Modelling and Simulation of hydrogen storage device for fuel cell using COMSOL Multiphysics

By: Akanji Olaitan
Supervised by: Professor Andrei Kolesnikov

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PRESENTATION OVERVIEW

- **Objective**
- **Introduction**
- **Mathematical Model**
- **Use of COMSOL**
- **Discussion**
- **Conclusion**

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OBJECTIVE

- To develop two- dimensional heat and mass transfer model for a packed bed metal hydride reactor

- To simulate the hydrogen absorption/desorption process in the reactor and compare simulation results with experimental data

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INTRODUCTION

- Due to the high demand and consistent usage of non- renewable carbonaceous fuels worldwide such as gasoline. There is need to provide an alternative energy source that will serve the same purpose as gasoline. Hydrogen has been considered as an alternative energy to be use in the fuel cell.
- Metal hydride technology uses metal alloys to adsorb hydrogen under moderate pressure and temperature, creating hydrides.
- It is important to simulate adsorption/desorption processes in the packed bed reactor as for design purposes as for operational control of reactor.

Metal hydride is a granular material with the size 10-50 μm. It is placed inside of the cylindrical container, in which hydrogen will be supplied from the centre and heat will be transferred through the reactor wall.

Metal hydride adsorbs hydrogen and releases it with the application of heat from Heat Transfer Fluid (HTF).

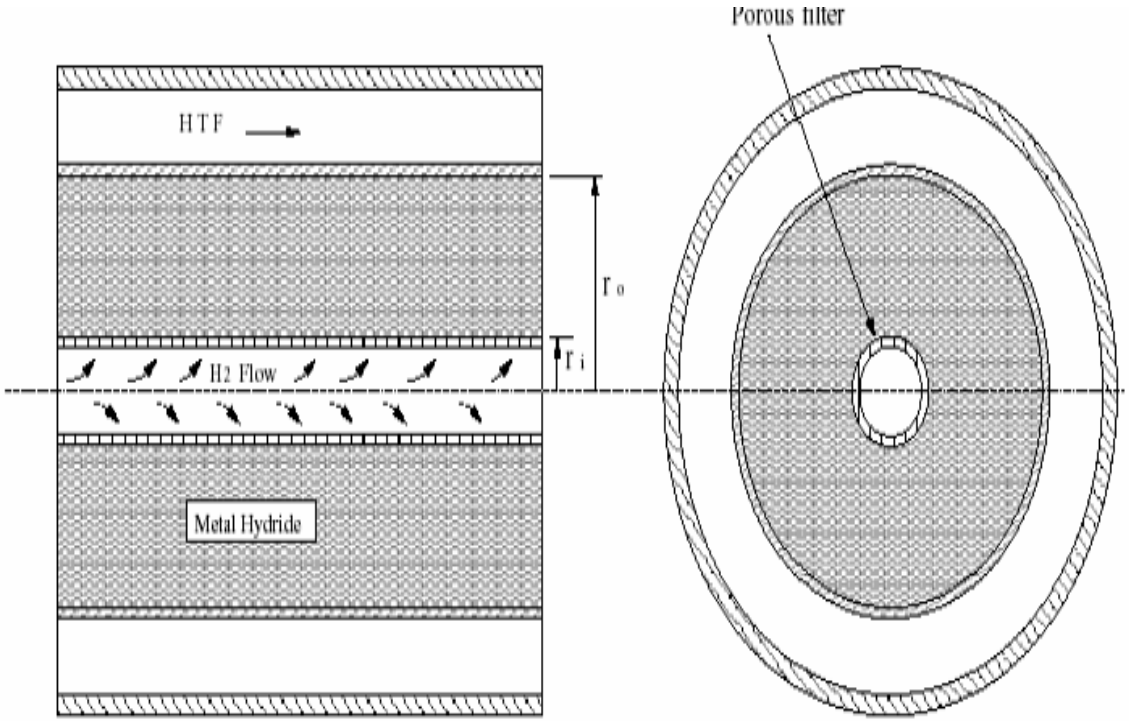

Figure1.Heat transfer in metal hydride hydrogen container

In general the model should incorporate multiphysics couplings between:

- Hydrogen adsorption/desorption kinetics
- Flow in porous media,
- Heat transfer in and between porous media and gas.

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Assumption

- Thermal equilibrium between the hydrogen gas and metal hydride exist
- The gas phase is ideal
- Velocity of Hydrogen gas is calculated by Darcy's law.
- Equilibrium gas pressure is calculated by Van't Hoff equation, disregarding hysteresis and plateau inclination of real pressure/concentration isotherms.

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- The assumption of thermal equilibrium implies that "effective properties" of gas-solid system such as thermal conductivity, heat capacity should be introduced.

- In this work the main thrust is given to the influence of correct expression for effective thermal conductivity on some important performance metrics such temperature, and pressure time variation.

MATHEMATICAL MODEL:

Mass balance

The mass conservation equation of the solid metal hydride:

$$(1-\varepsilon)\frac{\partial \ell_s}{\partial t} = m \qquad \text{.....(1)}$$

Mass balance equation for hydrogen gas

$$\varepsilon \frac{\partial \ell_s}{\partial t} + \nabla\left(\ell_g u_g\right) = m \qquad \text{.....(2)}$$

$$u_g = \frac{K}{\mu_g}\nabla P_g \qquad \text{.....(3)}$$

$$m = C_d \exp\left(-\frac{E_d}{R_g T}\right)\frac{P_g - P_{eq}}{P_{eq}}\ell_s \qquad \text{.....(4)}$$

