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Thermofluidynamic Modelling of Hydrogen Absorption and Desorption in a $LaNi_{4.8}Al_{0.2}$ Hydride Bed

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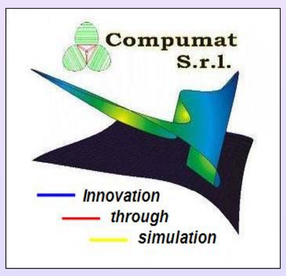


Model and geometry

A 2D-axial symmetry model for the prediction of heat and mass transfer in a metal-hydrogen reactor during charge and discharge has been modelled by means of finite element technique (FEM).

Equations solved are heat balance, mass-momentum balance and kinetic law.

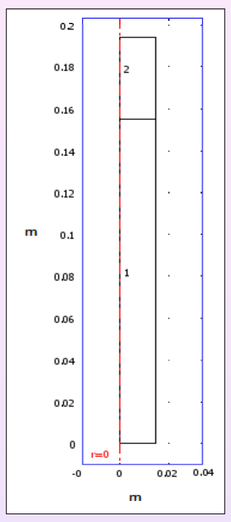
$$\left(\rho C_p\right)_e \frac{\partial T}{\partial t} - \nabla\cdot\left(k_e \nabla T\right) + \left(\rho_g C_{p_g}\right)\mathbf{v}_g \cdot \nabla T = Q_H$$

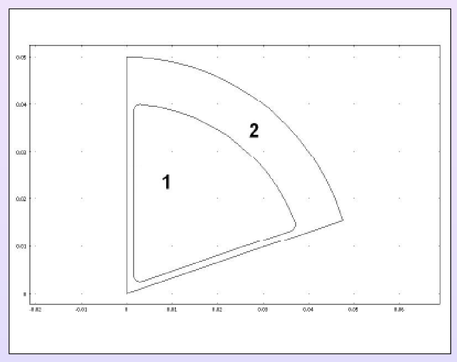
$$\frac{\partial \varepsilon \rho_g}{\partial t} + \nabla\cdot\left(\rho_g \mathbf{v}_g\right) = -m$$

$$m = C \cdot \exp\left(-\frac{E_a}{RT}\right)\cdot f\left(P\right)\cdot f\left(\rho\right)$$

Two different geometries have been considered.

The geometry used in modelling reactor 1 represents a longitudinal section with two subdomains: the first for the porous media and the second for the free space.





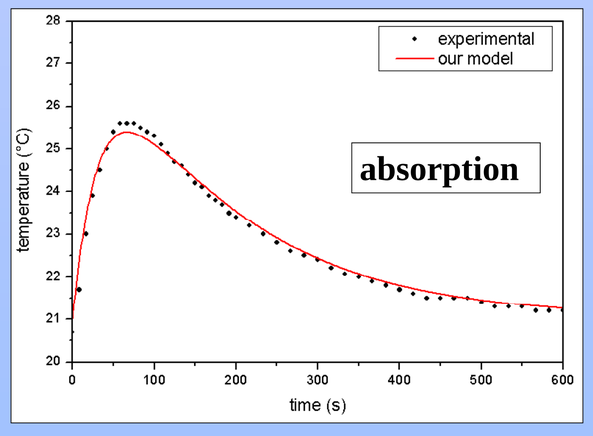
The reactor 2 was modelled by using symmetry properties; therefore only one sector of the vessel section has been considered

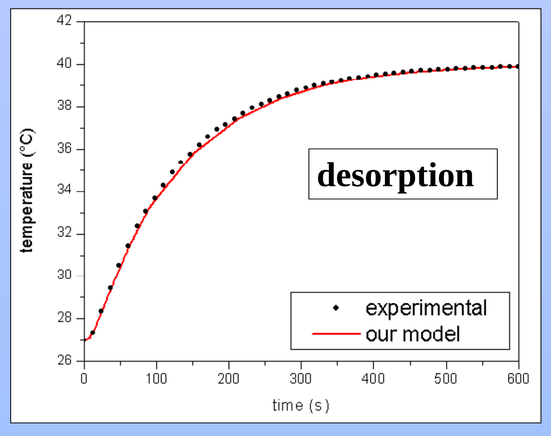
Results

Validation of model (reactor 1)

The experimental apparatus simulated consists of a metallic container collocated (reactor 1) into a water bath in order to keep constant temperature conditions. A source of H_2 is connected via a valve to the reactor and it is set at a constant pressure. Two series of 3 thermocouples (K-type) are located inside the vessel to register the temperature behaviour.

