Group of Energy Accumulating Processes & Materials

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Boreskov Institute of Catalysis

SORPTION FRIENDS

Taormina, Sicily,
May 2-4, 2023

Group of Energy Accumulating Processes & Materials

The staff

Doctor of Chemistry (Dr. hab.), Prof. Yuri Aristov

Doctor of Chemistry (Dr. hab.) Larisa Gordeeva

Dr. Alexandra Grekova

Dr. Marina Solovyeva

Dr. Michail Tokarev

Students

Ph.D. student Svetlana Strelova,

Bc. student at NSU Anastasiya Cherpakova.

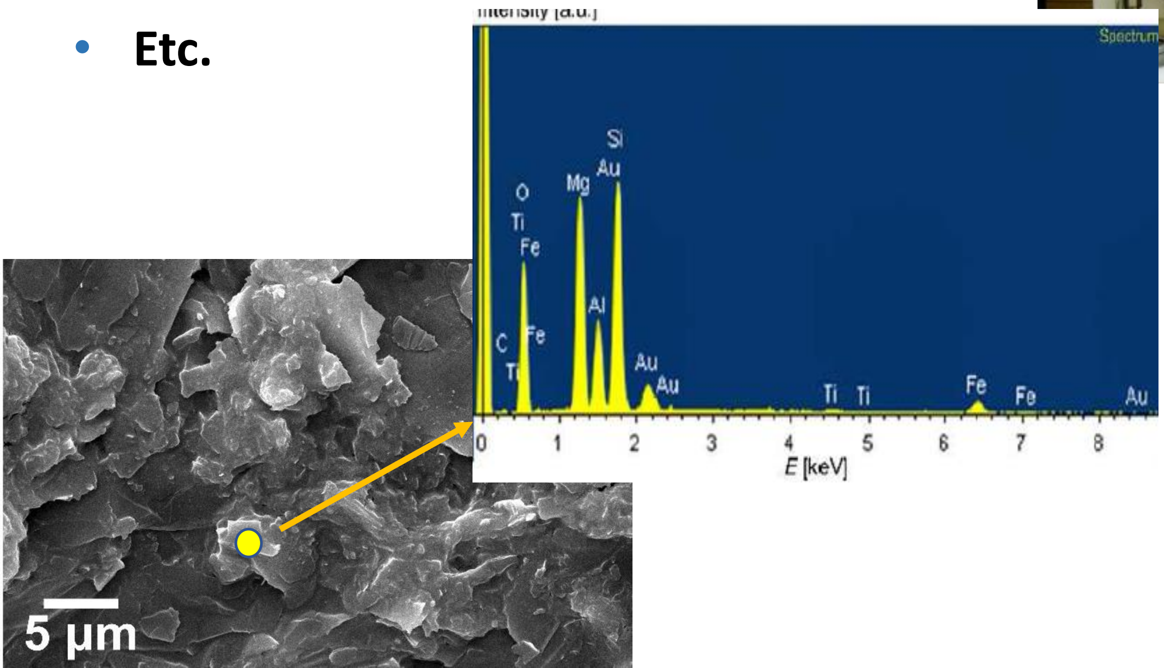
Research capabilities

- Synthesis of adsorbents
- Low temperature nitrogen adsorption
- IR - spectroscopy
- Thermogravimetry (Ruboterm, TGA 550)
- Differential Scanning Calorimetry
- Temperature/Pressure Jump

Research capabilities

Other methods available in BIC:

- XRD and synchrotron XRD in situ ,
- SEM,
- TEM,
- Energy-dispersive X-ray spectroscopy,
- NMR, including EFG
- Gas and liquid chromatography
- Elemental analysis
- Etc.



Current Projects

The adsorption heat conversion (AHC) is still being the main, but not the only field of research interests of the GEPM. Currently the researches in the GEPM are carried out in the following directions:

1. **Analysis of open adsorption cycles: combining the psychrometric chart of humid air with water adsorption isosters**

2. **Composites "LiCl/vermiculite" for adsorption thermal batteries: acceleration of sorption dynamics**

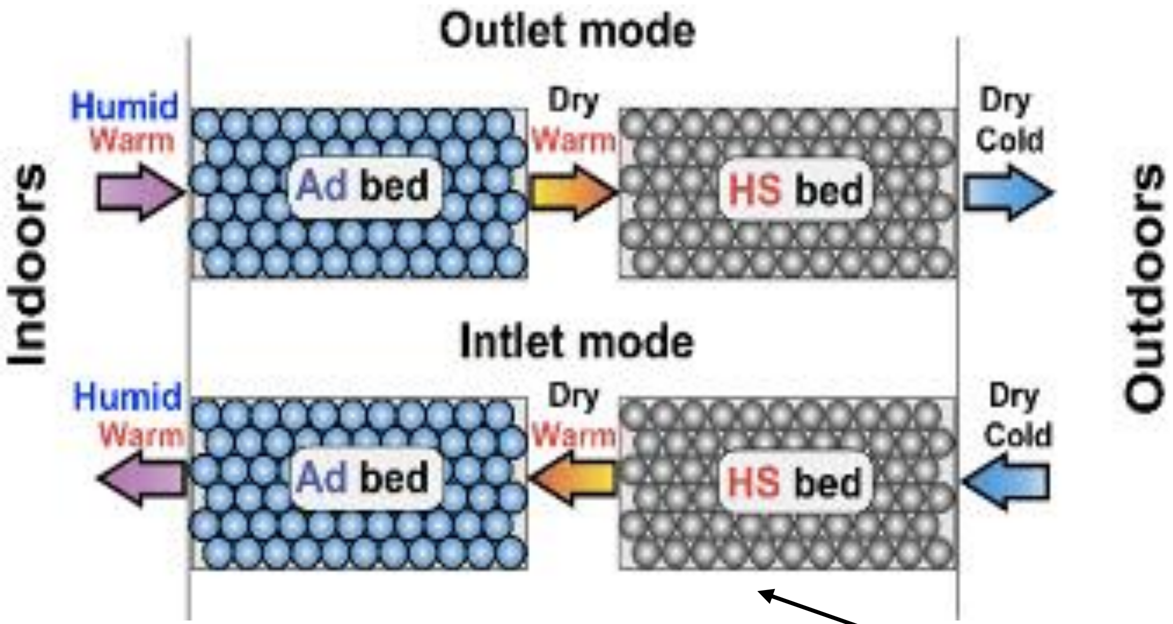
3. **Optimization of the adsorbent bed configuration**

