Multi-Scale Simulation Thermochemical District Network

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Abstract

Thermochemical-district-heating-cooling-networks provide an effective way to transport the excess heat and hygroscopic properties for long distances without suffering heat loss. Therefore, multinode thermochemical network components have been developed on two scales: 1) Demand-side application models for heating-cooling; 2) Thermochemical-district-network model, which transfers heat to the first-scale models.

In this paper, we propose a design and simulation approach for a thermochemical-district-heating-cooling-network and its components. Simulation results show the feasibility of the simulation approach, which uses multiscale modelling. Moreover, the thermochemical-fluid mass on the second-scale was defined based on buildings heating-cooling requirements. The electrical energies used to produce the required heating-cooling were 16% and 30% respectively.

Introduction

One aim of using water-based district heating and cooling (DH) networks is the reduction of pollutant and thermal emissions in the city area by removing combustion heating systems at the demand side; this has been presented by Ancona (2014). In addition, reduction of primary energy consumption comes at a lower cost, (Connolly, 2014).

Some aqueous salt solutions have hygroscopic properties that can store energy potential which is released it as soon as it absorbs humidity from air. The EU H2020 project H-DisNet examines how such thermochemical fluids (TCFs) can act as an energy carrier in district networks. The properties of these TCFs can be exploited for loss-free transport and storage of potential energy (Geyer, 2017). Moreover, thermochemical (TC) district networks can integrate different heat sources and it has the potential to exploit low excess heat.

The main objective of this paper modelling and simulating an approach to a TC district heating and cooling network, including heating and space cooling applications, and a TC district network that uses a TCF as the carrier. Most previous studies have focused on simulating district heating (DH), where the hot and cold sources are a combined heat and power (CHP) plant or excess heat from industries. None of the previous studies

simulating DH have used a TCF as the carrier. Component models, such as (Kim, 2015), have simulated the TC absorber for cooling as an individual application, but not as a complete TC district heating and cooling network. Moreover, none of previous studies have been simulated using a TCF as the absorber for heating.

In this paper, the modelling focuses on implementing multinode TC network components at different scales. Consequently, the model is broken down into two scales, as follows.

The first scale includes supply and demand models, which are developed as independent simulation models based on applications like heating and cooling of buildings.

In order to develop application models at the first simulation scale, we focus on modelling building heating and building cooling applications. A finite volume model, of the absorber by Fürst and Kriegel (2016), is used.

The second scale consists of a multinode district network model that transfers the TCF properties to the first scale models in both direction. TCF supply and return pipes were used to connect the nodes of the first level simulation to form a TC district network. Total TCF mass flow and pumping power were defined based on heating or cooling demand of the applications.

TC Process Fundamentals

The main TC process relies on two processes: Absorption and desorption, as shown in Figure 1a (Geyer, 2018).

The main advantage of the TC process is the production of heat and absorbing humidity in the air during the absorption process. Therefore, we employ it for heating applications to produce heat and control the humidity, while it is used to lower the humidity for the evaporative cooling application. Conversely, the TC process is used to absorb the heat and store it as latent heat during the desorption process.

For both processes, the following variables are considered: 1) Air relative humidity, 2) air temperature, 3) TCF concentration, 4) TCF temperature, 5) air flow and 6) TCF flow. Their relationships, including the velocities, are as presented by Chung, Ghosh, and Hines (1996).

$$Q = \alpha A \Delta T_m \quad (1)$$

$$M = \beta A \Delta X_m, \quad (2)$$

Where Q is heat flow W, α is heat transfer coefficient in W/m²K. M mass flow in kg/s, β is mass transfer

coefficient in $\text{kg}/(\text{m}^2\text{s})$, A is the surface area in m^2 , ΔT in $^\circ\text{C}$ and ΔX in g/kg are the average temperature, and humidity differences between air and TCF is the absolute humidity. The absorption process takes place once the humid air comes into contact with the concentrated hygroscopic TCF, if the air humidity is higher than the equilibrium level. As a result, the TCF absorbs the humidity until the equilibrium level is reached. The phase change from water vapor to water releases latent heat. The outcomes of this process are hot dried air and diluted TCF. The transfer of this heat between the air and TCF depends on the flows, conductivities, thermal capacities, and the initial conditions of both the air and TCF.

