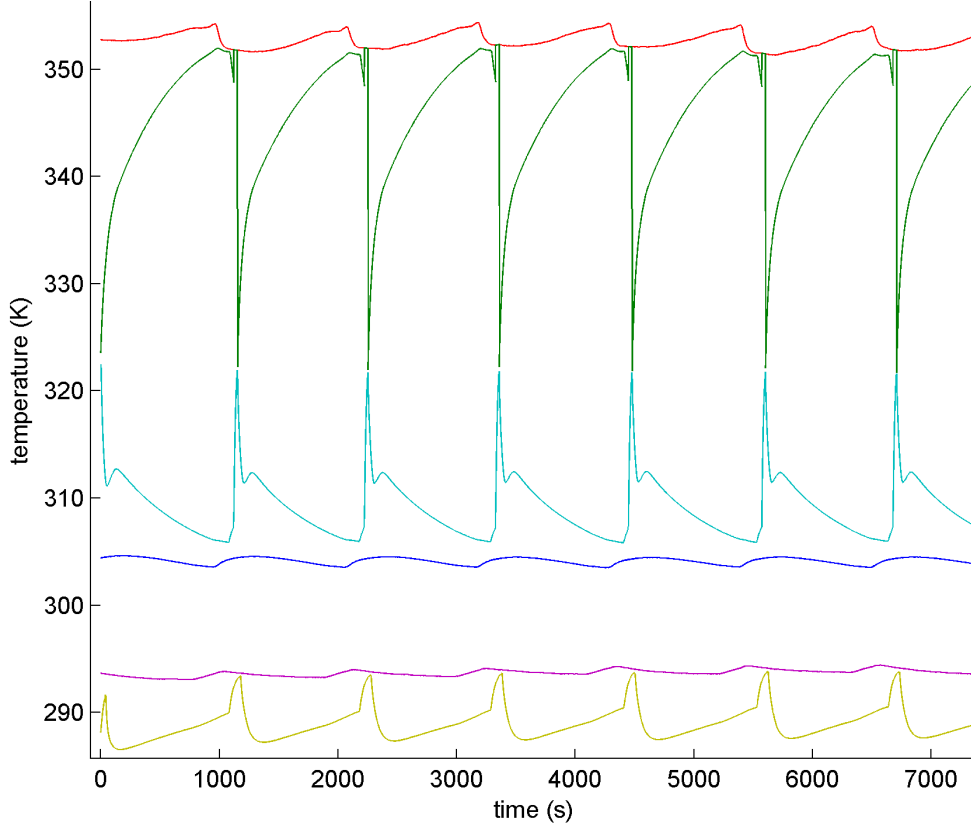


Figure 3.8: Simulation results with the basic inference system

The main reason for intelligent switching between the adsorption chiller phases resides in the variable heat source it uses. Solar heat varies during a day and a time based switching system doesn't take that into account. It is thus important to assess and improve the performance of the inference system during one day. A set of data covering 10 hours was generated. Besides the heat flow temperature variation, smaller variations of the cooling and chilling flow inputs were considered. The results of the simulation with the basic inference system are presented in fig. 3.9. The average COP is 0.41 and the refrigeration power 9.15 kW. In fig. 3.10 are shown the simulation results for the same set of input data, but for constant cycle times. The refrigeration power is an average of 9.2kW and the COP is 0.4. The similar performance is promising since the 900s – 180s – 30s phase times are considered optimal[21] for the chiller working with constant heat flow temperature of 80 – 85°C and the inference system used at this stage didn't reach its maximum potential.

