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ECC Refrigerator: Develop a system model using electrochemical (ECC) compressor and metal hydride (MH) heat exchangers- FY18 2nd Quarter Milestone Report

Bo Shen

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FY18 2nd Quarter Milestone Report

ECC Refrigerator: Develop a system model using ECC compressor and MH heat exchangers

Authors
Bo Shen

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Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831-6283
managed by
UT-BATTELLE, LLC
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Develop a system model using ECC compressor and MH heat exchangers
(Regular)

Executive Summary

This report describes equations for modeling electrochemical compressors and metal hydride heat exchangers. We developed two new component models into the HPDM model library. Two system simulations were conducted, one was a water heating system using LaNi5, and the other was a refrigeration system using V0.85Ti0.1Fe0.05. The simulations demonstrated that COPs of the electrochemical compression systems decreased drastically with increasing the electric current and capacity, due to reduced electrochemical compression efficiency at larger ohm resistance loss. Cyclic loss caused by the metal hydride and heat exchanger mass had a secondary effect on the system efficiency. Elimination of the heat exchanger cyclic loss could enhance the water heating COP of the LaNi5 system by 12% and increase the refrigeration COP of the V0.85Ti0.1Fe0.05 system by 7%.

Introduction

An electrochemical compression system is much different from a typical vapor compression system. It uses an electrochemical compressor to drive hydrogen and uses metal hydride powder to absorb and desorb hydrogen. When metal hydride absorbs hydrogen, it discharges heat to the environment; during the desorption process, it obtains heat from the surrounding. For this work, we added the electrochemical compressor and metal hydride heat exchanger models to the model library of ORNL HPDM, and reuse its system solving scheme and component-based platform.

Electrochemical Compressor Model

In an electrochemical compressor (ECC), the hydrogen flow is driven by the electrical current, which can be calculated using Faraday's Law [1],

$$\frac{dn}{dt} = \frac{I}{2F} \qquad (1)$$

Where *dn/dt* is the hydrogen molecule flow rate through the membrane, *I* is the electrical current, *F* is Faraday's number. It can be seen that the hydrogen flow rate is not affected by the inlet and outlet pressures.

The electrical voltage across a membrane consists of three parts,

$$U = U_{Nernst} + U_{ohm} + U_{ac} \qquad (2)$$

Where U_{Nernst} is Nernst potential, i.e. the actual force driving the hydrogen flow. U_{ac} is caused by the anode and cathode polarization, which is usually negligible for an ECC compressor using membranes. U_{ohm} is caused by the electrical resistance in the membrane, which is a loss factor and converts electrical energy to heat.

$$U_{ohm} = I \times R_i \qquad (3)$$

Where R_i is the internal electrical resistance of the membrane.

$$U_{Nernst} = \frac{R \times T_{EC}}{2F} \ln\left(P_{dis}/P_{suc}\right) \qquad (4)$$

Where R is the gas constant, T_{EC} is the ECC compressor's process temperature [K]. P_{dis} is the compressor's discharge temperature and P_{suc} is the suction pressure.

Thus, the electrochemical efficiency of the compressor is defined as Equation (5).

$$\eta_{EC} = U_{Nernst}/(U_{Nernst} + U_{ohm}) \qquad (5)$$

At constant suction and discharge pressures, U_{Nernst} doesn't change, while U_{ohm} increases with the current. Thus, η_{EC} decreases with increasing the electric current.

The total voltage and power consumption of an ECC compressor is a function of its electric current, equivalent to its hydrogen flow rate. They are insensitive to the suction and discharge pressures. Usually, an ECC compressor is characterized by a polariton curve, i.e. the total voltage as a function of the input current, in the form of polynomials, an example is given as below, which represents a prototype electrochemical compressor, provided by Xergy INC.

