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COMPUTATIONAL FLUID DYNAMIC (CFD) ANALYSIS OF A COLD-ADSORBED HYDROGEN TANK DURING REFILLING

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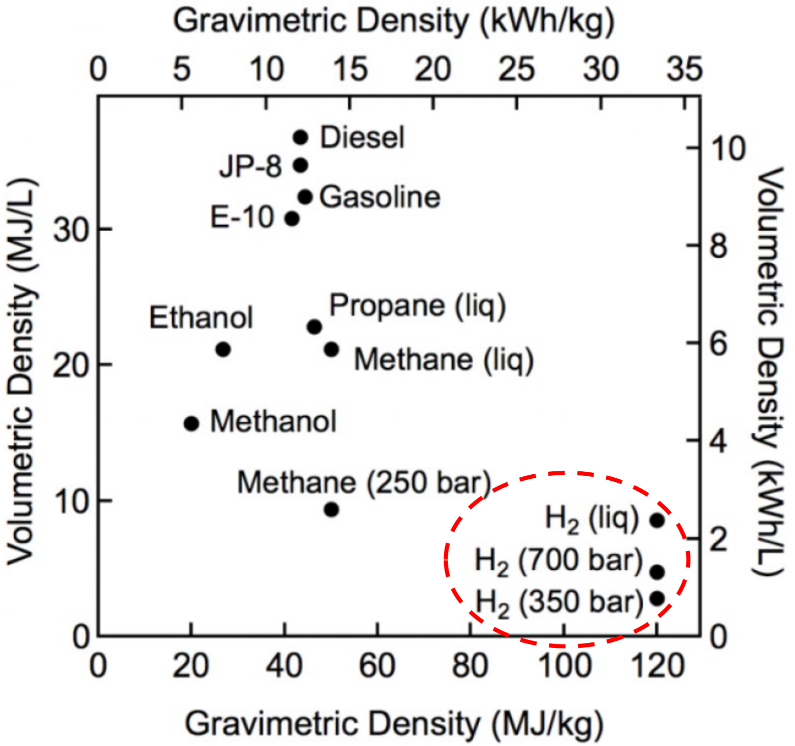
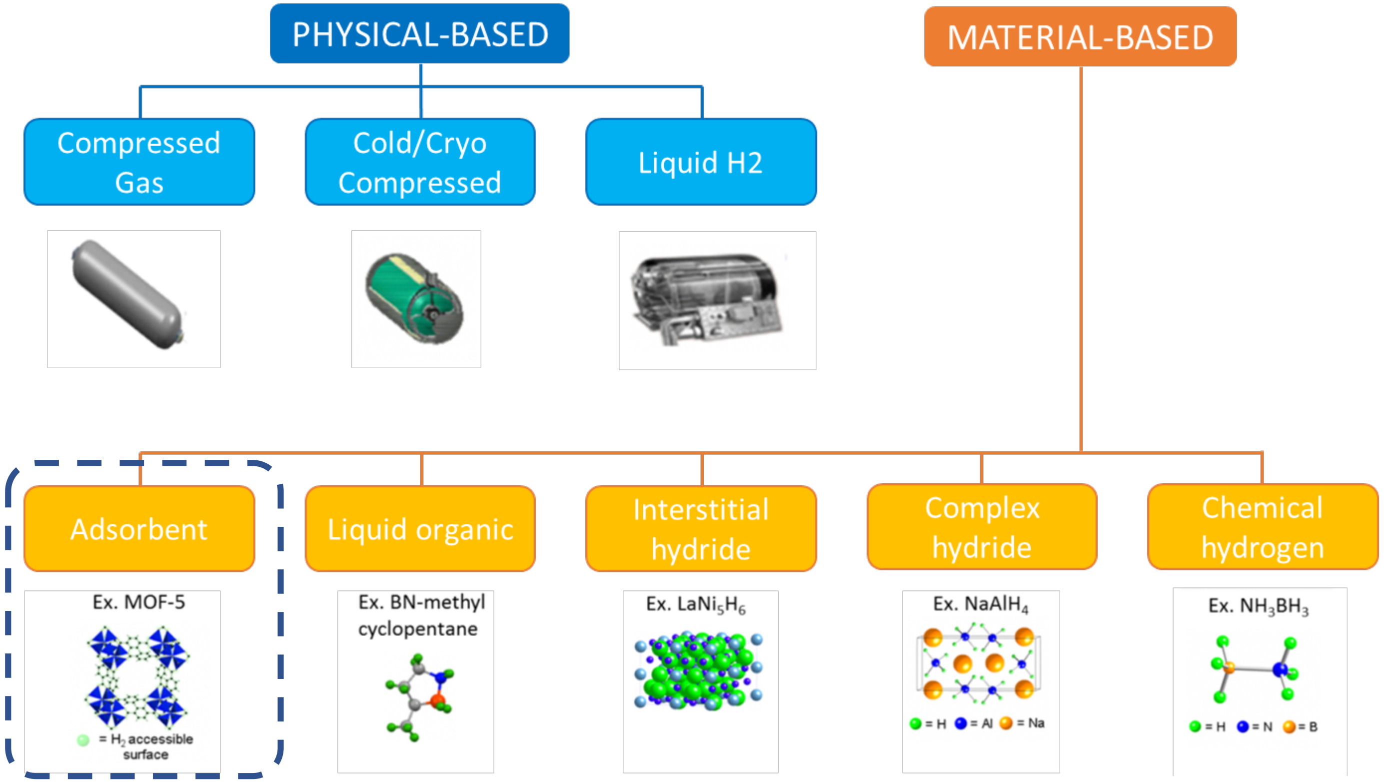
Why Study Hydrogen Storage

