MODELLING AN ADSORPTION SYSTEM FOR THE SEASONAL STORAGE OF HEAT IN RESIDENTIAL BUILDINGS

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ABSTRACT
A mathematical model of an adsorption storage unit has been developed and implemented into the ESP-r simulation environment. This paper briefly describes the mathematical model of the adsorption storage unit, its implementation in the ESP-r simulation program and the comparison of model results with published data. A case study of a house whose thermal requirements are met by a fuel cell cogeneration system coupled to a hot water tank for short term storage and an adsorption storage unit for long-term storage is presented in this paper. The overall performance of the proposed system, predicted by ESP-r, is presented, and conclusions are made with respect to model limitations and the long-term performance of coupling fuel cells and adsorption thermal storage systems.

INTRODUCTION
The research and development of new technologies to improve the efficiency of the energy use in buildings are important to help Canada meet its international commitment under the Kyoto protocol. The government of Canada has committed to reducing greenhouse gas emissions to six percent below 1990 levels during the first commitment period 2008-2012.

Residential fuel cell co-generation systems are an emerging technology and are considered as energy efficient alternatives to power and heat our homes. Ideally, fuel cell systems can satisfy all annual electric and thermal loads of a house, thereby increasing the overall efficiency of the cogeneration system. However, (Beausoleil-Morrison et al., 2002) have suggested that such systems can generate excess heat in the summer and do not generate sufficient heat in the winter if they are controlled to respond primarily to a house’s electrical demand. The mismatch in heat supply and demand can possibly be solved by the seasonal storage of heat. Adsorption storage systems seem advantageous since they can store a greater amount of energy per unit volume than sensible heat storage systems.

The adsorption process is a physico-chemical process that can be used to store heat. An adsorption storage unit essentially contains the following components: a container which contains the adsorbent, commonly referred to as the adsorber, a container that acts as a condenser or an evaporator, a valve and a pipe that connects the adsorber with the condenser/evaporator. The working principle of an adsorption storage unit can best be described by its three stages: charging, storage and discharge. Figure 1 illustrates the charging and discharge stages.

At the start of the charging process, the valve between the adsorber and the condenser/evaporator is closed and the adsorbent is wet, i.e. it contains the maximum amount of adsorbate vapour within its pores. As heat is supplied to the adsorber, via a fluid through the adsorber’s heat exchanger, the temperature and pressure in the adsorber increases, while the ratio of mass of adsorbate to mass of adsorbent remains constant (this stage is referred to as the isosteric heating of the adsorbent). When the adsorber pressure reaches the condenser pressure, the valve between the adsorber and the condenser is opened. Desorption of the adsorbent occurs and the vapour that is desorbed is directed to the condenser, where it is converted to liquid form. The charging process continues until the adsorber is dry, i.e. it contains the minimum amount of adsorbate vapour within its pores. The valve is now closed. The heat of condensation that is released as the adsorbate is condensed can be rejected or used. During the storage stage, the liquid adsorbate in the condenser/evaporator is kept separate from the adsorbent in the adsorber, by keeping the valve connecting the two components closed.
During the discharge stage, fluid at a lower temperature flows through the adsorber’s heat exchanger, recovering the adsorber’s heat and causing a pressure drop in the adsorber, while the ratio of mass of adsorbate to mass of adsorbent remains constant (this stage is referred to as the isosteric cooling of the adsorbent). When the pressure in the adsorber reaches the evaporator pressure, the valve connecting the adsorber to the evaporator is opened. The adsorbate in liquid form is evaporated with low temperature heat supplied to the evaporator. As it evaporates, the adsorbate in vapour form is directed to the adsorber where it is adsorbed by the adsorbent. This results in the release of the heat of adsorption that was stored in the unit. The discharge process continues until the adsorbent is wet, i.e. it contains the maximum amount of adsorbate vapour within its pores. At the end of the discharge process, the valve between the adsorber and evaporator is closed.