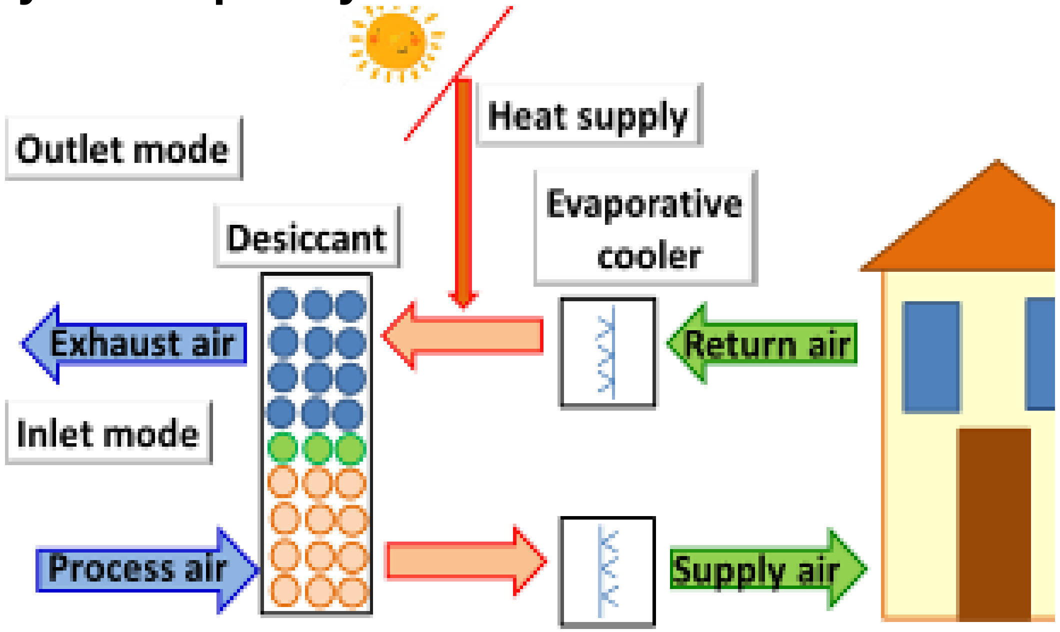
4. **Heat exchanger geometry optimization**

1. Analysis of open adsorption cycles: combining the psychrometric chart of humid air with water adsorption isosters

This is a new approach for a deeper analysis of adsorption processes in *__open__* systems for heat transformation and storage. Its idea is to plot adsorption isosters for a given adsorbent *directly* on the common psychrometric chart of humid air.

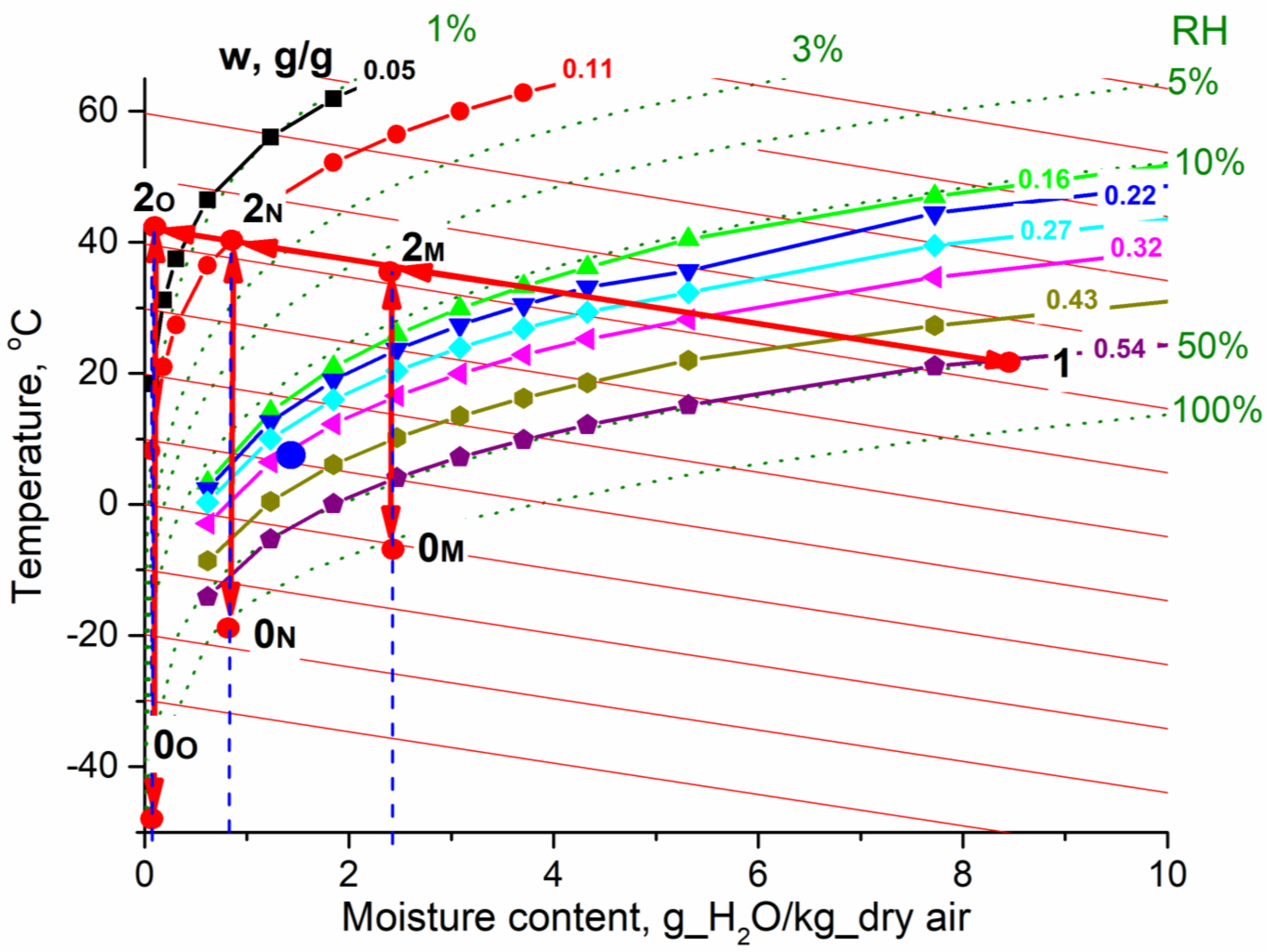
Such a combined diagram allows the states of air and the certain adsorbent to be analysed simultaneously. This may significantly simplifies the analysis of open systems.