Momentum balance

$$\ln\left(P_{eq}\right) = \frac{\Delta H}{RT} - \frac{\Delta S}{R}$$

$$+ \left(\phi - \phi_0\right)\tan\left[\pi\left(\frac{C}{C_m} - \frac{1}{2}\right)\right] + \frac{\beta}{2} \quad \text{.....(5)}$$

$$\frac{\partial\left(\ell_g \varepsilon\right)}{\partial t} + \nabla\left(-\ell_g \frac{K}{\mu_g} \nabla P_g\right) = 0 \qquad (6)$$

$$K = C_k \cdot d_p^2 \left(\frac{\varepsilon}{1-\varepsilon}\right)^2 \quad \text{.....(7)}$$

Permeability K and porosity ε are related by the equation (7) above, where d_p is metal hydride particle diameter and constant $C_k = 2.37*10^{-3}$

MATHEMATICAL MODEL (CONT)

ENERGY BALANCE

$$\frac{d}{dt}\left(\varepsilon \ell_s C_{pg} T + (1-\varepsilon)\ell_s C_{ps} T - \varepsilon \frac{\ell_g RT}{M_{H_2}}\right) + \nabla\left(\ell_g C_{pg} uT - \lambda_e \nabla T\right)$$

$$+ (1-\varepsilon)(-\Delta H)\ell_s m = 0 \ldots\ldots (8)$$

Effective thermal conductivity of metal hydride bed traditionally expressed as:

$$\lambda_e = \varepsilon\lambda_g + (1-\varepsilon)\lambda_s \ldots\ldots\ldots\ldots\ldots\ldots (9)$$

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USE OF COMSOL MULTIPHYSICS

COMSOL Multiphysics is use to simulate the absorption /desorption of metal hydride and hydrogen in a bed reactor, the procedures can be presented thus.

- Building of geometry using Boolean operator ,and allocating domain to both metal hydride and hydrogen
- Allocating boundaries conditions
- Set up the variables
- Incorporating the physics such heat transfer, mass transfer and momentum transfer
- Executing the meshing
- Allocating the solver
- Set up the time
- Run the simulation
- Plot the graphs

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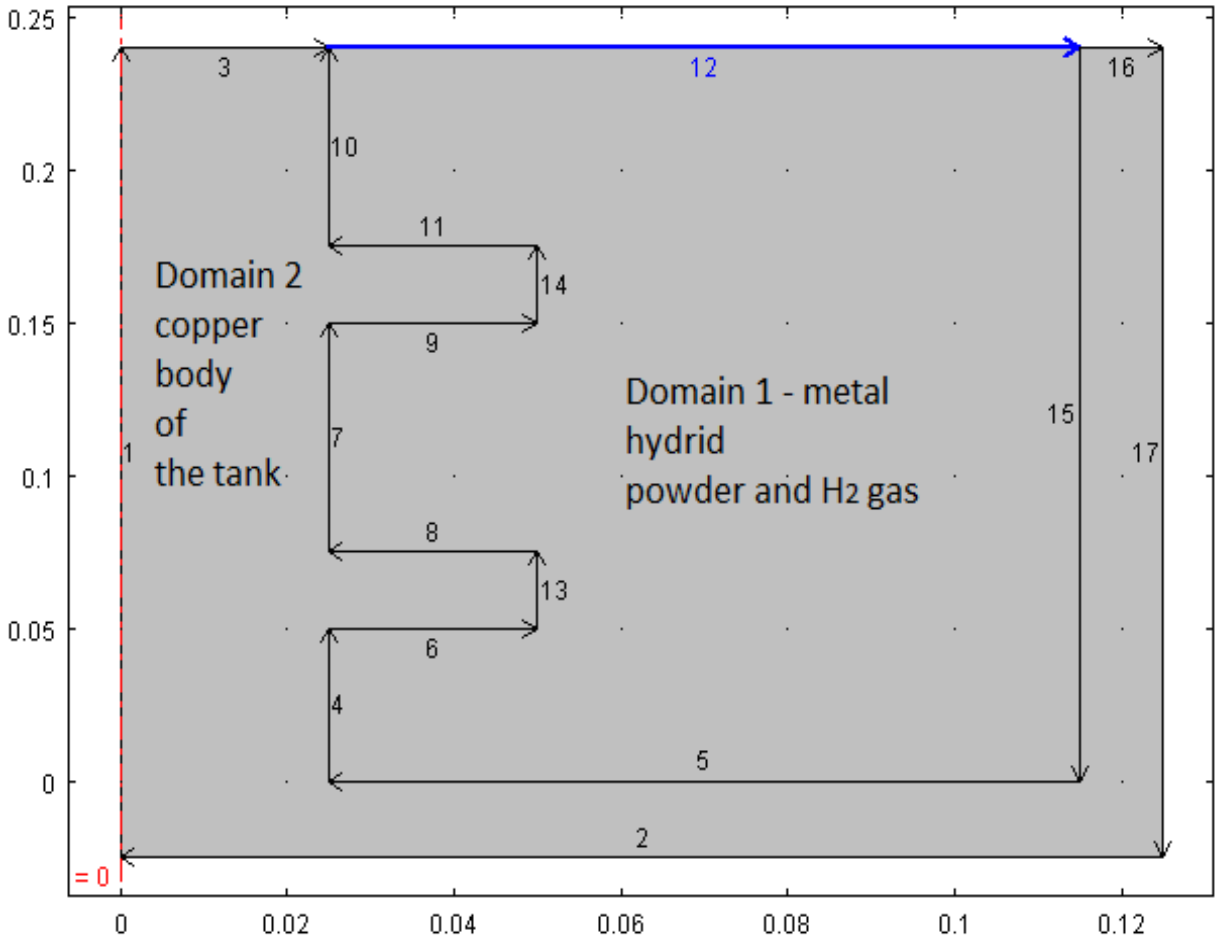

Figure 2 Boundaries within MHHST during hydrogen absorption and desorption

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DISCUSSION

- The graph of temperature variation in time at location z=45 mm from hydrogen inlet shows general trend agreement, however, the difference between experimental data and calculated temperature can reach up to 20% at times 1000-3000 sec, which is higher then accuracy of experimental method used to measure temperature.

