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Perforation Effect on a Rectangular Metal Hydride Tank at the Hydriding and Dehydriding Process

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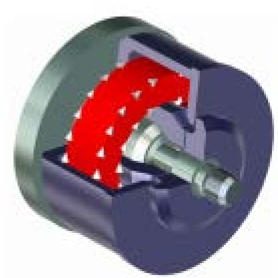

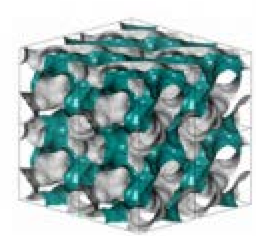

Agenda

- Introduction
- Mathematical Model
- Use of COMSOL Multiphysics
- Results & Discussion
- Conclusions

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Introduction Part

Available Candidates For the Post – Fossil Fuel Era:
Solar Power, Wind Power, Ocean Currents, Geothermal, **Hydrogen Energy**

Hydrogen

- Regarding Convenience for Transportation
- Versatility
- Safety
- Environmental Copatibility

- Occupies enormous Volume in Normal Conditions (1Kg H_2 at ambient temperature and atmospheric pressure, takes a volume $1m^3$)
- The Highest Energy per Unit Mass
- The most Abudant Element in Universe

BUT!

Low Energy Density per Unit Volume Under Atmospheric Conditions: Limitation of Effective Storage

Hydrogen storage

- Compressed Gas in High Pressure Tanks
- Liquid in Cryogenic Tanks
- Absorbed Element by Solid Materials in Porous Tanks

Alloys Used For Hydrogen Storage

AB – Alloys. (AB_2 and AB_5)
A – metals can absorb hydrogen (rare earth elements La, Ti, Zr, Mg, Ca)
B- metals can't absorb hydrogen (Fe Ni, Mn,Co)

Fe-Ti hydrides, La-Ni hydrides, Mg hydrides, Ti-Zr-V hydrides

Mathematical Model

Assumptions

- The media (H_2 and metal) are in local thermal equilibrium.
- Solid Phase is Isotropic and has uniform porosity
- Hydrogen is treated as an ideal gas.
- Van't Hoff Law
- Heat transfer by Radiation is Negligible.

Governing Equations: Energy, Mass and Momentum conservation and Kinetics of Absorption and Desorption of Hydrogen.

$$(\rho \cdot Cp)_e \cdot \frac{\partial T}{\partial t} + (\rho_g \cdot Cp_g) \cdot \overline{v}_g \cdot \nabla T$$
$$= \nabla \cdot (k_e \cdot \nabla T) + m \cdot (\Delta \mathrm{H} - T \cdot (Cp_g - Cp_s))$$

Energy Equation

$$(1-\varepsilon) \cdot \frac{\partial(\rho_s)}{\partial t} = -m$$

Hydride Mass Balance

$$\varepsilon \cdot \frac{\partial(\rho_g)}{\partial t} + div(\rho_g \cdot \vec{v}_g) = -m$$

Hydrogen Mass Balance

$$\vec{v}_g = -\frac{K}{\mu_g} \cdot grad(\vec{P}_g)$$

Darcy's Law

$$\ln P_{eq} = \frac{\Delta \mathrm{H}}{R_g \cdot T} - \frac{\Delta S}{R_g}$$

Van't Hoff Law

$$m = C_a \cdot \exp[-\frac{E_a}{R_g \cdot T}] \cdot \ln[\frac{p_g}{P_{eq}}] \cdot (\rho_{ss} - \rho_s)$$

Absorption Kinetic equation

$$m = Cd \cdot \exp[-\frac{E_d}{R_g \cdot T}] \cdot (\frac{P_{eq} - p_g}{P_{eq}}) \cdot (\rho_s - \rho_o)$$

Desorption Kinetic equation

Use of COMSOL Multiphysics (I)

Creating the model (Steps)

