



# Heat and Mass Transfer in Metal Hydride Systems for Hydrogen Storage and Purification

Dmitry Dunikov

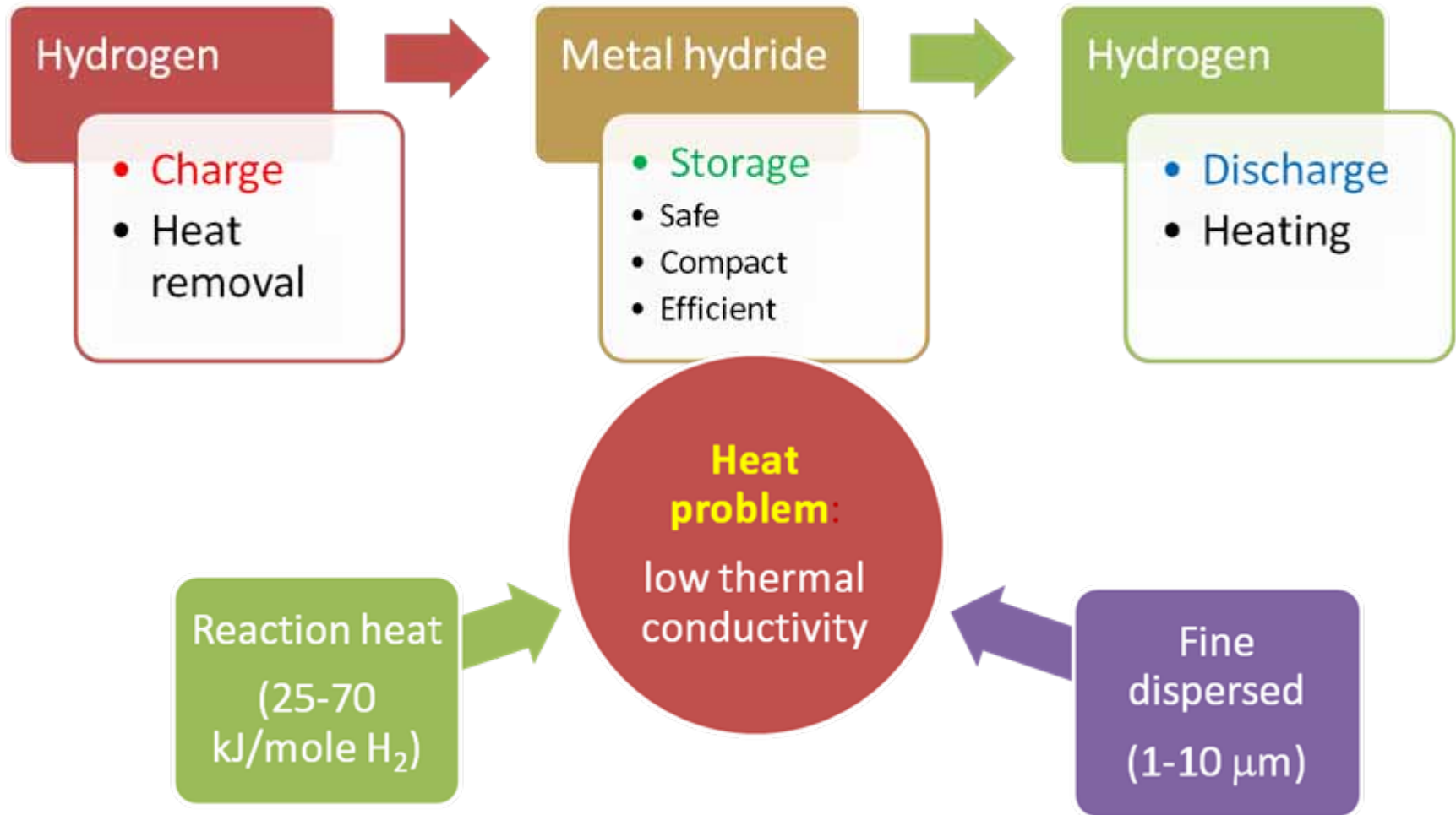
Joint Institute for High Temperatures of Russian  
Academy of Sciences

# System integration requirements for solid state hydrogen storage

- Operational requirements
  - Flow rate
  - Pressure
  - Purity
  - Temperature
- Material properties
  - Hydrogen capacity
  - PCT
  - Thermal properties
  - Impurity resistance
- Design features
  - Size and weight
  - Capital investment
  - Operational costs
  - Safety

