Thermochemical Energy Storage Using Salt Hydrates

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Thermochemical Energy Storage Using Salt Hydrates

Thermochemical phase change materials (TCM) for energy storage

TCMs impregnated into mesoporous materials like silica and zeolites

- Inorganic salt hydrates eg. MgSO\(_4\).7H\(_2\)O
- High volumetric heat capacity, low cost, easy availability
- Absorption of heat to release coordinated water
- Release of stored energy during hydration

Epsom Salt

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Seasonal thermal energy storage

\[
\text{Salt hydrate} \quad \xrightarrow{\text{Addition of heat(solar)}} \quad \text{Anhydrous salt} + \text{Water vapor}
\]

\[
\text{MgSO}_4 \cdot 7\text{H}_2\text{O} \quad \rightarrow \quad \text{MgSO}_4 + 7\text{H}_2\text{O}
\]
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Seasonal thermal energy storage

- Water released and heat stored when salt hydrates are heated above their dehydration temperature during warmer ambient periods
- Heat obtained from dehydrated salts by passing low temperature water vapor during cooler periods
Objectives of the investigation

- Design and optimize system geometry
- Characterize mechanisms
- Search for optimal material
- Compare performance of different potential TCMs using numerical and analytical experiments
- Predict optimum properties

Quantitative analysis

- Characterize total energy stored in dehydrated salts under different thermal conditions
- Energy loss by water vapor release from system
Configuration of the 2D simulation domain

- 2-dimensional square simulation box filled with porous MgSO$_4 \cdot 7$H$_2$O
- Heat flux applied from the top boundary
- Insulation of the other boundaries varied by introducing heat losses through them
Conservation of energy, mass and chemical species

Conservation of energy

\[
\frac{\partial}{\partial t} \left[ (M_h N_h C_h + M_s N_s C_s + M_g N_g C_g) T \right] = \nabla (K \nabla T) + r M_h N_h \Delta H
\]

\[ r = A \exp\left(-\frac{E}{RT}\right), \quad K = \beta_h K_h + \beta_s K_s + \beta_g K_g \]

The contribution of convective thermal and mass transport due to the movement of water vapor released from the salt hydrate is neglected.

Conservation of mass

\[
M_h \frac{\partial N_h}{\partial t} + M_s \frac{\partial N_s}{\partial t} + M_g \frac{\partial N_g}{\partial t} = 0
\]
Conservation of energy, mass and chemical species

\[ \frac{\partial}{\partial t} \left[ \left( M_h N_h C_h + M_s N_s C_s + M_g N_g C_g \right) T \right] = \nabla (K \nabla T) + r M_h N_h \Delta H \]  \hspace{1cm} (1)

\[ M_h \frac{\partial N_h}{\partial t} + M_s \frac{\partial N_s}{\partial t} + M_g \frac{\partial N_g}{\partial t} = 0 \]  \hspace{1cm} (2)

**Chemical kinetics**

First order chemical reaction

\[ \frac{\partial N_h}{\partial t} = -r N_h \]  \hspace{1cm} (3)

**Stoichiometry**

\[ \frac{\partial N_s}{\partial t} = - \frac{\partial N_h}{\partial t} \]  \hspace{1cm} (4)
Significant nondimensional parameters in the model

\[
\frac{\partial}{\partial t} \left[ (\eta_h + \eta_s + \eta_g) T \right] = K \nabla^2 T + D_m \eta_h \chi \exp \left( -\frac{E}{T} \right)
\]

\[
\frac{\partial \eta_h}{\partial t} = -D_m \eta_h \exp \left( -\frac{E}{T} \right)
\]

\[
\frac{\partial \eta_h}{\partial t} + \frac{C_h}{C_s} \frac{\partial \eta_s}{\partial t} + \frac{C_h}{C_g} \frac{\partial \eta_g}{\partial t} = 0
\]

\[
\frac{\partial \eta_s}{\partial t} = -\frac{M_s C_s}{M_h C_h} \frac{\partial \eta_h}{\partial t}
\]
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Significant nondimensional parameters in the model

\[
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\[
\frac{\partial \eta_h}{\partial t} = -D_m \eta_h \exp\left( -\frac{E}{T} \right)
\]

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<th>Symbol</th>
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| \(D_m\) | Modified Damköhler Number  
\(\frac{\text{Rate of thermochemical energy transfer}}{\text{Rate of heat diffusion}}\) |
| \(\chi\) | Dimensionless Thermochemical Heat Capacity  
\(\frac{\text{Enthalpy of dehydration of MgSO}_4 \cdot 7\text{H}_2\text{O}}{\text{Heat capacity of MgSO}_4 \cdot 7\text{H}_2\text{O per unit mass}}\) |
| \(\hat{q}\) | Dimensionless Heat Flux  
\(\frac{\text{Input heat flux}}{\text{Diffusive heat flux}}\) |
The local temperature of the uppermost boundary increases linearly (in region I) until the reaction temperature ($T = 1$) is reached after which there is an abrupt transition to a higher temperature during desorption (region II).
Transient evolution of concentration of different components

- The hydrated salt concentration decays as the temperature increases and its anhydrous form is produced.
- The increased concentration in the anhydrous component of the salt and the free water vapor are reflected in the $\eta_s$ and $\eta_g$ profiles.
The time required to initiate the desorption process for hydrated salts decreases nonlinearly as \( q \) increases.

**Performance ratio**

\[
\pi = 1 - \frac{\text{Energy lost}}{\text{Energy supplied}} = 1 - \frac{Q_g V}{\int_{t_r}^{t_e} q \, dt}
\]

As the input heat flux increases, the time required for the salt hydrate to undergo the reaction decreases.

When heat is lost from the insulated boundaries (\( \alpha \leq 0 \)), the effective energy available for the hydrate to undergo the chemical reaction is smaller.
A larger dehydration enthalpy ensures that all of the imposed flux is utilized towards the release of water vapor and a negligible fraction of the input energy diffuses through the system.

Heat diffusion in the system is enhanced by improving the thermal conductivity of the hydrate, resulting in smaller $D_m$ values.

Rapid thermal conduction implies that the hydrate layers take longer to retain sufficient energy to complete the thermochemical desorption reaction.
Thermochemical phase change materials could have significant implications for long-term energy storage applications

1. A mathematical model to investigate the capability of salt hydrates to store thermochemical energy during their dissociation into anhydrous salts and water vapor when they are supplied with external heat.

2. A parametric study provides suggestions to improve process performance, e.g., by properly selecting materials for thermochemical energy storage.

3. The process performance is improved by introducing a smaller heat flux and considering materials that have larger thermal conductivities, higher specific heat capacities, and lower thermochemical desorption rates.

4. A future approach to material design during the next phase of our research will use the parameter optimization method that we have developed.

Questions?