MATHEMATICAL MODEL

The mathematical model of an adsorption storage unit developed by (Mottillo, 2006) and used in this study is briefly described here. The model considers the three components of an adsorption storage unit: the adsorber, condenser and evaporator. A control volume surrounds each component, as illustrated in Figure 2.

![Figure 2. Control volumes of an adsorption storage unit](image)

The control volume surrounding the adsorber includes the adsorber vessel and the heat exchanger material within the adsorber. The energy balance on the adsorber is:

$$\left[ m_z C_p z + m_w X \cdot C_p w + \left( m_{vessel} C_p_{vessel} + m_h C_p h \right) \right] \frac{dT}{dt} = -Q_{loss} + \dot{Q}_{h / x} \pm m_z \frac{\Delta X}{\Delta t} \Delta H $$  \hspace{1cm} (1)  

The term on the left hand side of equation (1) is the variation of sensible energy stored in the adsorber. It is expressed as the sum of the energy variation in the dry adsorbent, in the vapour adsorbed within the adsorbent, in the adsorber vessel and in the heat exchanger contained within the adsorber.

The first term on the right hand side of equation (1), $Q_{loss}$, represents the heat losses from the adsorber to the surroundings by convection to the surrounding air and longwave radiation exchange.
with surfaces in the containing room. The second

term on the right hand side of equation (1), $\dot{Q}_{h/s}$, represents the heat exchanged with the adsorber’s heat source (positive term) or heat sink (negative term). Finally, the term $m_z \frac{\partial X}{\partial t} \Delta f$ represents the heat of adsorption stored or recovered from the unit. When the unit is charging, the term is a sink term and thus negative. When the unit is discharging, the term is a source term and therefore positive.

The condenser and the evaporator are modelled as a single component that acts as an air-cooled condenser when the adsorption storage unit is in charging mode and as an evaporator when the adsorption storage unit is in discharge mode. The model developed by (Mottillo, 2006) ignores the thermal transients within the condenser/evaporator. Also, the model assumes that the heat of condensation released during the charging mode is rejected to the outdoors and that the adsorbate in liquid form is directed to a reservoir where it is stored until it is needed at the evaporator for the discharge of the storage unit. The energy balance on the condenser (charging mode) is:

$$0 = −\dot{Q}_{c-e} - \dot{Q}_{\text{loss}} + \dot{m}_{\text{vap,flow}} h_{\text{vap}} - \dot{m}_{\text{liq}} h_{\text{liq}} = 0$$

(2)

The energy balance on the evaporator (discharge mode) is:

$$\dot{Q}_{c-e} - \dot{Q}_{\text{loss}} - \dot{m}_{\text{vap,flow}} h_{\text{vap}} + \dot{m}_{\text{liq}} h_{\text{liq}} = 0$$

(3)

The first term on the left hand side of equations 2 and 3, $\dot{Q}_{c-e}$, represents the heat of condensation that is removed from the condenser when the unit is in charging mode or the heat input at the evaporator when the unit is in discharge mode. The second term, $\dot{Q}_{\text{loss}}$, represents the sensible heat losses of the condenser/evaporator to the containing room due to convection to the surrounding air and longwave radiation exchange with surfaces in the containing room. The term $\dot{m}_{\text{vap,flow}} h_{\text{vap}}$ in equation 2 represents the heat contained in the vapour entering the condenser, while in equation 3, it represents the heat contained within the vapour leaving the evaporator. Similarly, the term $\dot{m}_{\text{liq}} h_{\text{liq}}$ in equation 2 represents the heat contained in the liquid leaving the condenser while in equation 3, it represents the heat contained in the liquid entering the evaporator.

Mass balance equations are applied to each control volume and combined with the energy balance equations 1-3 to fully describe the adsorption storage unit mathematically.

The mathematical model of the adsorption storage unit developed by (Mottillo, 2006) assumes that the solid and gas phases within the adsorber are in thermodynamic equilibrium, thus the resistance to mass transfer between the adsorbent and adsorbate is neglected. Also, the model assumes that the adsorbate, when in vapour form, behaves as an ideal gas and that the adsorption storage unit operates ideally. That is, during the isosteric heating and cooling phases, the ratio of adsorbate mass to adsorbent mass is constant and during the adsorption and desorption phases, the pressure is constant.