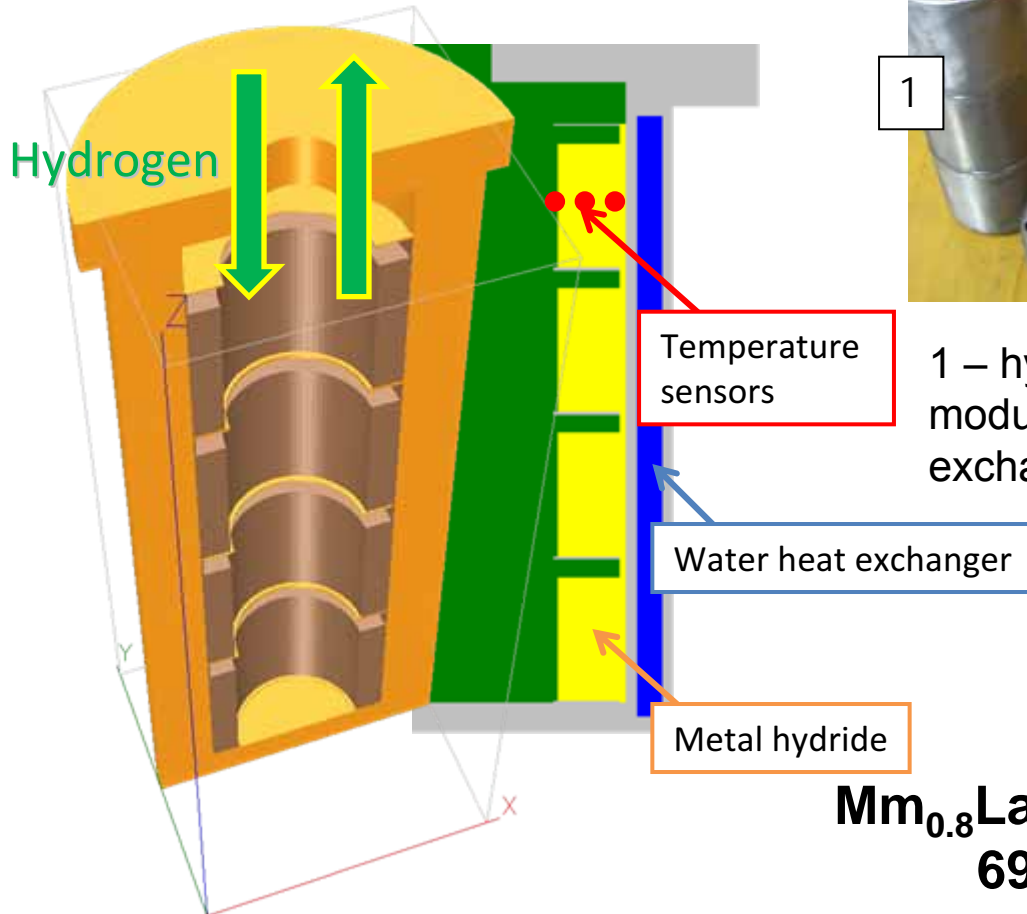
Objective of our research is to create basis for development of efficient hydrogen storage devices with optimized heat transfer

# Heat management is one of the most important limiting factors



# Experimental investigations: modular reactor

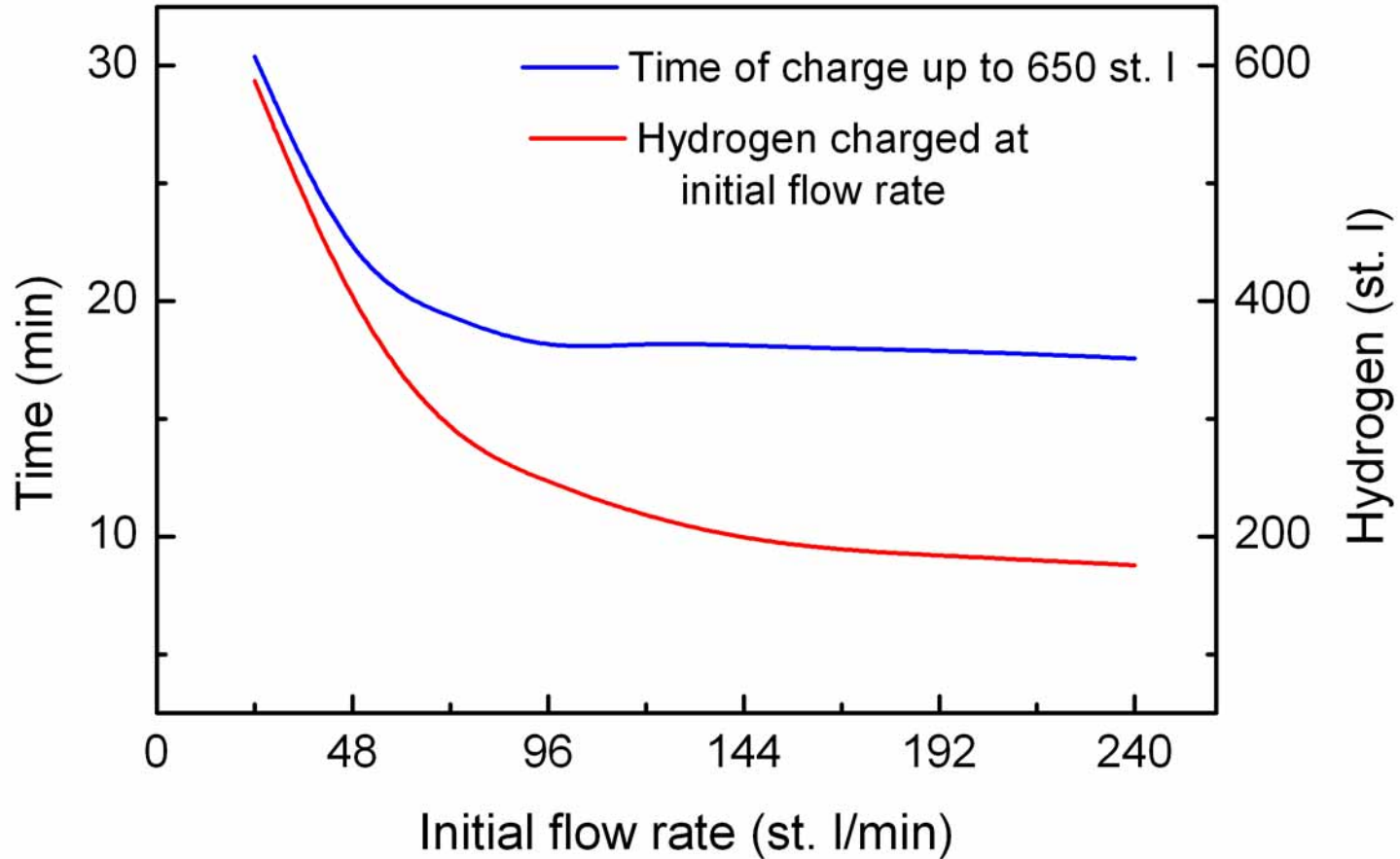
Charge and discharge with pure hydrogen at different flow rates from 240 st. l/min (regime 100%) down to 24 st. l/min (regime 10%)



