

# SIMULATION MODEL FOR ADSORPTION BASED HYDROGEN STORAGE

19. Symposium Energieinnovation 2026

HyCentA Research GmbH, Graz 2026

Viktoria Haberl, BSc.

# Austria's Research Center for Hydrogen Technologies



## HyCentA Research – Leading Hydrogen Innovation

- **120+ researchers** mechanical engineering, physics, chemistry, process engineering, electrical engineering
- **600+ projects** successfully completed
- **20+ years of R&D expertise**
- **State-of-the-art research**, testing and refueling infrastructure
- **International Cooperations**



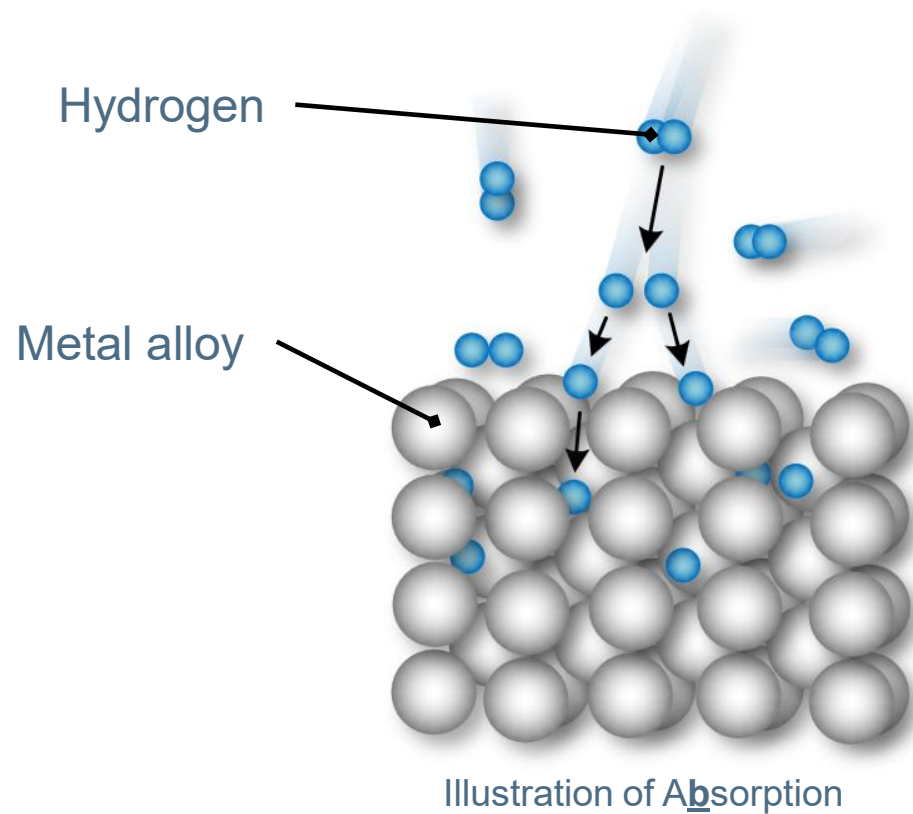
Extra-university research organization at  
Graz University of Technology (TUG)



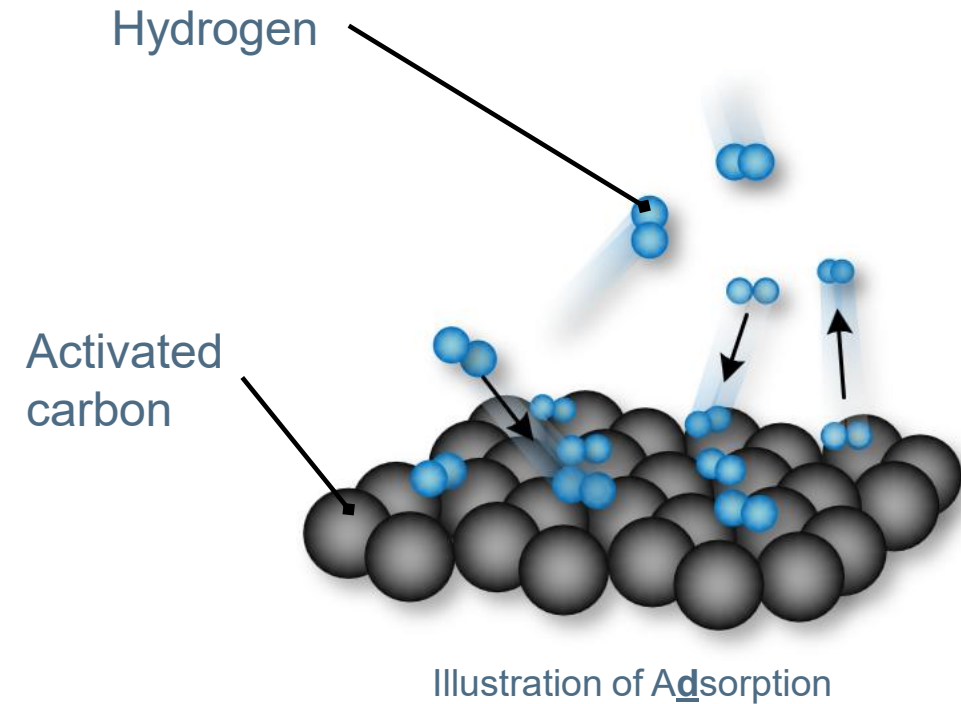
## Why use adsorption storage?

## Why create a simulation model?

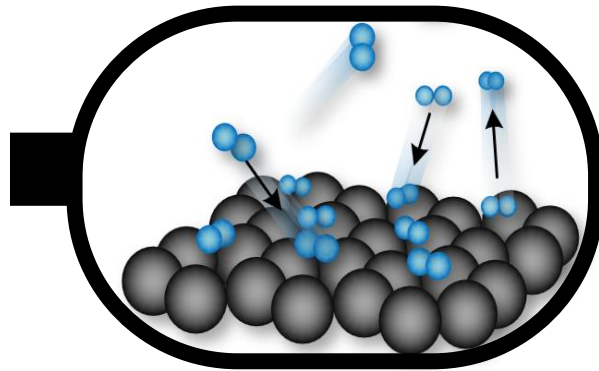
## Absorption in metal hydride



## Adsorption on activated carbon



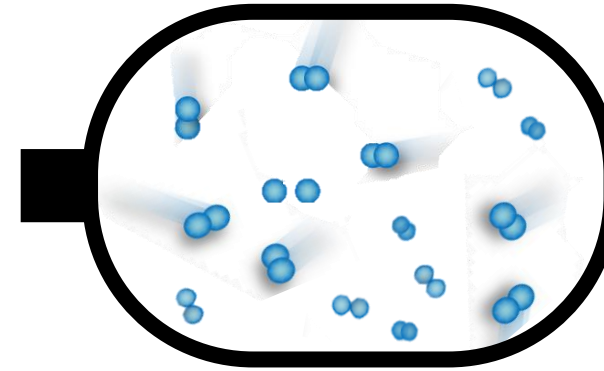
## Adsorption storage tank



V = 68 L  
Pressure = 40 bar  
Temperature = 77K

Storage capacity = 2 kg

## Compressed storage tank

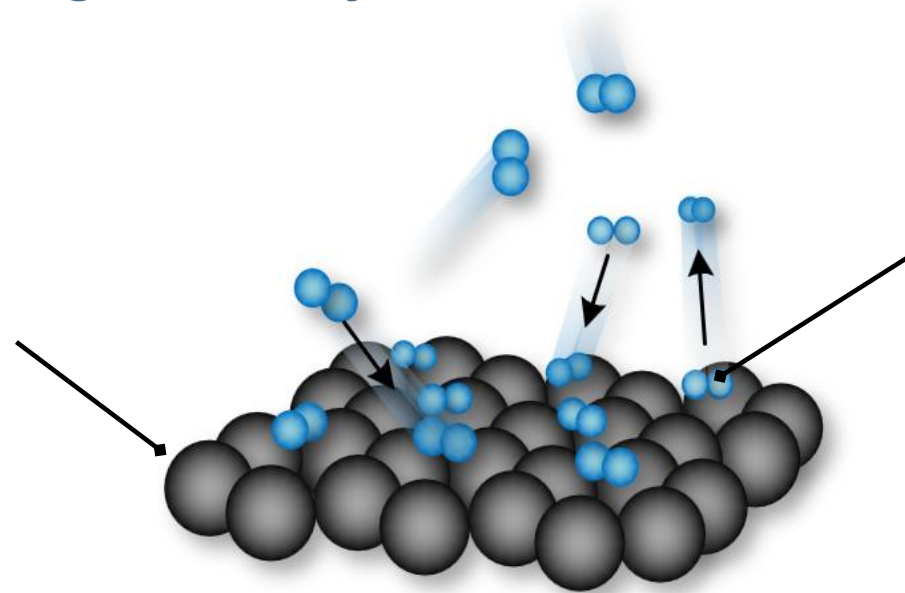


V = 68 L  
Pressure = 40 bar  
Temperature = 77K

Storage capacity = 0.9 kg

Operation pressures below  $\text{CH}_2$   
→ mitigated safety risks

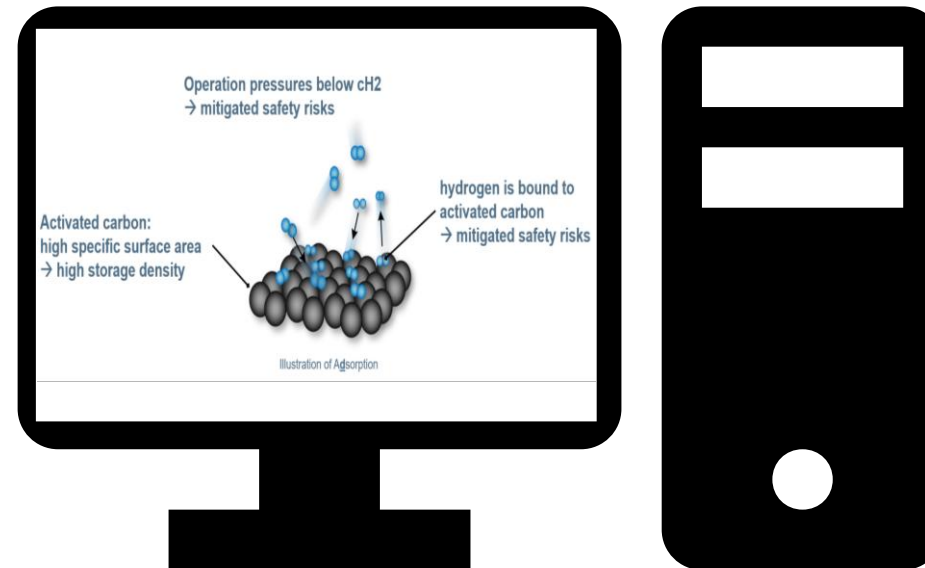
Activated carbon:  
high specific surface area  
→ high storage density