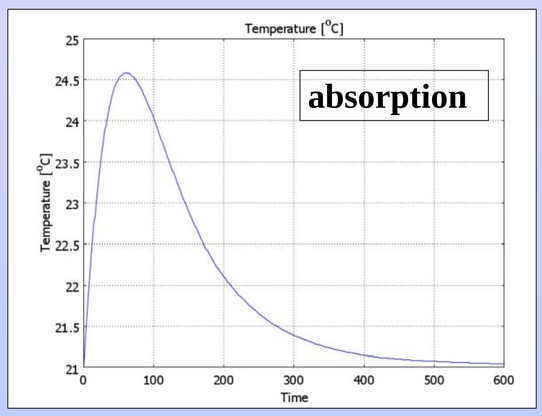
Results obtained by the model are compared with experimental data in order to validate the model. During absorption the temperature of the vessel increases until to reach about 26 °C, because of the exothermic process; then it decreases. During desorption the temperature increases slowly within the vessel, due to endothermic reaction.

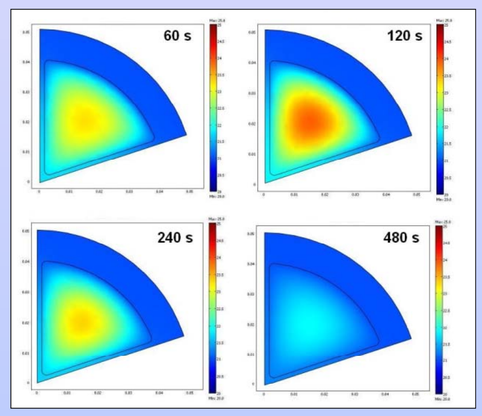




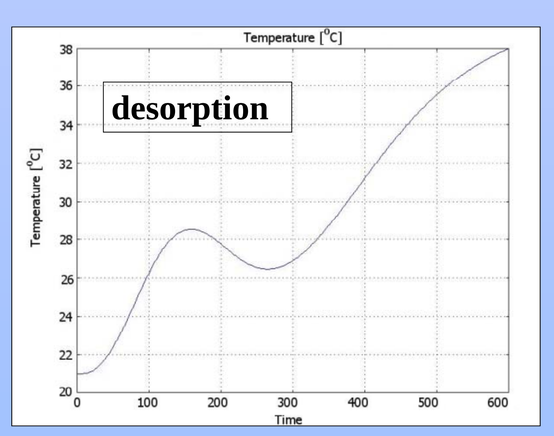
Theoretical prevision (reactor 2)

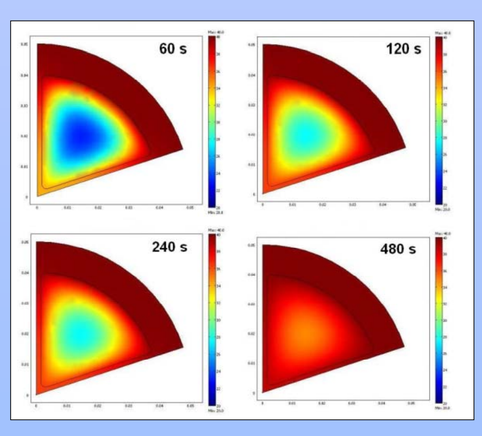
During absorption the temperature inside the reactor 2 (with fins) increases, showing the same behaviour as reactor 1 (without fins). Higher temperature values are observable in the internal zone due to the external cooling bath.





In desorption we observe a gradual increase in temperature, while the porous media is interested by the endothermic process. Higher temperature values are observable in the external zone due to the external heating bath.

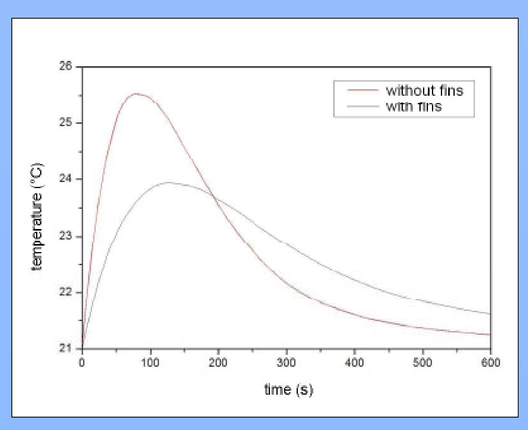




Discussion

The heat exchange in the system is correlated to two parameters: the effective thermal conductivity k_e (internal phenomena) and overall heat transfer coefficient h (external phenomena). The numerical results obtained were compared with experimental data in order to minimizing the error and evaluating the optimal heat transfer parameters.

For thermal conductivity the best value founded was about 1.32 W m^{-1} K^{-1}, both for absorption and desorption simulations. The best values of h founded are about 400 W m^{-2} K^{-1} for absorption and about 1000 W m^{-2} K^{-1} for desorption. The difference between the two cases is due to different external conditions.
Comparing the results obtained for reactors 1 and 2 it can be observed that the temperatures reached by the system are higher for the geometry without fins with respect to the geometry with fins (30 °C instead of 24 °C). This shows the utility of inserting fins in order to better the heat transfer in metal hydride vessels.



Work in progress

Actually the modeling of the connection between storage system and fuel cell is under investigation, using the software COMSOL Multiphysics. New kinetic laws are necessary in the case of small composition variations of the alloy used.

Acknowledgment

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