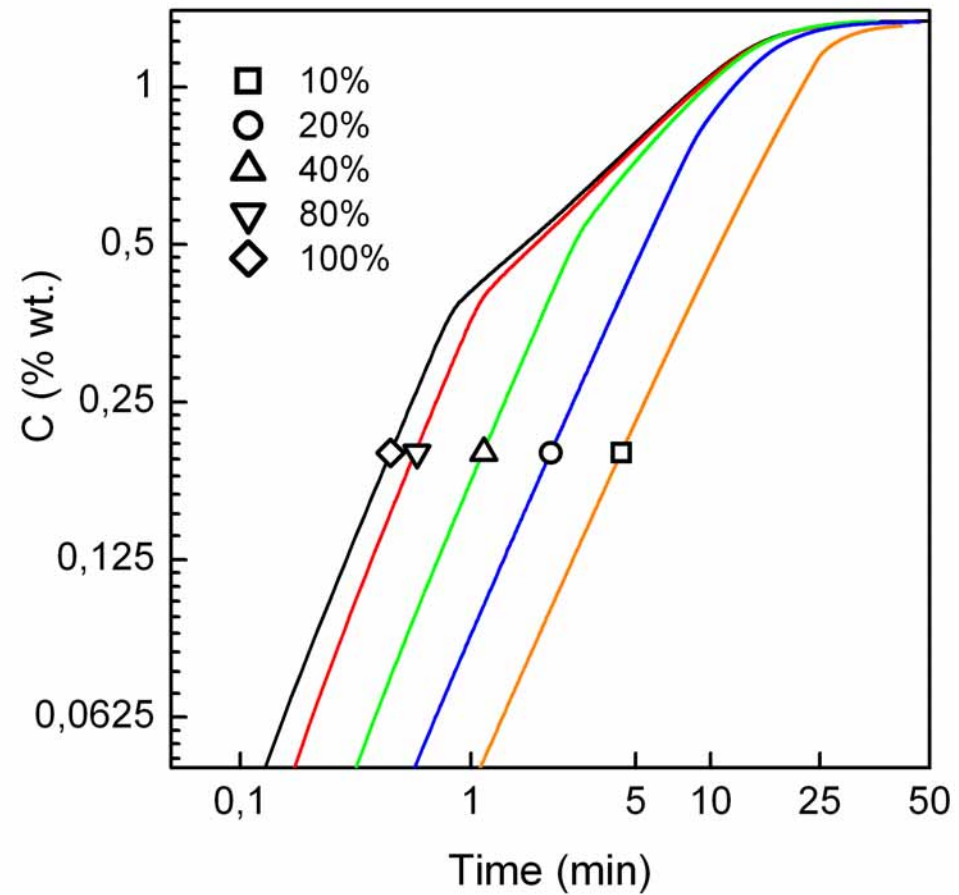
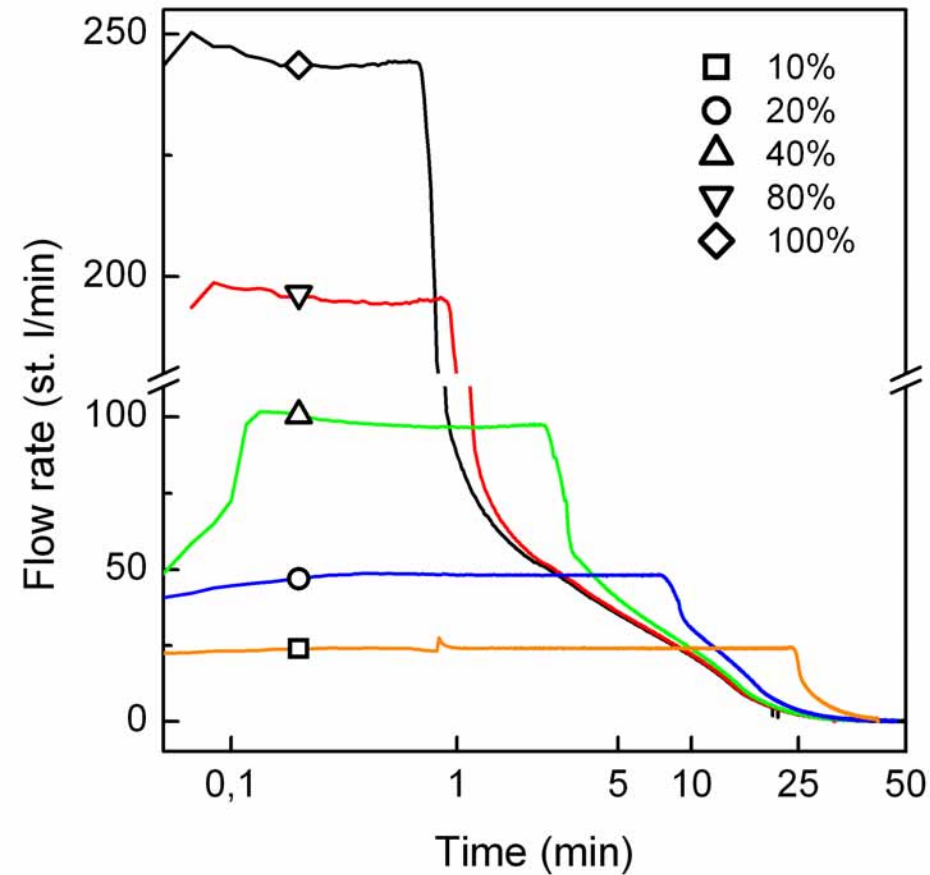
1 – hydride cartridge; 2 – MH module; 3 – casing with water heat exchanger; 4 – cover.