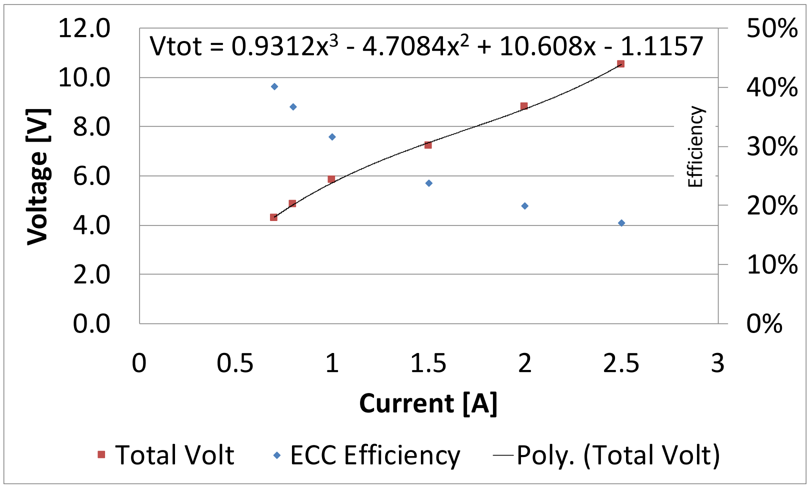


Figure 1: ECC Compressor's Total Voltage and Efficiencies Changing with Electric Current.

Metal Hydride Heat Exchanger Model

Metal hydrides are widely used to store hydrogen in automobile and power industries. As shown in the figure below, some alloys can be bonded with hydrogen and form metal hydrides. With increasing the hydrogen concentration, the material bond goes through the α phase, similar to the subcooled state of a refrigerant; in the α+β phase, the absorption/desorption temperature at a given plateau pressure doesn't change, similar to the two-phase state of a pure refrigerant; in the β phase, the hydride's temperature increases with the concentration, like the superheat state of a refrigerant. Major energy transfer of hydrogen absorption/desorption occurs in the α+β phase. The energy change is defined as formation heat absorbed per mole of hydrogen.

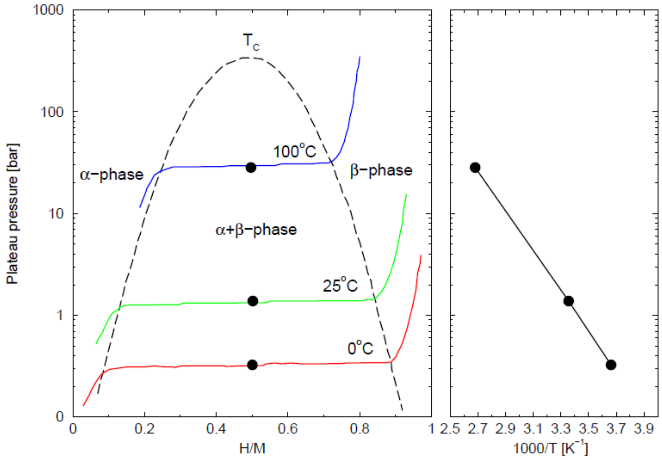


Figure 2: Left: Pressure-Composition-Isotherms (PCI) for a hypothetical metal hydride. Right: Van't Hoff's plot for a hypothetical metal hydride derived from the measured pressures at plateau midpoints from the PCI's, from Reference Andreasen (2004) [2].

During the absorption and desorption processes, the relationships between the hydrogen pressure and temperature are given in Equation (6) for desorption and Equation (7) for absorption, as introduced in Reference [1].

$$ln(P_e) = \frac{\Delta H}{RT_{process}} - \frac{\Delta S}{R} + f_s(C - C_{eq}) - \ln\left(\frac{P_a}{P_d}\right)_{T_{process}} \tag{6}$$

$$ln(P_c) = \frac{\Delta H}{RT_{process}} - \frac{\Delta S}{R} + f_s(C - C_{eq}) + \ln\left(\frac{P_a}{P_d}\right)_{T_{process}} \tag{7}$$

Where P_e is the desorption (evaporating) pressure [atm], and P_c is the absorption (condensing) pressure [atm]. ΔH is the formation heat per mole H_2, equivalent to latent heat of a refrigerant. ΔS is the formation entropy change. $ln(P_{e,c}) = \frac{\Delta H}{RT} - \frac{\Delta S}{R}$ is Van't Hoff's equation, to calculate the midpoint of plateau pressure. f_s is the plateau slope factor and $(C - C_{eq})$ is the change of hydrogen content in the MH alloy. $\ln\left(\frac{P_a}{P_d}\right)$ is the hysteresis factor at a given absorption/desorption temperature, $T_{process}$. The hysteresis factor causes lower pressure during desorption and higher pressure during absorption, in comparison to the midpoint plateau pressure predicted by Van't Hoff's equation.