hydrogen is bound to  
activated carbon  
→ mitigated safety risks

Illustration of Adsorption

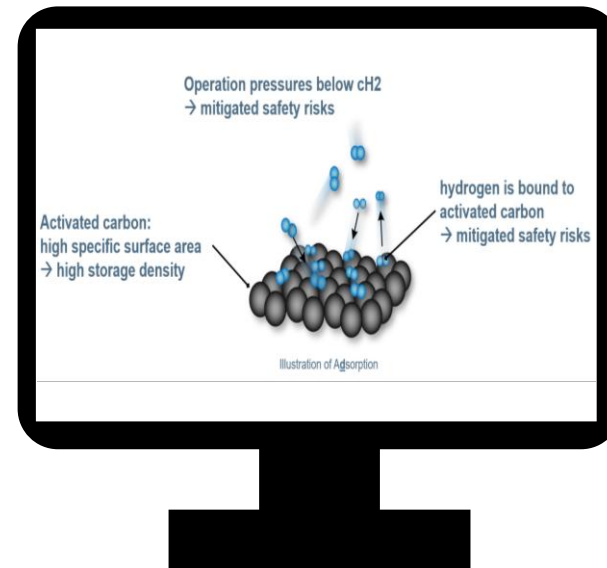
# Benefits of a simulation model



**Quick estimate of interrelations  
between system parameters**

**No safety risks**

**Vary system  
parameters  
independently**

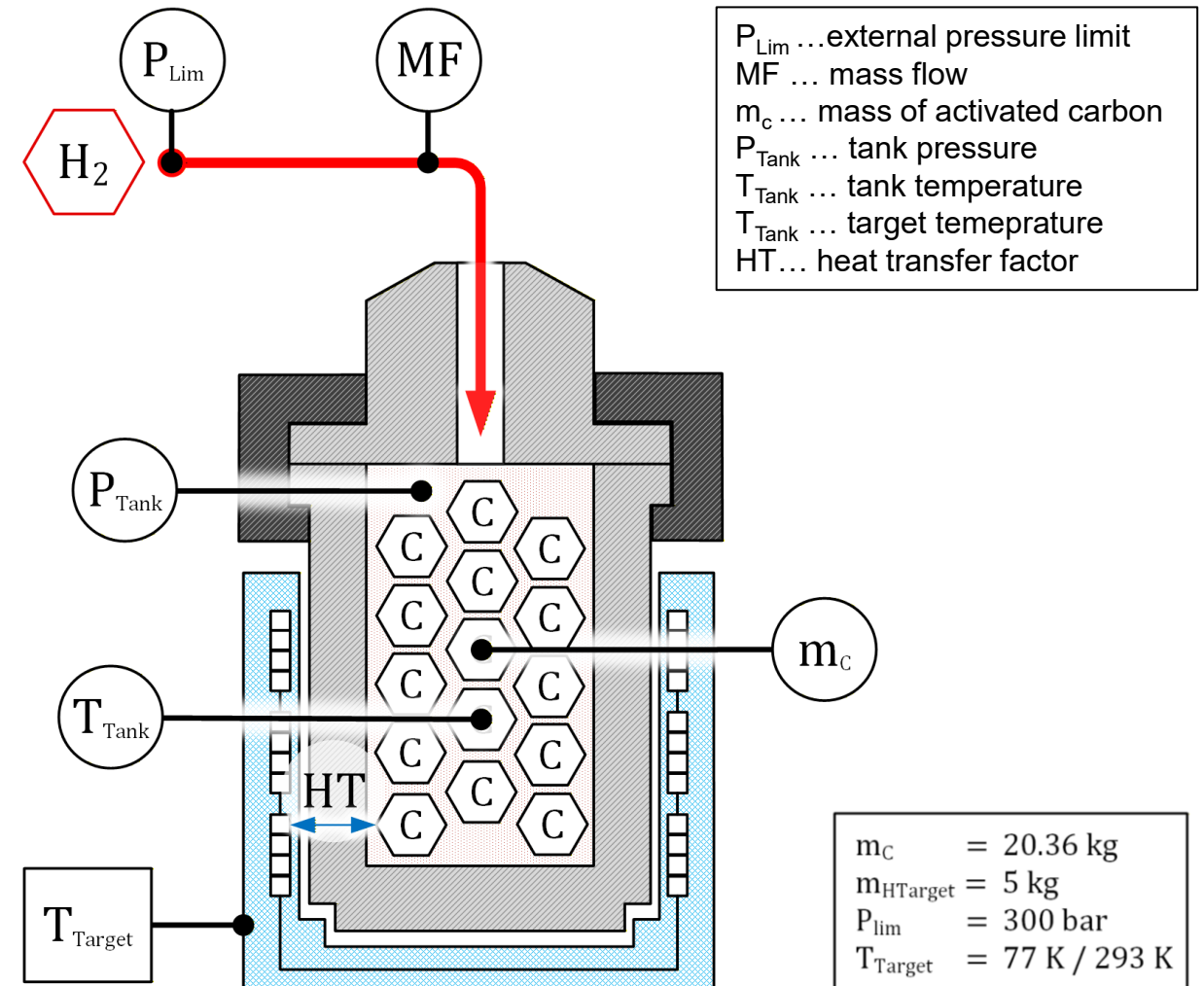


**Cheaper than  
conducting  
experiments**

# Schematic diagram of the simulated adsorption storage tank

## Parameter studies on hydrogen adsorption on activated carbon

- Fill adsorption tank with hydrogen  
→ observe its behaviour over time



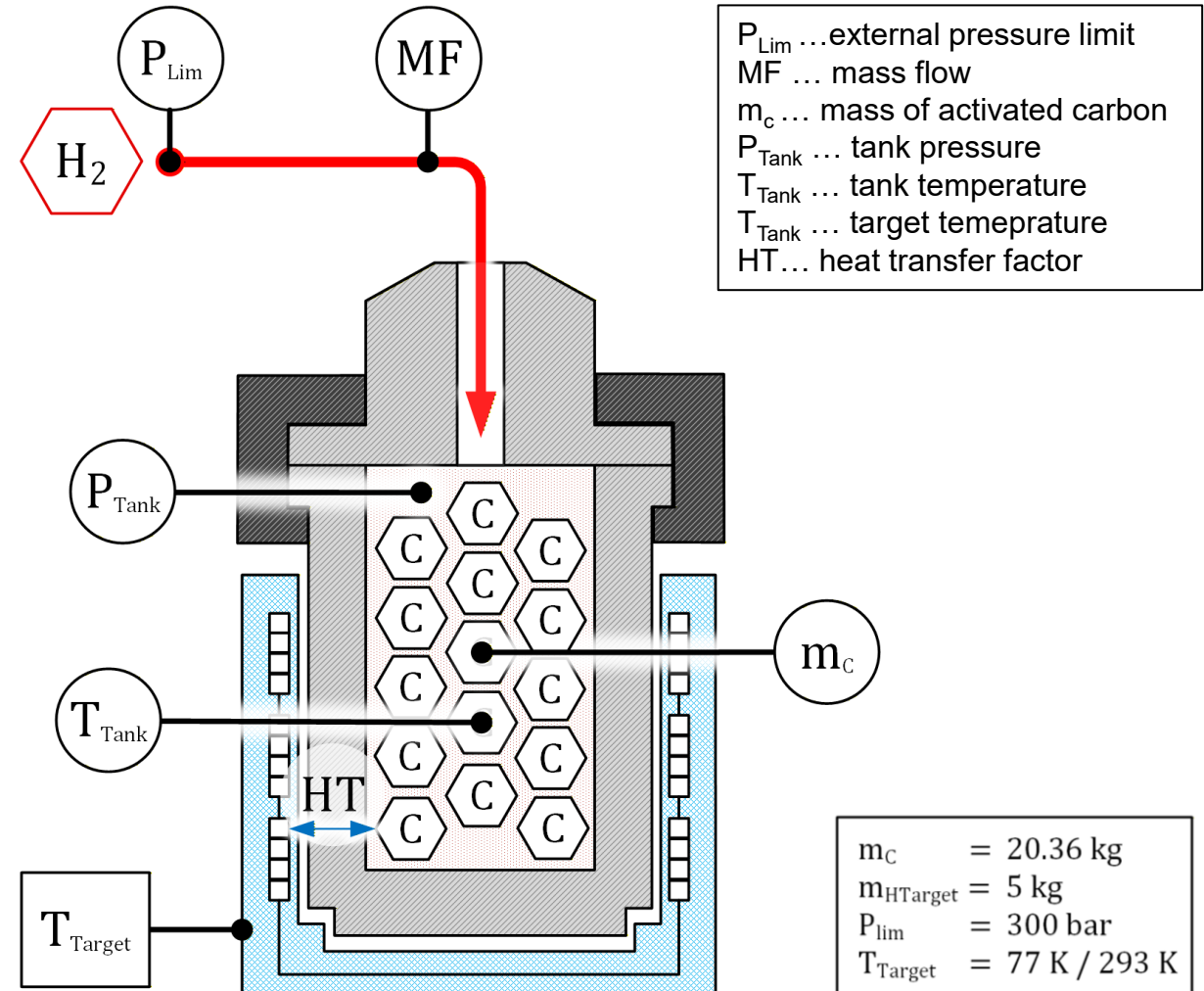
# Schematic diagram of the simulated adsorption storage tank

## Parameter studies on hydrogen adsorption on activated carbon

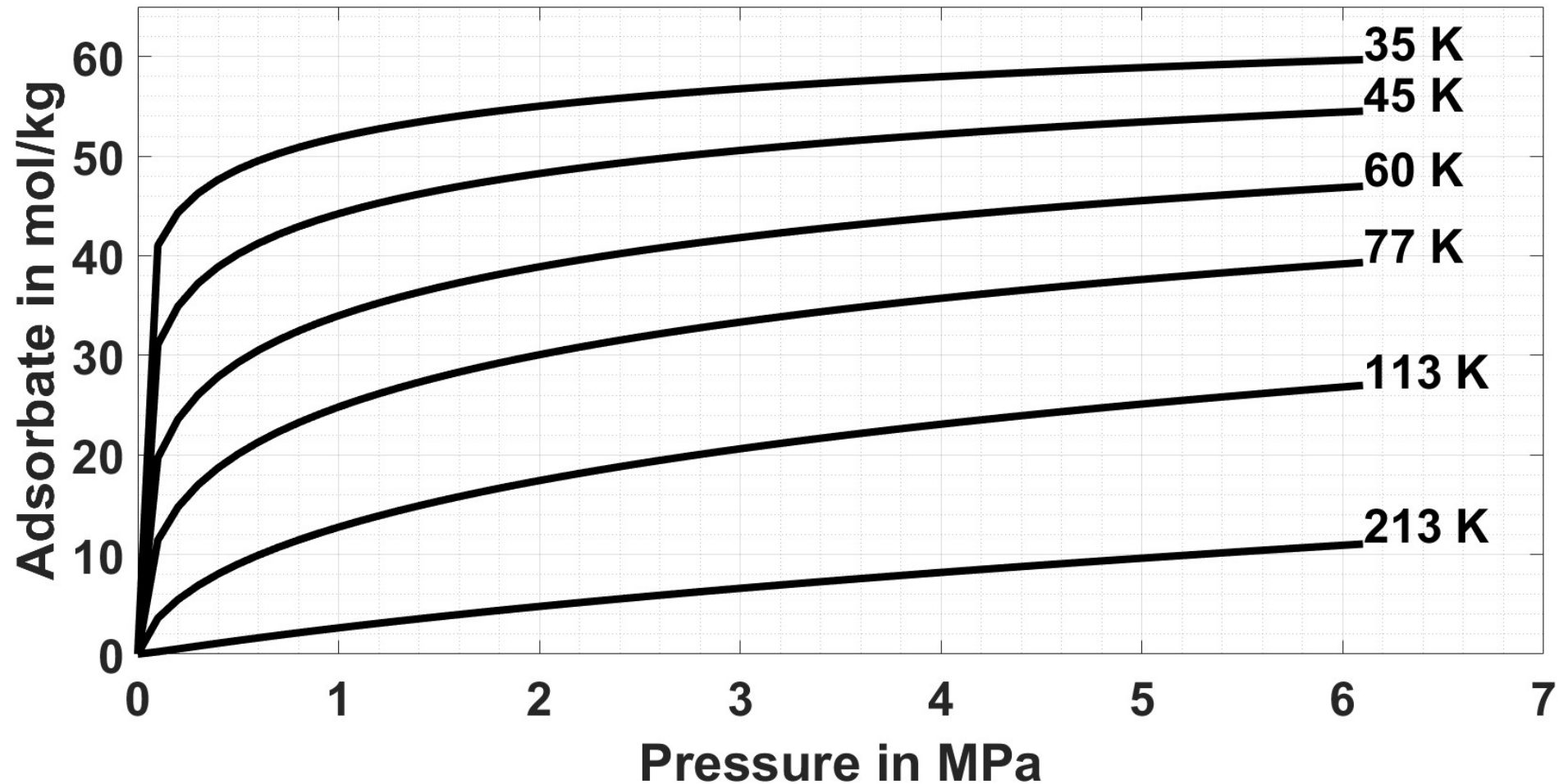
- Fill adsorption tank with hydrogen  
→ observe its behaviour over time