**4.69 kg of**  
 **$\text{Mm}_{0.8}\text{La}_{0.2}\text{Ni}_{4.1}\text{Fe}_{0.8}\text{Al}_{0.1}$  alloy**  
**690±5 st.l (1,33 % wt.)**

# Charging with pure hydrogen

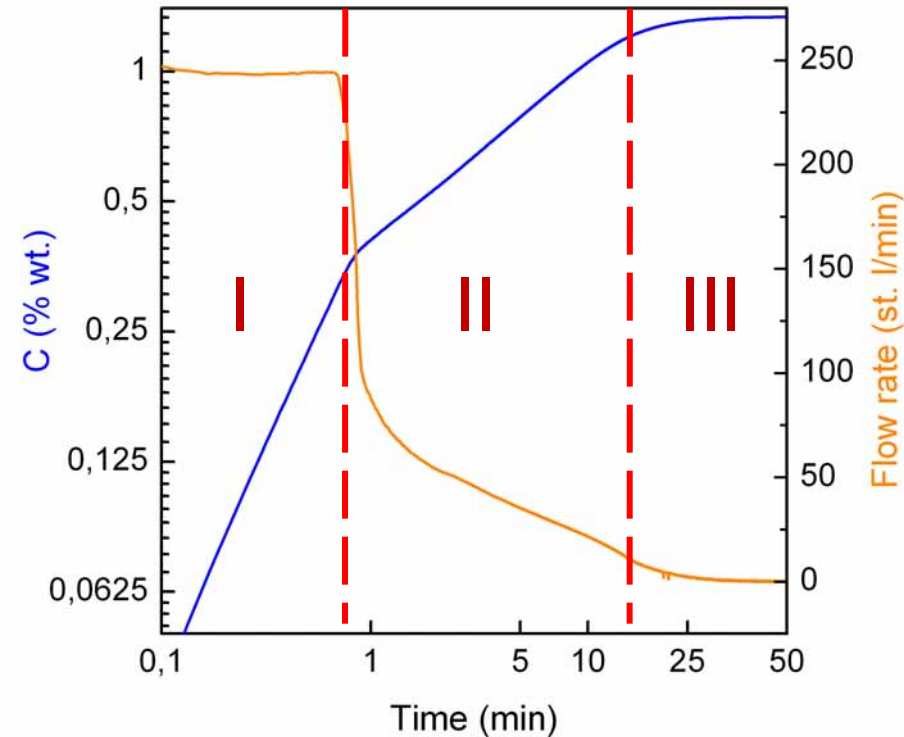


# Charging flow rate and hydrogen content

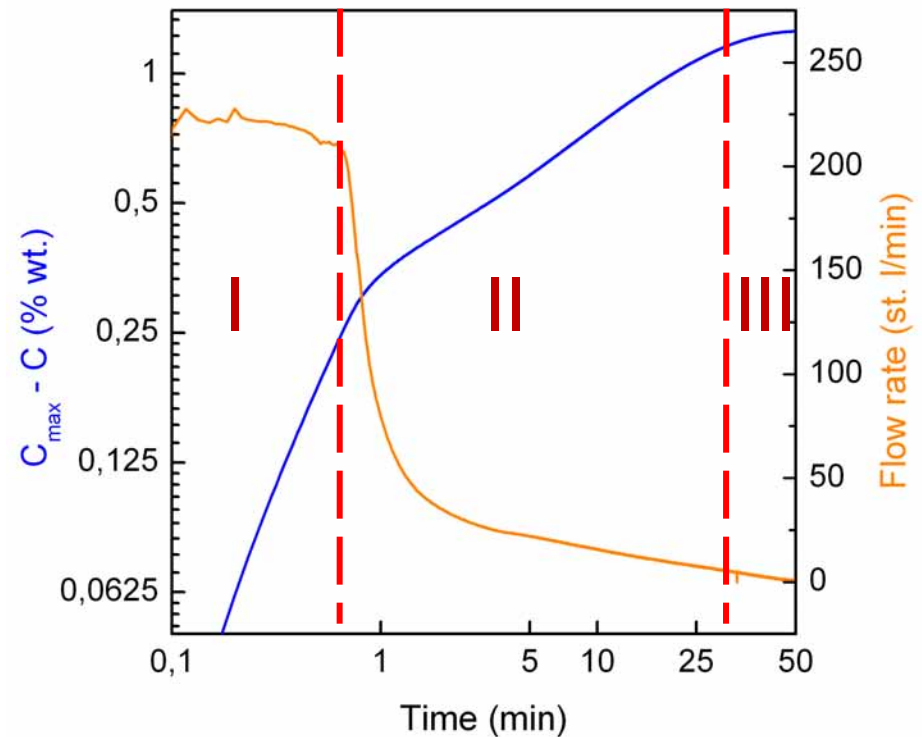


Results for discharging are similar. Main conclusion: the reactor can not be charged or discharged at constant hydrogen flow rate for the most of regimes.

# Three stages of process



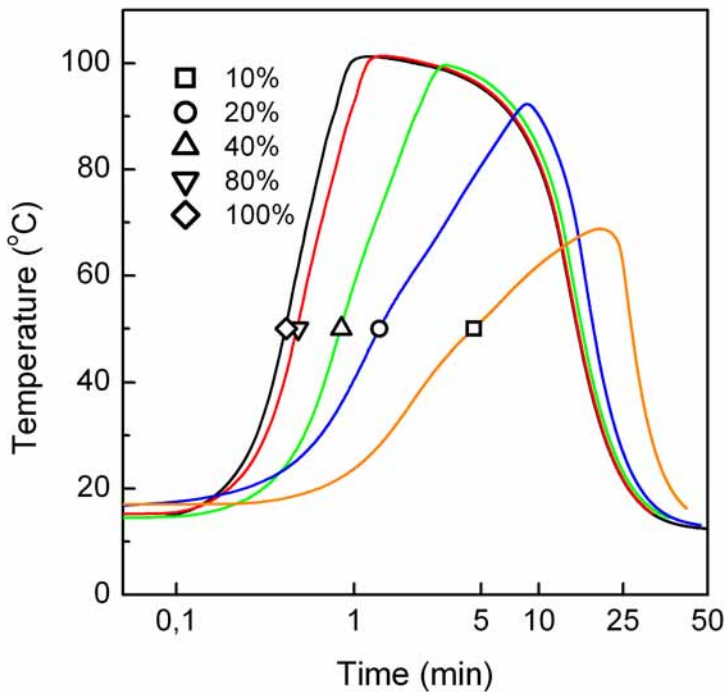
Charging at 100%



Discharging at 90%

We can divide the process of charging and discharging of MH reactor into three stages. Transition from the first to the second stage is connected with dramatic decrease of hydrogen flow rate at reactor inlet – and we can call this

