

STORHY FINAL EVENT HYDROGEN STORAGE SYSTEMS FOR AUTOMOTIVE APPLICATION

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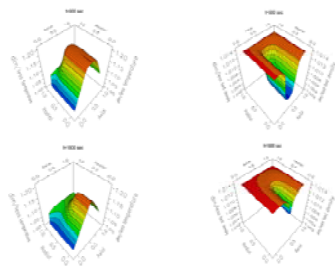


Modelling and Optimisation of Hydrogen Solid Storage Systems

Objectives

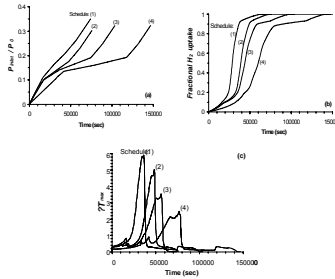
- ❖ An integrated modeling and optimization based approach and simulation tool has been developed for the efficient, safe and economic design of solid hydrogen storage tanks using advanced solid materials
- ❖ Recent advances on dynamic optimisation are utilized to develop optimal operating policies and novel cooling system design options for hydrogen storage in solids

Achievements



Time-space evolution of temperature profiles in the bed

Time-space evolution of solid density profiles in the bed



Optimal time scheduling of the pressure history, (a), and time evolution of: (b) H₂ mass uptake in the metal hydride reactor and (c) T_{max} in the metal hydride reactor

Macroscopic Simulation
2D Cylindrical Geometry

Conservation of mass
$$\epsilon \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) + (1-\epsilon) \rho_s \frac{\partial q}{\partial t} = 0$$

Conservation of Momentum (Darcy's law)
$$\mathbf{u} = -(\mathbf{K}/\mu) \nabla P$$

Conservation of Energy
$$\frac{d}{dt} \left(\epsilon \rho C_p T + (1-\epsilon) \rho_s C_p T - \epsilon \frac{\partial R T}{M_h} \right) + \nabla \cdot (\rho C_p \mathbf{u} T - \lambda \nabla T) + (1-\epsilon) (-\Delta H) \rho_s \frac{\partial q}{\partial t} = 0$$

Mass balance for the metal hydride
$$(1-\epsilon) \frac{\partial q}{\partial t} = C_s + \tau_m \exp(-\epsilon_s / \theta) \ln \left(\frac{p}{p_s} \right) (\lambda_m - \lambda)$$

Adsorption kinetics (LDF model)
$$\frac{\partial q}{\partial t} = k (q^* - q)$$

Definition of Equilibrium Pressure (Jemni and Nasrallah, 1995)
$$p_s = f(H) M_h \exp \left[\frac{\Delta H}{R} \left(\frac{1}{T_s} - \frac{1}{T} \right) \right]$$

Adsorption Isotherm (Langmuir)
$$q^* = \frac{q_m b P}{1 + b P} = \frac{q_m b_s \exp(-\Delta H / RT) P}{1 + b_s \exp(-\Delta H / RT) P}$$

Maximize hydrogen storage
 $\int_0^t P dt$

Maximize hydrogen storage capacity
 $\int_0^t q dt$

Constraints
 $m_{max} \geq 0.99$
 $P^* \leq P^{max}$
 $\Delta P \leq \Delta P^{max}$
 $\Delta T_{max} \leq \Delta T^{max}$
 $M_{max} \leq M^{max}$

Constraints
 $\Delta T_{max} \leq 0.99$
 $\Delta P_{max} \leq \Delta P^{max}$
 $q_{max}^* \leq q_s^*$
 $b_{max} \leq b_s$

Solve using advanced dynamic Optimisation techniques in gPROMS™

GCMC Simulation-Construction of a Database

Iterative Process
Heat of adsorption, ΔH_i depends on pore size

Optimum PSD for different constraints on the temperature rise

Case	ΔT_{max} (°C)	ΔP_{max} (bar)	τ_m (s)	ϵ_s	ΔH_i (kJ/mol)	Total Storage (mol)	ΔT_{max} (°C)
1	10	0.05	0.001	0.001	0.001	0.001	10
2	10	0.05	0.001	0.001	0.001	0.001	10
3	10	0.05	0.001	0.001	0.001	0.001	10
4	10	0.05	0.001	0.001	0.001	0.001	10

The approach takes into account realistic operating constraints related to maximum allowable tank temperature, maximum pressure drop and cooling fluid availability. A multi-scale modelling and optimisation framework is also investigated to explore the synergistic benefits between material design and storage processes, design and operation. Results indicate how process operating constraints, potentially expressing safety concerns, can affect material design. In particular:

- ❖ Significant improvements in the total storage time can be achieved when optimising the design of cooling systems in metal hydride beds.
- ❖ Optimal H₂ charging rate is an important control variable to ensure satisfaction of maximum temperature limitations inside the bed.
- ❖ Process operating constraints, expressing safety considerations, can significantly affect optimal Pore Size Distributions in nanoporous carbons.

Future Perspectives

- ❖ The tool is available for further testing and use in realistic tank design environments and applications

Partners

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