### Investigate influence of:

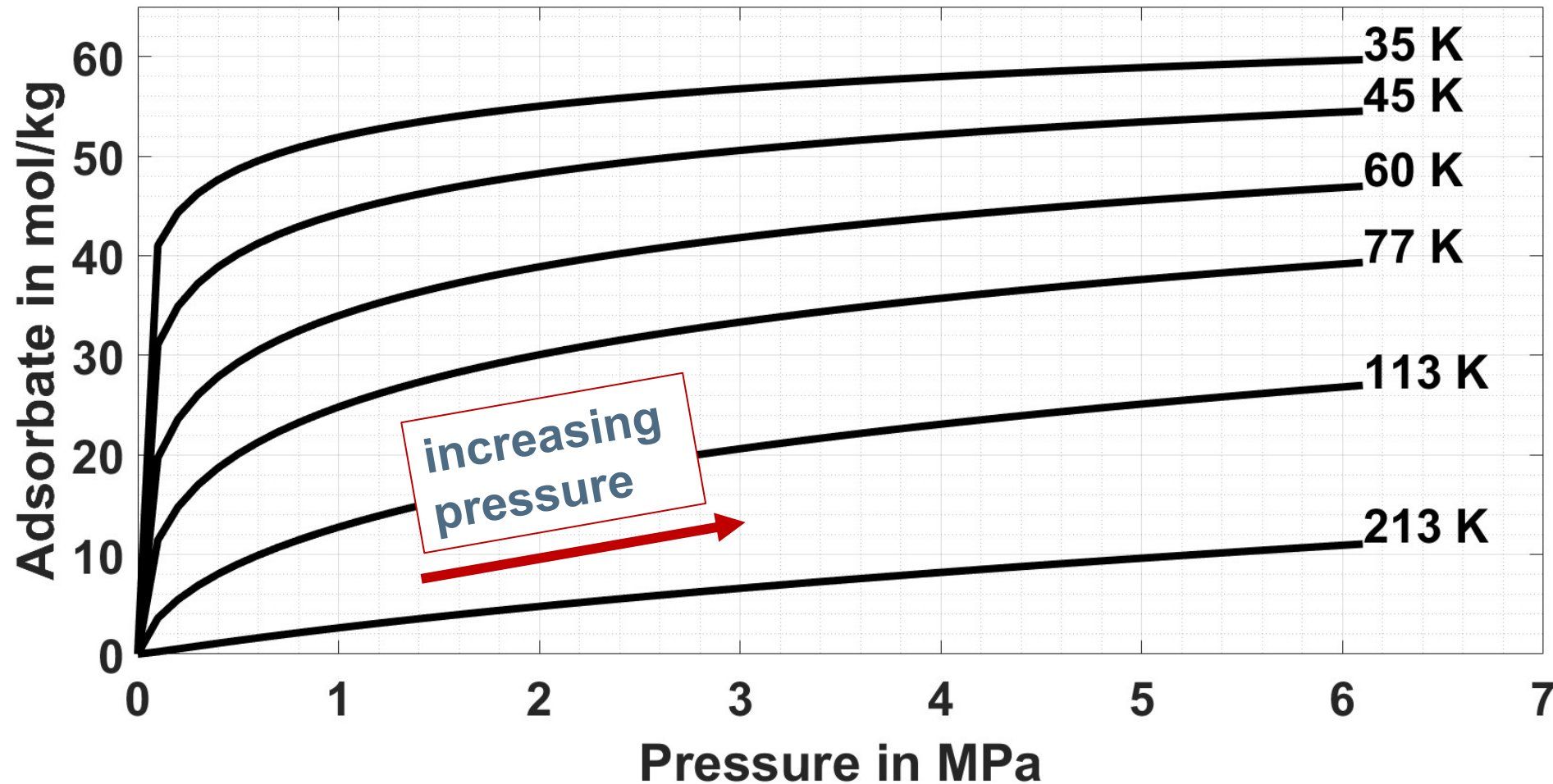
1. Target temperature on storage capacity
2. Temperature control on storage capacity
3. Mass flow on filling time