**crisis of heat and mass transfer**



## I stage

Rapid heating with pressure increasing

## I – II transition (crisis)

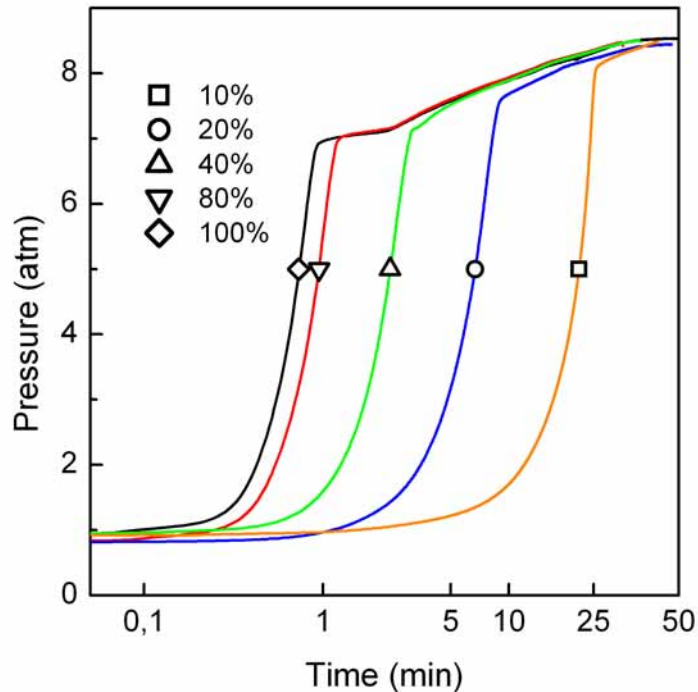
Maximum temperature reached

## II stage

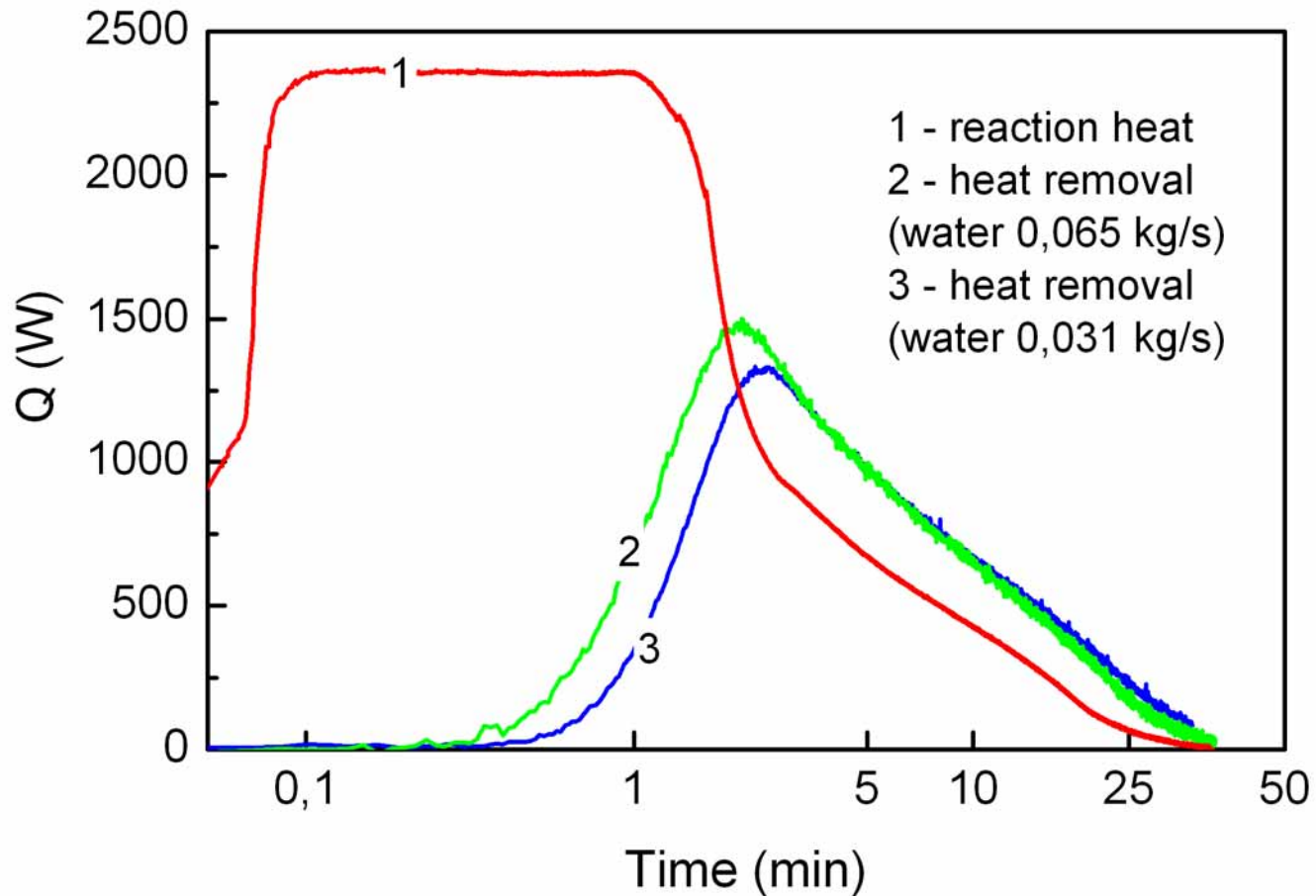
Steady temperature and pressure changing