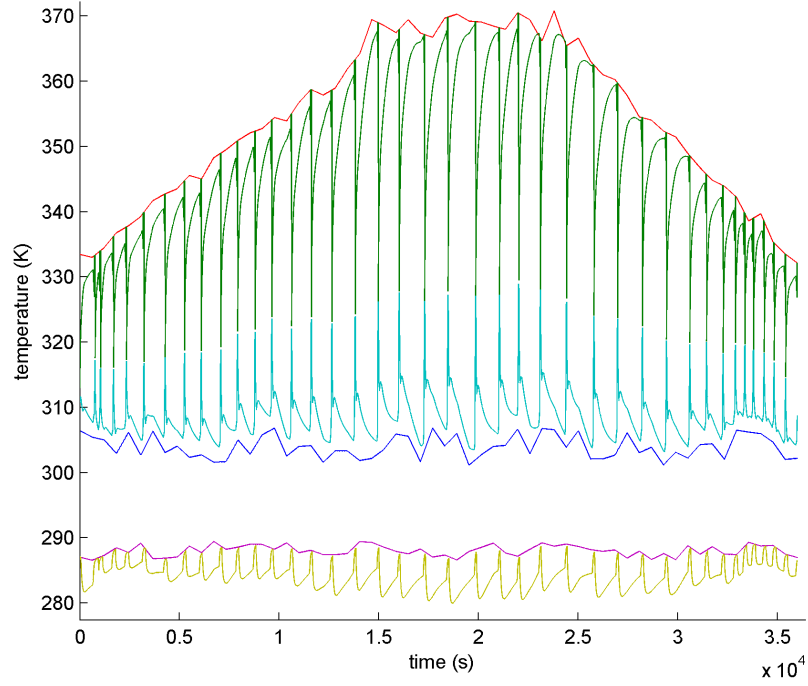


Figure 3.9: Simulation over 10 hours during a day with basic inference system

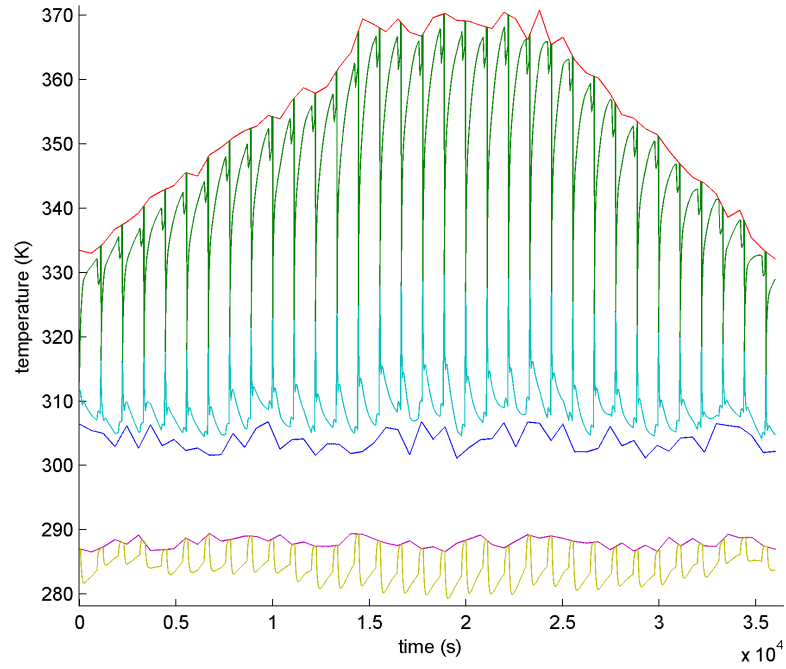


Figure 3.10: Simulation over 10 hours during a day with constant cycle times (adsorption/desorption time - 900 s; mass recovery - 180 s; heat recovery - 30 s)

3.4 Improved inference module

As stated in the previous section, a longer mass recovery phase improves the performance of the system for lower heat flow temperatures. Moreover, experimental results suggest that the adsorber should be heated to the highest temperature available² and cooled down close to a 2°C difference between cooling water input and output[20].

The fuzzy inference procedure for switching from adsorption/desorption phase to mass recovery phase becomes:

```

if AdsorptionRate is High then Wait
if AdsorptionRate is Low then Switch
if DesorptionRate is High then Wait
if DesorptionRate is Low then Switch
if Theatin-Theatout is High then Wait
if Theatin-Theatout is Low then Switch
if Tcoolout-Tcoolin is High then Wait
if Tcoolout-Tcoolin is Low then Switch

```

Figure 3.11 presents the new structure of the fuzzy inference system. Extra non-fuzzy rules are included, one for increasing by 60s the mass recovery phase at temperatures lower than 70°C, and one for modifying the **Theatin-Theatout** membership functions for temperatures higher than 80°C.

The data set covering 10 hours of a day was used to test the new inference system. The results are presented in fig. 3.12. The average COP obtained is 0.49 with an average refrigeration capacity of 9.18 kW. The performance improvement relative to the fixed phase time control version is of 22.5%.