The mathematical model of the adsorption storage unit has been implemented into the ESP-r simulation environment (ESRU, 2002), where it is represented as an explicit plant component.

In order to verify the mathematical model of the adsorption storage unit and its implementation in ESP-r, (Mottillo, 2006) considers a simple plant network that consists of the adsorption storage unit, circulating pumps and pipes. It is assumed that the heat source and heat sink connected to the adsorber are at a constant temperature, as is the evaporator’s heat source and the liquid adsorbate stored in the reservoir. Finally, the air entering the condenser is assumed to be at the outdoor temperature for the particular time of year considered for the simulation.

Simulation results that are obtained using the new proposed model of the adsorption storage unit are compared to the simulation results provided by (Leong and Liu, 2004) in their investigation of an adsorption heat pump.

Figure 3 presents the variation of the adsorber temperature with time obtained using the proposed model. Figure 4 presents the variation of average temperature with time obtained by (Leong and Liu, 2004). They presented the average temperature of the adsorbent bed, metal tube and heat exchanger fluid as in their model each of these components is represented by several control volumes. The results of Figure 3, however, were obtained by incorporating the adsorbent bed, metal tube and heat exchanger fluid in one single control volume. The letters A, B, C and D in Figures 3 and 4 denote the isosteric heating, desorption, isosteric cooling and adsorption phases of the cycle, respectively. The shape of curves presented in Figures 3 and 4 are similar. Both studies predict that the adsorbent bed reaches about 470 °C at the end of the desorption phase (B) and the charging phase (A+B) lasts for approximately 3300 seconds.
PLANT NETWORK

The plant component model of the adsorption storage unit is combined with existing plant component models within ESP-r to form the plant network presented in Figure 5. The plant network consists of a solid oxide fuel cell (SOFC), a main water storage tank, an adsorption storage unit, a reservoir which contains the liquid adsorbate, an auxiliary water storage tank, an air-handling unit, circulating pumps and controls. A zeolite adsorbent and water adsorbate working pair is assumed for the adsorption storage unit.

The main water storage tank meets the house’s space heating load via an air-handling unit. The air-handling unit contains a heating coil served by the main water storage tank (loop E in Figure 5) and a fan that circulates air to the house. The circulating fan and the loop E pump operate only when the temperature in the house is below the thermostat setpoint temperature. A heat recovery ventilator (HRV) operates continuously to supply the required ventilation (not shown in Figure 5). The main water storage tank also serves the house’s domestic hot water requirement. The main water storage tank receives heat exhausted by the fuel cell (loop A) and/or heat recovered from the adsorption storage unit (loop C) to meet the thermal loads (space heating and domestic hot water) imposed on it.

The adsorption storage unit stores heat on a seasonal basis. It is expected that most of the exhaust heat available from the SOFC will not be required in the summer as no space heating load exists during this period. Excess heat is stored in the adsorption storage unit during the cooling season and is recovered during the heating season when the SOFC is not able to meet the space heating and domestic hot water requirements of the house. The unit is only permitted to switch into the charging mode of operation during the cooling season and into the discharge mode of operating during the heating season.

During the cooling season, the adsorption storage unit switches into the charging mode if all of the following conditions are met:

- the temperature in the main water storage tank is above the upper set-point temperature for more than 25 minutes. A reset period of 25 minutes is chosen to avoid the cycling on and off of the adsorption storage unit;
- the temperature of the adsorber is less than the maximum value. The maximum temperature of the adsorber can be set to the temperature of the water leaving the SOFC’s heat exchanger (this implies that no further heat can be transferred) or slightly lower so as to account for the temperature difference between the heat source and adsorber that is required for proper heat transfer (Restuccia and Cacciola, 1999);
- the temperature of the water leaving the SOFC’s heat exchanger is greater than the minimum charging temperature required by the adsorber. The charging temperature required by the adsorption storage system depends on the adsorbent/adsorbate pair chosen for the system;
- the fuel cell is operating.
The SOFC’s thermal output is directed to the adsorption storage unit so that the excess heat available can be stored (loop B in Figure 5) when the latter is in the charging mode of operation.