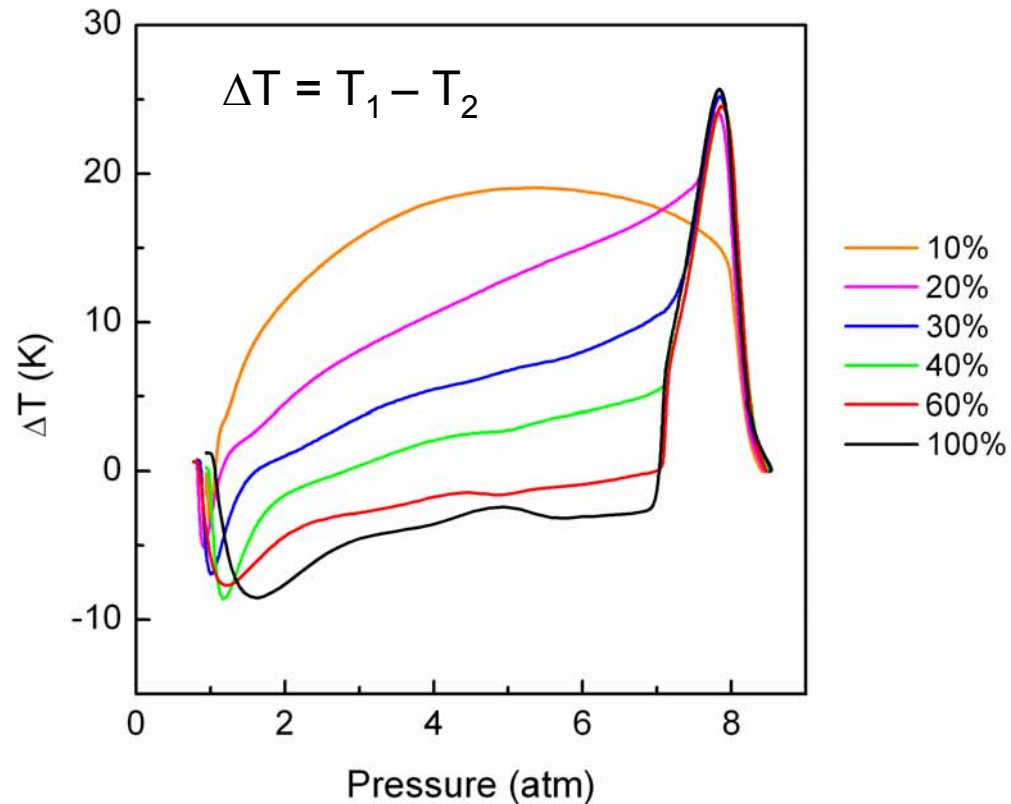
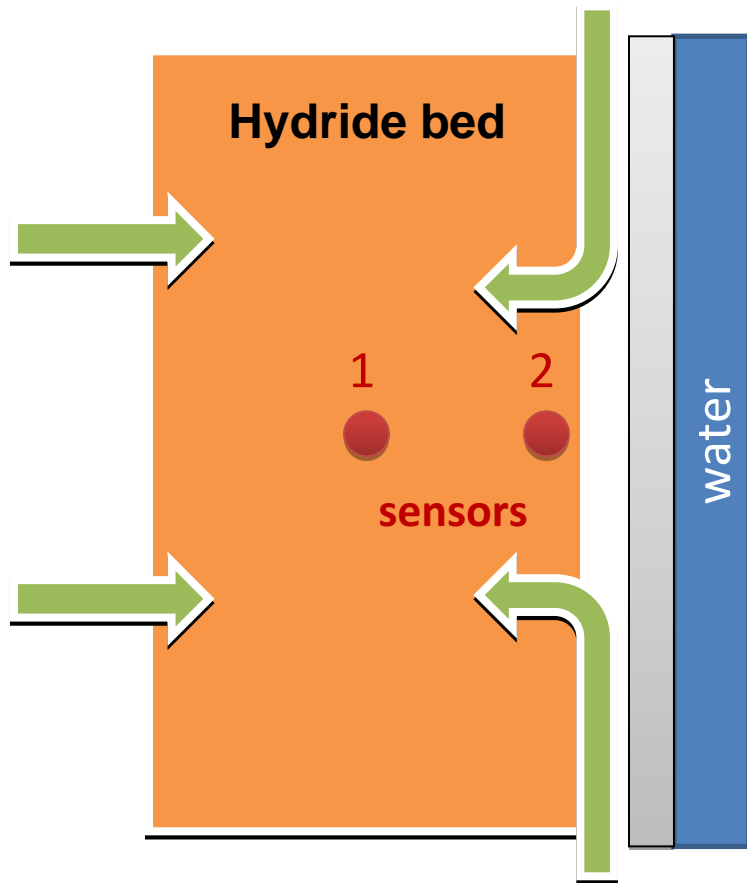
## III stage