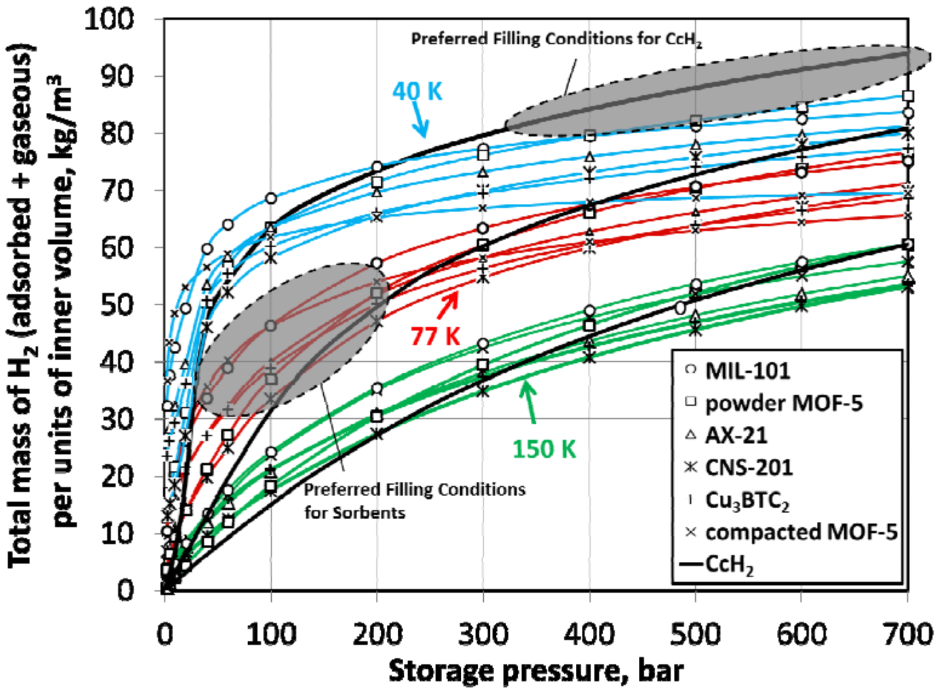




Adsorption of hydrogen using nonporous materials

H2 molecules are physically adsorbed within the pores of substances that have substantial surface areas and extensive gas-solid interfaces, such as zeolites, activated carbons (AC), and metal-organic structures (MOFs)

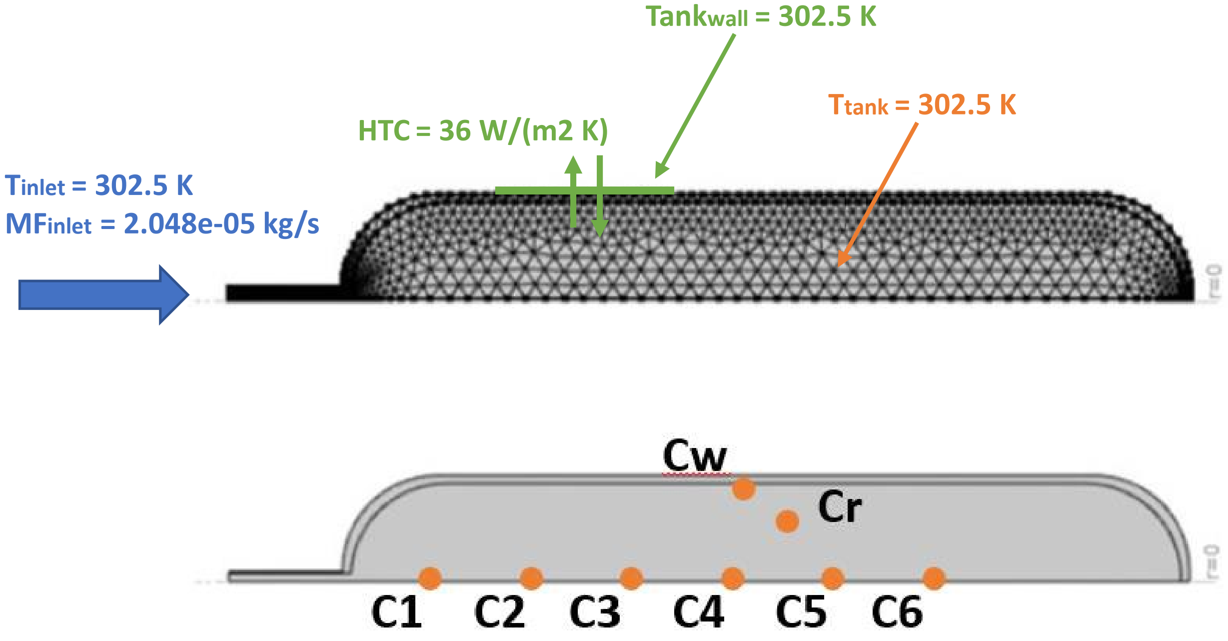
- H2 can be stored at lower pressures, (i.e. 100 bar), in comparison to compressed hydrogen gas storage
- H2 can be stored at higher temperatures, (e.g. 77° K), as opposed to the temperatures required for liquid hydrogen storage
- Compared to chemical hydrogen storage, this adsorption approach offers quicker absorption and requires lower temperatures



The important measurements for this application are:
(1) amount adsorbed as a function of pressure
(2) temperature dependence of adsorption
(3) the enthalpies of adsorption
(4) the adsorption/desorption characteristics

CFD model validation

- Initial and boundary condition:



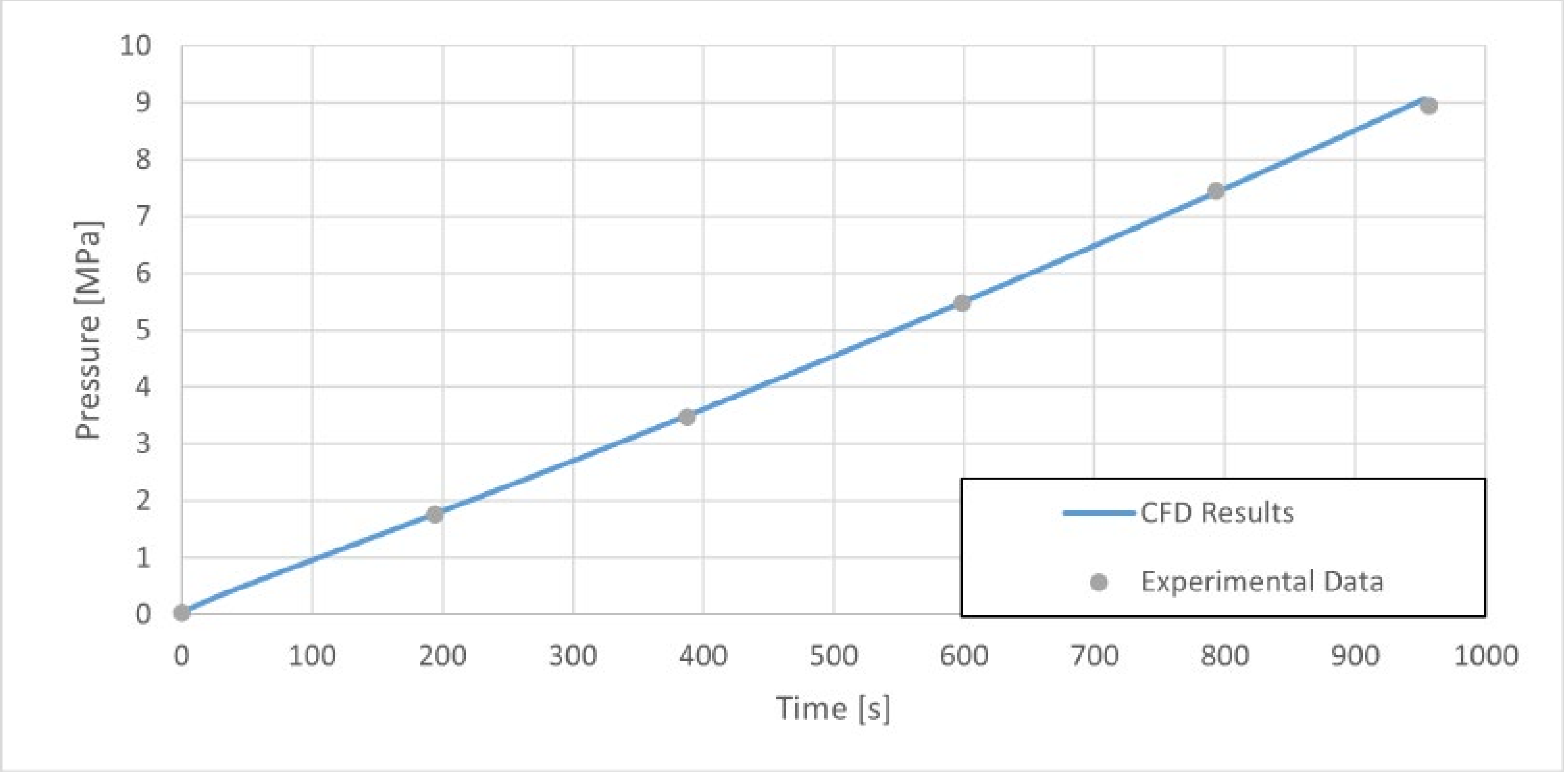
2.5 L tank with activated carbon

Properties	Hydrogen	Steel wall
Bulk density ρ_b kg/m^3	Ideal gas	7830
Specific Heat Cp J/kgK	14700	468
Conductivity k W/mK	0.206	13
Dynamic viscosity μ Pa·s	8.411e-6	-

Properties	Activated Carbon
Bulk density ρ_b kg/m^3	269
Specific Heat Cp J/kgK	825
Conductivity k W/mK	0.764
Bed porosity ϵ	0.49
Particle diameter d_p mm	2.0

A modified Dubinine-Astakhov (MDA) adsorption model is used to describe the adsorption:

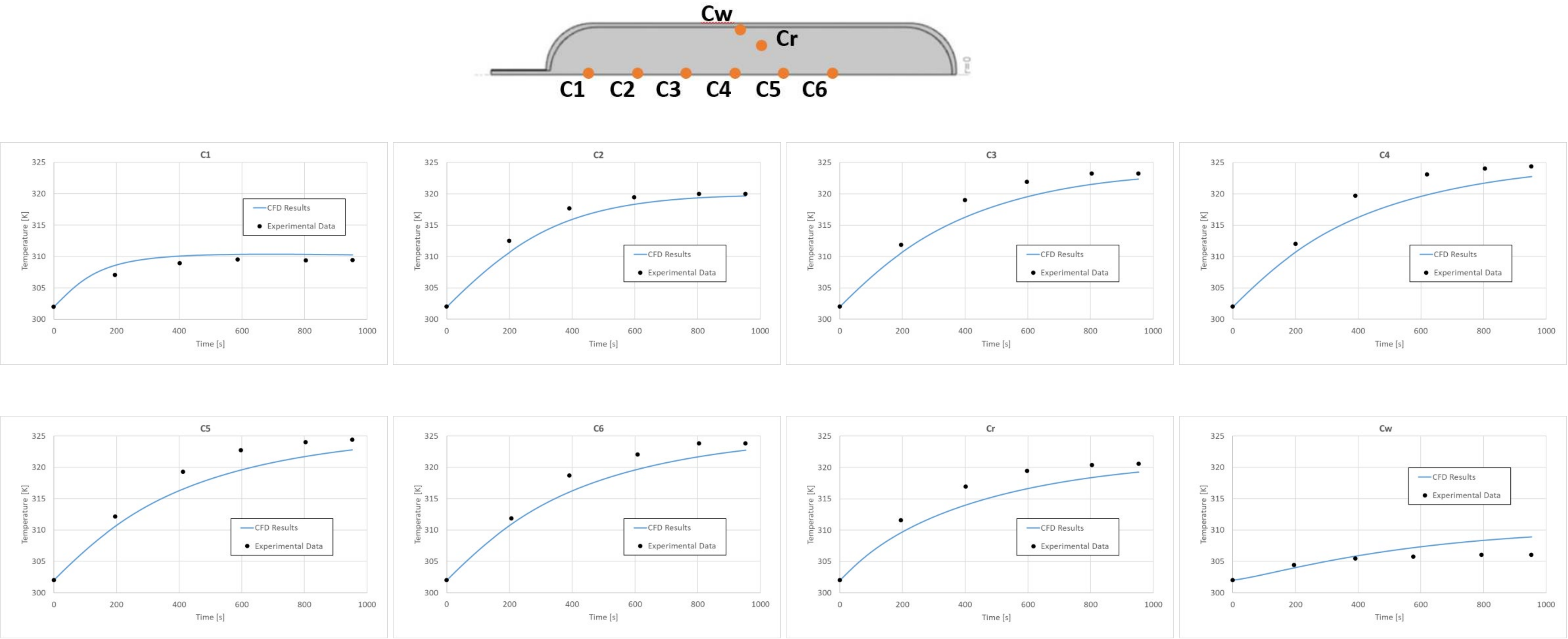
CFD model validation - Results



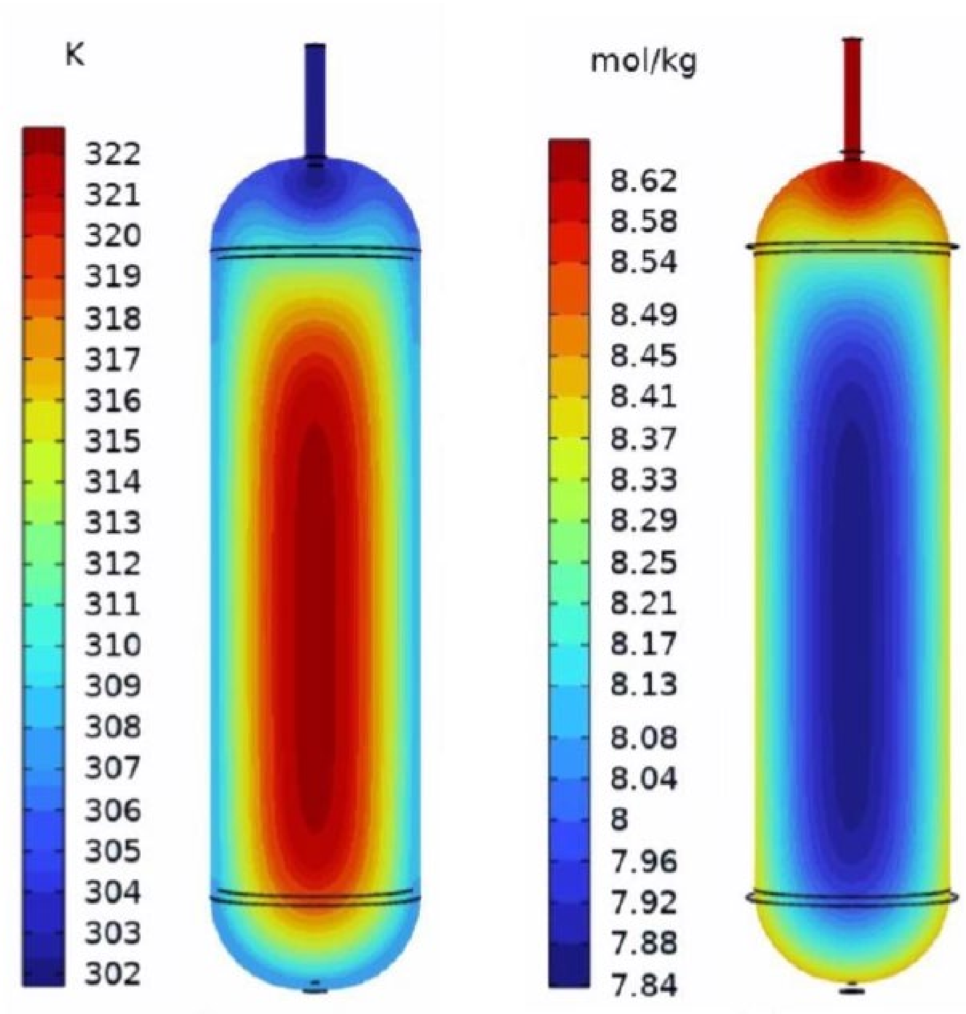
Xiao J, Wang J, Cossement D, Bénard P, Chahine R. *Finite element model for charge and discharge cycle of activated carbon hydrogen storage*. Int J Hydrogen Energy 2012;37:802–10. https://doi.org/10.1016/j.ijhydene.2011.04.055.

Xiao J, Peng R, Cossement D, Bénard P, Chahine R. *CFD model for charge and discharge cycle of adsorptive hydrogen storage on activated carbon*. Int J Hydrogen Energy 2013;38:1450–9. https://doi.org/10.1016/j.ijhydene.2012.10.119

CFD model validation - Results

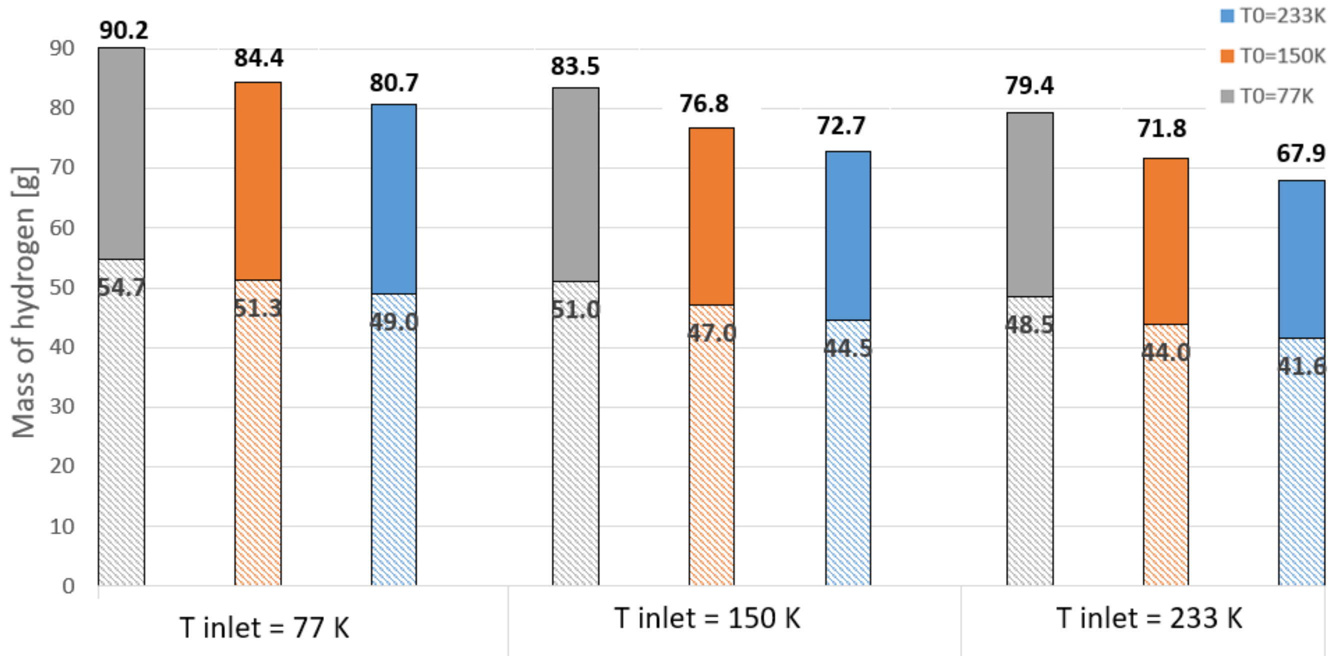


CFD model validation - Results



a) b)