I. Choose the appropriate equations (Heat Transfer – Darcy's Law – Diffusion in Diluted Species)

II. Choose the analysis (Time Dependent)

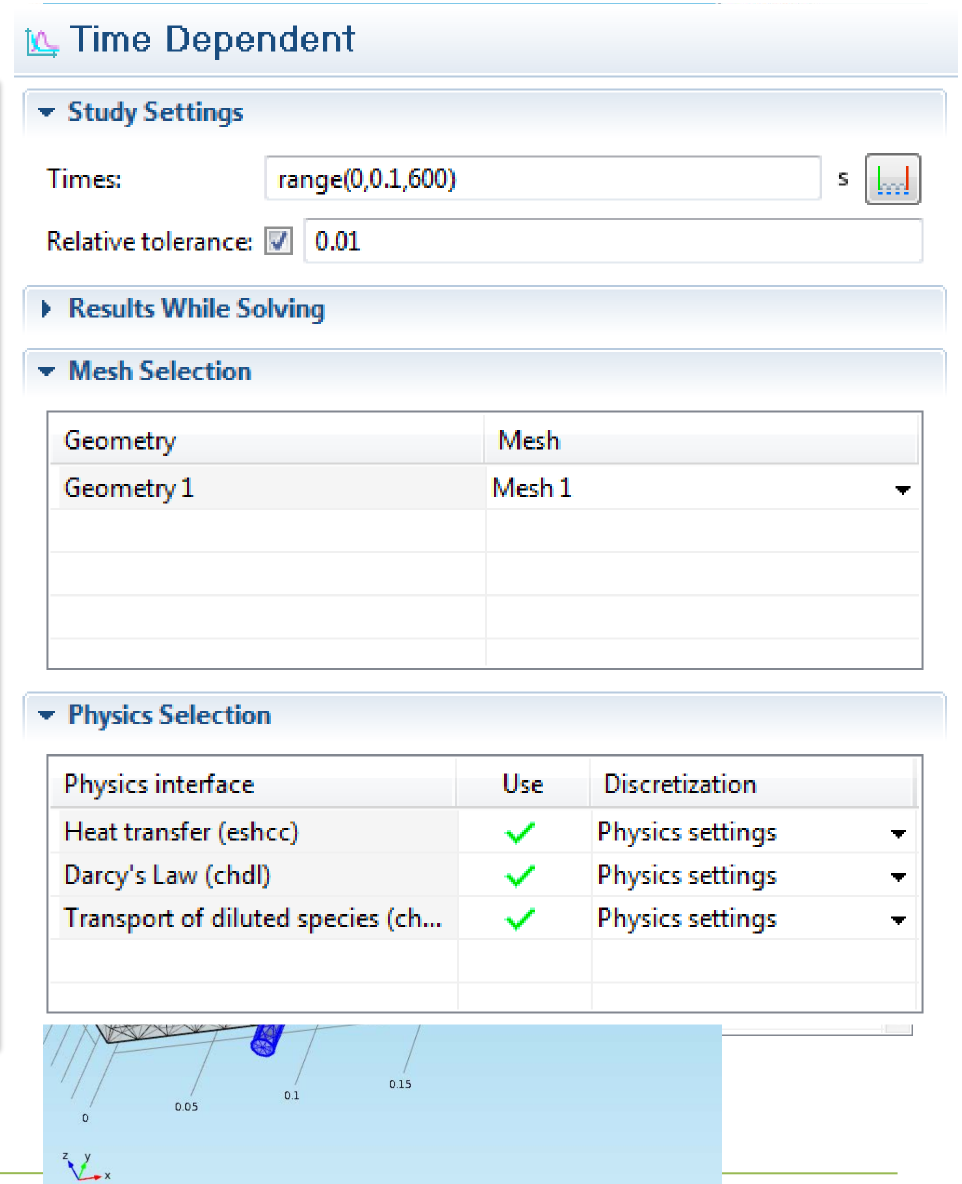
III. Create the geometry (Perforated Rectangular – Conventional Rectangular)

IV. Input all variables of the model (Gas Global Constant, Metal's density, Gas density…)

V. Input the model's parameters, initial and boundary conditions. Further input of the heat, mass and concentration sources

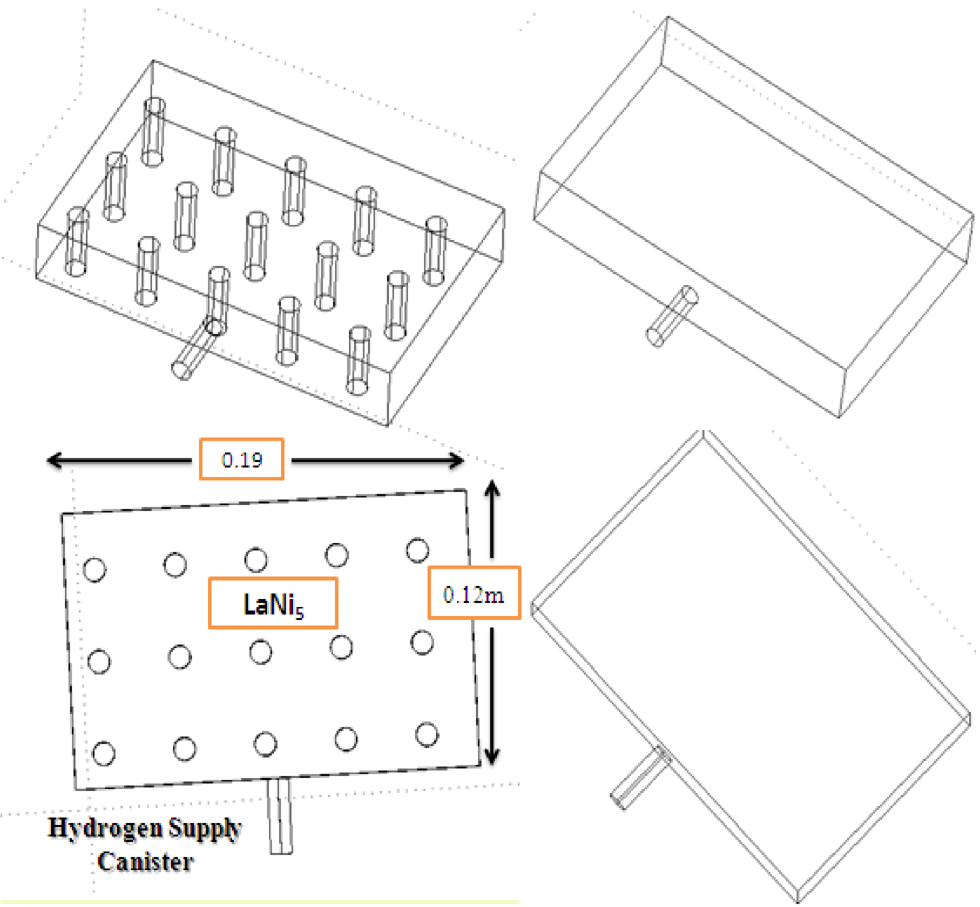
VI. Create a mesh (130000 degrees of freedom)