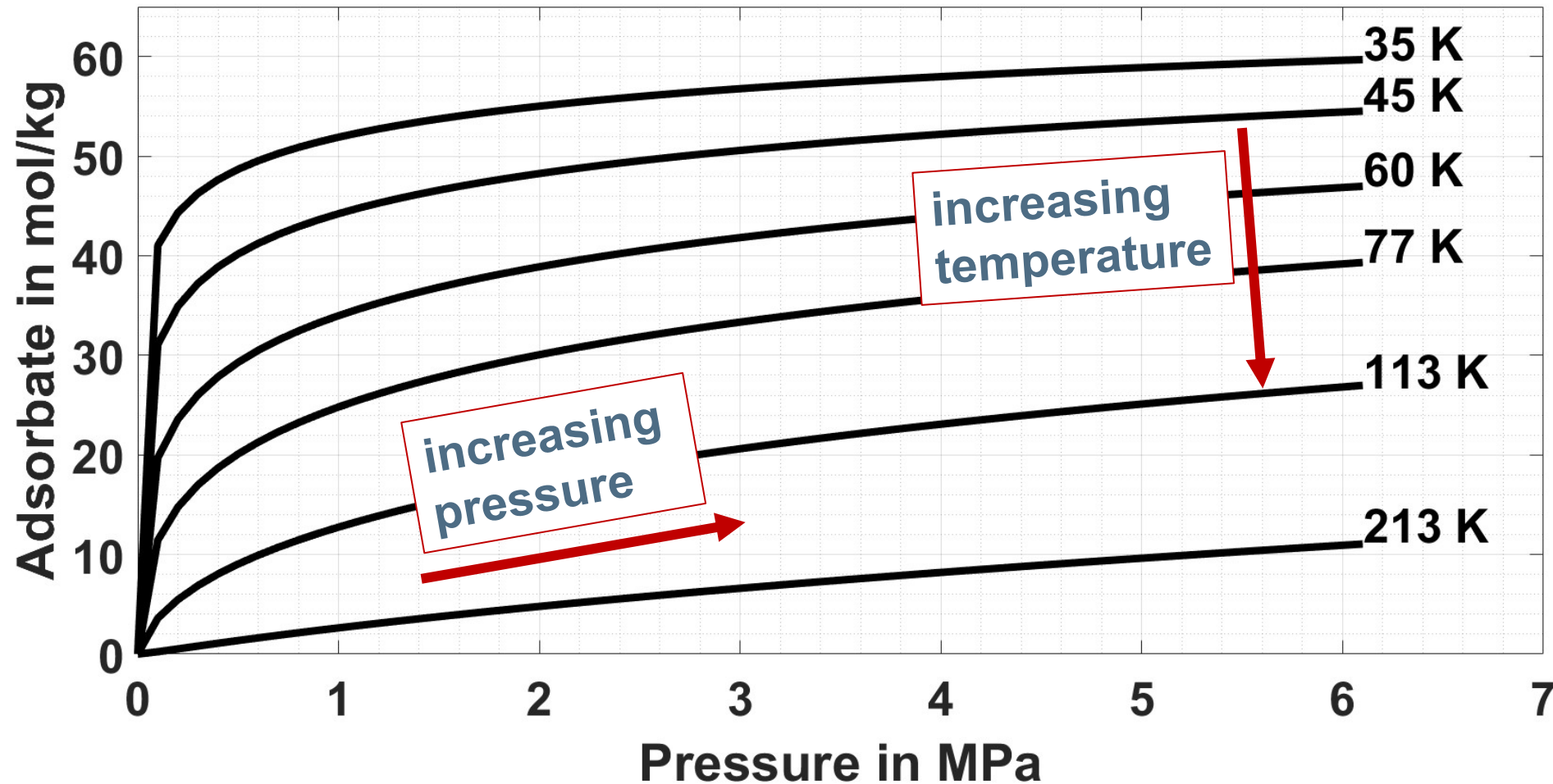
# Adsorption isotherms



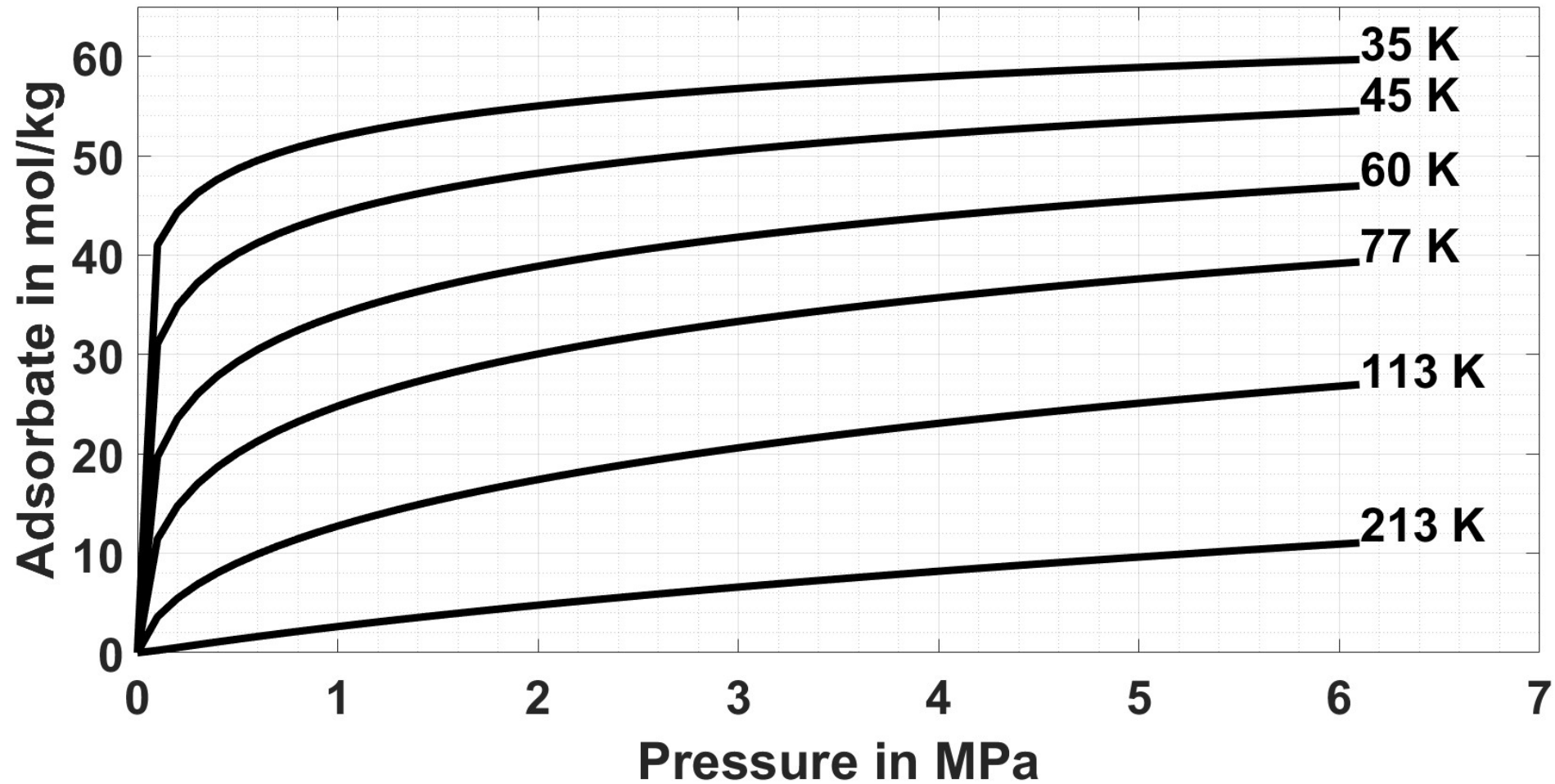
# Adsorption isotherms



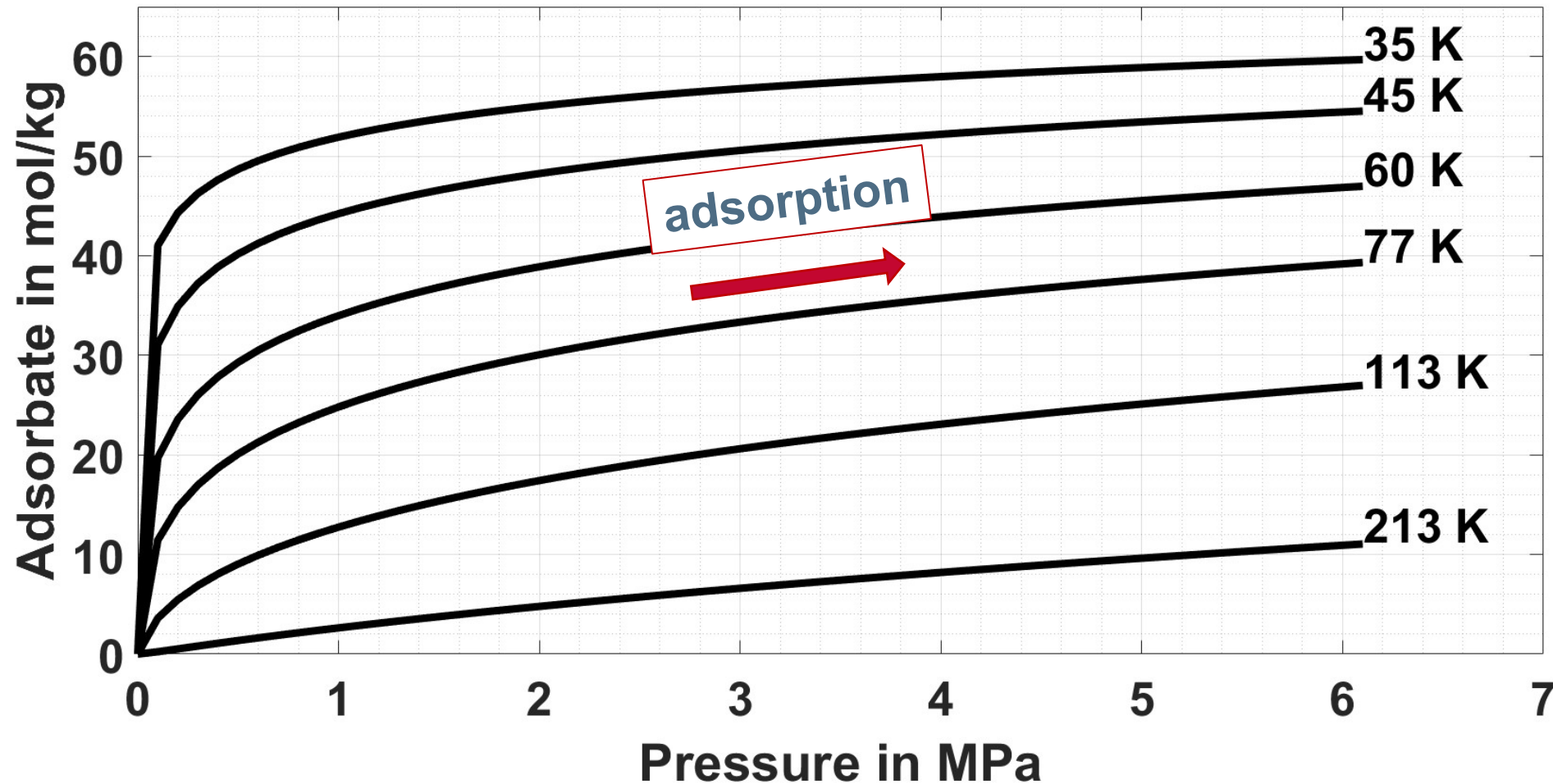
# Adsorption isotherms



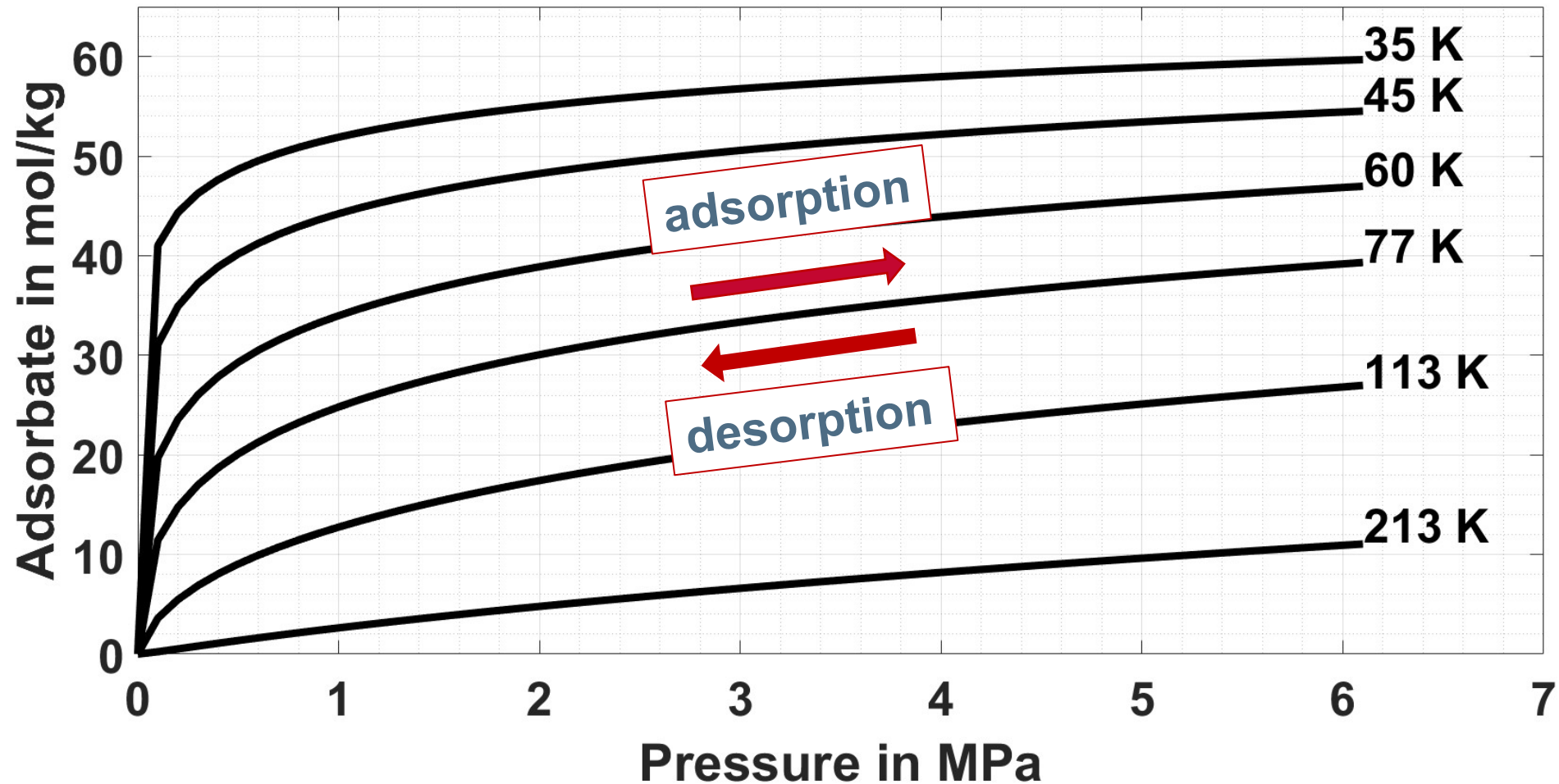
# Adsorption isotherms



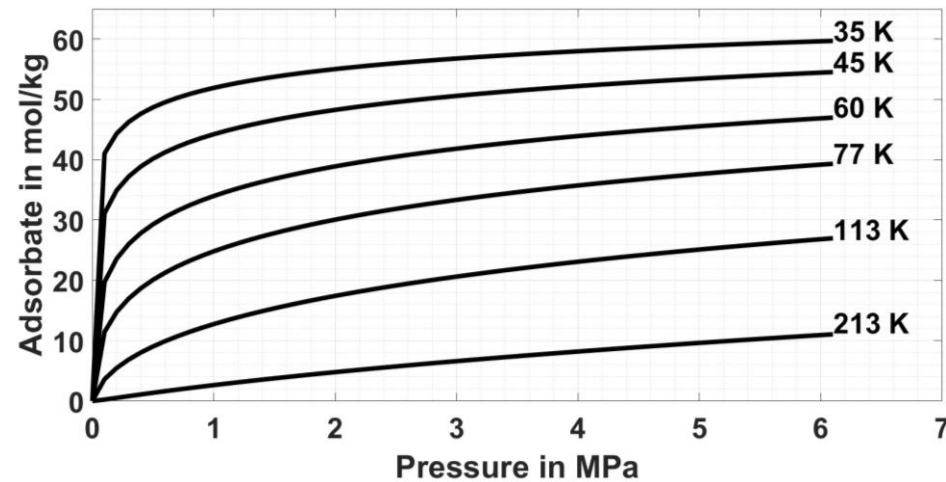
# Adsorption isotherms



# Adsorption isotherms



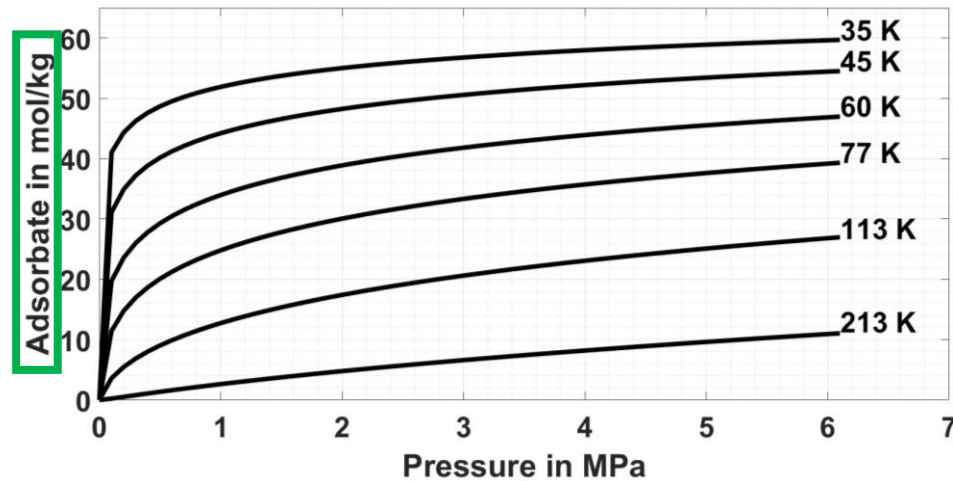
$$n_{ads} = n_{max} * \exp\left[-\left[\frac{RT}{\alpha + \beta T}\right]^2 \ln^2\left(\frac{P_0}{P}\right)\right]$$