Effect of different initial tank and H2 inlet T



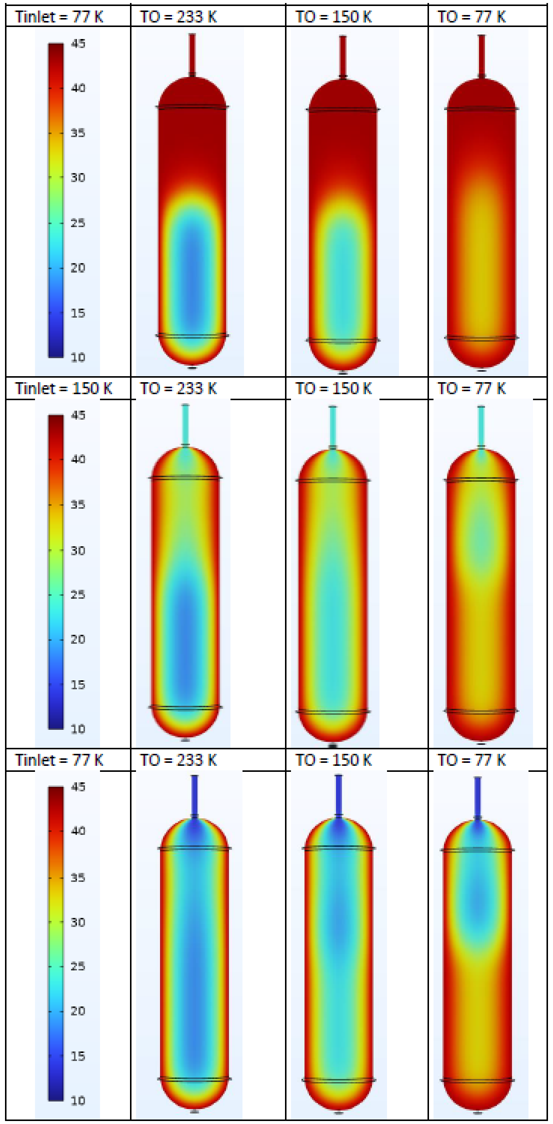
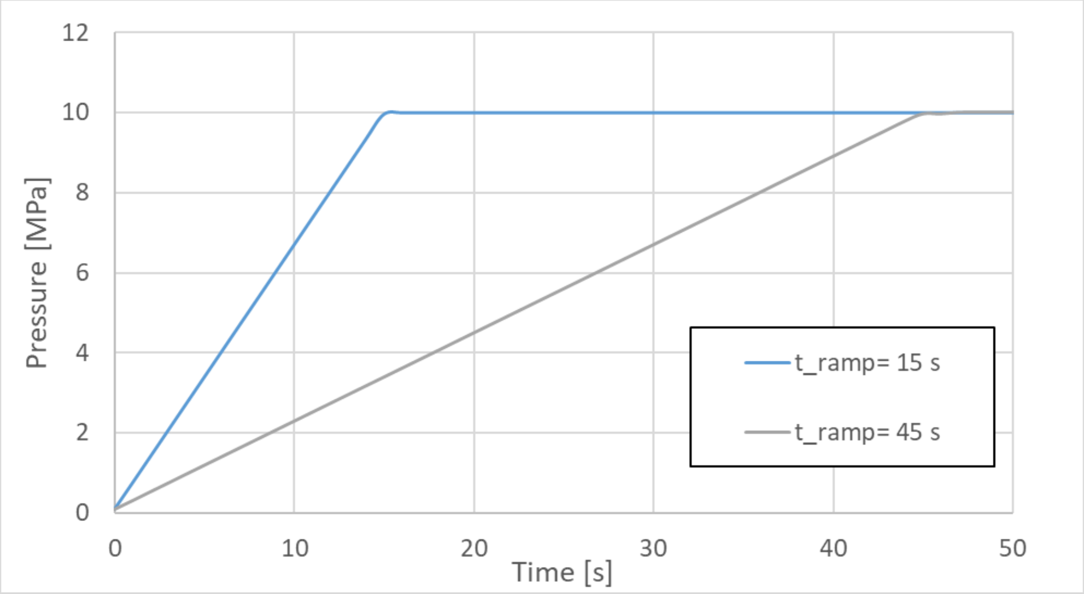
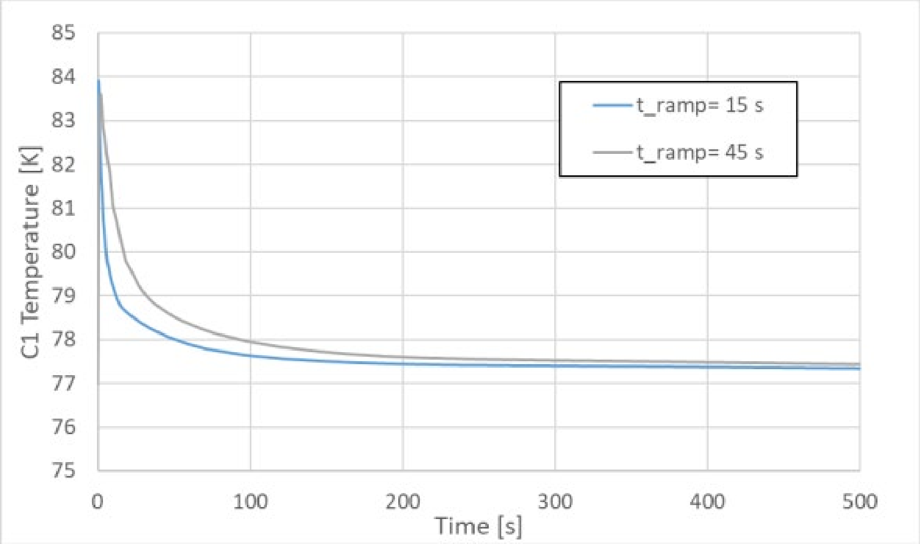
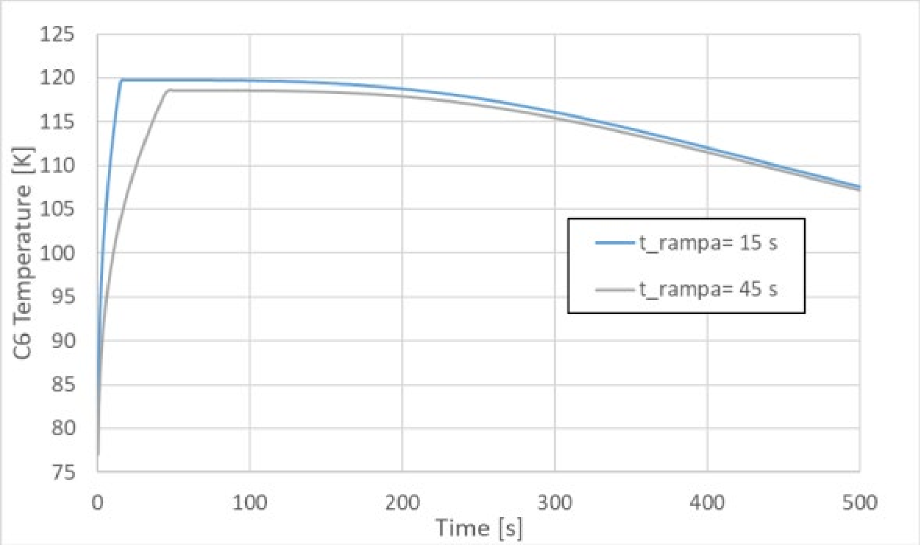