In a MH heat exchanger, the absorption/desorption temperature is dictated by the heat exchanger effectiveness, which is calculated using a UA-LMTD method as shown in Equation (8).

$$Q = UA * \frac{(T_{ci} - T_{process}) - (T_{co} - T_{process})}{\ln\left[\frac{(T_{ci} - T_{process})}{(T_{co} - T_{process})}\right]} \tag{8}$$

Where Q is the heat transfer rate, UA is the heat transfer unit number of the MH heat exchanger. T_{ci} and T_{co} are the coolant inlet and outlet temperatures. The energy change rate at the coolant side is given in Equation (9).

$$Q = \dot{m}_c Cp_c (T_{ci} - T_{co}) \tag{9}$$

Where $\dot{m}_c$ is the coolant mass flow rate, Cp_c is the specific heat.

A MH alloy is a solid refrigerant, switching its role from evaporation to condensation, and thus, cyclic loss, due to the MH and heat exchanger mass, has to be considered. The energy balance at the MH side is given in Equation (10).

$$Q = \dot{m}_{H_2} \Delta H_{mass-based} - (\dot{M}_{MH} Cv_{MH} + \dot{M}_{HX} Cv_{HX})(T_{process} - T_{balance}) \tag{10}$$

Where $\dot{m}_{H_2}$ is the hydrogen mass flow rate, $\Delta H_{mass-based}$ is the formation heat per unit hydrogen mass flow rate, $\dot{M}_{MH}$ and $\dot{M}_{HX}$ are the switched mass rates of the MH alloy and heat exchanger, respectively, incurred along with the hydrogen mass flow rate. Cv_{MH} and Cv_{HX} are the specific heat of the MH alloy and the heat exchanger material, respectively. $T_{balance}$ is the system balance temperature when the ECC compressor is off. The required $\dot{M}_{MH}$ is determined by the absorption mass ratio of hydrogen in the alloy, i.e. $\dot{M}_{MH} = \dot{m}_{H_2}/H_2MassRatio$. $\dot{M}_{HX}$ is the heat exchanger mass switched with the alloy.

Simulation Cases

Various MH alloys are suitable for hydrogen compression system. It shall be noted that formation heat ranges from 20 to 50 kJ/mole H_2. Larger formation heat and hydrogen mass ratio absorbed by a MH alloy lead to higher system efficiency. The condensing and evaporating temperatures (pressures) don't directly impact the ECC compressor power consumption, but, affect the cyclic loss due to switching the MH alloy and heat exchange mass between the desorption and absorption. We assessed two cases, one uses LaNi5 for water heating, and the other uses V0.85Ti0.1Fe0.05 for refrigeration. The table below depicts their properties.

Table 1: Properties of LaNi5 for water heating and V0.85Ti0.1Fe0.05 for refrigeration

	ΔH	ΔS	T_L	T_H	P_L	P_H	P_a/P_d	Cv_{MH}	H_2 Ab Ratio
Unit	kJ/molH2	kJ/molH2/K	C	C	atm	atm	-	J/kg/K	-
LaNi5	31.8	110.0	25	200	1.49	171.9	1.25	440	1.5%
V0.85Ti0.1Fe0.05	42.9	148.0	-20	100	0.08	53.14	2.0	440	1.5%

In the table, T_L and T_H are minimum and maximum working temperatures of one alloy. P_L and P_H are the corresponding pressures. H_2 Ab Ratio is the hydrogen absorption mass ratio in an alloy. f_s in Equations (6) and (7) was treated as zero.

We used the polarization curve shown in Figure 1. The ECC cycle consists of two operations. During one operation, the ECC compressor drives the hydrogen flow and generates cooling/heating capacity; in the other operation, the ECC compressor is off, when the MH alloy and heat exchangers recover to a balance temperature of 80°F, i.e. the surrounding air temperature. It is assumed that each period takes half of the cycle time.

When running the water heating (WH) cycle using LaNi5, the evaporating/desorption temperature was controlled at 77°F, and the condensing/absorption temperature varied from 120°F to 180°F. Figures 3 and 4 illustrate the water heating COP and capacity changing with the driving electric current and absorption temperature. We assumed that the cyclic loss caused by the heat exchanger mass was equal to that of the MH alloy, i.e. $\dot{M}_{MH}Cv_{MH} = \dot{M}_{HX}Cv_{HX}$. It can be seen that, the WH capacity increases proportionally with the driving current, however, the WH COP degrades significantly. The rising absorption temperature minorly impairs the COP and capacity, due to the increased cyclic loss.