$n_{ads}$	Absolute H <sub>2</sub> uptake [mol/kg]
$n_{max}$	Max. H <sub>2</sub> uptake [mol/kg]
$P$	Pressure [MPa]
$P_0$	Saturation vapor pressure [MPa]
$T$	Temperature [K]
$R$	Universal gas constant [J/mol K]
$\alpha$	Enthalpy factor [J/mol]
$\beta$	Entropy factor [J/mol K]

$$n_{ads} = n_{max} * \exp\left[-\left[\frac{RT}{\alpha + \beta T}\right]^2 \ln^2\left(\frac{P_0}{P}\right)\right]$$

Adsorbed amount

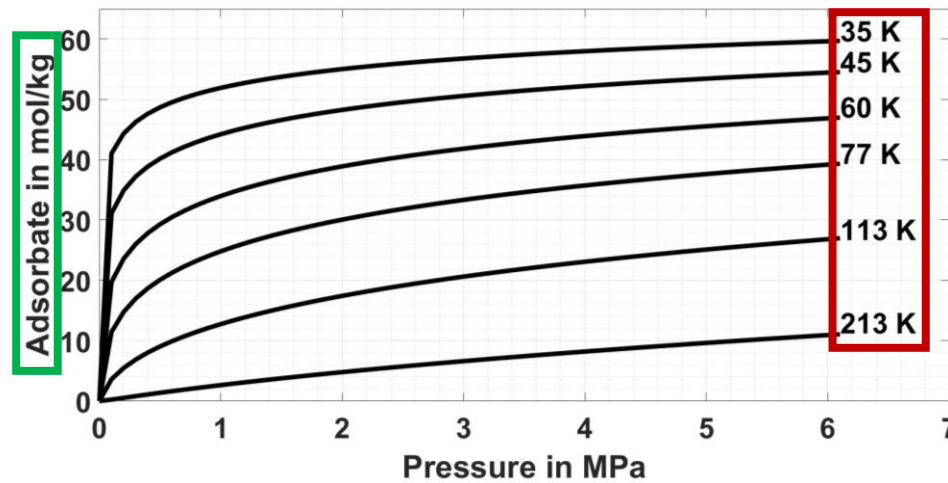


$n_{ads}$	Absolute H <sub>2</sub> uptake [mol/kg]
$n_{max}$	Max. H <sub>2</sub> uptake [mol/kg]
$P$	Pressure [MPa]
$P_0$	Saturation vapor pressure [MPa]
$T$	Temperature [K]
$R$	Universal gas constant [J/mol K]
$\alpha$	Enthalpy factor [J/mol]
$\beta$	Entropy factor [J/mol K]

Temperature dependent term

$$n_{ads} = n_{max} * \exp\left[-\left[\frac{RT}{\alpha + \beta T}\right]^2 \ln^2\left(\frac{P_0}{P}\right)\right]$$

Adsorbed amount



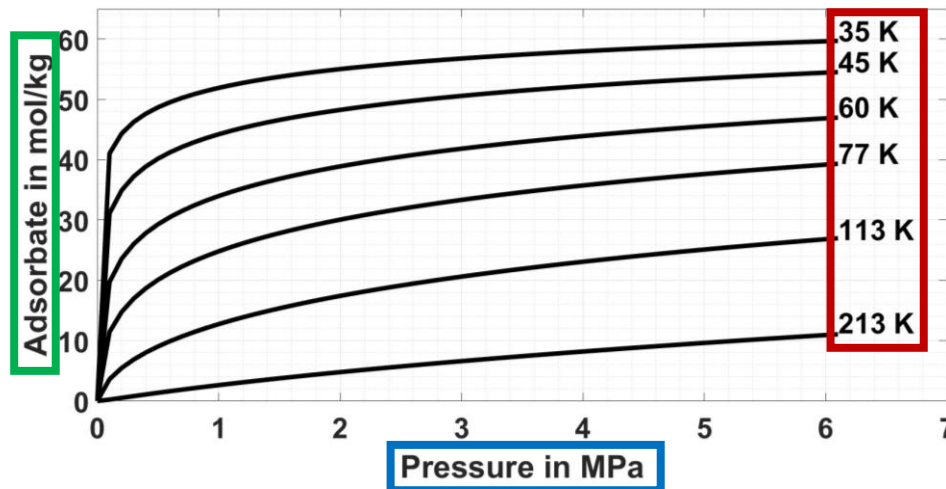
$n_{ads}$	Absolute H <sub>2</sub> uptake [mol/kg]
$n_{max}$	Max. H <sub>2</sub> uptake [mol/kg]
$P$	Pressure [MPa]
$P_0$	Saturation vapor pressure [MPa]
$T$	Temperature [K]
$R$	Universal gas constant [J/mol K]
$\alpha$	Enthalpy factor [J/mol]
$\beta$	Entropy factor [J/mol K]

Temperature dependent term

$$n_{ads} = n_{max} * \exp\left[-\frac{RT}{\alpha + \beta T} \ln^2\left(\frac{P_0}{P}\right)\right]$$

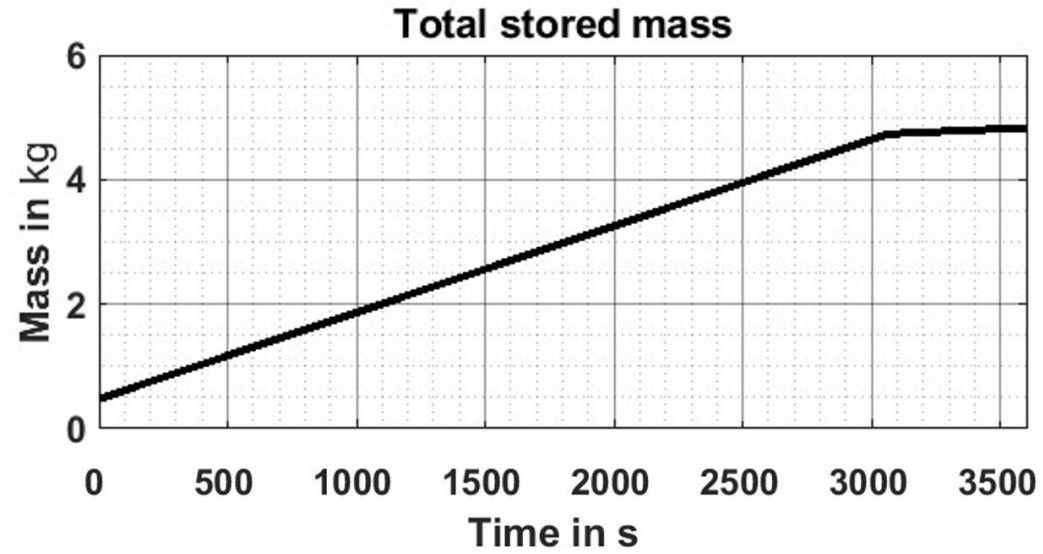
Adsorbed amount

Pressure dependent term

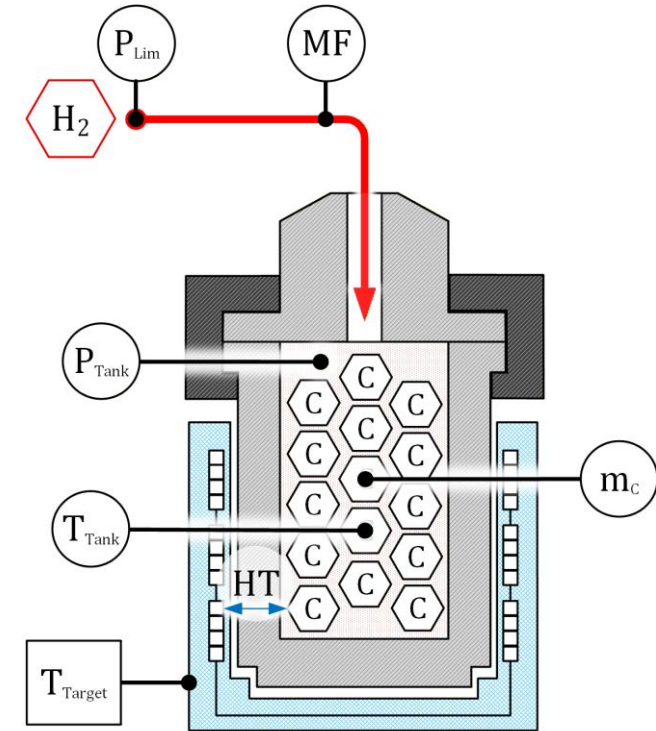


$n_{ads}$	Absolute H <sub>2</sub> uptake [mol/kg]
$n_{max}$	Max. H <sub>2</sub> uptake [mol/kg]
$P$	Pressure [MPa]
$P_0$	Saturation vapor pressure [MPa]
$T$	Temperature [K]
$R$	Universal gas constant [J/mol K]
$\alpha$	Enthalpy factor [J/mol]
$\beta$	Entropy factor [J/mol K]

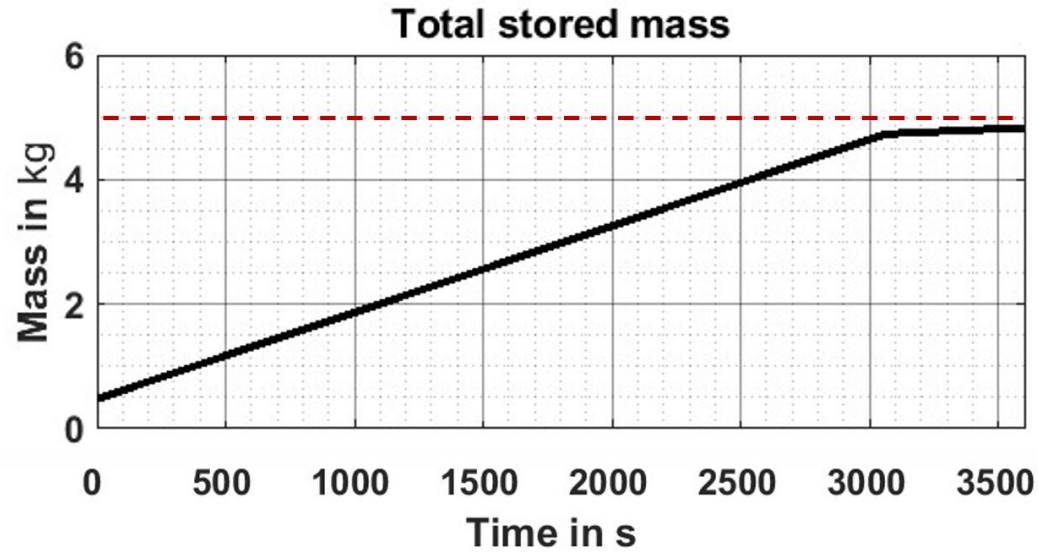
# Adsorption storage tank – total stored mass