VII. Solve the problem

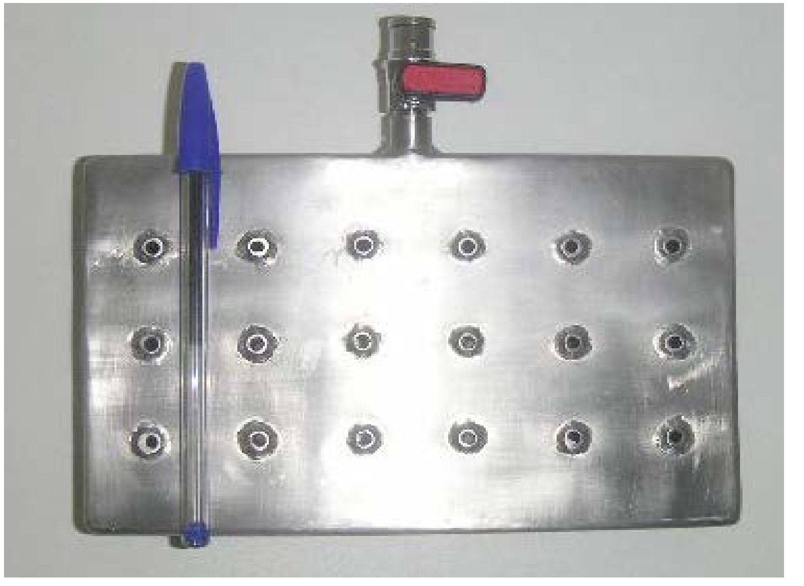


Use of COMSOL Multiphysics (II)

Geometry of the Model



Geometry of the real Hydride Tank



External L-Dimension (mm)	**190**
External W- Dienmsion (mm)	120
External H-Dimension (mm)	33

Use of COMSOL Multiphysics (III)