RESULTS

Absorption/Desorption process was simulated for hydrogen storage tank filled with metal hydride. The geometry of the tank and boundary conditions are developed. the simulation results of the model described above were presented. The distribution of gas pressure, density of the gas in metal hydride and hydrogen desorption rate temperature, and Flow rateof hydrogen are shown in the figure 3,4,5 ,6,7,8 and 9.figure 10 shows temperature profile.

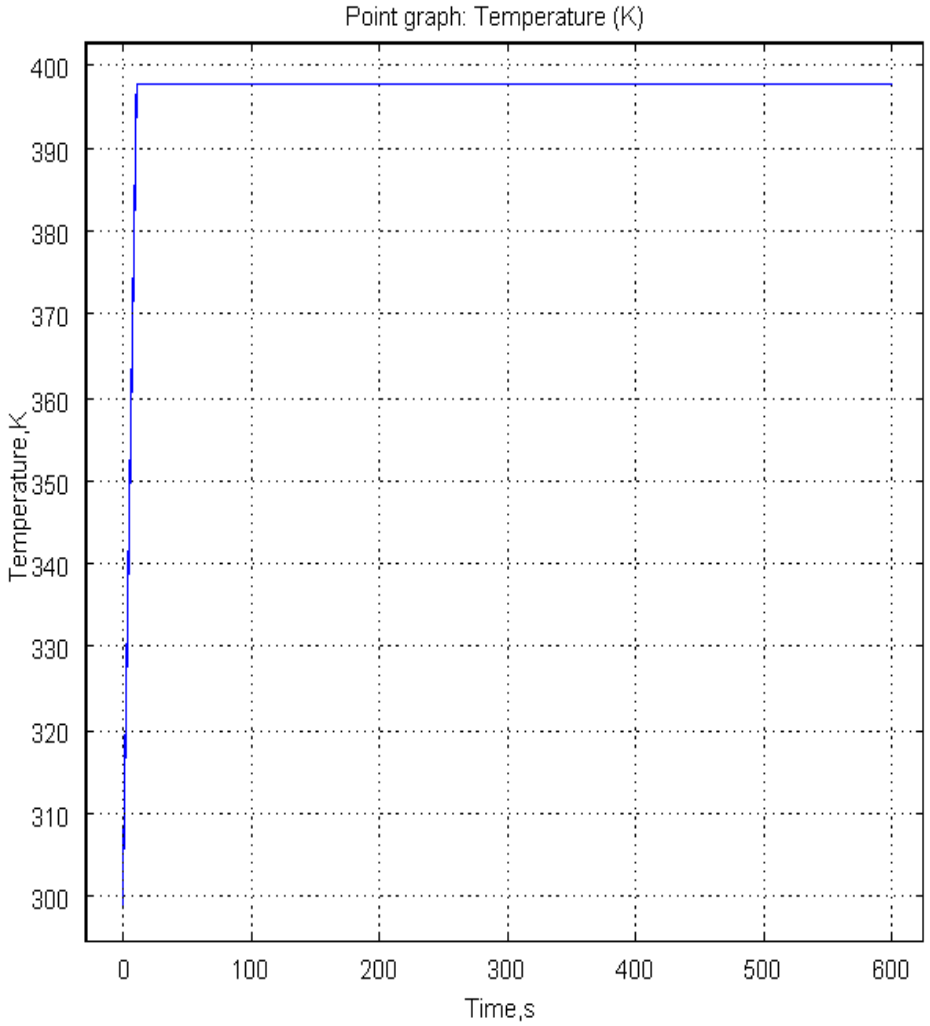

Figure 3.Time evolution of temperature in metal hydride reactor at point with coordinates [0.08, 0.14] during 600s period.

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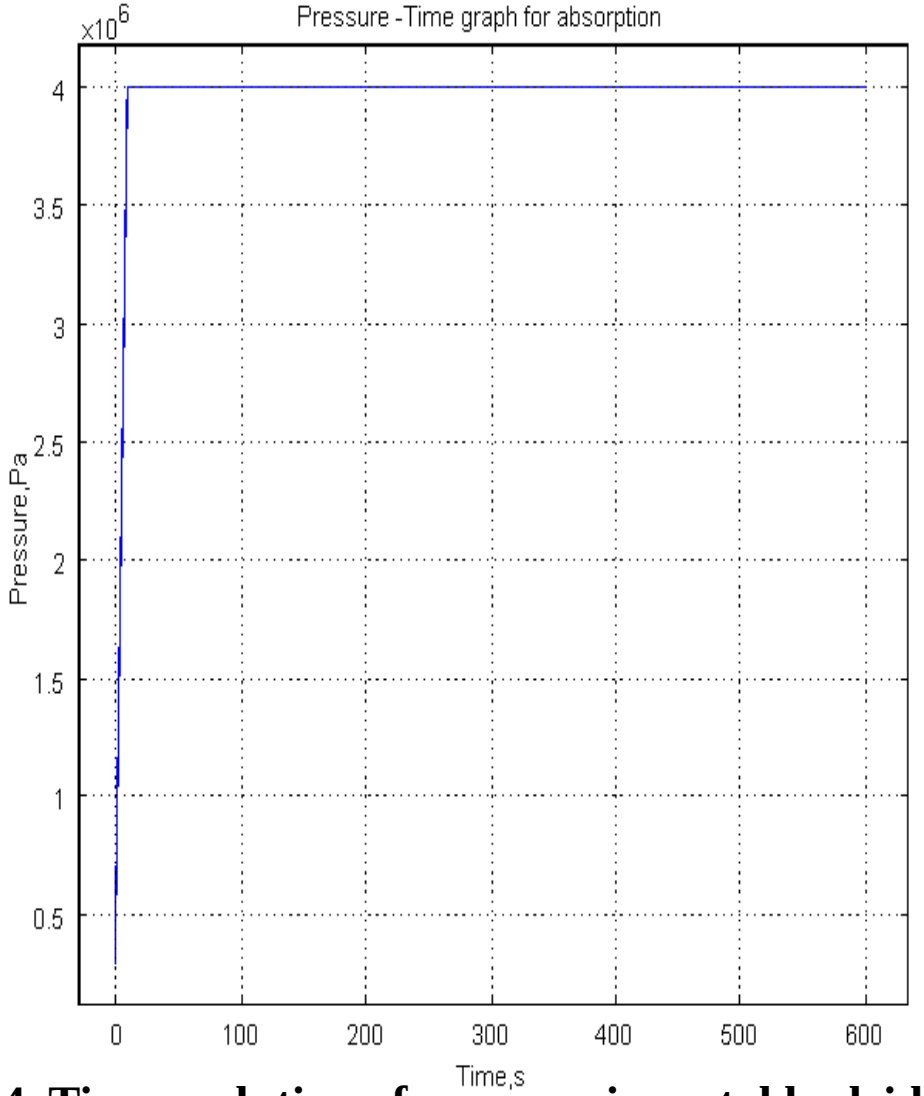