Schemes of open cycle for Ventireg process and cooling & dehumidification

1. Combining the psychrometric chart of humid air with water adsorption isosters



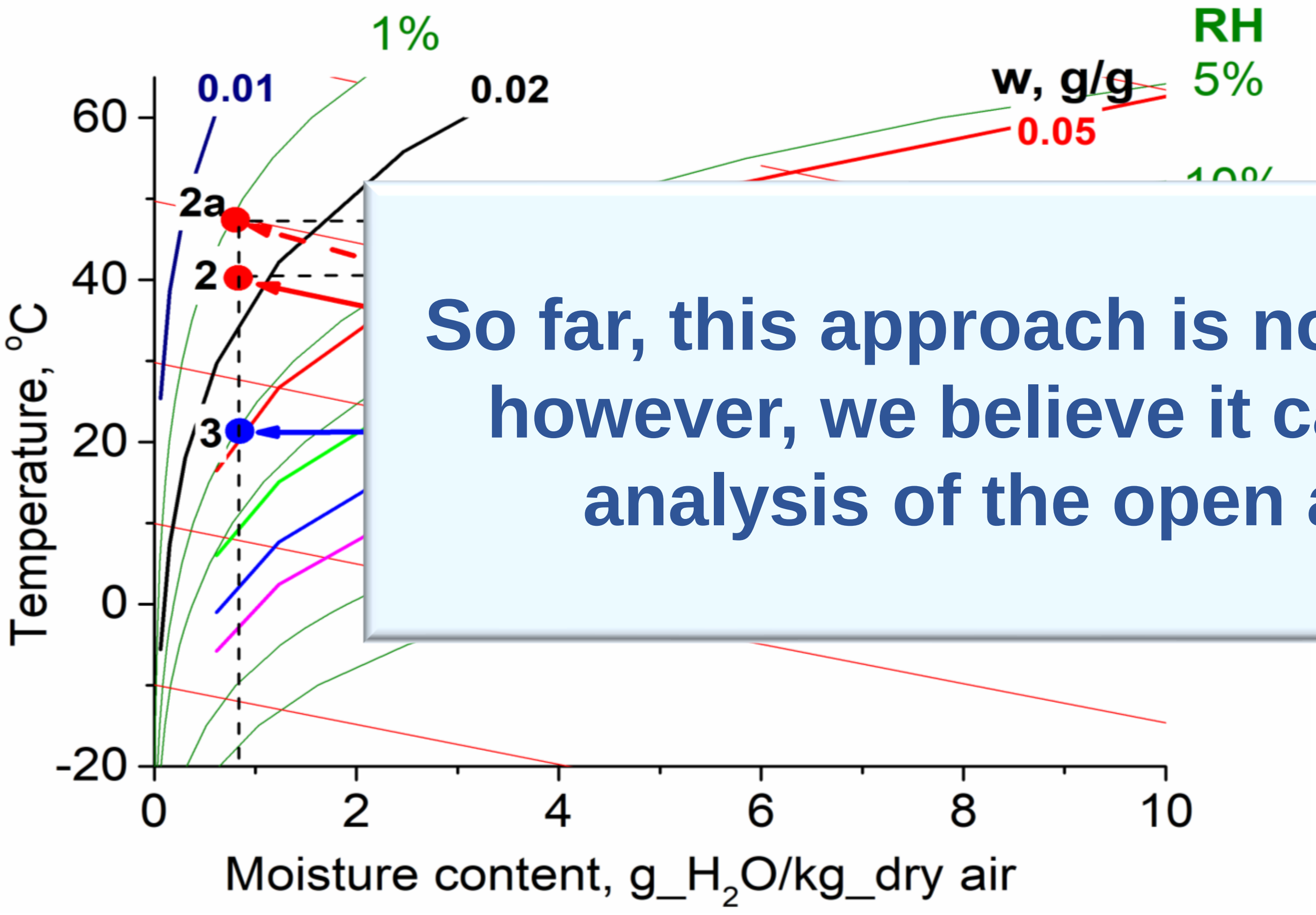
Schematics of the VentireG process in the selected locations of Russia. Adsorbent – composite $CaCl_2$/silica.

Here the lines with constant RH of psychrometric chart is presented by dotted lines and the isosters of water adsorption on a $CaCl_2$/silica composite - by solid lines. Of course, it may be done for any adsorbent which follows the Polanyi potential theory.

<u>This approach affords</u>:

- **analysis of the suitability of adsorbent for Ventireg**
- **evaluation of adsorption swing in the cycle under conditions of various climatic zones**

1. Combining the psychrometric chart of humid air with water adsorption isosters



Schematics of the different modes of the VentireG process.
Adsorbent – silica gel Siogel.

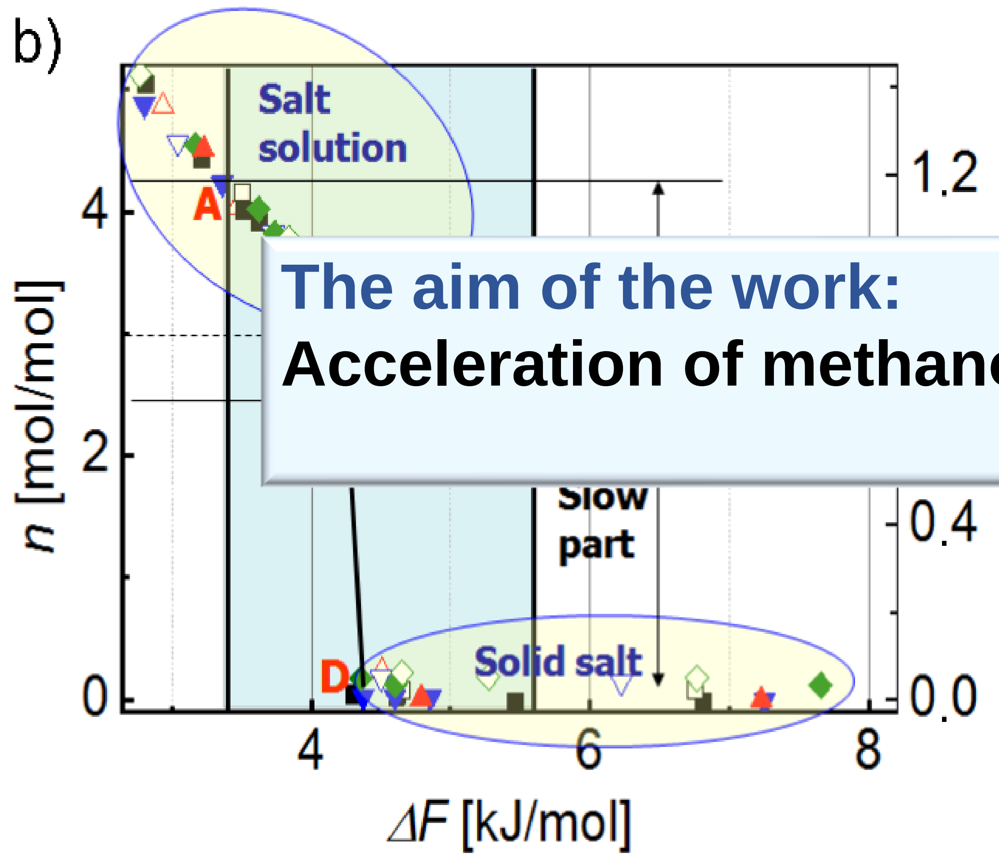
isothermal
atic (1-2)

So far, this approach is not famous and popular; however, we believe it can be very fruitful for analysis of the open adsorption cycles.