On the other hand, in Figure 1b, the desorption process takes place as soon as the dry air comes in contact with the diluted TCF and if the relative air humidity is lower than the equilibrium level. As a result, TCF desorbs the humidity to reach the equilibrium state and takes in heat during the phase change from water to water vapor—water evaporation. The outcomes of this process are humid warm air and concentrated TCF.

Figure 1: a) absorption and b) desorption processes.

The performance varies from one absorber design to another, based on the packing surface form and material. The absorber geometry and the air flow direction are as presented by Chung, Ghosh, and Hines (1996), and Sadasivam and Balakrishnan (1991). Moreover, it relies on the ratio between both TCF and air flow.

Thermochemical fluids

By means of experiment and analysis of several salt solutions or thermochemical fluids (TCFs), the physical and thermochemical properties were written as a function of temperature and concentration.

$\text{MgCl}_2\text{-H}_2\text{O}$ and $\text{LiCl-H}_2\text{O}$ were evaluated in order to have a comparison of fluids already used in absorption processes, and representing candidates for TC district heating and cooling networks. However, in Modelica, the $\text{LiCl-H}_2\text{O}$ model was used at lower concentration to meet the heat capacity of $\text{MgCl}_2\text{-H}_2\text{O}$.

System Description

Technical Equipment and Material of TC Technology

The main equipment used in the TC process are defined based on two major processes: 1) The absorption process, where it is used at the demand side for heating and cooling applications; and 2) the desorption process, where it is

used at the supply side for TCF regeneration (concentration). The equipment required is:

Absorber/Desorber: A device that provides a direct exchange surface between the TCF and air to achieve the absorption or desorption processes. The TCF flow is always driven by gravity from the top to the bottom, while in this study the air flow ran in the opposite direction to the TCF.

Concentrated/diluted TCF: TCFs exploit the hygroscopic properties of a salt solution as a function of temperature and concentration for the absorption of moisture from the air. This occurs until its vapour pressure reaches equilibrium with the incoming air.

Fan/pump: In this study, both a fan and a pump were required to move the TCF and air, respectively, using on-off controls.

TCF–TCF/air–air heat exchangers: This is a device used to transfer the heat between two fluids. The heat exchanger effectiveness in this work was taken to be 80%.

Humid air source: There are many humid air sources, such as greenhouses, swimming pools or humidifiers.

Indirect adiabatic evaporator: The main principle of the indirect evaporator is that the outside surface is kept wet. Once the exterior air passes over this surface, the water evaporates and the outside surface cools. As a result, the interior hot air next to the inside surface cools down, but without increasing its humidity.

First scale—system description of the applications

Building heating application: The design of this model is based on the initial design presented by (Geyer, 2018). Here, the model is developed by adding more components to increase the efficiency. We also consider a dynamic simulation, where the outdoor conditions are applied to the building model. Moreover, a TCF storage tank model was added in order to use the concentrated TCF until it becomes diluted. Consequently, the same TCF will be used in the absorption process until the concentration drops to a level that cannot generate a significant amount of heat, for example, from 30% to 27%. As shown in Figure 2, the space heating model consists of two parts. The TCF part contains the components that use the TCF as a medium. The air part contains the components that use the air as a medium. The first part contains the components *Supply and Return TCF* from the network, *Heater* for TCF preheating, and *TCF Storage tank*. The second part contains the components *Humid air source*, *Heat exchanger*, and *Building*. Both partial streams meet in the absorber to achieve the absorption process. Moreover, a snapshot at time t during the heating period of the components variable values of the building heating case is presented in the same figure.

Building space cooling application: There are several space cooling designs that use the principle of evaporative cooling with TCF system. They have been presented by Geyer (2018), and Kim (2015). In this work we present an alternative design for space cooling using evaporation and TC technology.

Figure 2: System model of building space heating application.