Figure 8. Adsorption [mol/Kg] inside the tank at the end of the filling

Effect of Pressure ramp rate



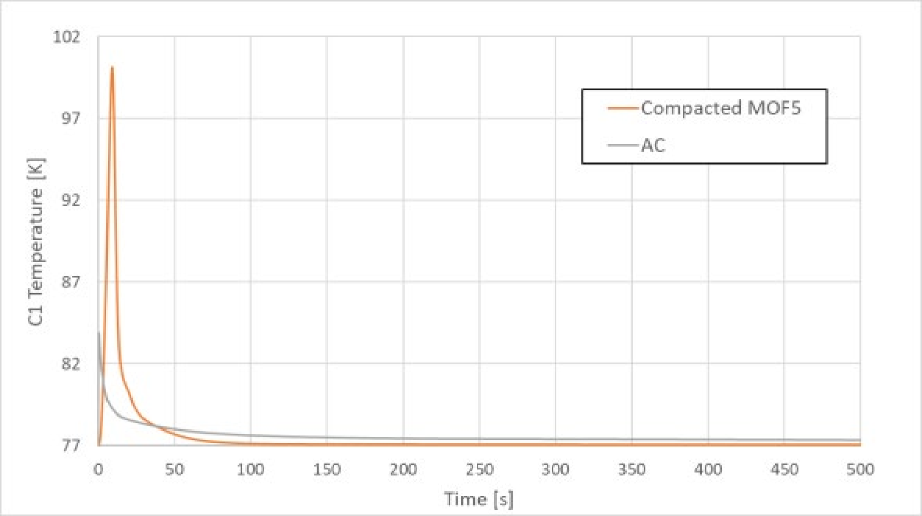


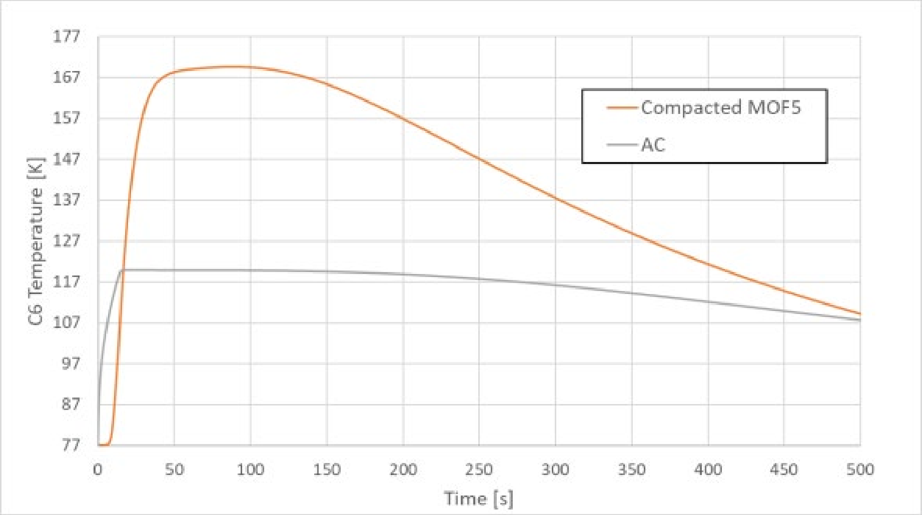


Effect of different adsorbent material (1/2)

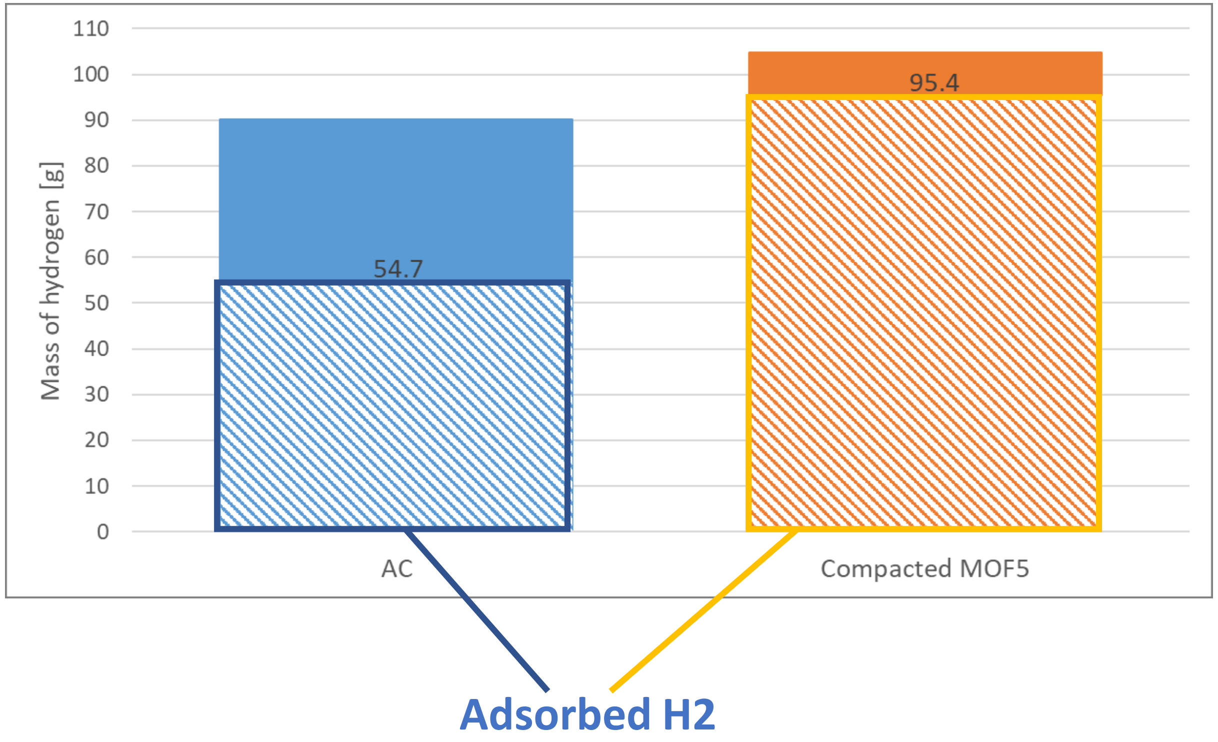
Properties	Activated Carbon	Compacted MOF-5
Bulk density ρ_b kg/m^3	269	406
Specific Heat Cp J/kgK	825	742.5
Conductivity k W/mK	0.764	0.3
Bed porosity ϵ	0.49	0.1266
Particle diameter d_p mm	2.0	0.038
Permeability m^2	1.7e-08	2e-13