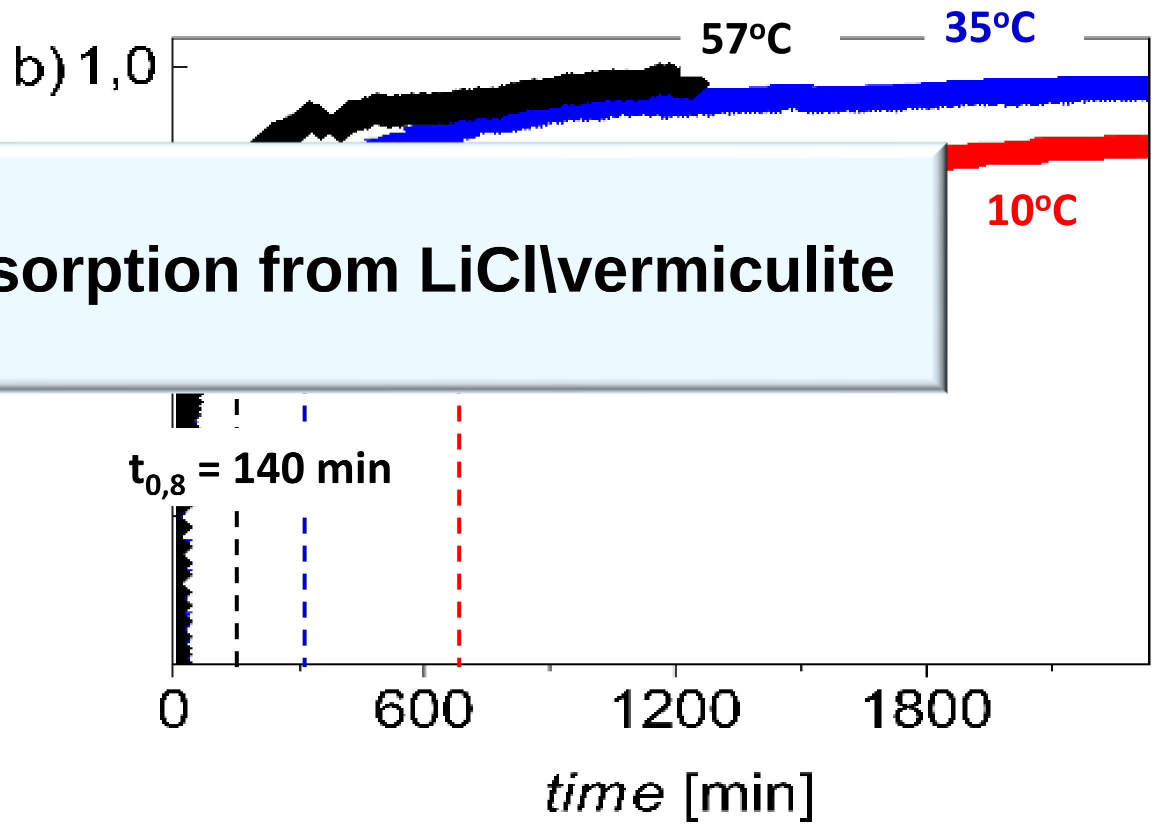
Yu. I. Aristov, L.G. Gordeeva, *Energy*, 239 (2022) 122278,
https://doi.org/10.1016/j.energy.2021.122278

2. Composites "LiCl/vermiculite" for adsorption thermal batteries: acceleration of sorption dynamics

Problem: extremely slow ad/desorption dynamics



Characteristic curve of methanol sorption on LiCl/Vermiculite.

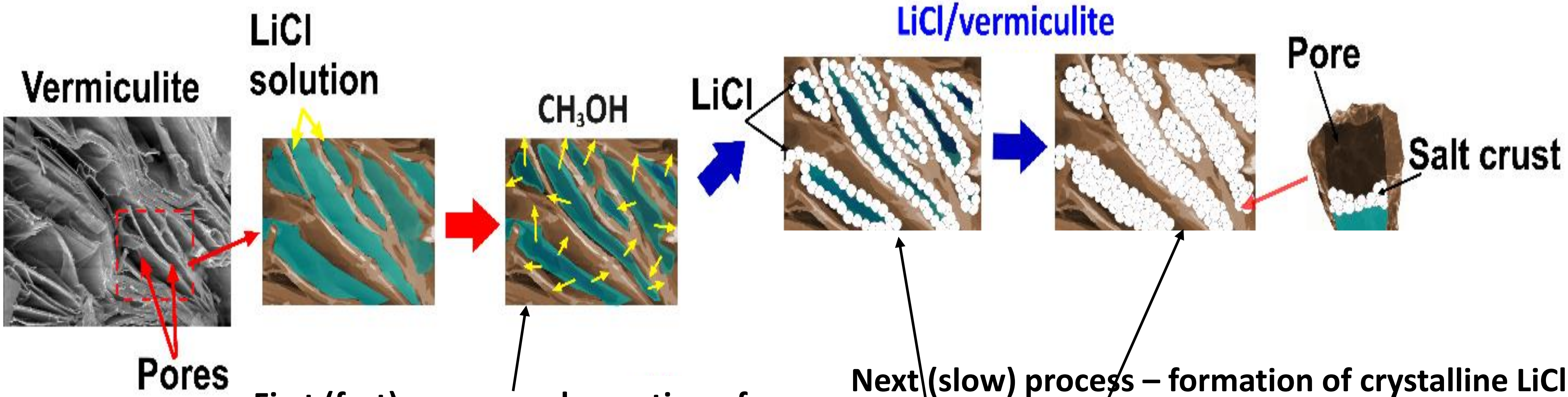


Dimensionless kinetic curves of the methanol desorption from LiCl/vermiculite

The aim of the work:

Acceleration of methanol desorption from LiCl\vermiculite

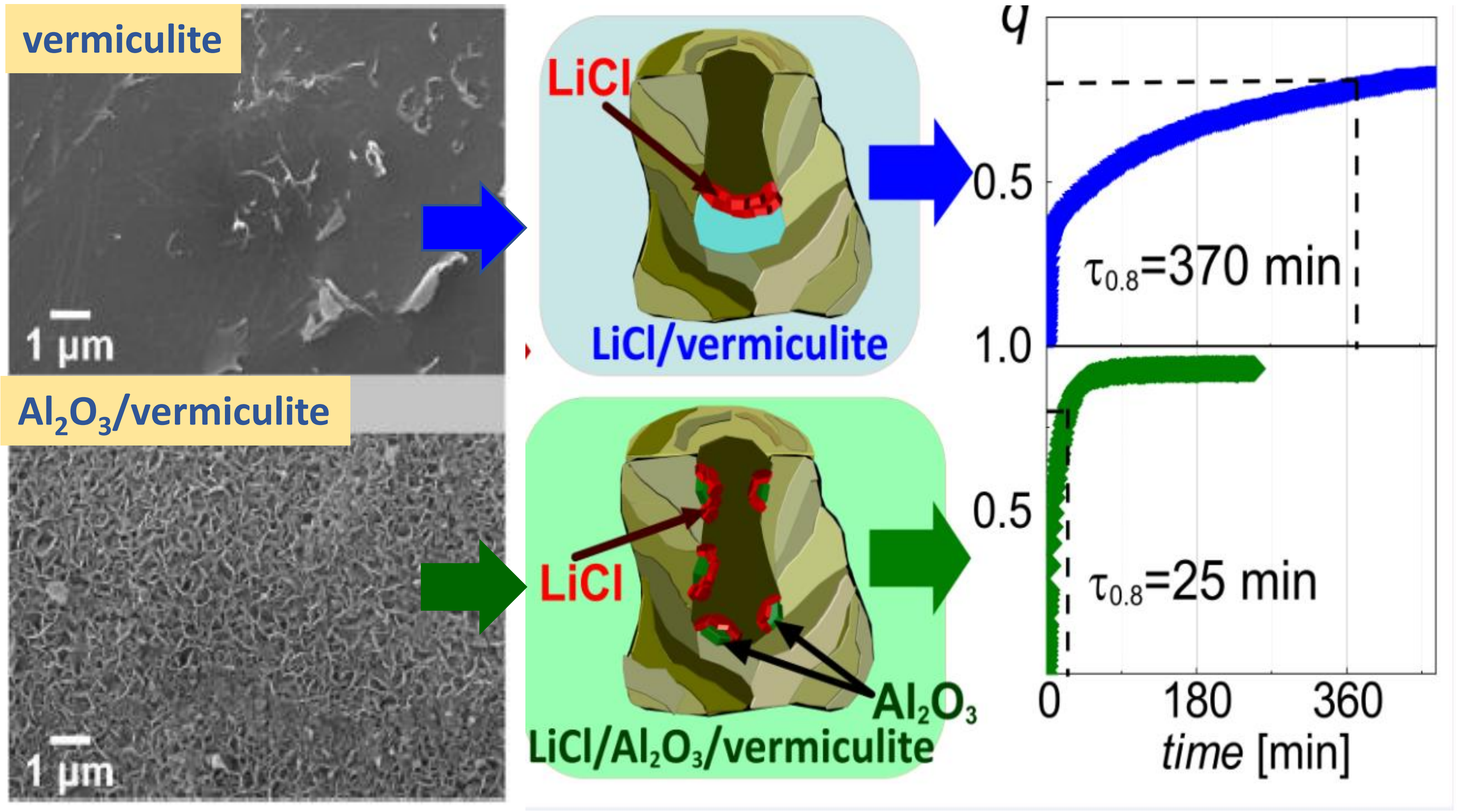
2. Composites “LiCl/vermiculite” for adsorption thermal batteries: acceleration of sorption dynamics



First (fast) process – desorption of methanol from the LiCl-methanol solution inside pores

Next (slow) process – formation of crystalline LiCl:
- Nucleation
- Nuclei growth

2. Composites “LiCl/vermiculite” for adsorption thermal batteries: acceleration of sorption dynamics

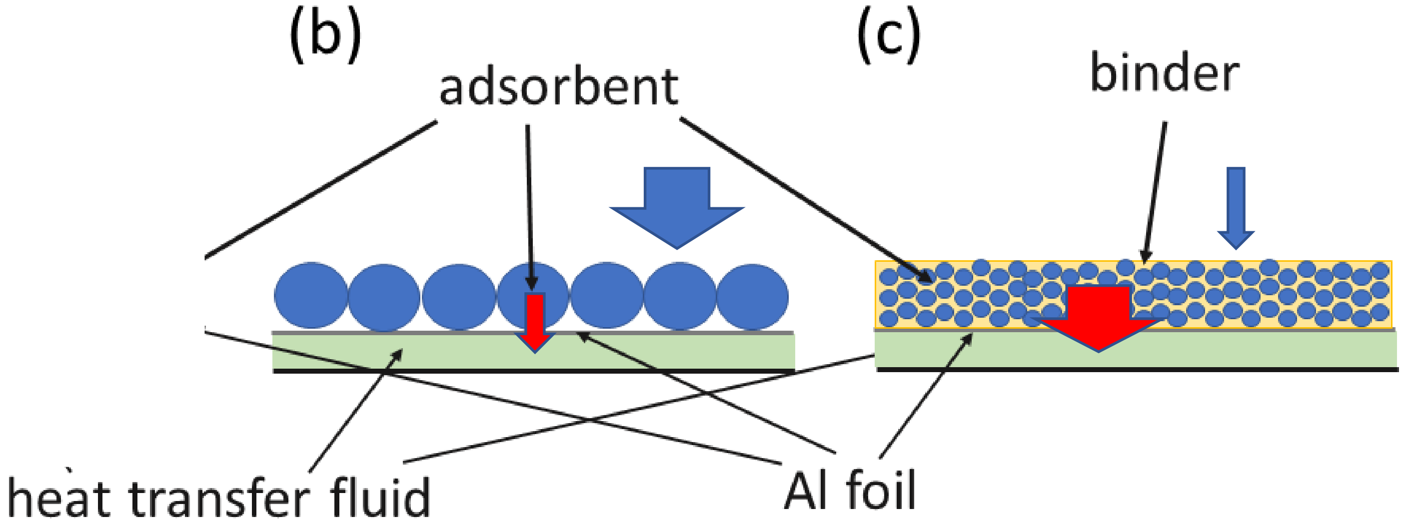


The addition of 2-9% of dispersed Al_2O_3 leads to giant acceleration of methanol desorption: the characteristic desorption time $t_{0.8}$, corresponding to the conversion q=0.8, decreases by 2-12 times. A acceleration mechanism includes the adsorption of Li^+ ions on it, the formation of Li^+-Al_2O_3 surface complexes, which, being LiCl nucleation centers, accelerate the LiCl crystallization.

S.Strelova, L.Gordeeva, A.Grekova, A.Salanov, Yu.Aristov, Energy 263 (2023) 125733

3. Optimization of the adsorbent bed configuration

Loose grains loaded between fins of the HEx	Thin adsorbent coting on the HEx surface