Figure 4. Time evolution of pressure in metal hydride bed at point with coordinates [0.08, 0.14] in 600s

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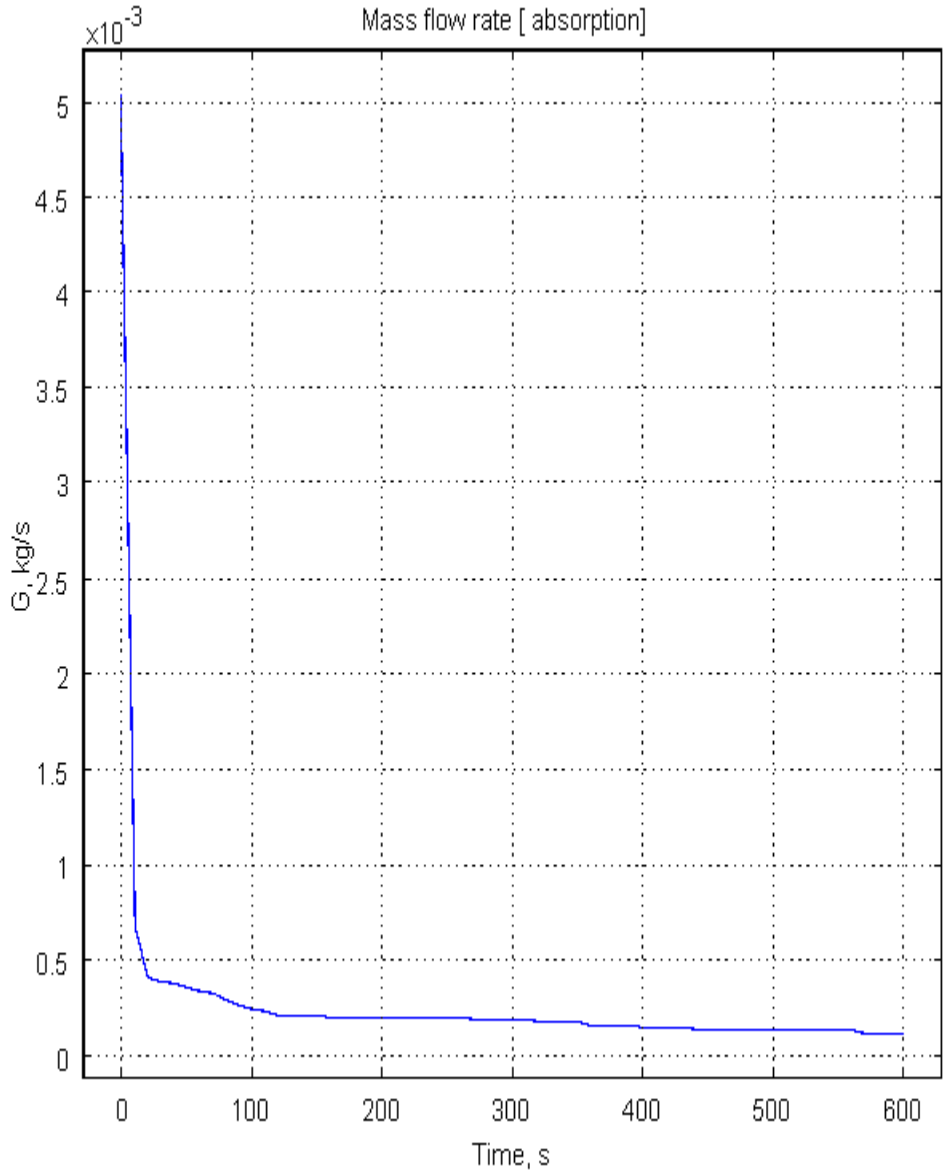

Figure 5. Flow rate of hydrogen in metal hydride during absorption in simulation time 600s.