Boundary Conditions

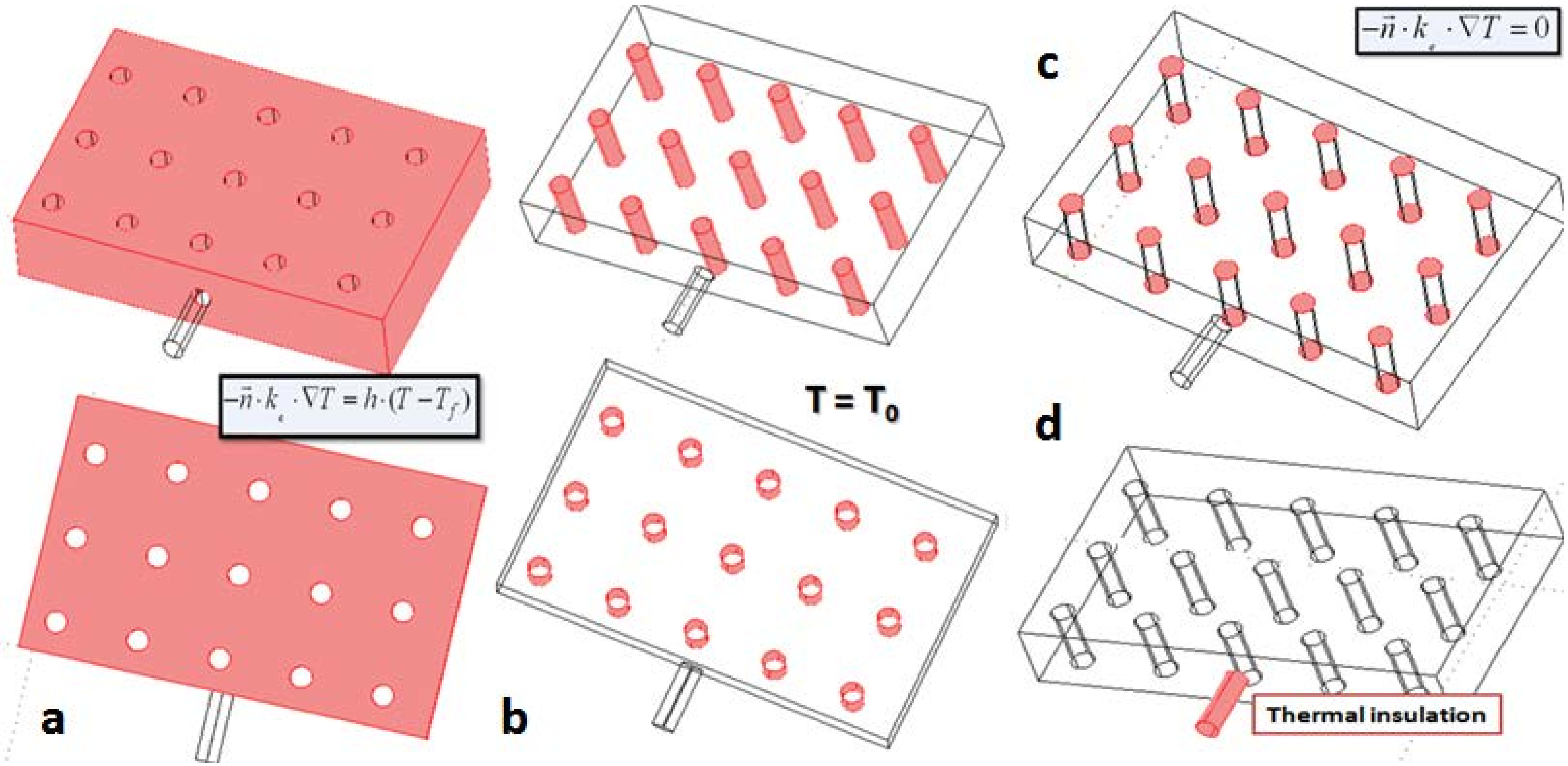


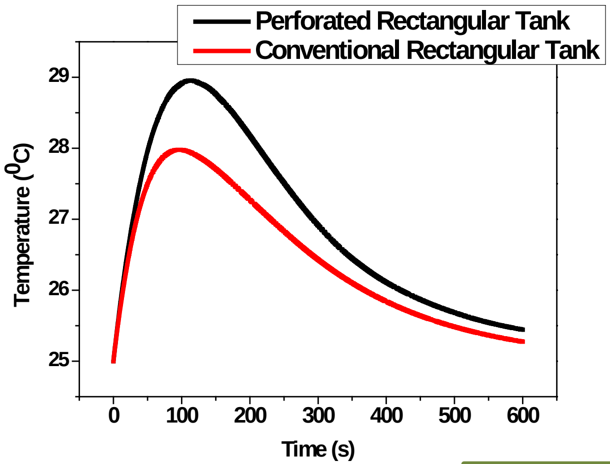
Figure a. Heat Transfer with External Heating/Cooling Source

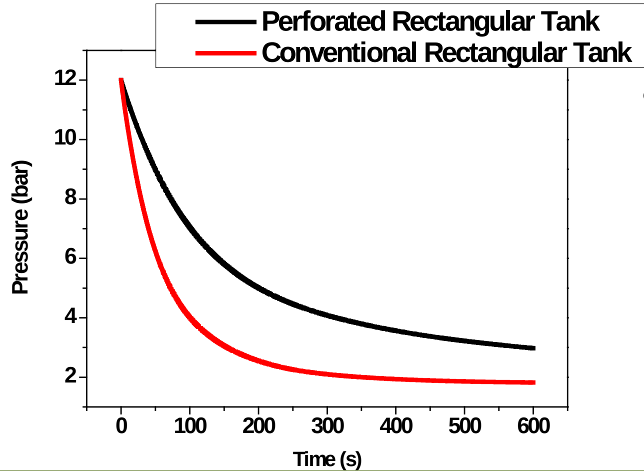
Figure b. the boundary condition between the tube and the metal hydride tank $T = T_0$

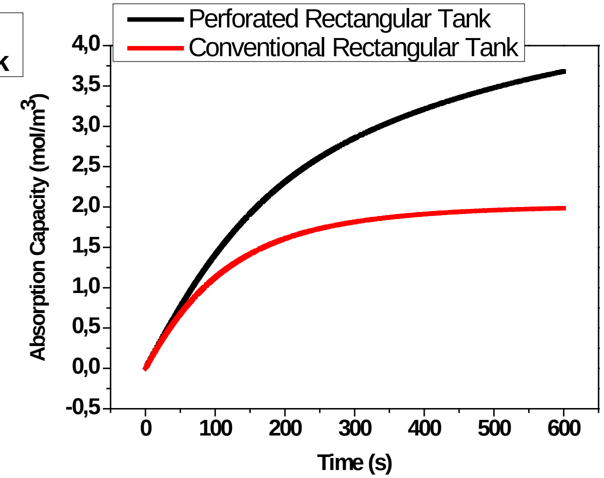
Figure c. The Boundary Condition has set as Convective flux

