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COMSOL CONFERENCE 2018 BOSTON

3D Unsteady CFD Simulations of Heat and Mass Transfer with Chemical Reaction of Seasonal Solar Thermochemical Heat Storage System for Buildings

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Introduction

Solar energy storage has been an extensive research topic among the several thermal energy applications over the past three decades. Thermal energy storage (TES) systems in general, improve the energy efficiency of systems and sustainability of buildings by reducing the mismatch between supply and demand, and can substantially increase the solar fraction. They expand the use of solar collectors and result in enhanced solar coverage of the space heating demand.

TES systems using thermochemical materials are particularly attractive and provide a high energy storage density at a constant temperature. Chemical energy storage has unique advantages of high energy storage and low heat losses over other storage technologies and is considered as the most promising alternative.

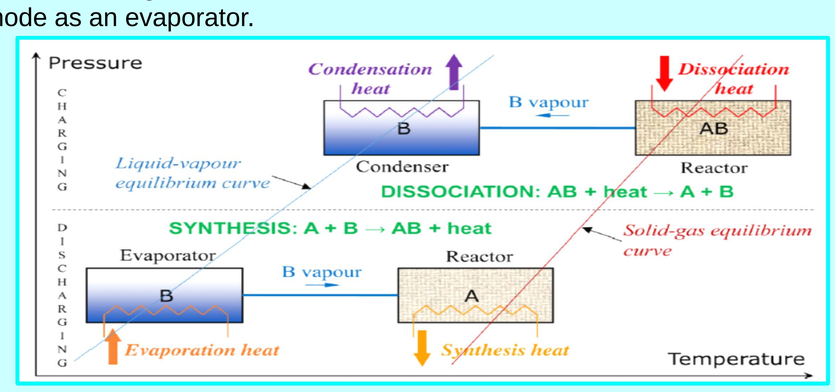
The principle of chemical reaction is based on the reversible reaction between two substances, for instance a solid such a salt and a gas or water vapour, with endothermic decomposition (charging mode in summer), and exothermic synthesis (discharging mode in winter) processes.

Heat, mass transfer and momentum transport processes are coupled with chemical reactions in a thermochemical heat storage system. The endothermic and exothermic reactions in a chemical reactor in closed or open system are strongly integrated by heat transfer from adjacent heat exchanger.

In this investigation, a three-dimensional unsteady CFD model of a solid/gas thermochemical porous reactive bed with a plate-fin heat exchanger operating in a close system is developed to simulate and analyse the thermal synthesis of the exothermic hydration reaction of pure salt during the discharging process for seasonal heat storage in building application.

Operating Principles

Fig. 1 illustrates the operating principles of a thermochemical heat storage system using solid-gas chemical reaction. The heat exchanger that is used in dissociation mode as a condenser is the same, which is used in synthesis mode as an evaporator.



$$Salt \cdot xH_2O_{(s)} + Heat \leftrightarrows Salt \cdot (x-y)H_2O_{(s)} + yH_2O_{(g)} \qquad MgCl_2 \cdot 2H_2O_{(s)} + 4H_2O_{(g)} \leftrightarrow MgCl_2 \cdot 6H_2O_{(s)} + 4\Delta H_r$$

Fig. 1. Schematic diagram of a thermochemical heat storage system [1]

Model Geometry

Figs. 2a,b illustrate the geometric models of the thermochemical heat storage (TCHS) reactor based on $MgCl_2 \cdot 2H_2O$ for the synthesis (hydration) mode for discharge process for the validation case and the study. 3D unsteady models were built in the CFD commercial software COMSOL. The unsteady simulations were run for a time period, which corresponds to the time required to complete the chemical reaction in the TCHS reactor. This corresponds to a residence time of 14 hours and a time step of 20 s, which was considered to be acceptable in terms of accuracy and efficiency.

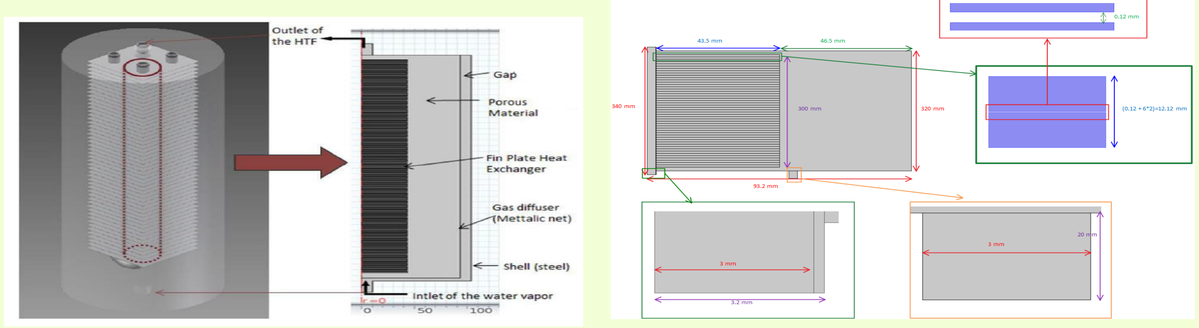


Fig. 2. Reactor geometry with 2D asymmetric view for the : (a) validation case [2] and (b) the simulated reactor