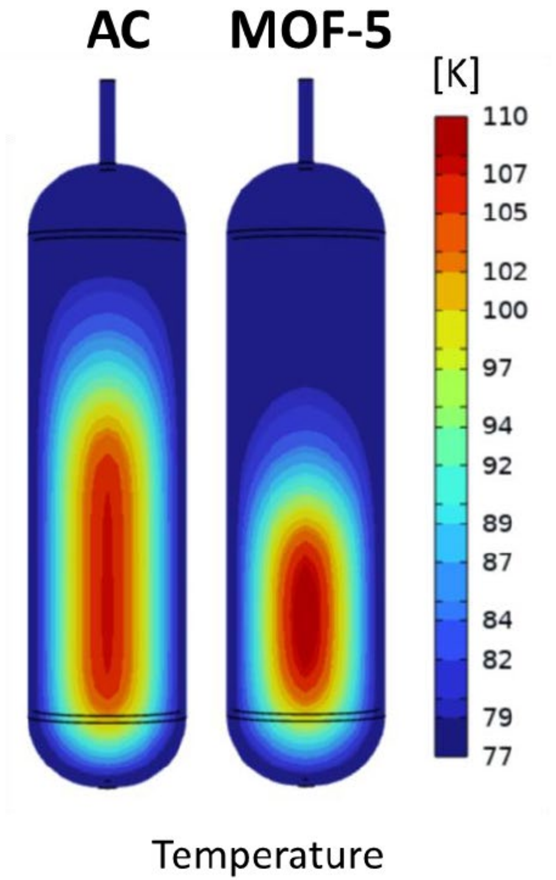
Parameters	Activated Carbon	Compacted MOF-5
n_{max} mol/kg	71.6	70.178
P_0 MPa	1470	1927.3
α J/mol	3080	2541.5
β J/molK	18.9	8.0691

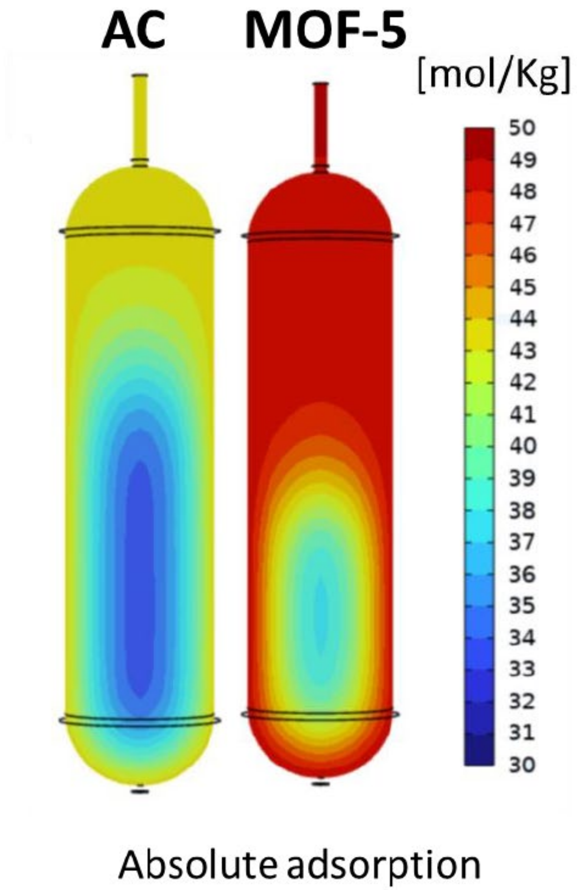




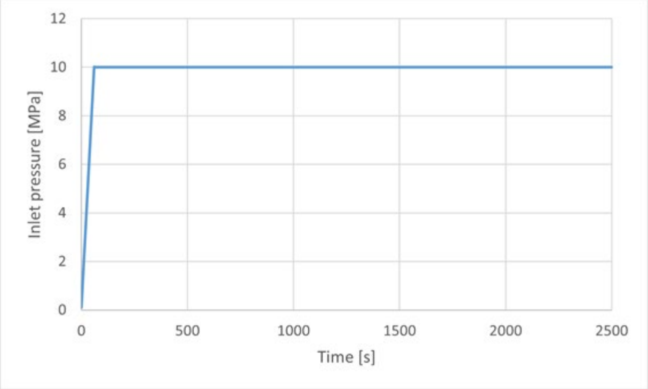
Effect of different adsorbent material (2/2)