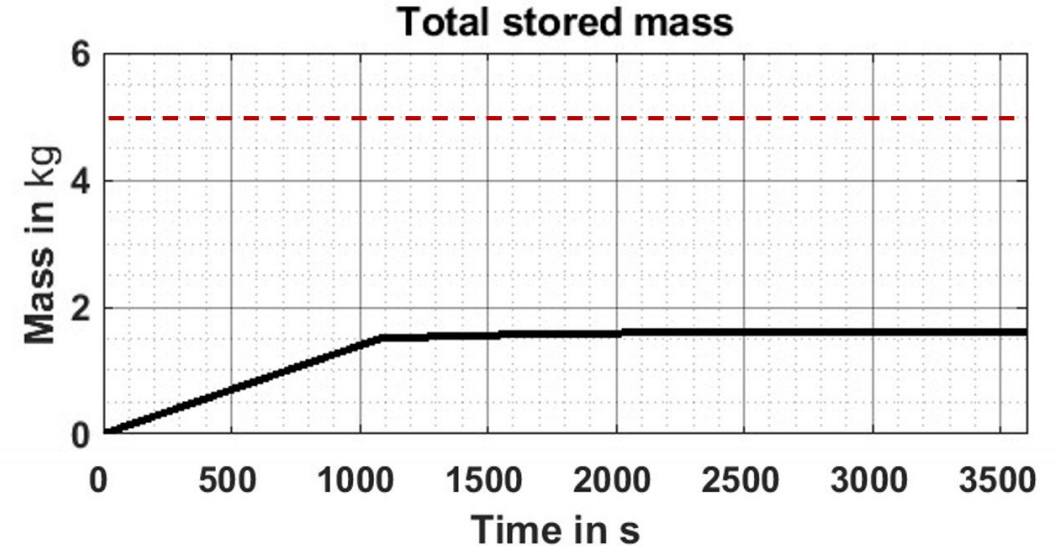
**Target temperature: 77 K**



# Influence of the target temperature on the storage capacity



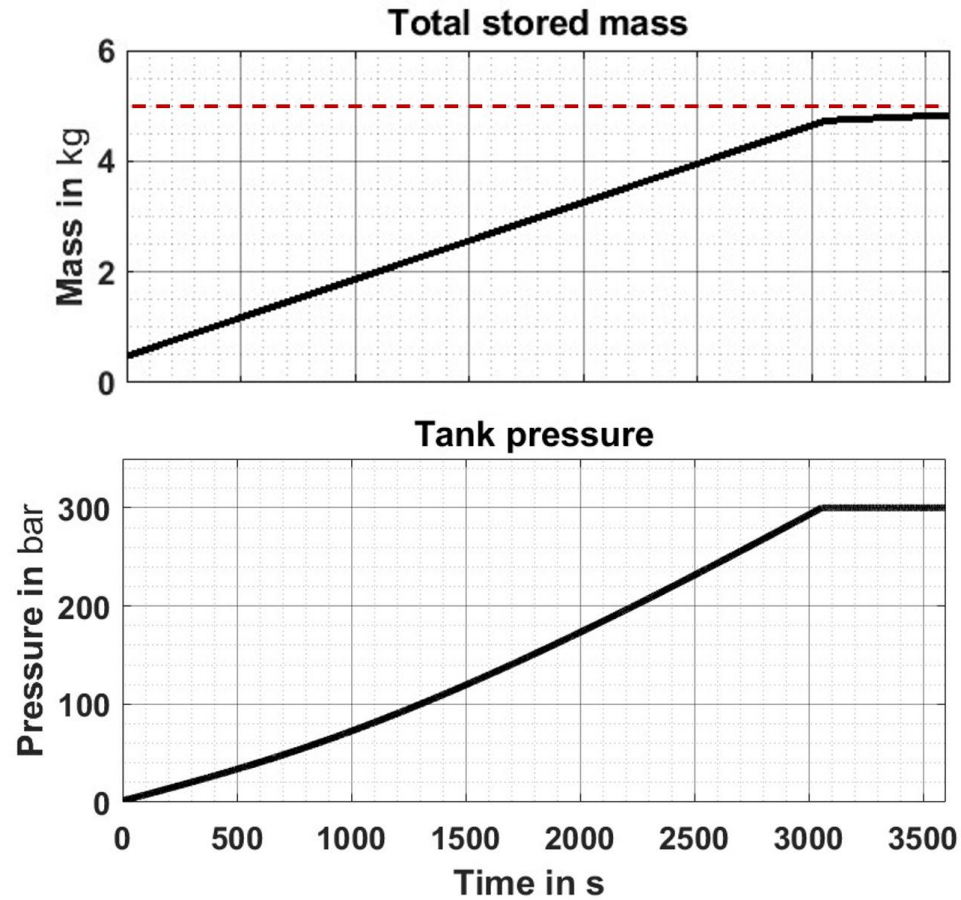
Target temperature: 77 K



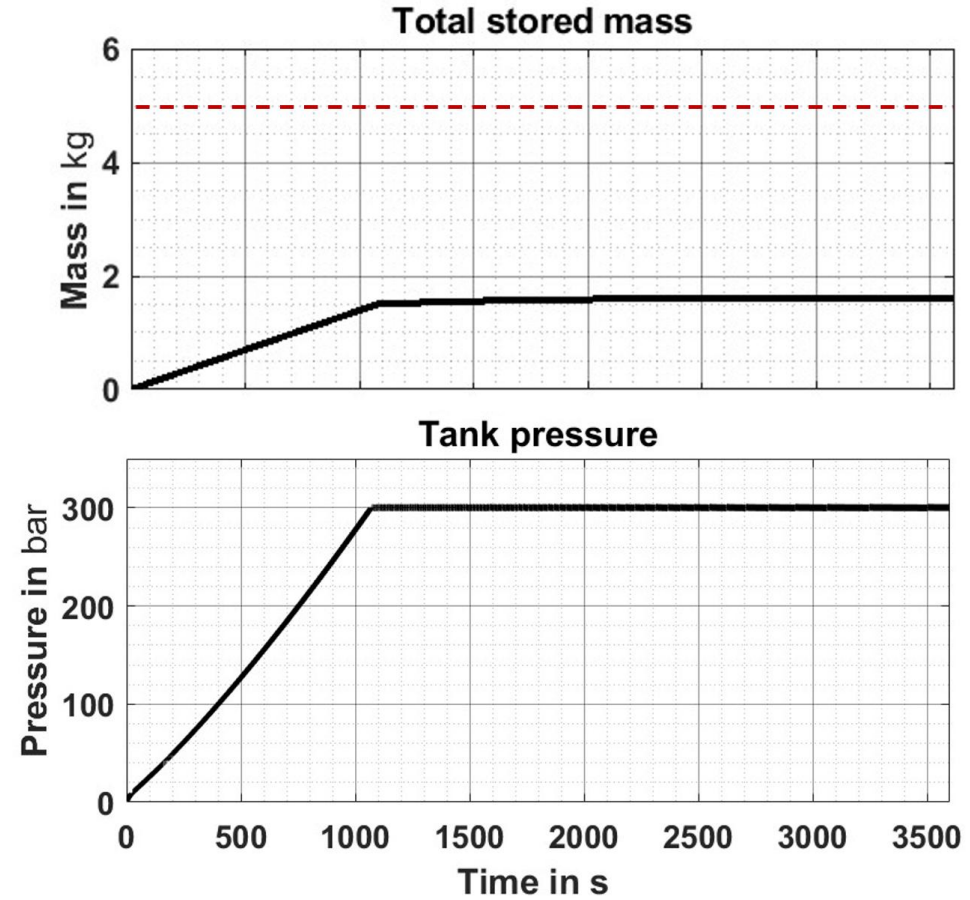
Target temperature: 293 K

Storage target, 5 kg - - -

# Influence of target temperature on storage capacity – the two filling phases

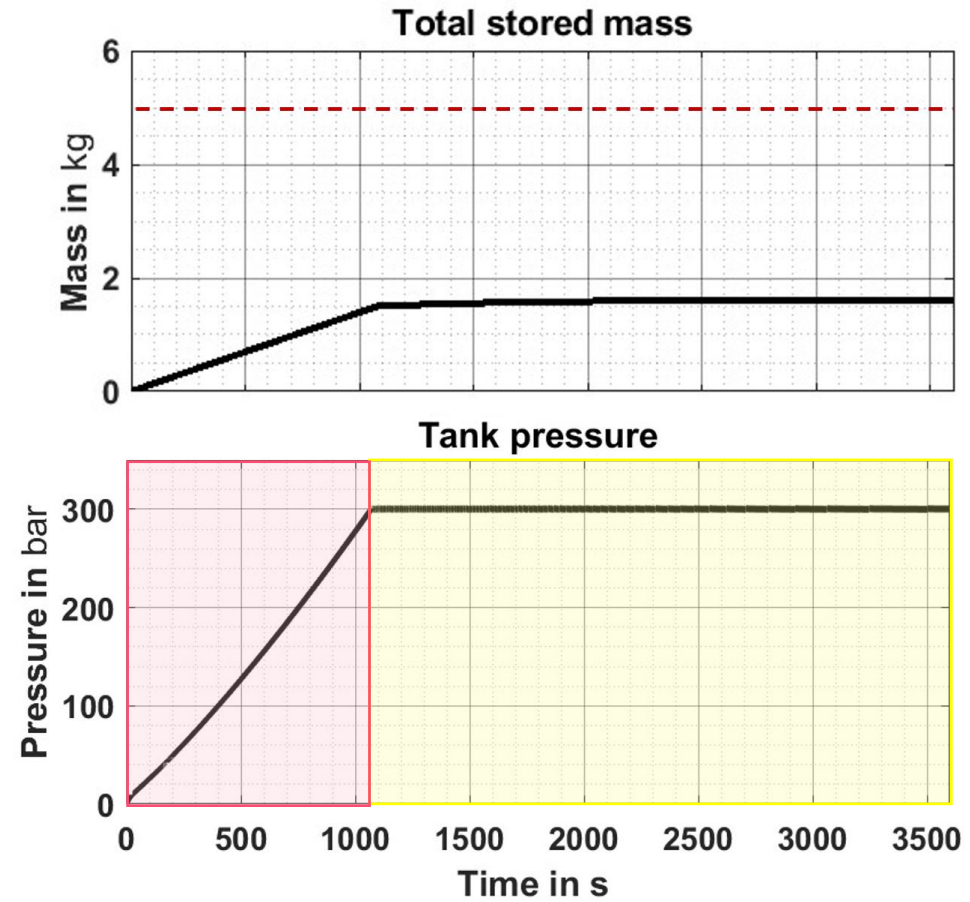
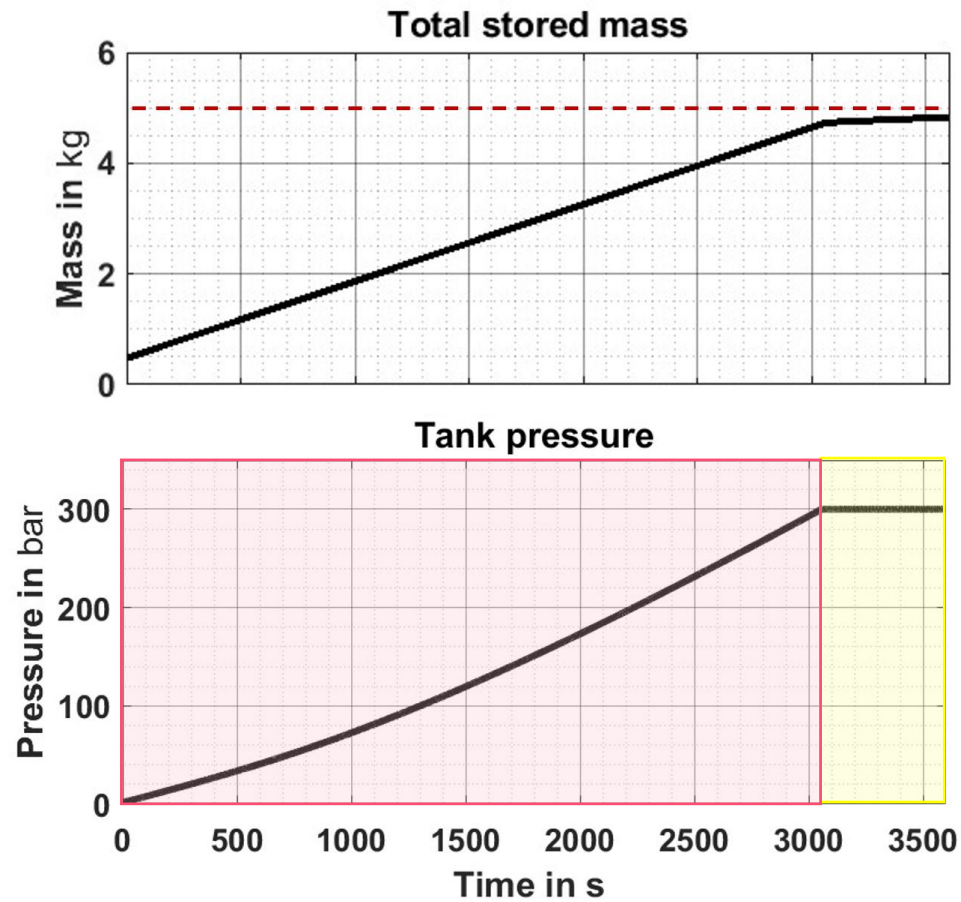