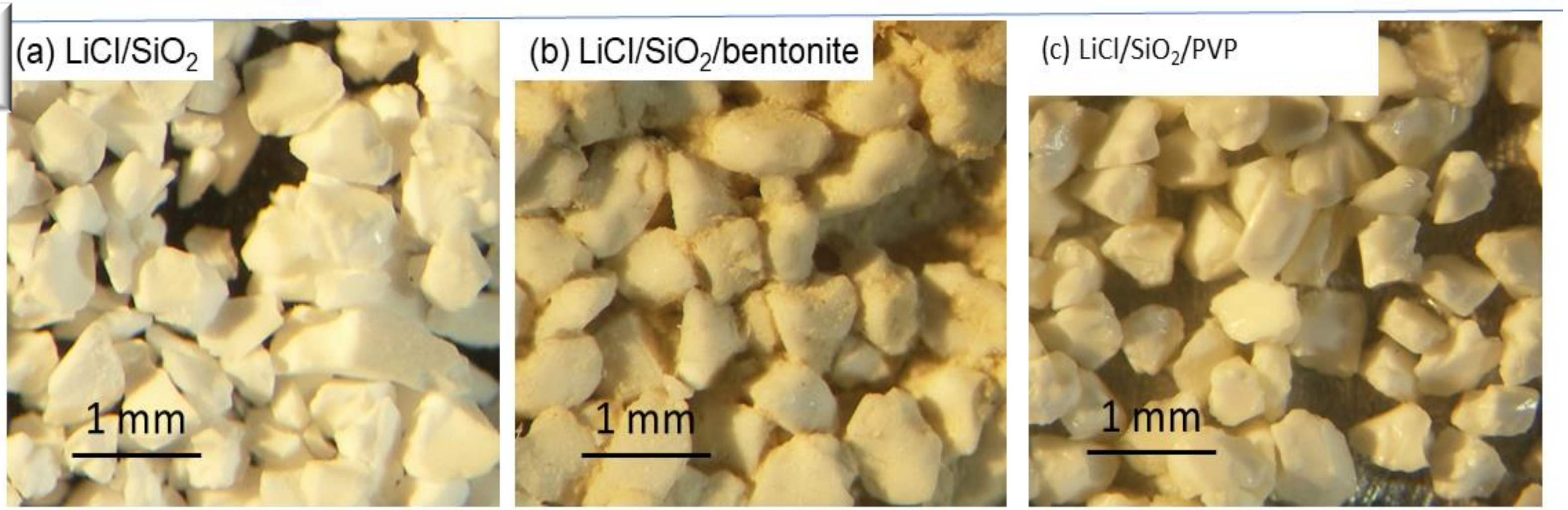


• Fast mass transfer • Poor heat transfer	• Poor mass transfer • Fast heat transfer

Problem: Compromising between the heat and mass transfer is prerequisite!

3. Optimization of the adsorbent bed configuration: LiCl\silica

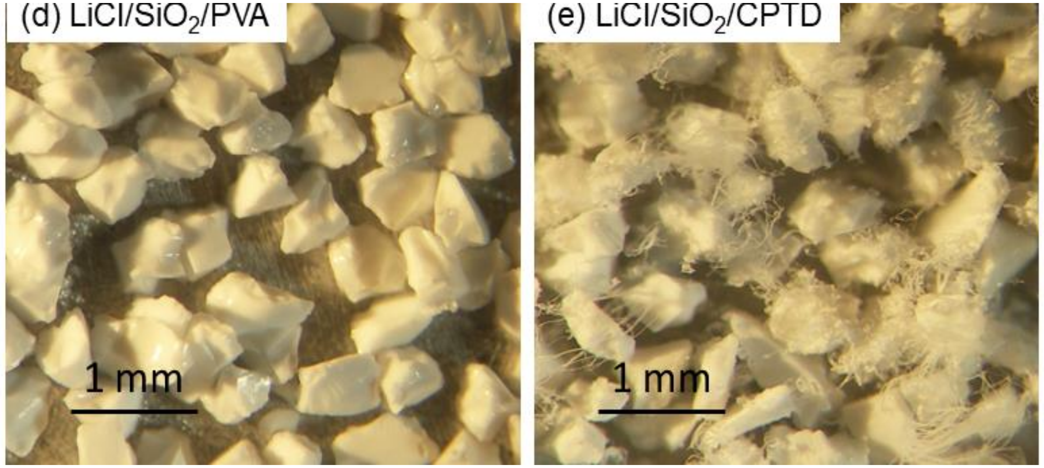
Effect of the binder nature



<u>Organic binders:</u>
PolyVinylPyrrolidones (PVP)
PolyVinyl Alcohol (PVA)
PolyAnyline (PA)