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Pressure Profile

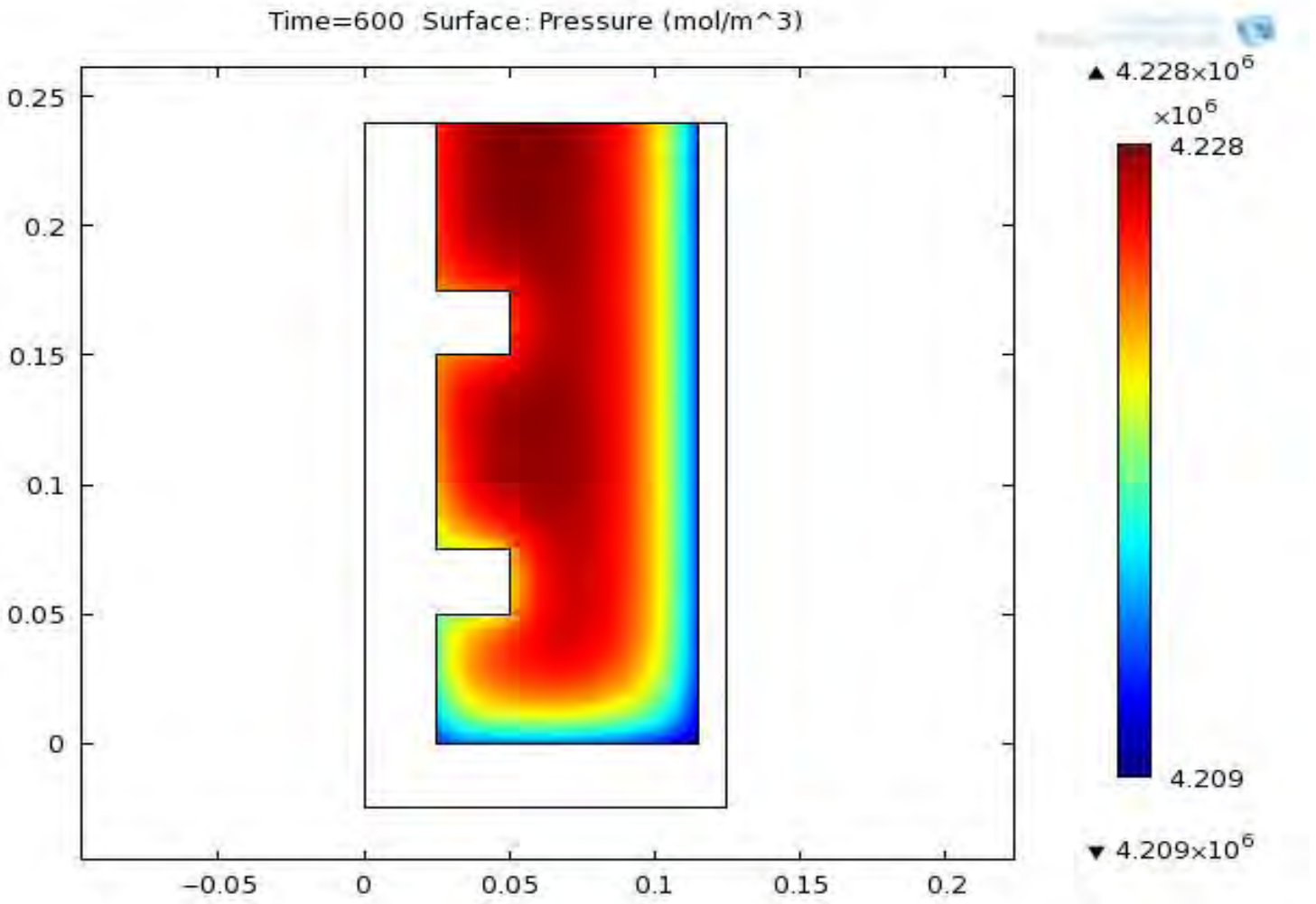

Figure 6. Pressure variation along metal hydride hydrogen storage tank

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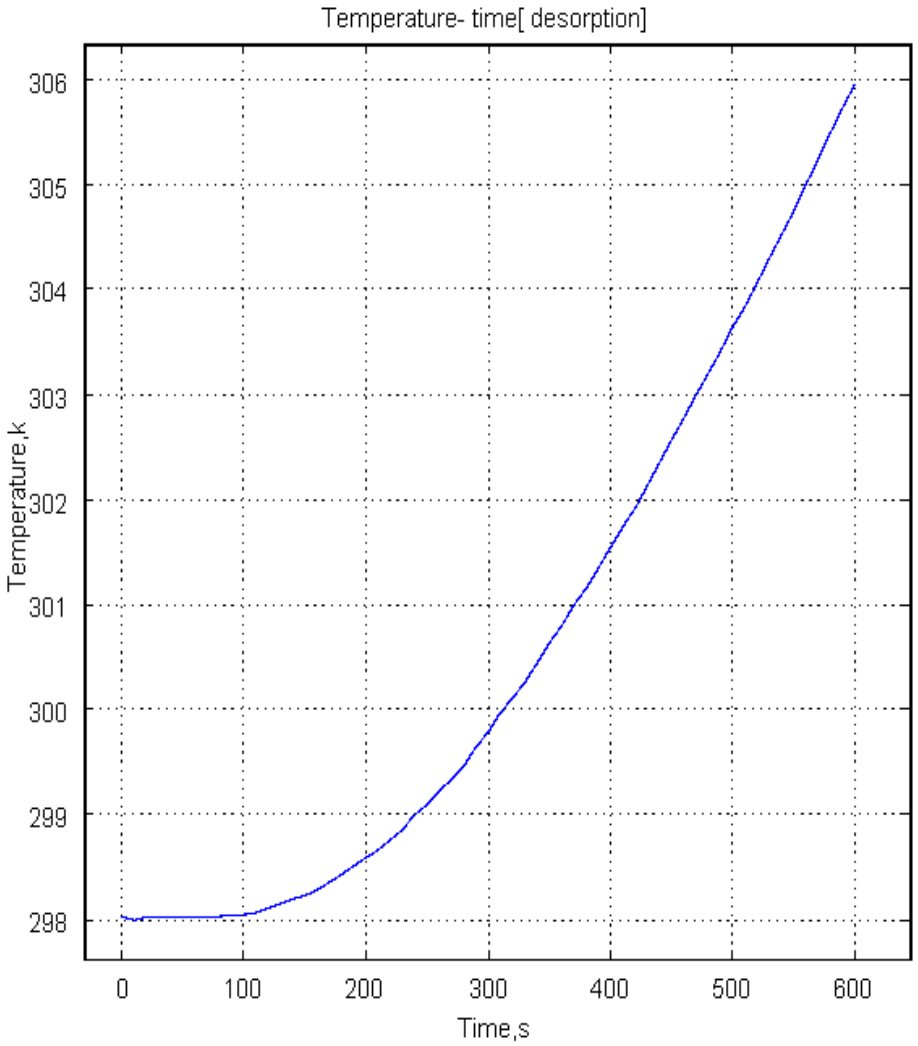