The charging of the adsorption storage unit ends when any of the following conditions is met:

- the temperature in the main water storage tank is less than the lower setpoint temperature;
- the temperature of the adsorber is greater than or equal to the maximum temperature of the adsorber;
- the temperature of the heat source is below the minimum charging temperature required by the adsorbent/adsorbate pair;
- the fuel cell is switched off.

For periods when the temperature in the main water storage tank is above a maximum setpoint temperature and excess heat cannot be stored, a safety device rejects heat from the water storage tank (loop F in Figure 5) to prevent scalding.

During the heating season, the adsorption storage unit switches into the discharge mode if both of the following conditions are met:

- the temperature in the main water storage tank is less than the lower set-point temperature for more than 25 minutes;
- the temperature of the adsorber is greater than the minimum value. The minimum temperature of the adsorber can be set to the water tank’s temperature (this implies that no further heat can be transferred) or slightly greater so as to account for the temperature difference between the heat sink and adsorber that is required for proper heat transfer.

The discharge of the adsorption storage unit ends when any of the following conditions is met:

- the temperature in the main storage tank is above its upper set-point temperature;
- the temperature in the adsorber is less than the minimum adsorber temperature;
- the adsorbent is wet and cannot contain any more adsorbate.

The main water storage tank contains a backup natural gas burner that operates when the SOFC or the adsorption storage unit cannot meet the house’s heating demands.
The purpose of the auxiliary water tank is to provide the low-temperature heat that is required at the evaporator during the discharge phase.

The SOFC cogeneration system depicted in Figure 5 is similar to the system considered by (Beausoleil-Morrison et al., 2002), except that in the latter case there is no adsorption storage system for the seasonal storage of the SOFC's excess thermal output. (Beausoleil-Morrison et al., 2002) defines the total (electrical plus thermal) efficiency of a SOFC cogeneration system, \( \eta_{\text{cogen}} \), in terms of the lower heating value of natural gas, \( \text{LHV}_{\text{nat-gas}} \) [GJ/m³]:

\[
\eta_{\text{cogen}} = \frac{\text{SOFC}_{\text{elec-out}} + \text{SOFC}_{\text{thermal-out}} - \text{Tank}_{\text{ref-heat}}}{\text{SOFC}_{\text{nat-gas}} \cdot \text{LHV}_{\text{nat-gas}}} \tag{4}
\]

where
- \( \text{SOFC}_{\text{elec-out}} \) is the SOFC’s annual electrical output (GJ);
- \( \text{SOFC}_{\text{thermal-out}} \) is the SOFC’s annual thermal output (GJ);
- \( \text{Tank}_{\text{ref-heat}} \) is the annual energy rejected from the water storage tank by the safety device (GJ) and \( \text{SOFC}_{\text{nat-gas}} \) is the annual natural gas consumption of the SOFC (m³).

**APPLICATION**

The plant network described in the previous section is configured to provide the space heating and domestic hot water requirements of a modern energy-efficient house built to the R-2000 standard (Natural Resources Canada, 2005) and located in Montréal. The domestic hot water (DHW) loads and non-HVAC electrical loads were selected to be typical of a family of four.

The SOFC operates to meet the house’s electrical load and its thermal output is either transferred to the adsorption storage unit or to the main water storage tank, depending on the sensed control parameters.

Several characteristics of the plant network components are listed in Table 1. The parameters specified for the adsorption storage controller are specified in Table 2.