Inlet pressure reached, temperature goes down



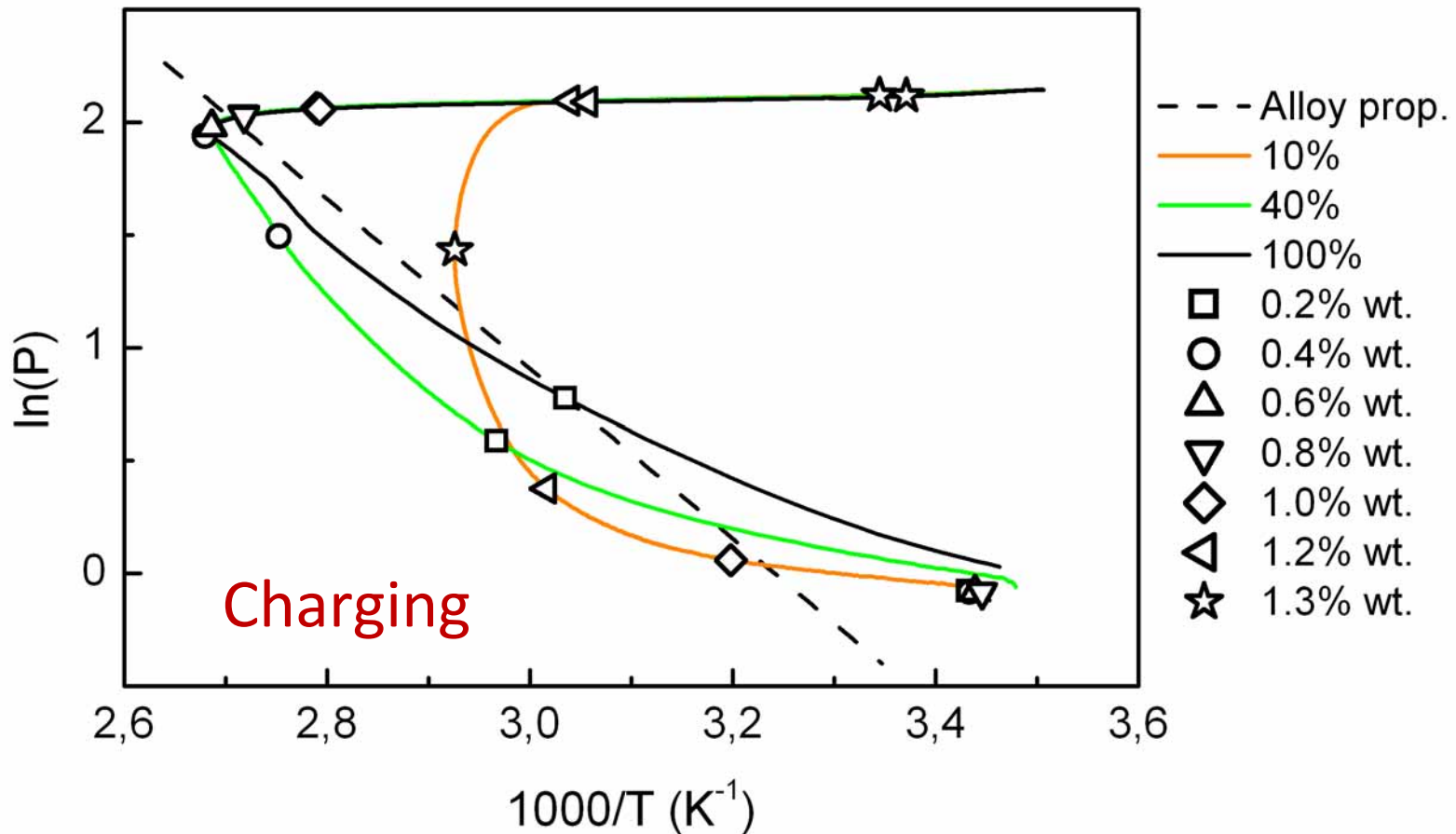
# Heat balance at charging





## I stage – heating to reaction temperature

Hydrogen sorption in hydride bed is limited only by regulator at reactor inlet. Heat of reaction cannot be efficiently removed from the bed.