Results and Discussion

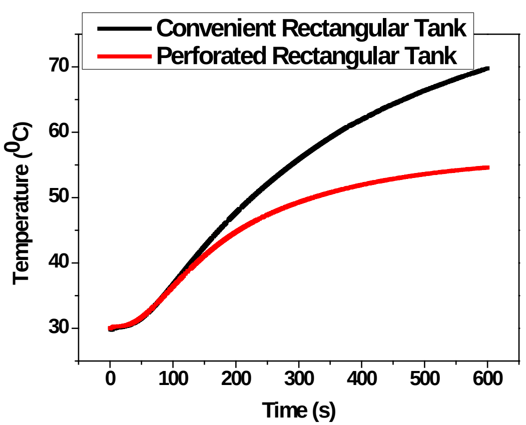
Hydrogen Absorption Procedure

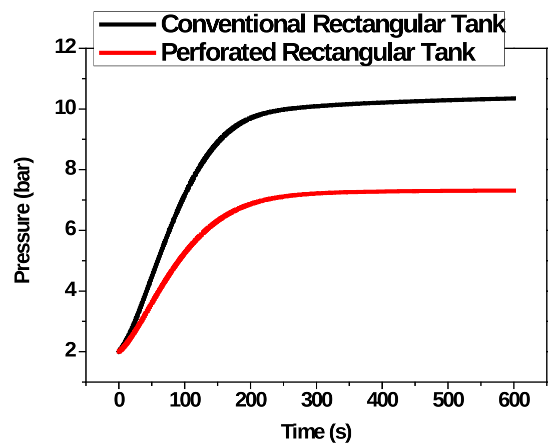


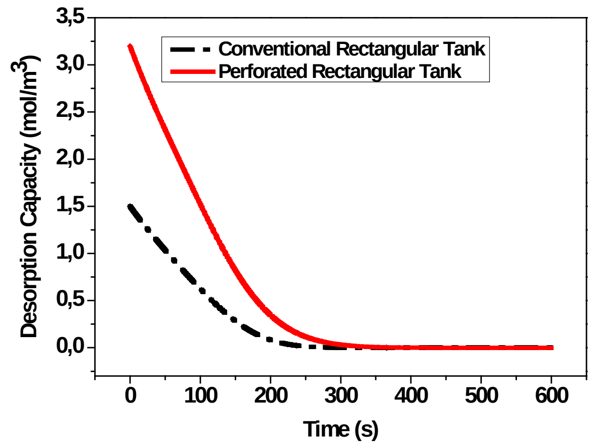




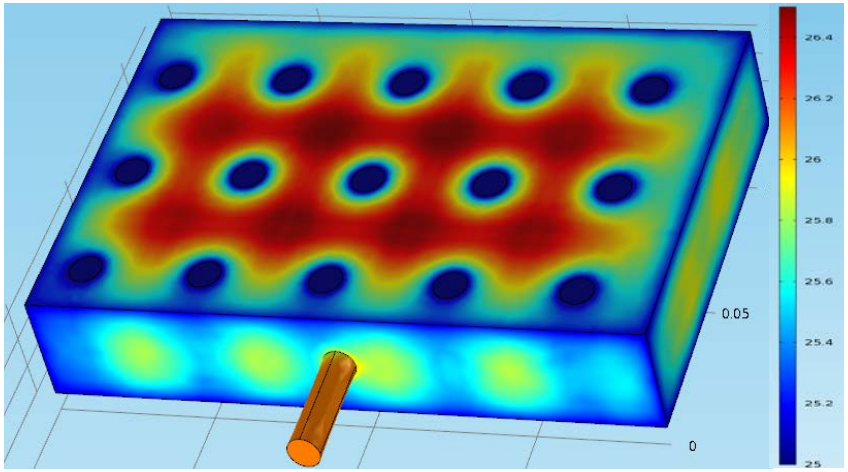