Acknowledgement: *Funding for this work was provided by Natural Resources Canada through the Program of Energy Research and Development.*

Model Set-up

The Navier-Stokes and energy equations in three-dimensional form were used to solve for the transient hydrodynamic, reacting and thermal fields. Therefore, the resulting governing equations can be written as follows:

Energy balance:

$$(\rho C_p)_{bed} \cdot \frac{\partial T}{\partial t} = \nabla \cdot (\lambda_s \nabla T) + \dot{q} \quad \text{with} \quad \dot{q} = \Delta H_r \cdot \frac{\partial \alpha}{\partial t} \cdot \frac{\rho_s}{M_s}$$

where $(\rho C_p)_{bed} = (1-\varepsilon_s)(\rho C_p)_s + \varepsilon_s (\rho C_p)_v$

Mass balance:

$$\frac{\partial (\varepsilon_d \rho_v)}{\partial t} = D \cdot \Delta \rho_v - \nabla \cdot (\rho_v \boldsymbol{u}) \qquad \frac{\partial (\varepsilon_s \rho_v)}{\partial t} = \dot{m} - \nabla \cdot (\rho_v \boldsymbol{u}) + D \cdot \Delta \rho_v$$

$$\boldsymbol{u} = -\frac{k}{\mu}(\nabla p - \rho_v g) \quad \text{with} \quad \frac{\mu}{\mu_i} = \left(\frac{T}{T_i}\right)^{1/2} \left\{ \frac{1 + S/T_i}{1 + S/T} \right\}$$

$$\frac{\partial (\varepsilon_d \rho_v)}{\partial t} = -\nabla \cdot \left(\rho_v \frac{k_d}{\mu} (\nabla p) \right) \quad \text{with} \quad k_d = \frac{\varepsilon_d^3 \cdot d_d^2}{36 \cdot \tau^2 \cdot f_{CK} \cdot (1-\varepsilon_d)^2}$$

$$\frac{\partial (\varepsilon_s \rho_v)}{\partial t} = D \cdot \Delta \rho_v - \nabla \cdot \left(\rho_v \frac{k_s}{\mu} (\nabla p) \right) - \chi \frac{\partial \alpha}{\partial t} \frac{M_v}{M_s} \rho_s$$

Chemical kinetics [3-5]:

$$\frac{\partial \alpha}{\partial t} = A_f \exp\left(-\frac{E_a}{RT}\right) \cdot (1-\alpha) \cdot \left(1 - \frac{p_{eq}}{p}\right) \qquad \frac{\partial \alpha}{\partial t} = R_{kin} \cdot (1-\alpha) \cdot \left(1 - \frac{p_{eq}}{p}\right) = A_f \cdot exp\left(-E_a/RT\right) \cdot (1-\alpha) \cdot \left(1 - \frac{p_{eq}}{p}\right)$$

The above Equations are solved together with an energy balance in unsteady 3D.

Table 1. Thermophysical properties of heat storage system used in this work

Parameter	Value	Unit	Description
d_p	$2 \cdot 10^{-3}$	m	Salt grain diameter
β	10	K·min^{-1}	Heating rate
ε_s	0.76	-	Porosity of the salt bed
ε_d	0.89	-	Porosity of the diffuser
k_d	$1.13 \cdot 10^{-10}$	m^2	Permeability of the diffuser
k_0	$0.11 \cdot 10^{-11}$	m^2	Permeability of the anhydrous salt
k_1	$2.10 \cdot 10^{-10}$	m^2	Permeability of the hydrated salt
p_i	1230	Pa	Inlet pressure of vapour/steam
μ	$8.9 \cdot 10^{-4}$	Pa.s	Dynamic viscosity of the vapour
$(\rho C p)_s$	1.940	MJ·m^{-3}·K^{-1}	Volumetric heat capacity of the solid salt
$(\rho C p)_v$	2.080	MJ·m^{-3}·K^{-1}	Volumetric heat capacity of the vapour
C_i	500	mol·m^{-3}	Initial concentration
x	4	-	Stoichiometric coefficient
M_v	0.018	kg·mol^{-1}	Molar mass of vapour
M_{s1}	0.203	kg·mol^{-1}	Molar mass of hydrate salt
M_{s0}	0.131	kg·mol^{-1}	Molar mass of anhydrous salt
ΔH_r	63,800	J·mol^{-1}	Reaction enthalpy
ΔS_r	158	J·mol^{-1}·K^{-1}	Reaction entropy
R	8.314	J·mol^{-1}·K^{-1}	Ideal gas constant