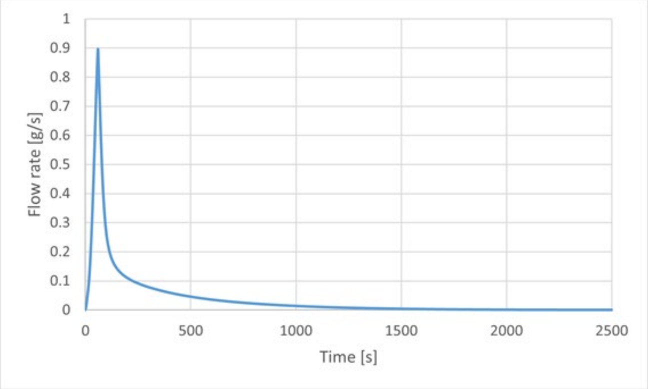


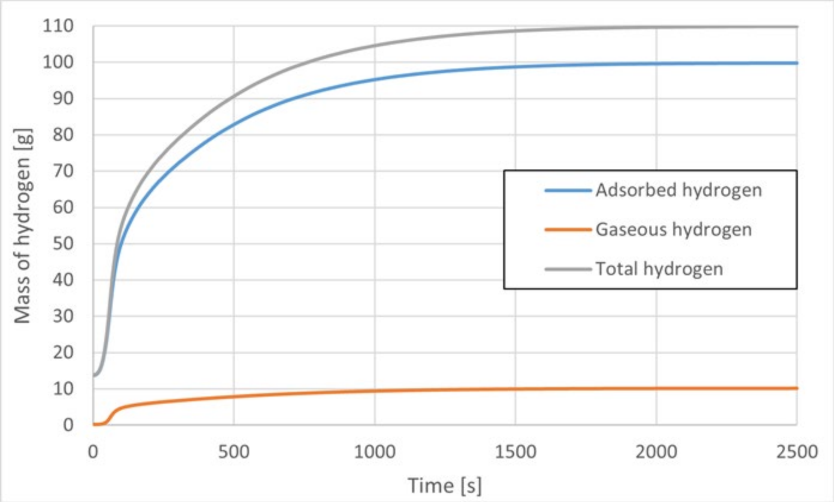


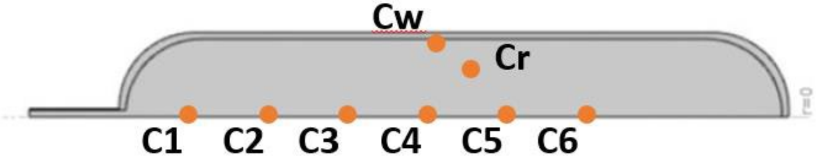


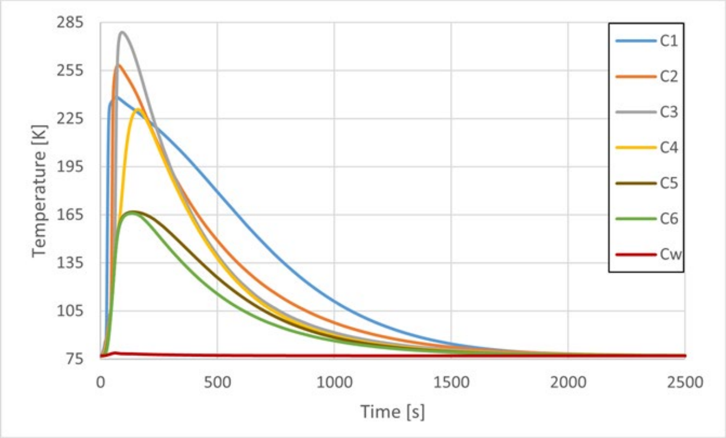
Pressure imposed at the inlet (1/2)











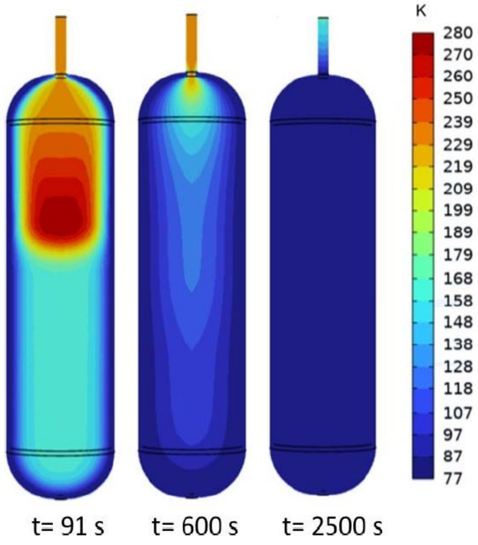


Figure 9. Temperature contours at 91, 600 and 2500 seconds

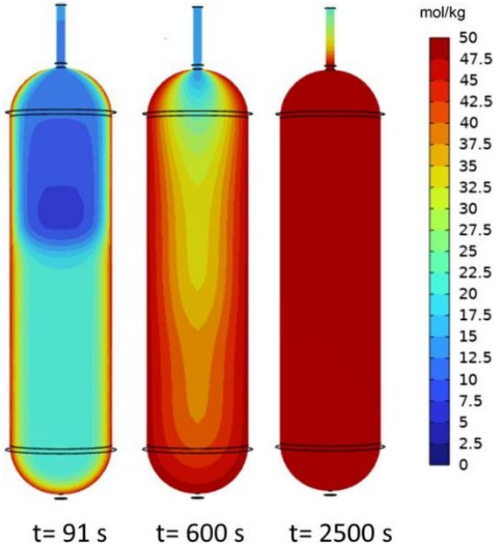
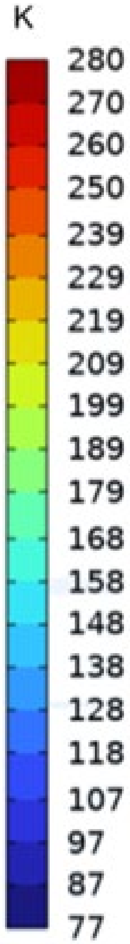
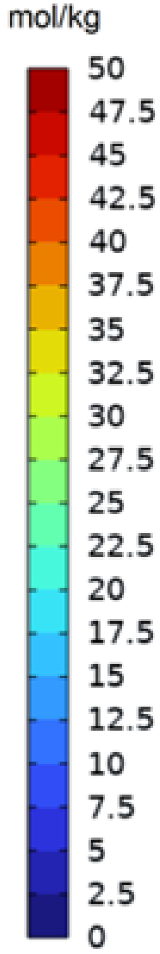


Figure 10. Absolute adsorption at 91, 600 and 2500 seconds

Pressure imposed at the inlet (2/2)

Temperature **Absolute adsorption**





Conclusions

- A validated CFD model has been used to simulate a 2.5-litre hydrogen tank filling process in the presence of adsorbent materials, using COMSOL Multiphysics 6.1
- The same model has been utilized to investigate the impact of various factors, including inlet temperature, inlet pressure ramp rate, and initial tank temperature, on the quantity of hydrogen stored at the end of the filling process
- The effect of two type of adsorbent material (i.e. AC and MOF-5) have been also studied: for the case studied, MOF-5 has higher absolute adsorption than the AC.
- The hydrogen temperature inside the tank and the absolute adsorption has been analyzed:
  - it has been observed that lower temperatures led to higher absolute absorption of hydrogen
  - the total quantity of hydrogen stored in tank for a filling time of 2500 s is 110 g, with the adsorbed mass 10 times bigger than the hydrogen accumulated in the empty portions of the material

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