**Target temperature: 77 K**



**Target temperature: 293 K**

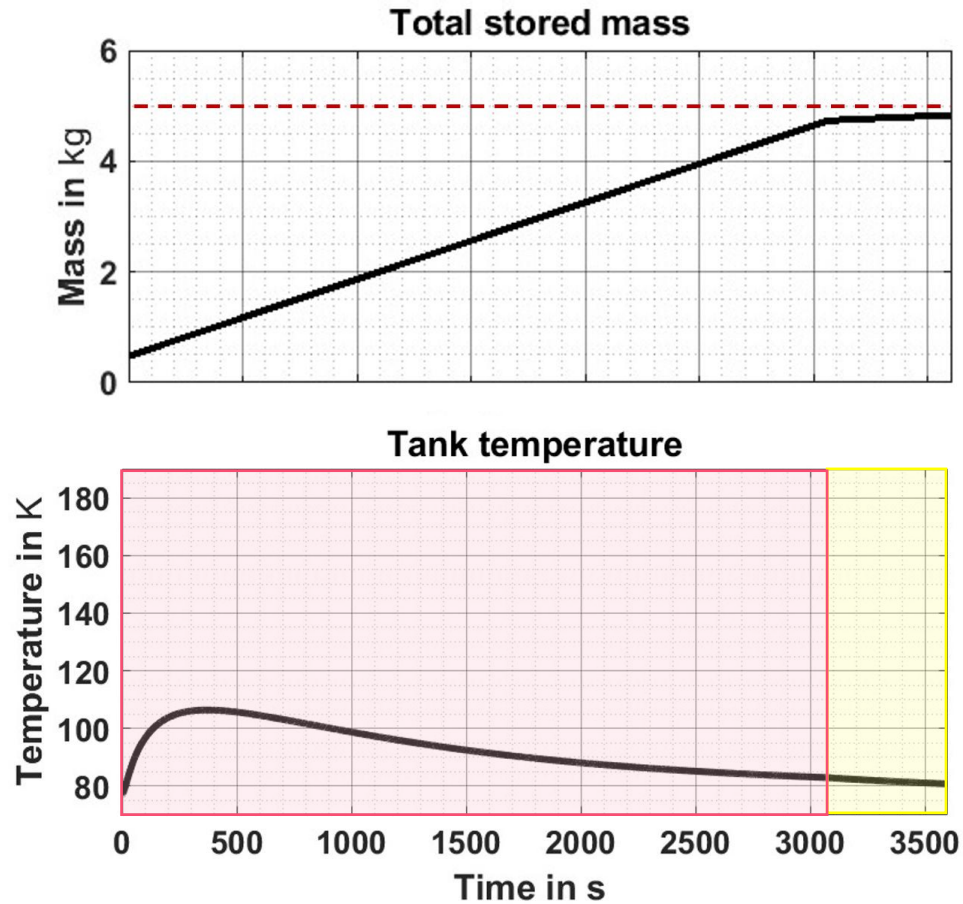
# Influence of target temperature on storage capacity – the two filling phases



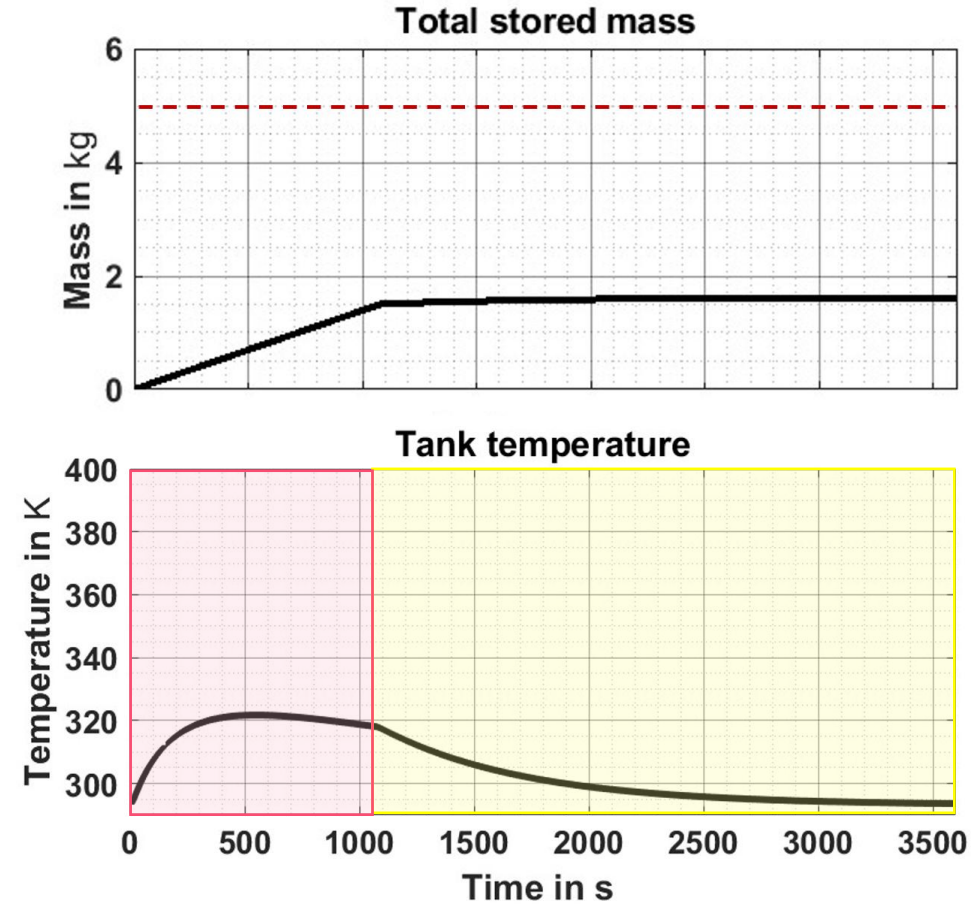
**Regular filling phase: mass flow driven**