The input parameters that are required by the plant component model of the adsorption storage unit are based on data available in the literature. It should be noted that most of the published data that is available pertains to adsorption systems used in heat pump applications and therefore the input parameters may not represent the actual operating characteristics of an adsorption system used for a storage application. No attempt is made in this analysis to optimize the characteristics of the adsorption storage unit, or of any of the components within the plant network.

| Table 1. Characteristics of plant network components |
|-----------------|------------------|
| SOFC            | Fuel source | Natural gas |
| Minimum net electric output (W) | 500          |
| Maximum net electric output (W) | 5000        |
| Water storage tank | Fuel source | Natural gas |
| Total (water and tank) mass (kg) | 300          |
| Nominal burner capacity when ON (W) | 29300        |
| Combustion and flue efficiency (%) | 80           |
| Natural gas burner ON set-point (°C) | 50           |
| Natural gas burner OFF set-point (°C) | 60           |
| Heat-dump set-point (°C) | 90           |
| Adsorption storage unit | Mass of adsorbent (kg) | 7500        |
| | Mass of adsorber vessel (kg) | 20           |
| | Mass of adsorber heat exchanger (kg) | 50           |
| | Adsorber/fuel-cell heat-exchanger effectiveness (-) | 0.5          |
| | Adsorber/water tank heat-exchanger effectiveness (-) | 0.5          |
| | Minimum temperature difference between adsorber and heat source/sink (°C) | 5            |
| | Condenser pressure (kPa) | 10           |
| | Condenser heat exchanger effectiveness (-) | 0.5          |
| | Condenser fan power rating (W) | 200          |
| | Evaporator pressure (kPa) | 1            |
| | Evaporator heat exchanger effectiveness (-) | 0.5          |

For this analysis, heat losses from the adsorption storage unit to the surroundings are not modelled, for several reasons: (1) input data such as the overall heat transfer coefficient and the surface area of the unit’s individual components (adsorber, condenser and evaporator) are not available; (2) although the heat losses from the unit’s individual components to the ambient are taken into account in the mathematical model, it is not known, in the actual operation of the system, if and how the pressure in the unit would be kept constant when the temperature of the unit decreases due to heat losses to the ambient; (3) the simulation results show that even for the ideal case in which the heat losses from the unit’s individual components to the ambient are ignored, the adsorption storage unit is not able to store or recover sufficient thermal energy; hence this case
study shows that the adsorption storage unit will likely not be feasible in these conditions.

Table 2. Characteristics of adsorption storage unit controller

<table>
<thead>
<tr>
<th>Period during which charging is permitted</th>
<th>May 1 - September 30</th>
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<tbody>
<tr>
<td>Period during which discharging is permitted</td>
<td>October 1 - April 30</td>
</tr>
<tr>
<td>Water tank upper (ON) set-point temperature for charging of unit (°C)</td>
<td>65</td>
</tr>
<tr>
<td>Water tank lower (OFF) set-point temperature for charging of unit (°C)</td>
<td>55</td>
</tr>
<tr>
<td>Water tank lower (ON) set-point temperature for discharging of unit (°C)</td>
<td>65</td>
</tr>
<tr>
<td>Water tank upper (OFF) set-point temperature for discharging of unit (°C)</td>
<td>75</td>
</tr>
</tbody>
</table>

A simulation is carried out for an entire year (January 1 – December 31) using a 5-minute time-step and a 3-day start-up period. The house’s annual heating load is 56.5 GJ/year.

ESP-r predicts the house’s annual energy consumption to be 147.4 GJ. The adsorption storage unit delivers 6.0 GJ of energy during the heating season and stores 0.5 GJ of energy during the cooling season. Figure 6 presents the energy flows into and out of the adsorption storage unit for each month.

The adsorption storage unit discharges most of its stored energy in January; the amount of thermal energy discharged to the water tank decreases between January 1 and April 30. An examination of the simulation results shows that on April 30, the temperature of the adsorber is 59.2°C, suggesting that the adsorption storage unit is no longer a significant source of thermal energy for the water storage tank which is maintained at a temperature above 50°C.

Although the adsorption storage unit is available for charging between May and September, only 0.5 GJ of energy is stored in the unit, all in May. An analysis of the simulation results shows that the adsorption storage unit has sufficient capacity to store more heat however the temperature of the water leaving the SOFC’s exhaust-to-water heat exchanger is not high enough to complete the charging of the adsorption storage unit. An examination of the simulation results shows that the adsorber reaches a temperature of 94.5°C on May 27. However, the temperature of the water leaving the SOFC’s heat exchanger does not exceed 94.5°C and therefore no thermal energy is directed to the absorber. An analysis of the simulation results also shows that only sensible heat is stored in the adsorption storage unit and no desorption takes place in the adsorber.