Parameter	Value	Unit	Description
T_{eq}	298	K	Equilibrium temperature
ρ_v	1,000	kg·m^{-3}	Density of water
ρ_s	1,980	kg·m^{-3}	Density of salt bed
λ_v	0.025	W·m^{-1}·K^{-1}	Vapour thermal conductivity
λ_{s0}	0.55	W·m^{-1}·K^{-1}	Anhydrous salt thermal conductivity
λ_{s1}	0.77	W·m^{-1}·K^{-1}	Hydrate salt thermal conductivity
A_f	$7.45 \cdot 10^{-4}$	s^{-1}	Pre-exponential factor
E_a	5,000	J·mol^{-1}	Activation energy of water
E_{de}	541	kWh·m^{-3}	Storage energy density of salt hydrate
T_i	293.15	K	Initial temperature

Simulation Results

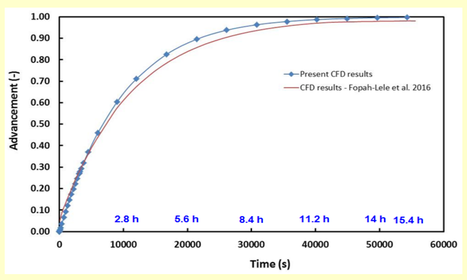


Fig. 3. Reaction advancement profiles of the reactive porous bed reactor during discharging

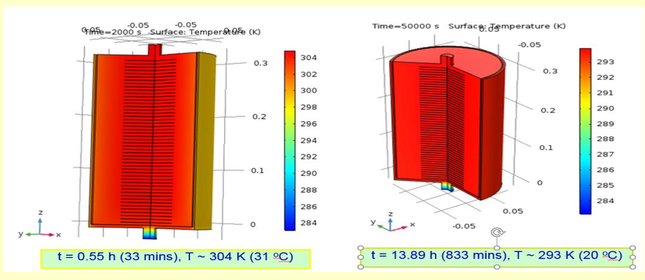


Fig. 4. 3D view of the reactive spatial view of the reactor temperature during discharging at 0.5 h and 14 h

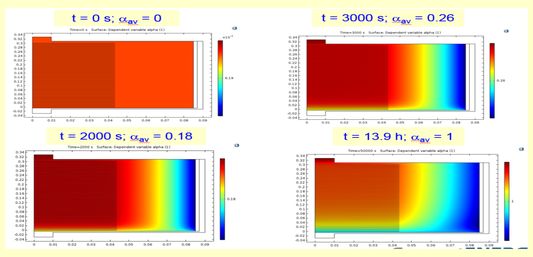


Fig. 5. Reaction advancement profiles of the reactive porous bed reactor during discharging

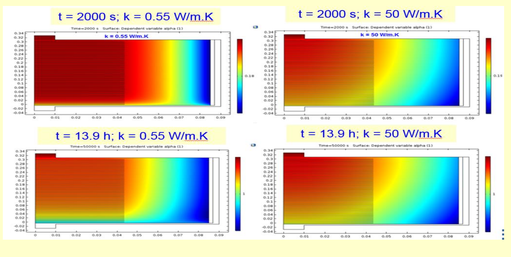


Fig. 6. Reaction advancement profiles of the reactive porous bed reactor during discharging for different thermal conductivities

Conclusion

In this investigation, a three-dimensional unsteady CFD model of a solid/gas thermochemical porous reactive bed with a plate-fin heat exchanger operating in a close system is developed to simulate and analyse the thermal synthesis of the exothermic hydration reaction of pure salt during the discharging process. Validation of the unsteady reacting flow computation results with data found in the literature has shown a good agreement. Different temporal and spatial dimensional distribution maps of temperatures, velocities and reaction advancements have been obtained. The effect of the reactive bed thermal conductivity on the performance of the system has shown small increase in the system performance for thermal conductivities up to 50 W/m.K. The CFD model may serve as a valuable design tool for future simulation and optimisation of TCHS for both charge and discharge modes.

References

[1] K.E. N'Tsoukpoe, N. Mazet, P. Neveu, The concept of cascade thermochemical storage based on multimaterial system for household applications, Energy and Buildings 129 (2016) 138–149.
[2] A. Fopah-Lele, F. Kuznik, T. Osterland, W.K.L. Ruck, Thermal synthesis of a thermochemical heat storage with heat exchanger optimization, Applied Thermal Engineering 101 (2016) 669–677.
[3] B. Michel, P. Neveu, N. Mazet, Comparison of closed and open thermochemical processes, for long-term thermal energy storage applications, Energy, 72 (2014) 702–16.
[4] H.B. Lu, N. Mazet, B. Spinner, Modelling of gas-solid reaction—coupling of heat and mass transfer with chemical reaction, Chemical Engineering Science, 51 (1996) 3829–3845.
[5] N. Mazet, M. Amouroux, B. Spinner, Analysis and experimental study of the transformation of a non-isothermal solid/gas reacting medium. Chemical Engineering Communications 99 (1991) 155–74.

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