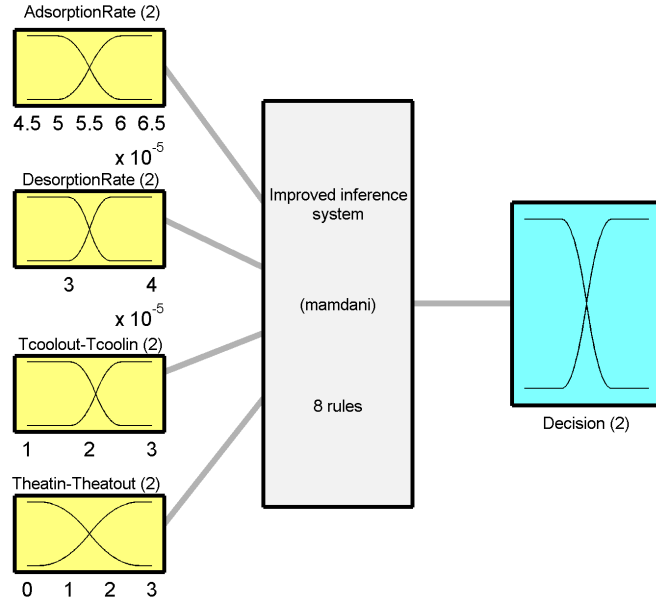


Figure 3.11: The improved inference system structure

²In [21] is mentioned that above 80°C the COP cannot improve significantly.

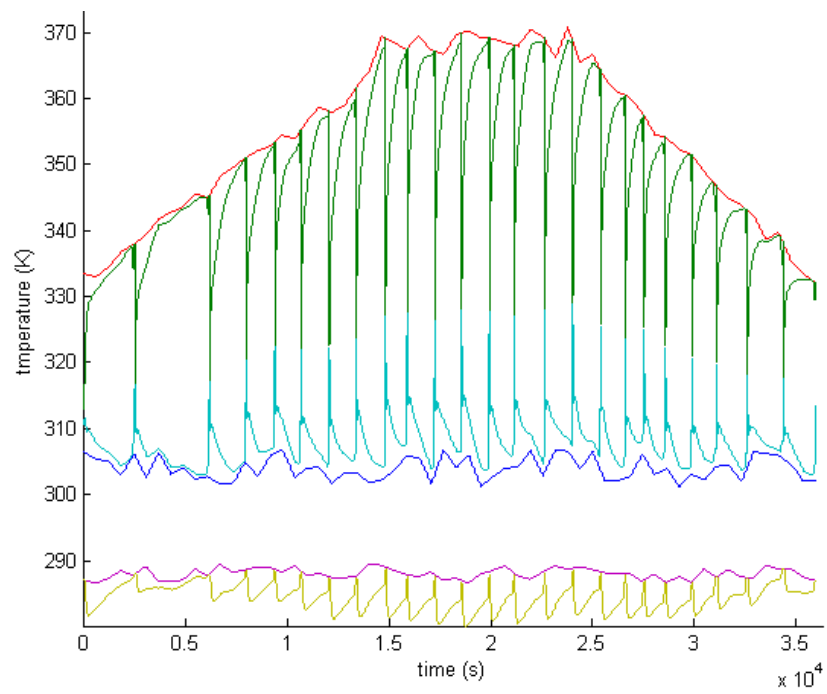


Figure 3.12: Simulation results with the improved inference module

Chapter 4

Conclusions

A review of sorption based systems used in space technology revealed their increasing importance in thermal control of instruments and a mature and essential presence in Life Support Systems. Space industry uses sorption processes for obtaining sub-Kelvin temperatures, for cooling instruments and for providing a clean and comfortable environment for humans in space. Limited control is used for sorption processes, being it in space or on ground. Most of these systems work on timed cycles with good enough results for not requiring better control solutions. Nonetheless, it was proved in the previous chapter that a basic control system that takes advantage of the expert knowledge could increase the performance of such systems. Timed cycles may offer excellent results for (more or less) constant inputs, but they can do little when it comes to large variations in the inputs or perturbations.

The main reason for using only timed based cycles as control solutions for sorption systems is their strong nonlinearity. Time based cycles can be optimized with very good results on an experimental basis for very specific working conditions, whereas developing an intelligent control system requires surpassing the obstacles raised by the strong nonlinearity. Moreover, mathematical models are difficult to extract due to the highly empirical characteristic of sorption theory. More control possibilities could appear if a better system identification is available. Thus, further studies regarding nonlinear system identification (using neuro-fuzzy methods) of sorption processes are required to improve the results of these paper.

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