Figure 7. Time evolution of temperature in metal hydride reactor at point with Coordinates [0.08, 0.14] during 600s period.

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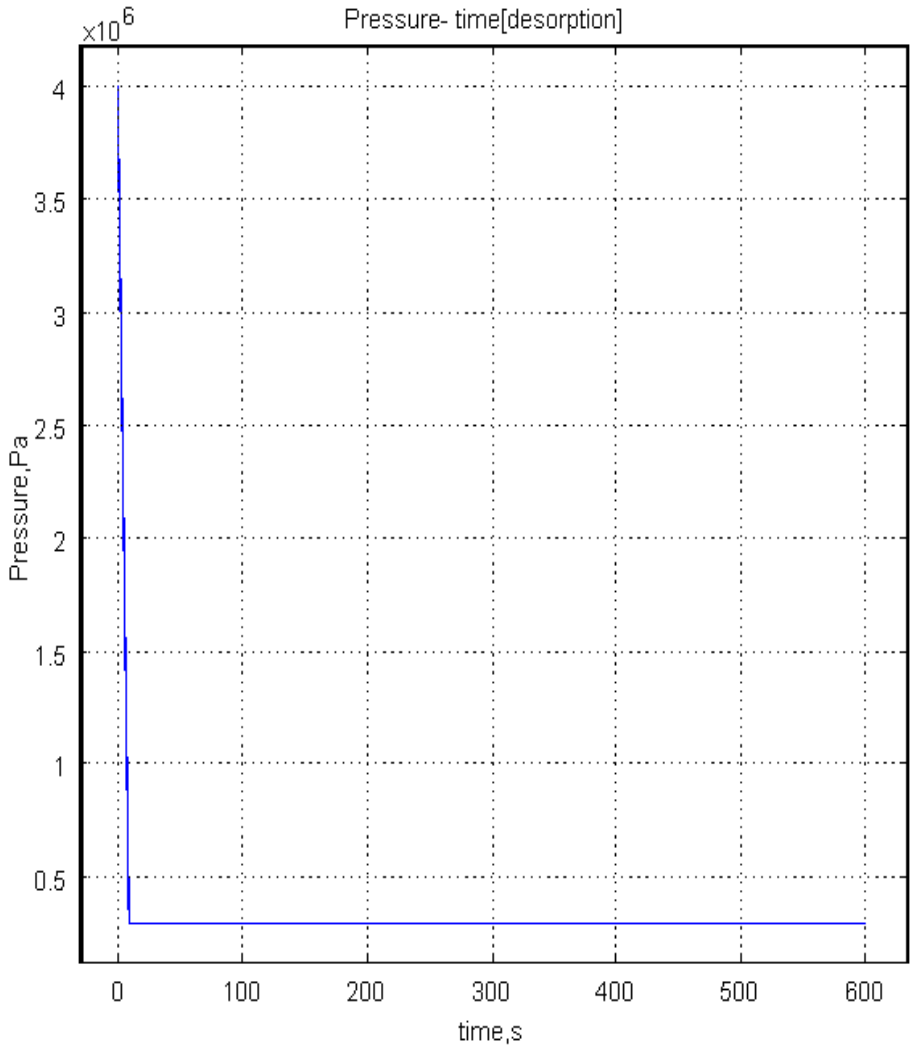

Figure 8.Pressure distribution of hydrogen from metal hydride at [0.08, 0.14] in simulation time 600s during desorption.