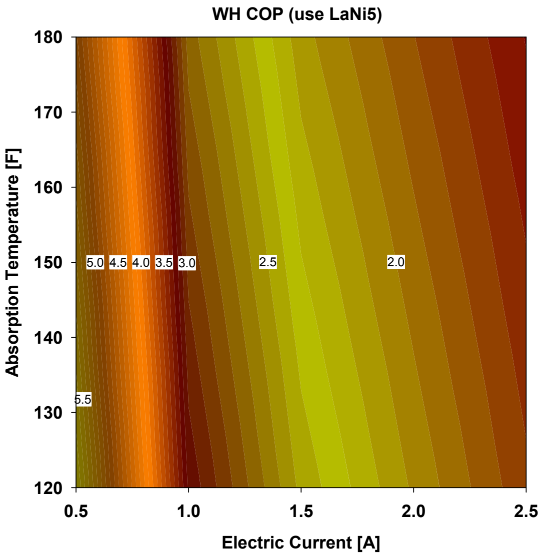


Figure 3: water heating COP (LaNi5) changing with driving electric current and absorption temperature

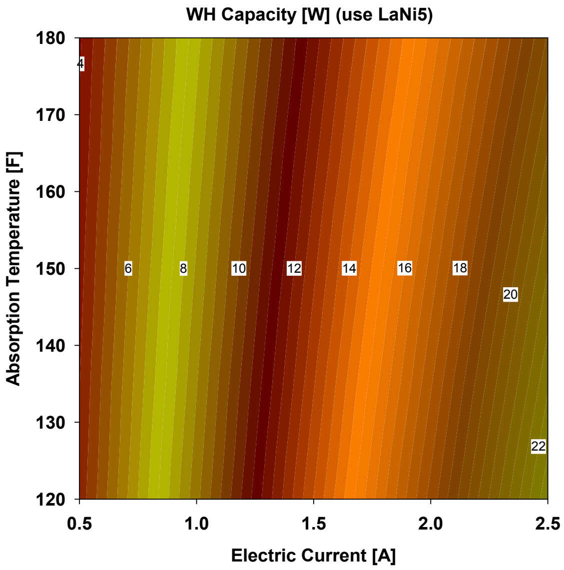


Figure 4: water heating capacity (LaNi5) changing with driving electric current and absorption temperature

When running the refrigeration cycle using V0.85Ti0.1Fe0.05, the condensing/absorption temperature was controlled at 100°F, and the evaporating/desorption temperature varied from 0°F to 30°F. Figures 5 and 6 illustrate the refrigeration COP and capacity. It was assumed that the cyclic loss caused by the heat exchanger mass was equal to that of the MH alloy. In the figures, the refrigeration capacity increases proportionally with the driving current, however, the refrigeration COP degrades significantly. The decreasing desorption temperature impairs the COP and capacity in a less noticeable way.

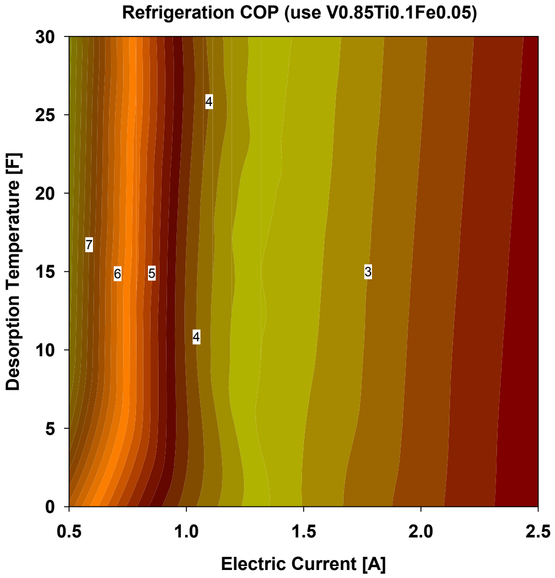


Figure 5: refrigeration COP (V0.85Ti0.1Fe0.05) changing with driving electric current and desorption temperature