<u>Inorganic binders</u>:
Bentonite
Pseudoboehmite
Aluminium oxynitrate

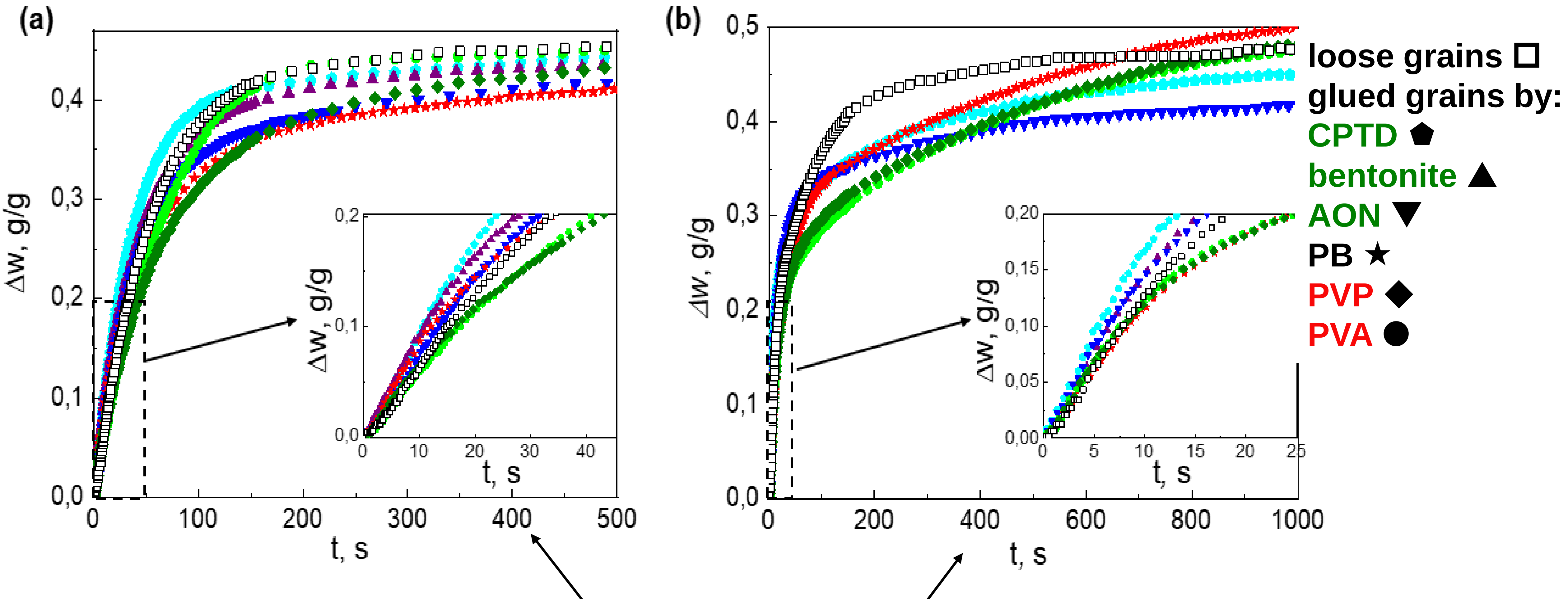
LiCl/silica gel
D_{gr} = 0.4-0.5 mm



<u>Hybrid binders</u>:
ceramic-polymer heat-conducting compound CPTD 1/3T

3. Optimization of the adsorbent bed configuration: LiCl\silica

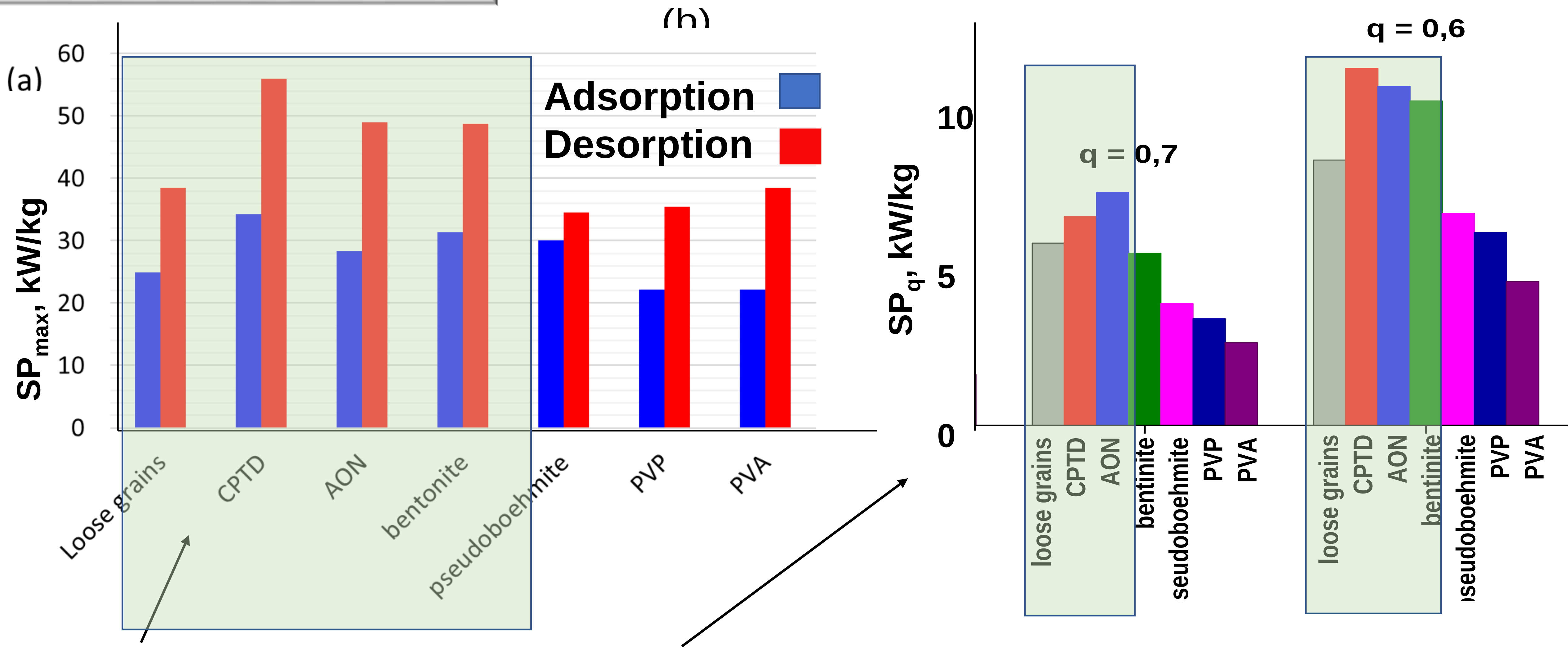
Effect of the binder nature



Kinetic curves of water adsorption and desorption

3. Optimization of the adsorbent bed configuration: LiCl\silica

Effect of the binder nature



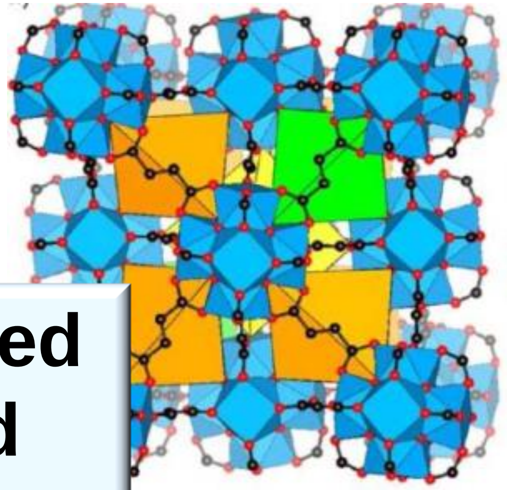
Maximum SP_{max} and average SP_q specific power restricted by conversion q

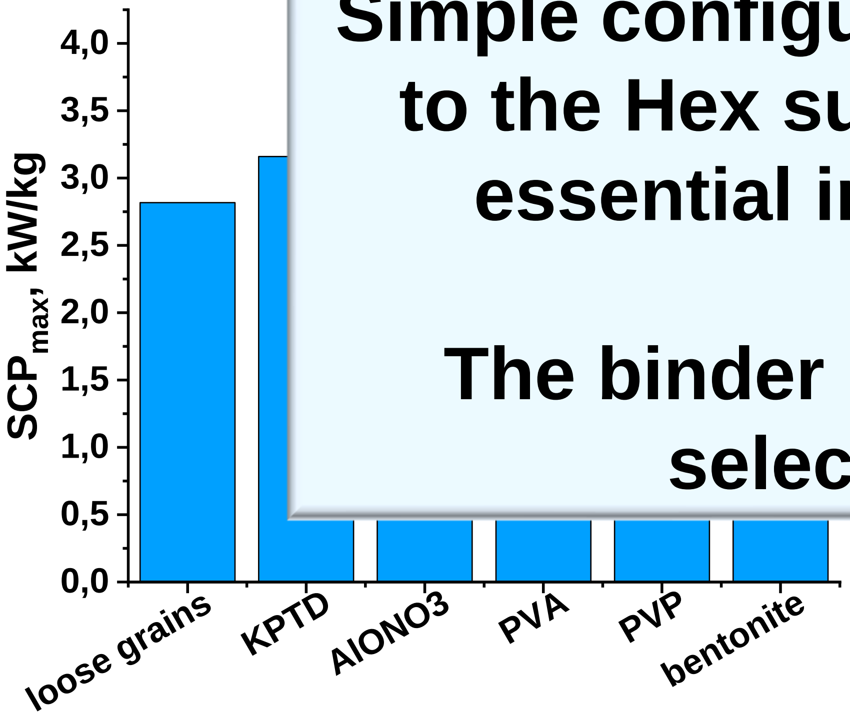
3. Optimization of the adsorbent bed configuration: MOF-801