Hydrogen Desorption Procedure



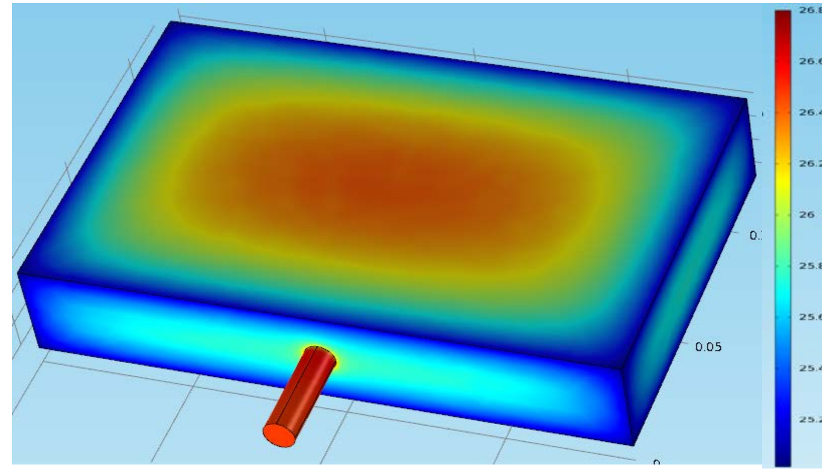




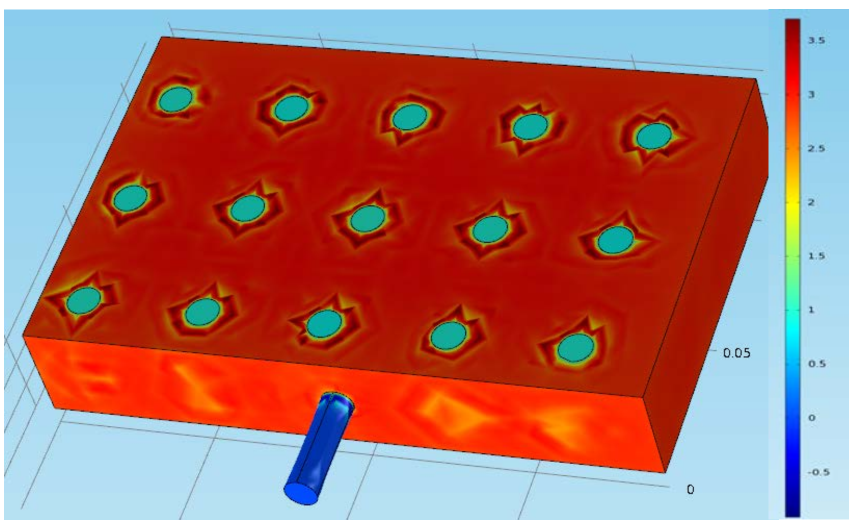
Results and Discussion (II)



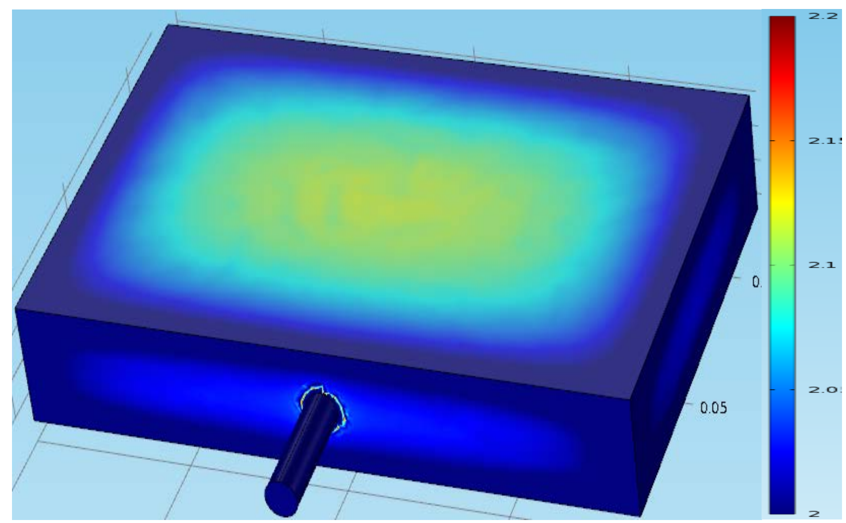
Temperature distribution After 235s of Absorption