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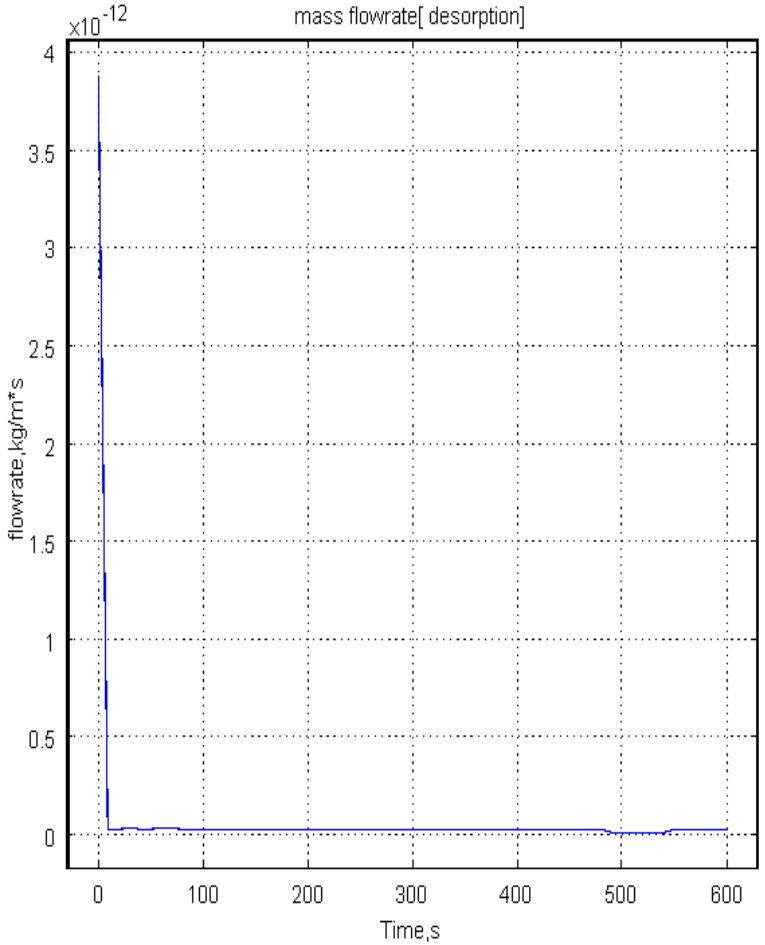
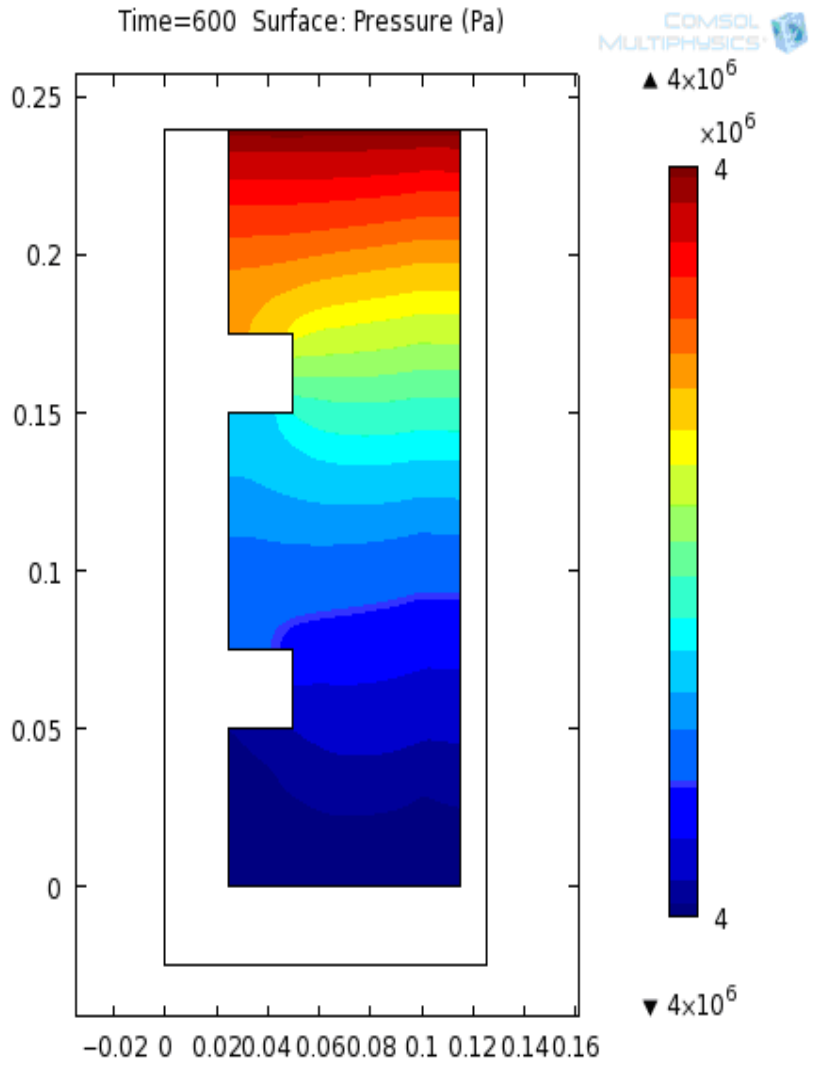


Figure 9. Hydrogen flow rate from metal hydride in simulation time 600s during desorption