Figure 3: System model of Building space cooling application

Figure 4: TC district network components

Similar to the space heating application, the system consists of two parts, a TCF part and an air part, as shown in Figure 3. In this work we present an alternative design for space cooling using evaporation and TC technology. Similar to the space heating application, the system consists of two parts, a TCF part and an air part, as shown in Figure 3. The first part only contains *Supply and Return TCF* from the network. The second part contains the *Heat exchanger* component used to precool the incoming air (the relative humidity increases to a suitable level for the absorption process, as the air is already humid during summer), *Indirect evaporator*, and *Building*. Both partial streams meet in the absorber to realize the absorption process. A snapshot at time t during the cooling period of the components variable values of the building cooling case are presented in Figure 3.

The second scale—system description of TC district network

TC district network TCF storage: The TC district network system, as shown in Figure 4, consists of three parts and connects the first scale with the second scale. The components are as follows. 1) Supply side: the main pieces of equipment are the *desorber*, *heat exchanger* and *heat source*, the latter of which comes from an industrial source in this case. 2) Demand side: including the building heating and cooling applications. 3) The pipe network and TCF storage transports the TCF from a heat source, to TCF storage, then to the buildings. The main advantage of using a TC district pipe network is the possibility of transporting excess heat and hygroscopic properties for long distances from the supply to the

demand sides without heat loss, because the heat is stored as latent potential. The values presented in Figure 4 represent the TC district network component variable values range during the heating and cooling period.

Methodology and Modelling and Simulation Approach

To determine the potential of TCF and absorption technology, a large simulation model of a TC district network was developed, covering the whole network. This simulation approach requires multiservice modelling based on applications such as heating and cooling. To create the district network model, the pipe network models connect the first level nodes. The models and submodels were developed based on applications from the object-oriented language “Modelica” Modelica Association (2017) and the IDEAS library (Baetens, 2015). These libraries are suitable for dynamic simulation of a district network as they are flexible and able to use multidomain modelling.

Modelica component model description and boundary conditions

Modelica absorber/desorber model: This component was modelled by a finite volume model, with a counter-flow configuration, it was developed by Fürst and Kriegel (2016). The model was based on correlations developed for heat and mass transfer coefficients derived from experimental data. It is represented by a nonlinear regression, as presented by Chen, Zhang and Yin (2016).

Modelica TCF models: The dynamic medium Modelica model of $\text{MgCl}_2\text{-H}_2\text{O}$ developed in this work to use it with the absorber model for the absorption process is based on the work of ZHAW laboratory. The experimental equations for the thermodynamic properties of temperature, concentration, and enthalpy were not validated in this work. Therefore, $\text{LiCl-H}_2\text{O}$ Modelica model was used at lower concentrations to meet the heat capacity of $\text{MgCl}_2\text{-H}_2\text{O}$. The $\text{LiCl-H}_2\text{O}$ model has already been developed by Fürst and Kriegel (2016), based on the thermodynamic properties and its equations, as presented by Pátek and Klomfar (2008).

Modelica humid air source model: We considered a constant humid warm air model based on the average temperature and humidity of a green house, which are around 16.5 °C and 80% respectively. In future work, a derived greenhouse dynamic model will be considered.

Modelica fan/pump model: The fan and pump models are for a centrifugal pump or fan with ideally controlled mass flow rate or pressure. They are already available in the Modelica library Modelica Association (2017).

Modelica heat exchanger models: The heat exchanger model is based on a constant effectiveness, where it transfers an amount of heat $Q = Q_{\max} \cdot \varepsilon$, where ε is a constant effectiveness and $Q_{\max}$ is the maximum heat that can be transferred.

Modelica building model: To develop a set of models that are representative for a typical building stock, we

modelled several building configurations with different insulation types and different floor area sizes, to cover several heating and cooling demands. The outdoor temperature during the heating period (October to April) was taken from the weather data of Brussels, Belgium, while the outdoor temperature during the cooling period (June to August) was taken from the weather data of a random city that has a real summer like Madrid, Spain. Table 1 shows the building model conditions.

The weather data was chosen from two city because the heating and cooling are considered as two different cases with real conditions regardless the city. Thus, Brussels was chosen for heating case as the study run in Belgium, and because there is no need for cooling there, Madrid was chosen for cooling application as it is warm.

Table 1: Building characteristics and conditions.