Temperature distribution After 185s of Absorption

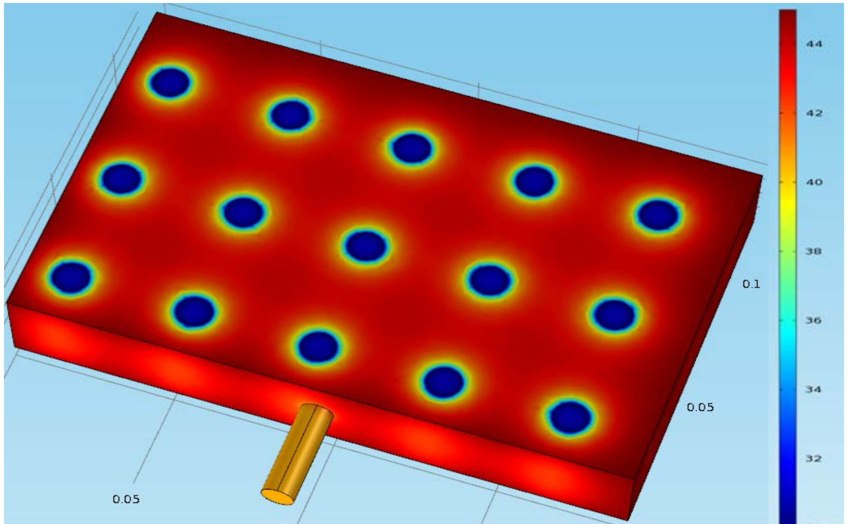


Concentration distribution at the end of the process

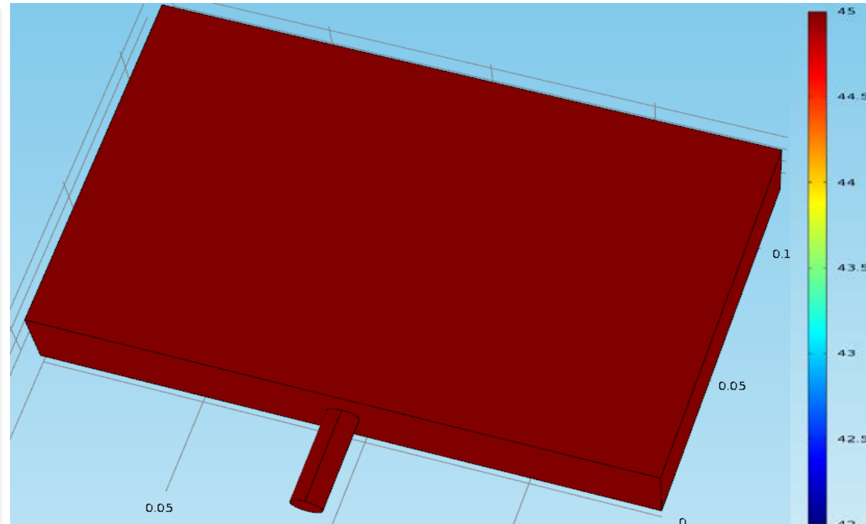


Concentration distribution at the end of the process

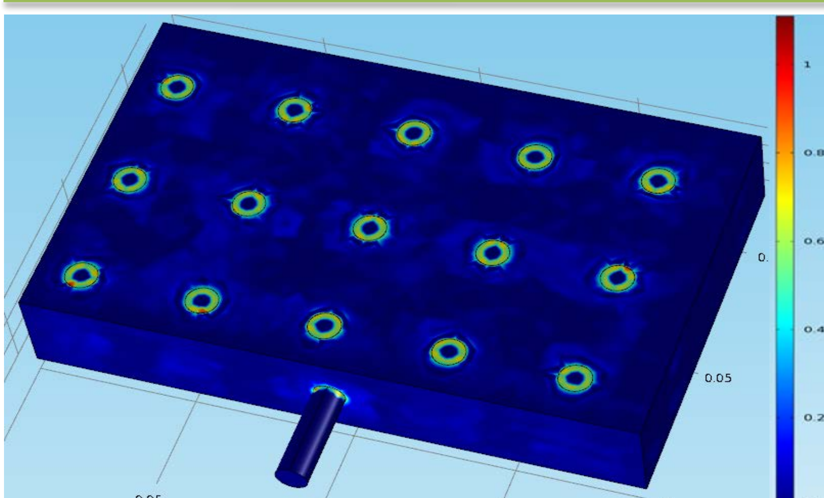
Results and Discussion (III)



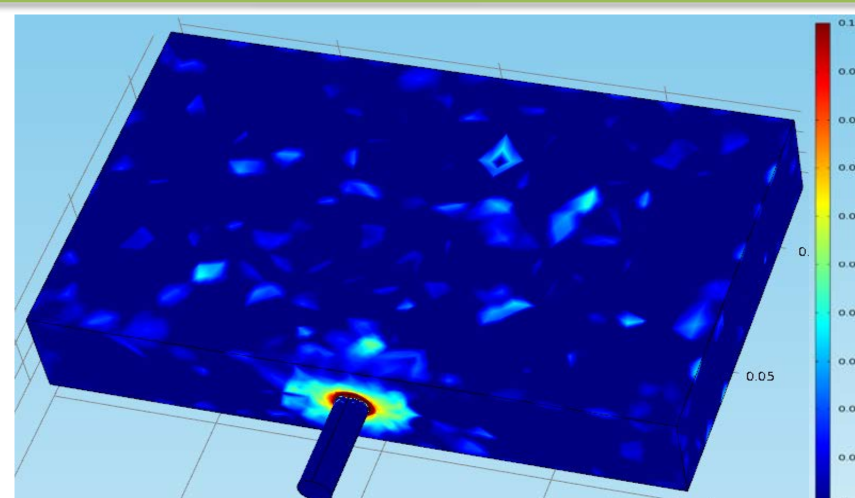
Temperature distribution at the end of Desorption Process