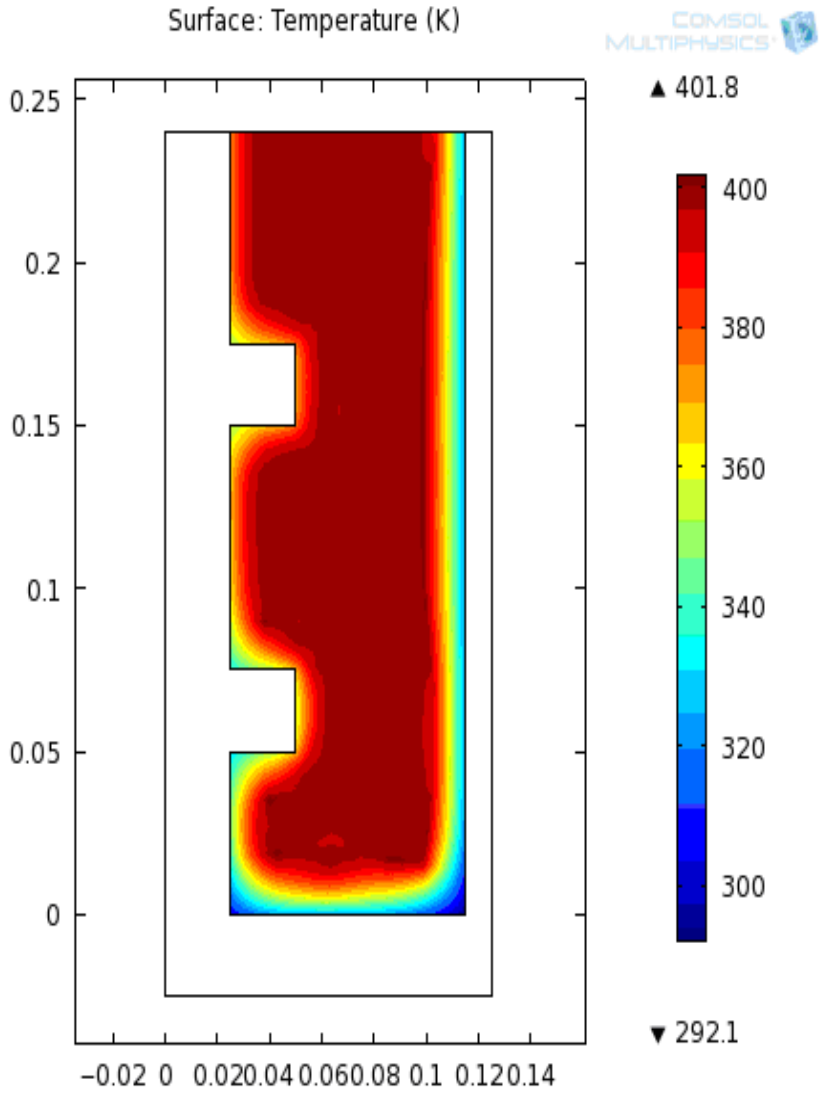


Figure 10. Pressure and Temperature distribution during desorption

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Temperature Profile

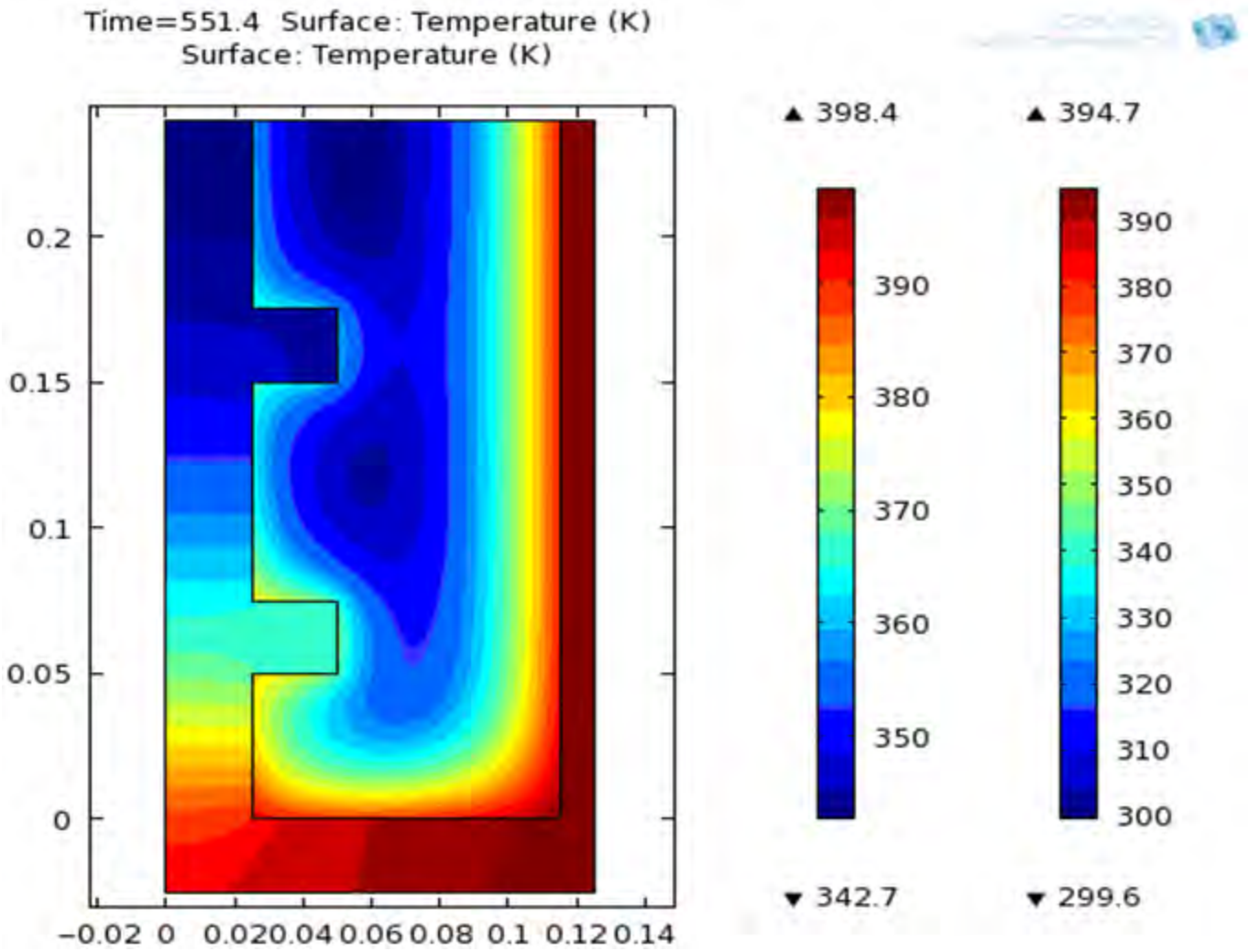

Figure11.Temperature profile during Absorption/Desorption

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Conclusions

- Dynamic mathematical model for the metal hydride hydrogen storage was developed
- In order to verify the model, the numerical model presented above was compared to experimental results of Jemni et al.,1995.the influence of all the operating parameters such as Temperature, Pressure, Density and Flow rate was investigated
- Temperature, pressure and density non-steady distributions inside the metal hydride porous bed were revealed.

COMSOL User Conference2011,Stuggart, Germany.

Thanks

Questions!!!

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