Building Set	No. of Buildings	Volume, m ³	Heating Demand, MWh	Cooling Demand, MWh	Specific Heating, Cooling Demand, kWh/m ² a
1	2	540	11.8	8.3	122/86
2	2	540	14.4	8.6	149/89
3	1	350	18.6	8.4	248/134
4	1	540	10.2	7.9	106/82
5	1	400	10.7	8	150/112
6	3	700	10.1	8.1	81/65

Modelica indirect evaporator model: This model performs as a heat exchanger with 75% efficiency. The first air stream uses the outgoing air from the building to evaporate the water from the outside surface and cool it down. The second air stream comes from the absorber to make contact with the cold surface and cool it down without gaining humidity; it then goes into the building.

Modelica application models and simulation approach

Space heating Modelica model and Operation mode: Figure 5 illustrates the Modelica model of the air and TCF flow modes for the space heating model, which consist of the following.

Air cycle operation mode: As shown Figure 5, The humid warm air is provided from a *constant humid air source*. The incoming air temperature is around 16 °C and the relative humidity around 80%, The humid warm air is move by *Fan1* to the air–air *heat exchanger* with a defined air flow, which depends on the maximum heat demand, the size of the building, and the design of the absorber. In this case, the air flow is around 2 to 3 kg/s. As a result, the temperature of the humid warm air increases typically 2–3 °C because of exchange of heat with the warm outgoing air from the building. Next, the preheated humid air enters the *Absorber* to exchange heat and humidity with the TCF. Therefore, the preheated humid warm air releases humidity and gains heat because of the absorption.

Figure 5: Illustration of the air and TCF flow modes in the Modelica space heating model.

Figure 6: Illustration of the air and TCF cycle operation modes in the Modelica space cooling model.

Finally, the heated warm air goes to the *Building* for heating, with a final temperature of between 21 and 24 °C. However, there is another fan, *Fan2*, to provide fresh air to building at a very low rate of flow. Both fans are controlled by the indoor thermostat to maintain the indoor temperature at between 20 and 22 °C.

TCF cycle operation mode: As shown Figure 5, TCF enters the demand side from the pipe network with the outdoor TCF temperature around 4–6 °C and 30% concentration. The network supply pump *pump1* moves the TCF to a *Heater* to preheat it to around 18 °C. Next, the preheated TCF enters the TCF *Storage tank* to guarantee supply TCF to the tank with a set initial temperature, to have an efficient absorption process. The TCF temperature should be between 18–20 °C. Once the tank is full, the network supply pump *pump1* stops and the *local pump* works to move the TCF to the *Absorber*, to absorb the humidity from the humid air and release heat. As a result of this absorption process, the TCF concentration—circulated via the storage tank—decreases. This operation lasts until the concentration of the TCF in the tank reaches the lower limit of 27%. At this point, the *local pump* stops and the network return *pump2* transports the diluted TCF to the network to reconcentrate it at the supply side. The network supply *Pump1* delivers newly concentrated TCF from the pipe network. Both *Pump1* and *Pump2*, are controlled by a TCF concentration sensor; they open when the TCF concentration is below 27% and close when the TCF concentration is above 30%, and vice versa for the *local pump*.

Space cooling Modelica model and operation mode:

The air and TCF cycles in the cooling case are, in principle, similar to the heating absorption process, although the main purpose is to absorb humidity from the air while rejecting heat. Thus, the TCF concentration should be lower than the heating case, to avoid releasing greater amount of heat at high concentration, which is not required in the cooling case. Thus, the TCF concentration is considered to be 27% in this study Figure 6, illustrates the Modelica model of the air and TCF flow modes for the space cooling model, which consist of the following.

Air cycle operation mode: As shown Figure 6, the initial incoming air temperature is around 33 °C and the relative humidity is 50%, which is equivalent to the outdoor temperature and humidity during the cooling period. The hot humid air is moved by the *Fan* to the air–air *Heat exchanger* with a defined air flow that depends on the maximum cooling demand and the size of the building. In this case, the air flow is around 1.5 to 3 kg/s. As a result, the temperature of hot humid air decreases to around 25.3 °C, because of exchange of heat with the cold outgoing air from the building. Next, precooled humid air enters the *Absorber* to exchange heat and humidity with the TCF. Therefore, the precooled humid air releases humidity and gains heat during absorption process; the temperature, relative humidity, and absolute humidity become respectively around 26.5 °C, 57%, and 12.3 g/kg. Afterwards, the precooled dry air goes to the *indirect evaporator* to cool down the precooled dried air without exchanging humidity. Finally, the cold air with temperature around 20–21 °C and relative humidity around 70% goes to the *Building* for cooling. The *Fan* is

controlled by the indoor thermostat to maintain the indoor temperature at between 20 and 23 °C.