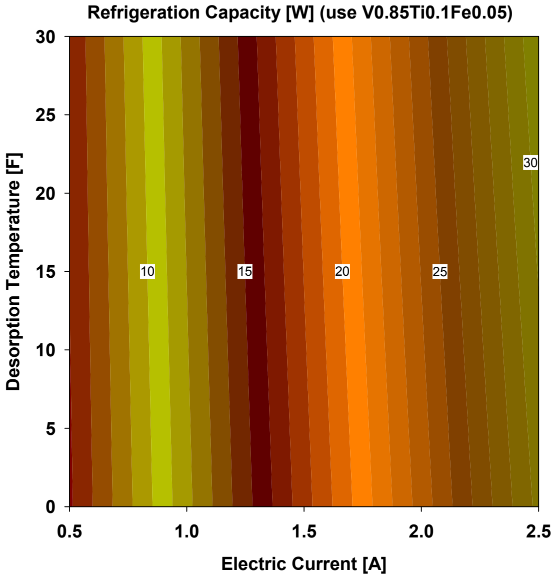
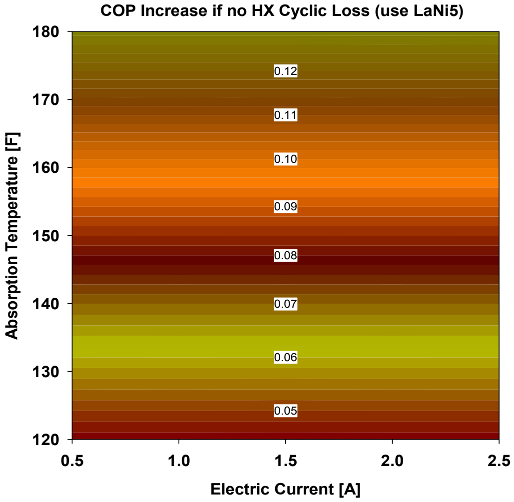


Figure 6: refrigeration capacity (V0.85Ti0.1Fe0.05) changing with driving electric current and desorption temperature

In Figures 7 and 8, we evaluated the effect of cyclic loss due to the heat exchanger mass. Gains in COPs were predicted for the WH system and refrigeration system when the heat exchanger cyclic loss was eliminated. The simulations demonstrate that the COP of the WH system can be enhanced by 12% at the highest absorption temperature, and the COP of the refrigeration increases by 7% at the lowest desorption temperature.



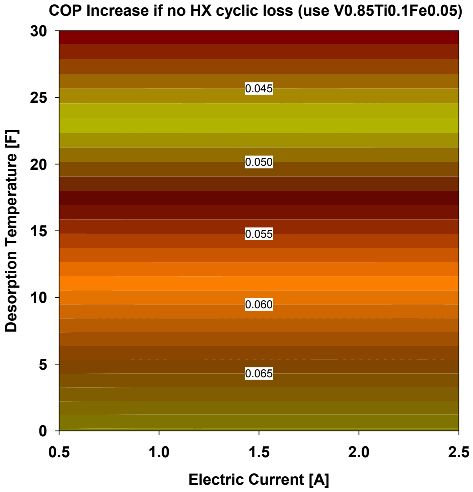


Figure 7: water heating COP increase (LaNi5) changing with driving electric current and absorption temperature, assuming no cyclic loss of heat exchanger

Figure 8: refrigeration COP increase (V0.85Ti0.1Fe0.05) changing with driving electric current and desorption temperature, assuming no cyclic loss of heat exchanger

Summary

We developed new component models for ECC compressors and MH heat exchangers. Two system simulations were conducted, one was a water heating system using LaNi5, and the other was a refrigeration system using V0.85Ti0.1Fe0.05. The simulations demonstrated that COPs of the electrochemical compression systems decreased drastically with increasing the electric current and capacity, due to reduced electrochemical compression efficiency at larger ohm resistance loss. Cyclic loss caused by the metal hydride and heat exchanger mass had a secondary effect on the system efficiency. Elimination of the heat exchanger cyclic loss could enhance the WH COP of the LaNi5 system by 12% and increase the refrigeration COP of the V0.85Ti0.1Fe0.05 system by 7%.

References

[1] Ye Tao, Hoseong Lee, Yunho Hwang, Reinhard Radermacher, Chunsheng Wang, Electrochemical compressor driven metal hydride heat pump, In International Journal of Refrigeration, Volume 60, 2015, Pages 278-288, ISSN 0140-7007

[2] Andreasen, A. (2004). Predicting formation enthalpies of metal hydrides. (Denmark. Forskningscenter Risoe. Risoe-R; No. 1484(EN))., http://orbit.dtu.dk/files/7711359/ris_r_1484.pdf