In October, the adsorption storage unit is allowed to discharge but of course, can only discharge a limited amount of energy since a small amount of energy was stored in the unit during the previous summer. The adsorption storage unit discharges approximately 0.6 GJ of energy between October and December. The temperature of the adsorber on December 31 is 56.1°C.

Figure 7 presents the thermal energy added to the water tank by the SOFC, the thermal energy added to the water tank by the natural gas burner, the thermal energy added to the water tank by the adsorption storage unit and the thermal energy rejected from the tank by the safety device on a monthly basis.

The SOFC delivers 34.3 GJ of thermal energy to the water tank over the year. However, 12.4 GJ of energy is rejected from the water tank to maintain the temperature in the water tank below its maximum set-point temperature. Therefore, the SOFC’s net thermal contribution is 21.9 GJ. The water tank’s burner must provide 32.1 GJ of thermal energy during the year to maintain the water in the tank above its minimum set-point temperature. The
adsorption storage unit provides 6.0 GJ of thermal output to the tank. Therefore, for this specific case the SOFC provides 36.5% of the house’s thermal loads while the adsorption storage unit provides 10.0% of the house’s thermal loads.

The total cogeneration efficiency of the system, calculated using equation (4), is 62.9%.

CONCLUSION

For the set of operating conditions considered in this study, the adsorption storage unit was able to provide energy that would otherwise be required by the backup heating system in the winter. However, the adsorption storage unit did not store sufficient amounts of thermal energy in the summer since the temperature of the unit’s heat source, the water leaving the SOFC’s exhaust gas-to-water heat exchanger, was not at a high enough temperature to fully charge the unit. Therefore, a significant amount of thermal energy is rejected from the water storage tank by the safety device during the summer.

It is recommended that different operating conditions be investigated in future work to obtain the optimal performance of the adsorption storage unit during the summer. In particular, the pump flow rates for loops A and B (Figure 5) should be optimized since they affect the temperature of the water leaving the SOFC’s heat exchanger. Also, it may be feasible to control the SOFC to operate at a constant electrical output during the summer – this will increase both the electrical and thermal output of the SOFC, which will lead to higher exhaust gas temperatures.

The mathematical model of the adsorption storage unit that has been developed and implemented in the ESP-r simulation program is appropriate for studying the feasibility of coupling a SOFC cogeneration system to an adsorption system for seasonal heat storage. Further analyses are recommended to determine the feasibility of the concept and the optimal operating parameters of the system components.

Further validation of the mathematical model of the adsorption storage unit is needed and recommended; preferably with actual experimental data obtained for an adsorption system used in a storage application.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tr>
<td>Cp</td>
<td>Specific heat</td>
<td>J/kg°C</td>
</tr>
<tr>
<td>h</td>
<td>Enthalpy</td>
<td>J/kg</td>
</tr>
<tr>
<td>m</td>
<td>Mass</td>
<td>kg</td>
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<td>kg/s</td>
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<tr>
<td>Q</td>
<td>Heat flow rate</td>
<td>W</td>
</tr>
<tr>
<td>t</td>
<td>Time</td>
<td>s</td>
</tr>
<tr>
<td>T</td>
<td>Temperature</td>
<td>°C</td>
</tr>
<tr>
<td>X</td>
<td>Ratio of adsorbate mass to adsorbent mass</td>
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</tr>
<tr>
<td>ΔH</td>
<td>Enthalpy of adsorption</td>
<td>J/kg</td>
</tr>
<tr>
<td>η</td>
<td>Efficiency</td>
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</tr>
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</table>

Subscripts

- c-e: Condenser/Evaporator
- cogen: Co-generation
- h/x: Heat exchanger
- liq: Liquid
- vap: Vapour
- vap,flow: Vapour flow
- w: Water
- z: Adsorbent (zeolite)

REFERENCES