TCF cycle operation mode: As shown Figure 6, TCF enters the demand side from the pipe networks with ~26 °C outdoor temperature and 27% concentration, where the network supply pump *pump1* moves the TCF to the *Absorber*, to absorb humidity from the humid pre-cooled air and release heat. As a result of this absorption process, the TCF concentration decreases and it goes back to the pipe by network return pump *pump2* to reuse it with another building or reconcentrate it on the supply side. Both *Pump1*, *Pump2*, are controlled by indoor thermostat to maintain the indoor temperature at between 20 - 23 °C.

Modelica TC district network simulation approach:

The TC district network Modelica model contains the pipe network and the demand side consisting of 10 different buildings with different heating and cooling demands, and sizes, as presented in Table 1. This number of buildings was chosen to cover different heat demands and building characteristics. In addition, there are two large external TCF storage tanks connected to the pipe network, as shown in Figure 7, to supply and return the TCF to and from the supply and demand sides.

Figure 7: Illustration of TC district network in Modelica.

To transfer the heating energy from the supply side to the demand side, we used the TCF as carrier, to store the thermal energy as latent heat. Therefore, it does not matter how far the distance between the supply and demand sides is, as there is no heat loss because the pipe model deals only with pressure loss and flow. To define the total TCF mass flow profile and total TCF, mass and therefore pumping energy, a full simulation model of the TC district network was run. However, running the simulation with the full physical component models of the TC district network and with such a large number of buildings can take few days, as there are many complex models, which makes the simulation time longer. Therefore, another approach was applied, as shown in the Figure 8. By running individual simulations for the heating and cooling applications, we could obtain the heating and cooling demand, as well as the supplied heat to the buildings. As a result, the TCF mass flow profiles were defined and the data model with these mass flow profiles were used in the TC district network model to obtain the total pumping energy and total TCF mass.

Figure 8: Model and simulation approach of a simplified TC district network.

Simulation Results and discussion

Simulation results for the space heating application

The simulation results during the heating period from October to April demonstrated the hygroscopic and heating potential of using TC technology during the absorption process. Figure 9 and Figure 10 show the temperature and relative humidity before and after the absorber, and the indoor temperature and its relative humidity during three days in January, taking *building 5* as an example (see Table 1).

Figure 9: Indoor/outdoor temperature, Air temperature before/after the absorber during three days in January.

Figure 10: Relative humidity of indoor air, and before/after the absorber for three days in January.

The outdoor temperature oscillates between 7 and -8°C . The temperature difference before and after the absorber becomes around 2°C , while the relative humidity drops from 70% to 55%. However, the indoor temperature and its relative humidity are maintained to between $\sim 19.8^{\circ}\text{C}$ to $\sim 22^{\circ}\text{C}$ and 55% to 65%, respectively. Also it is clear that the indoor temperature drops quickly in some periods, the reason behind that is because the main heat source is coming from the ventilation air after the absorber, thus once the temperature after the absorber drops, the indoor temperature drops as well, to solve this problem a better control strategy is needed, which will be developed in the future work.

Figure 11: TCF tank concentration during three days in January.

Figure 12: supply pump mass flow of three days in January.

Figure 11 shows the concentration in the TCF tank. Because of the absorption process, the concentration drops from 30% to 27.5% over the course of about 10 hours, with the dropping period varying based on the tank size and heating load. However, it takes only 0.5 hour to evacuate the diluted TCF and fill it with a newly concentrated TCF. Figure 12, shows the network supply pump mass flow during three days, with a maximum mass flow of 1.5 kg/s. The maximum air mass flow in *building 5* was 2 kg/s, while the maximum TCF mass flow was 0.3 kg/s. The fan is controlled by the indoor thermostat setpoint between 19.5°C and 22°C , and the local pump is controlled by the tank concentration sensor with setpoint between 0.3 and 0.275 concentration.