Temperature distribution at the end of Desorption Process



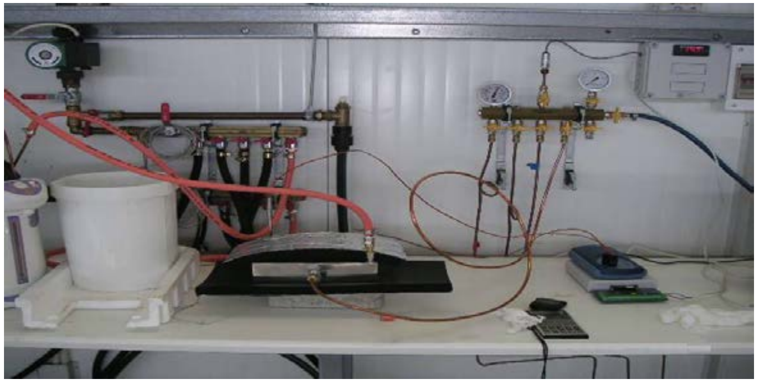
Concentration at the first 20s of desorption



Concentration at the first 20s of desorption

Results and Discussion (IV)

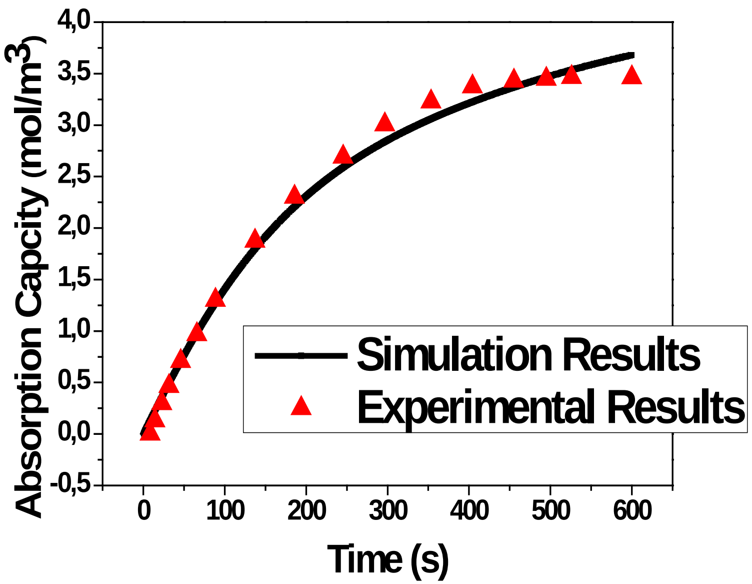
Comparison Between Experimental and Simulation Results

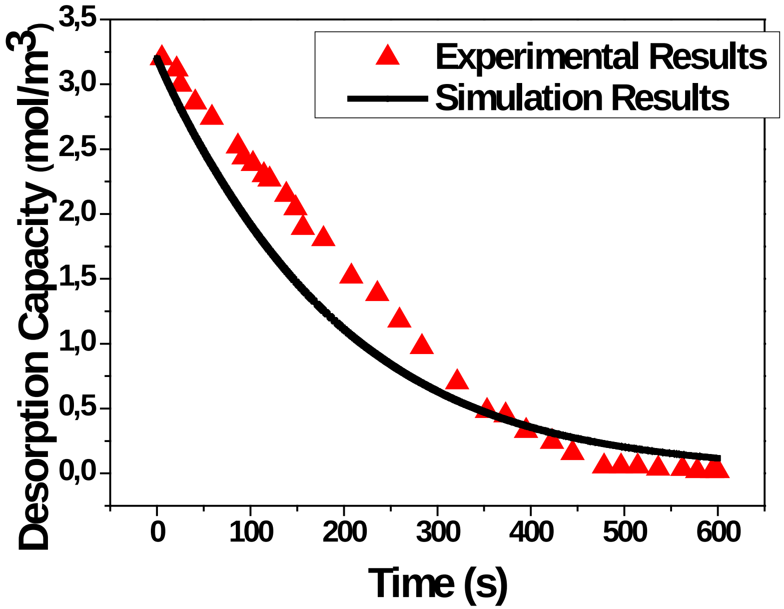


Versus??

or

Combination!!!





Conclusions

- ❖The presence of a cooling material inside a reactangular tank, greatly influences the hydriding reaction.

- ❖The presence of a cooling material inside a reactangular tank, greatly influences the dehydriding process. It seems that the reaction gets weaker but can be controlled more easily.

- ❖The experimental data matching heavily on the simulation results, and confirms our simulation model.

- ❖Combining our simulation model with experimental data, we can define some parameters such as Activation energy for Absorption and Desorption, Thermal Conductivities, Absorption and Desorption Constants

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Thank you very much!!!

Any Questions????

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