**Convergence phase: temperature driven**

# Influence of target temperature on storage capacity – temperature evolution

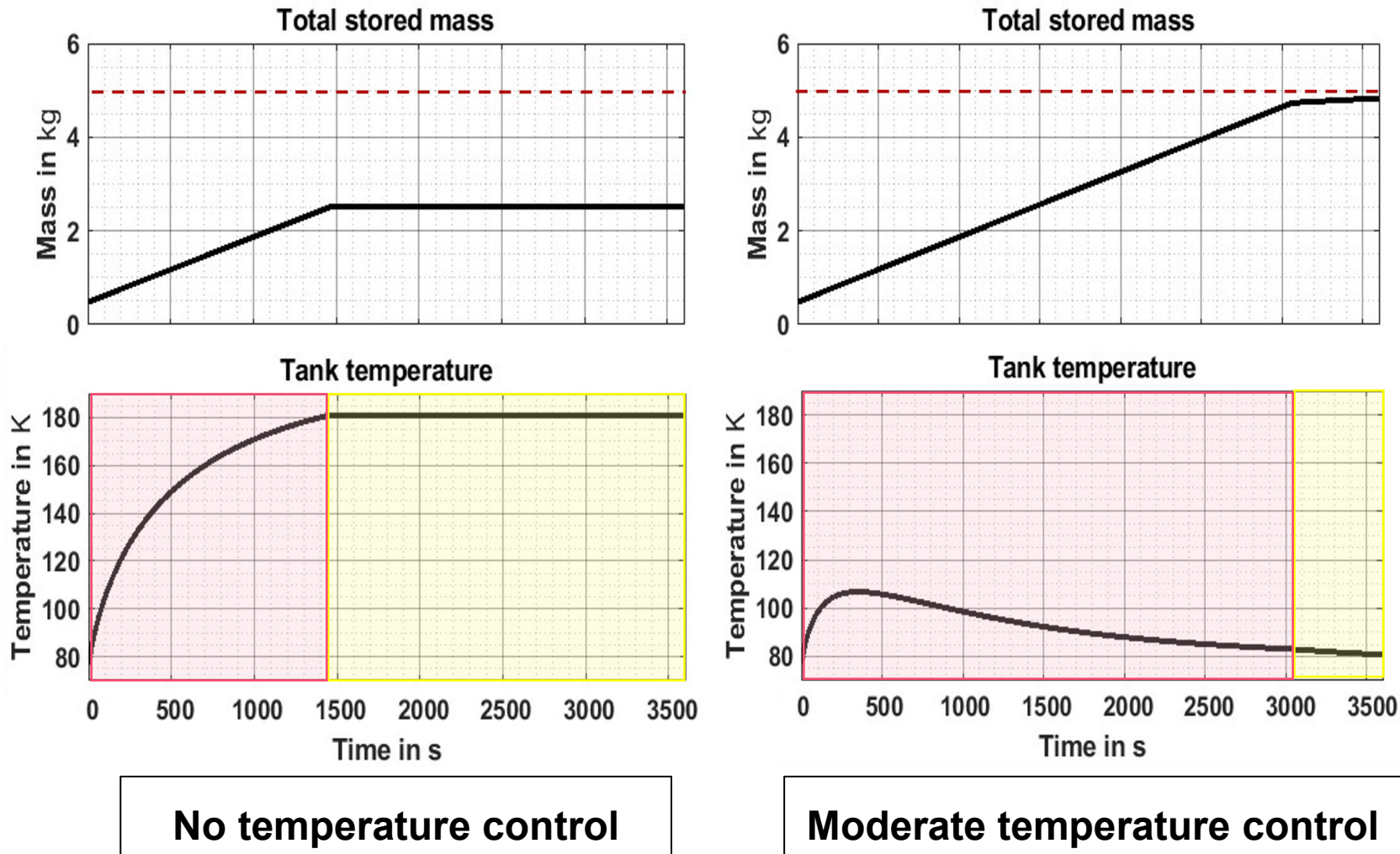


**Target temperature: 77 K**



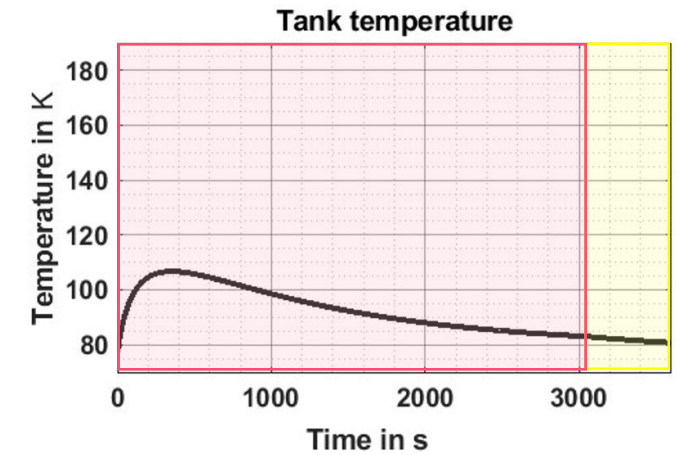
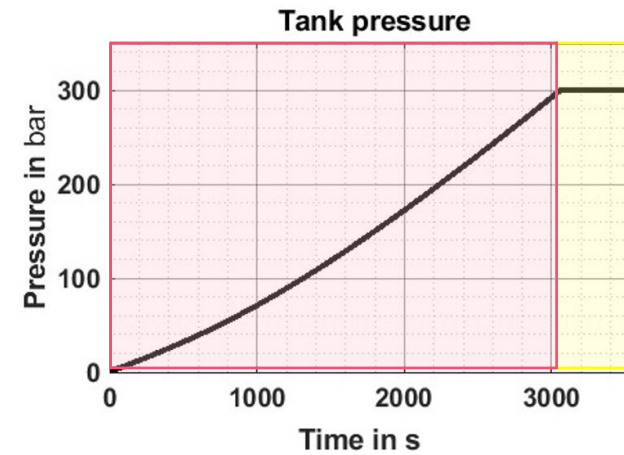
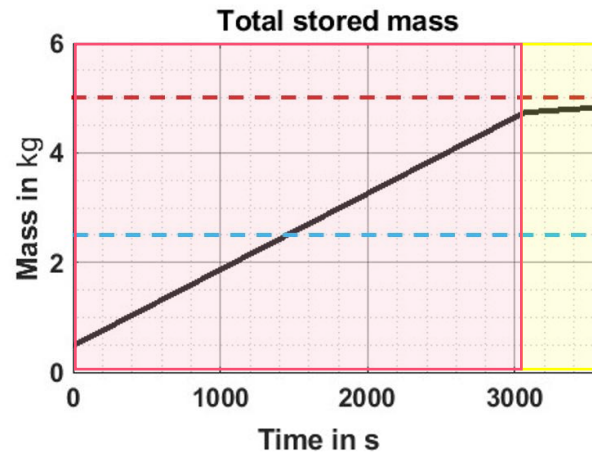
**Target temperature: 293 K**

# Influence of the temperature control on the storage capacity



# Influence of the mass flow on the filling time

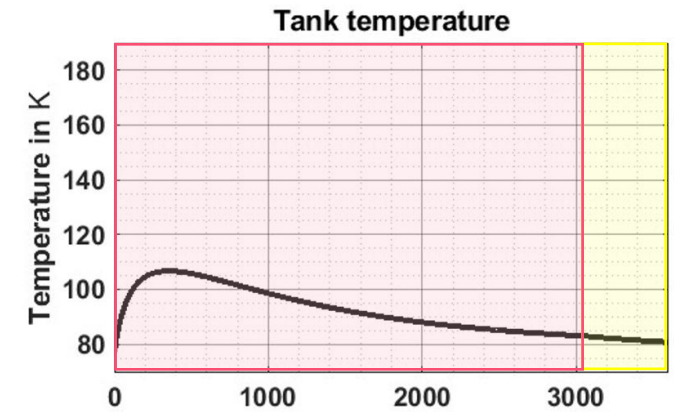
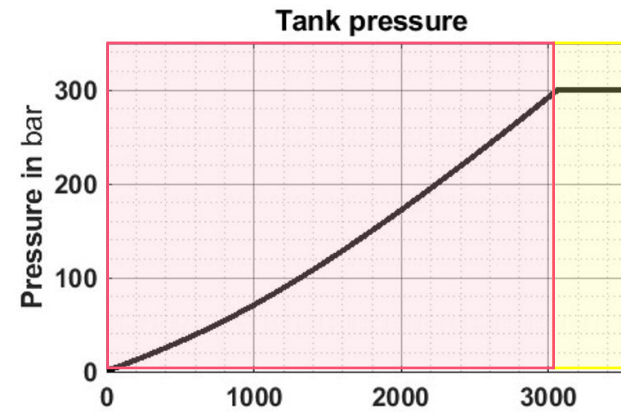
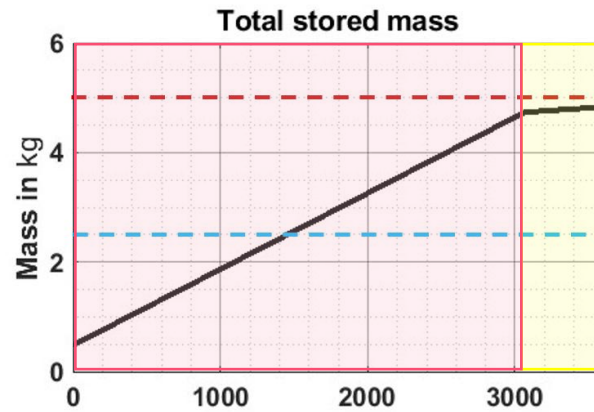
Initial mass flow: 5 kg/h



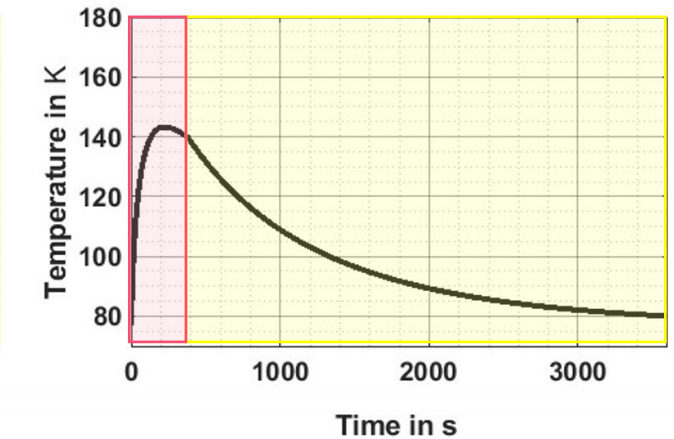
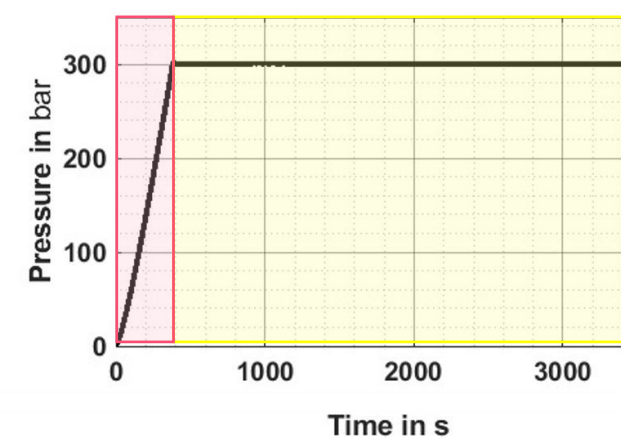
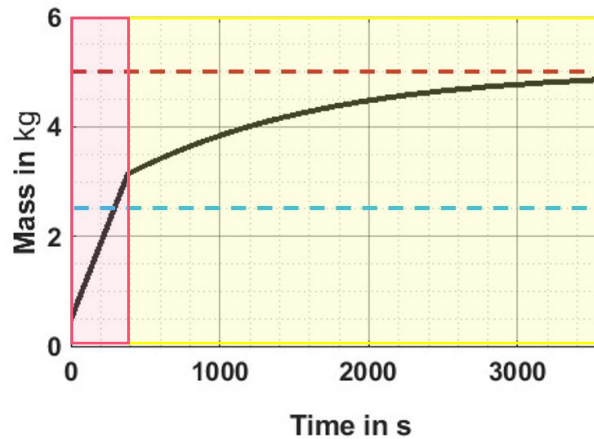
Storage target, 5 kg - - -  
Half filling, 2.5 kg - - -

# Influence of the mass flow on the filling time

Initial mass flow: 5 kg/h

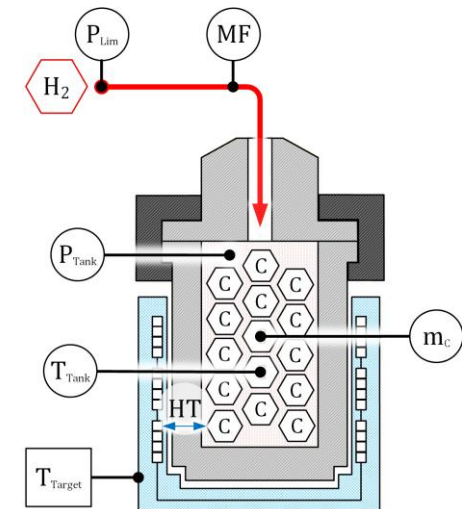


Initial mass flow: 25 kg/h



Storage target, 5 kg - - - -  
Half filling, 2.5 kg - - - -

- To reach high storage capacities temperatures below room temperature are required
- The temperature control of the storage tank has to be optimized towards high thermal conductivity to reach these low temperatures
- Even with temperature control higher mass flows do not result in faster filling time when loading the tank fully – the system is self-inhibiting



Join us in shaping the future of hydrogen technology!


**HyCentA Research GmbH**

Inffeldgasse 15

A-8010 Graz

- Phone: +43 316 873 9500
- [office@hycenta.at](mailto:office@hycenta.at)
- [www.hycenta.at](http://www.hycenta.at)



 Bundesministerium  
Innovation, Mobilität  
und Infrastruktur

 Bundesministerium  
Wirtschaft, Energie  
und Tourismus