Space cooling application results

The simulation results represent the cooling period from June to August. Figure 13 and Figure 14 show the temperature and the absolute humidity of the cooling system components of *building 5* during three days in August (see Table 1). The initial outdoor temperature and absolute humidity were 31°C and 12 g/kg, respectively. It is obvious that the temperatures and the absolute humidities changed based on the heat or mass exchange process. Whereas the air temperature decreases because of the heat exchanger from the initial outdoor temperature to the temperature before the absorber, it increases a little after the absorber while the absolute humidity decreases. It is obvious that the temperatures and the absolute humidities changed based on the heat or mass exchange process. Whereas the air temperature decreases because of the heat exchanger from the initial outdoor temperature to the temperature before the

absorber, it increases a little after the absorber while the absolute humidity decreases.

Figure 13: Air temperature of indoor air, before/after the absorber and after the evaporator for three days in August

Figure 14: Absolute humidity of indoor air, before/after the absorber and after the evaporator during three days in August

Then, the air temperature drops again without exchanging humidity after the evaporator because of the indirect evaporation. Finally, both air temperature and absolute humidity increase, with the indoor air to be maintained at between 21°C and 25°C , and 9.6 g/kg to 9.8 g/kg respectively, with relative humidity 63% to 50%

TC district network simulation results

Figure 15 shows the total heating energy supplied to the buildings, total energy used by the fans, and the local pumps' energy consumption for the buildings of the TC district heating network.

Figure 15: Total supplied heat energy and total fan and local pump energy during heating period.

It is obvious that the total supplied heat energy is sufficient to cover the 10 buildings heat demand (Table 1). The total electrical energy consumption of fans and local pumps energy to produce the supplied heat energy, are 16%, 0.007% respectively.

The entire TC district heating network is controlled by the concentration sensors in the TCF tanks.

The energy density of the TCF depends on the concentration, concentration difference during the absorption process, the TCF and Air flow and the ratio between them. For example, the energy density of the TCF for the building 5 is around 65 kW per ton, the concentration difference is from 30% to 27.5%, the TCF and air flow and the ratio between them are 0.3 kg/s, 2 kg/s and 0.15, respectively. However, by increasing the TCF concentration difference the energy density will increase as well, by optimize the system, which could be the case in the future work.

Figure 16 shows the total supplied cooling energy or the used dehumidification energy in the absorber and total fans and local pumps energy consumption of the TC district cooling network. The total supplied cooling energy was sufficient to cover the 10 buildings' demands (Table 1). The total electrical energy consumption for the fans and local pumps to produce the supplied cool or dehumidification energy of the absorber were 30% and 0.04%, respectively.

Figure 16: Total supplied cooling energy and total fan and local pump energy during the cooling period.

The energy consumption of the local pumps in cooling case was higher than the heating case because of the need to pump more TCF mass to meet the cooling requirements. The entire TC district cooling network was controlled by the building thermostat sensors.

The curves in both Figure 15 and Figure 16 seem to be linear. However, it is not linear and there are sudden increments of the energy curve; they do not appear in these plots because the time step is quite large.

Conclusions

This paper investigates a multiscale modelling and simulation approach at the level of applications on the demand side, and the level of the district network that transfers TCF to the first level. Moreover, the total energy consumptions of the demand side pumps and fans are evaluated with supplied heat or cooling energy.

The simulation results of the first level, which contains the heating application, demonstrated the benefit of using the hygroscopic and heating/cooling potential of TC technology. The produced heat in the absorption process was sufficient for the demand side of the TC district network sector with specific initial conditions. Similarly, the space cooling application demonstrated the benefit of using TC technology with an evaporative cooling design,

mainly by reducing of the humidity during the absorption process. However, the results show that in some moments the indoor temperature increases or decreases above or below the temperature set-point. The main reason behind that is the need to use a better control.

The simulation results of the second level, which contains the TC district heating and cooling networks, showed the feasibility of using two levels. The simulation data results of the first level were used to form the TC district heating and cooling network model. The simulation time for this simplified TC district network model is quite fast comparing with running a full physical TC district network model simulation over an entire year, which was estimated to take more than 6 days for 10 buildings. Based on the results, the total network pumping energy and the total TCF mass were defined.

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