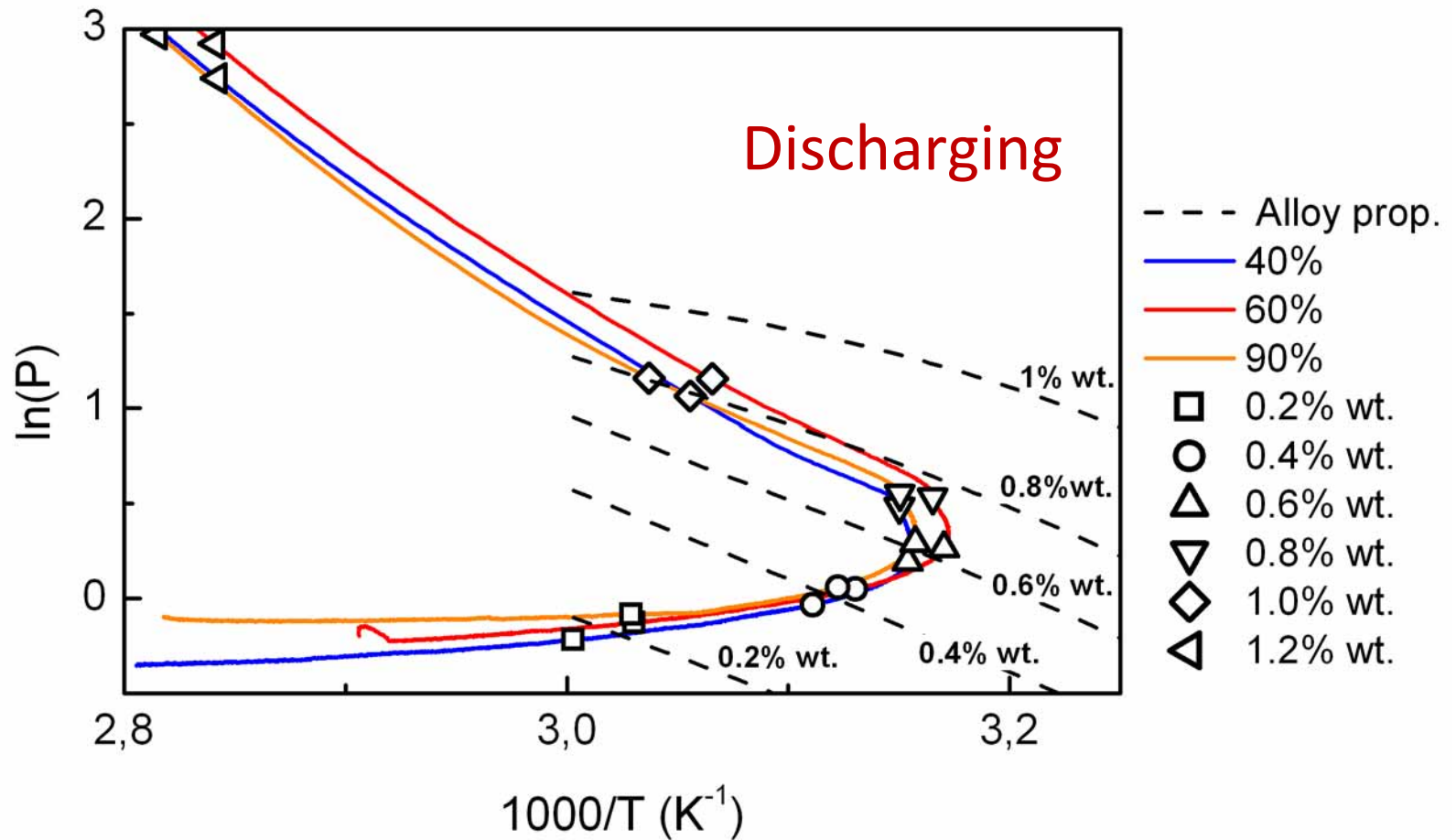


## II stage – equilibrium sorption

Most of hydrogen (>50%) is charged at II stage, and it corresponds to plateau of PCT diagram

## Heat-balanced regimes

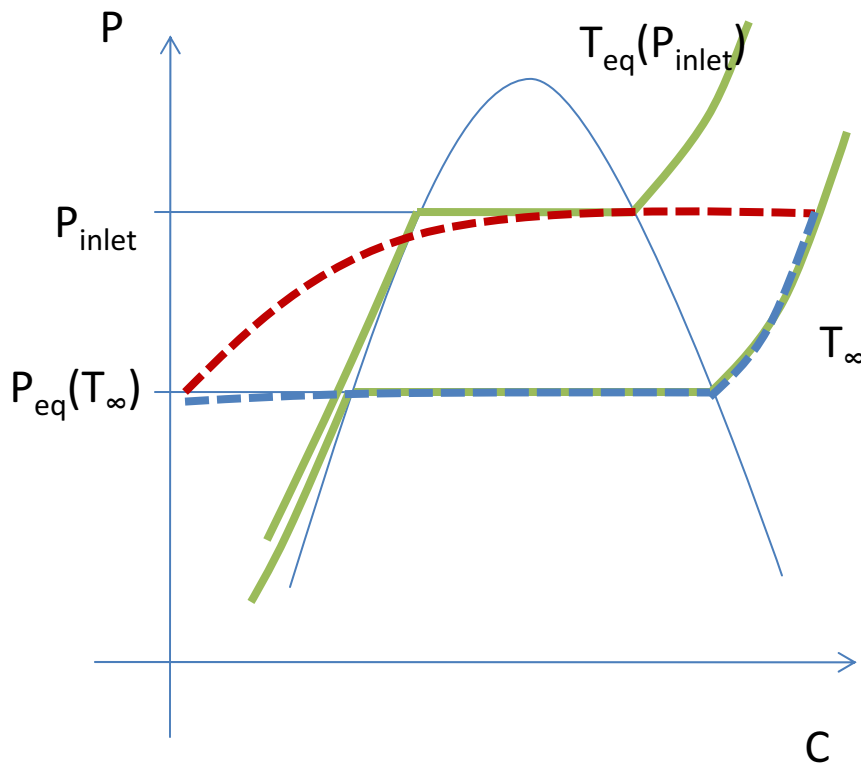
If heat removal is higher than heat generation for given hydrogen flow rate the I and II stages unite and there's no crisis



### III stage – finishing

Most of hydrogen (>50%) is charged at II stage, and it corresponds to plateau of PCT diagram

# Criteria of balanced heat regime



- - - Unbalanced regime  
- - - Balanced regime

$$Q_{\text{reaction}} = m_{\text{MH}} g \Delta H$$

$m_{\text{MH}}$  - mass of hydride bed

$g$  - flow rate,  $\Delta H$  - heat of reaction

$$Q_{\text{heat exchanger}} = \alpha F (T_{\text{MH}} - T_{\infty})$$

$\alpha$  - heat transfer coefficient

$F$  - heat transfer surface

$$Q_{\text{heat exchanger}} > Q_{\text{reaction}}$$

$$g < \alpha F (T_{\text{eq}}(P_{\text{inlet}}) - T_{\infty}) / m_{\text{MH}} \Delta H$$

$$\alpha = 120 \text{ W/m}^2 \text{ K (AB}_5 \text{ alloy)}$$

# Conclusions

- Charging and discharging of MH reactor is three stage process:
  - I – Heating/cooling to reaction temperature  $T_{eq}(P_{inlet})$
  - II – Equilibrium sorption/desorption
  - III – Finishing (cooling/heating to  $T_{\infty}$ )
- I – II transition is connected with heat and mass transfer crisis
- Crisis is connected with insufficient cooling or heating of MH bed
- Heat-balanced regimes with sufficient heat transfer and assure constant flow rate at reactor inlet
- Heat-balanced regimes criteria:

$$g < \alpha F (T_{eq}(P_{inlet}) - T_{\infty}) / m_{MH} \Delta H$$

Thank you!