Effect of the binder nature

MOF-801

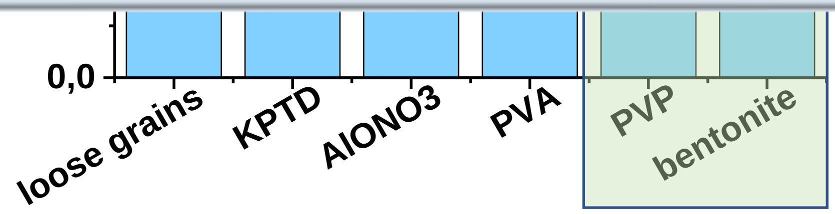
$Zr_6O_4(OH)_4(^{-}O_2C\text{-}CH{=}CH\text{-}CO_2^{-})_6$





Simple configuration of adsorbent grains glued to the Hex surface with a binder may afford essential increase in the specific power

The binder nature is a matter of thorough selection for each adsorbent

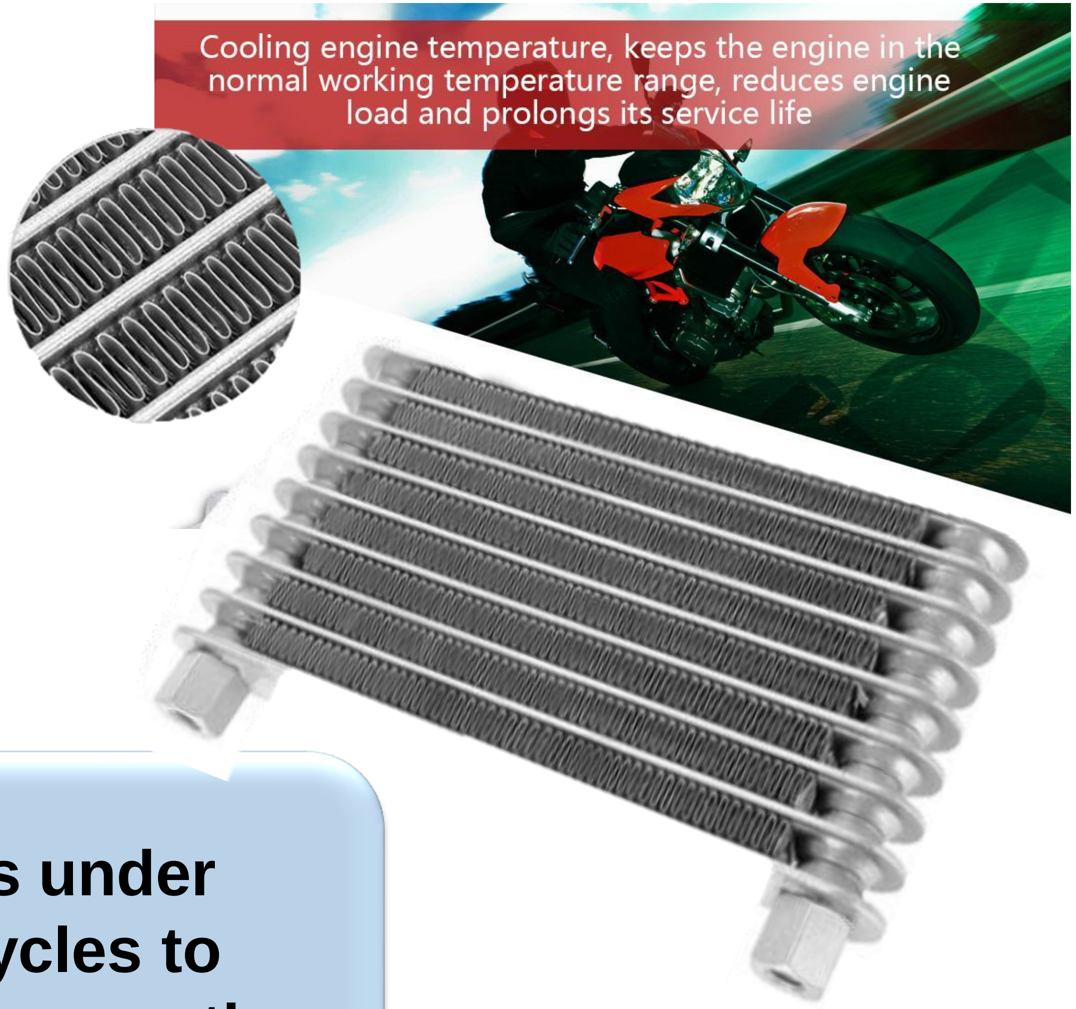


Maximum and average specific power

4. Heat exchanger geometry optimization

The problem

AHC commonly uses commercial gas-to-liquid automobile and motorcycle HExs, which geometry is not optimized for AHC.



The aim of the work

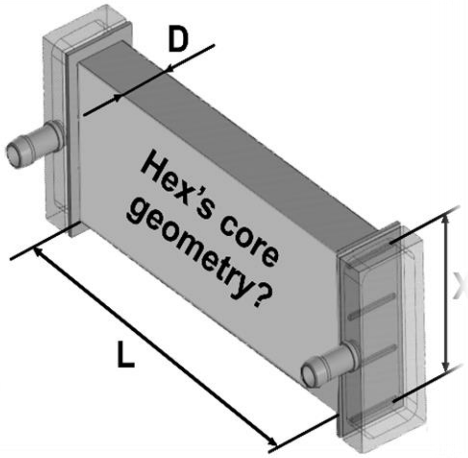
The study of various HEx configurations under typical working conditions of the AHT cycles to identify the optimal HEx geometry, which ensure the most efficient operation of AHC.

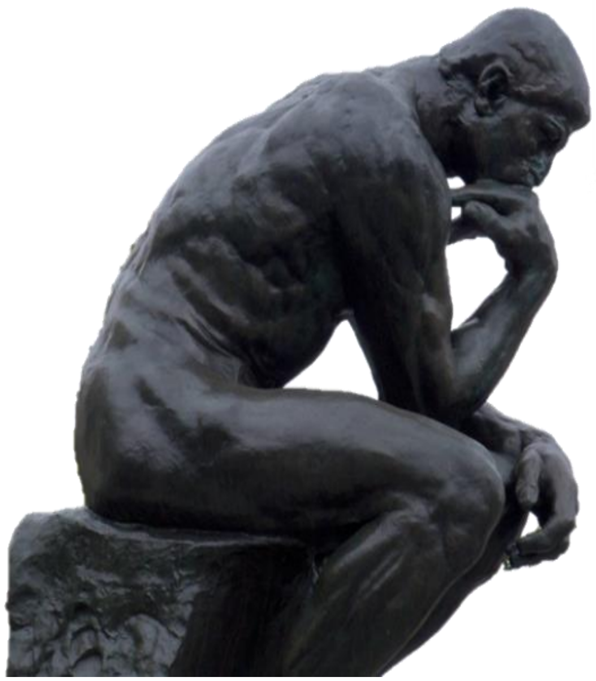
4. Heat exchanger geometry optimization

Two directions

Search for the most promising FFT Hex <u>produced by industry</u>

Search for <u>new Hex</u> geometries



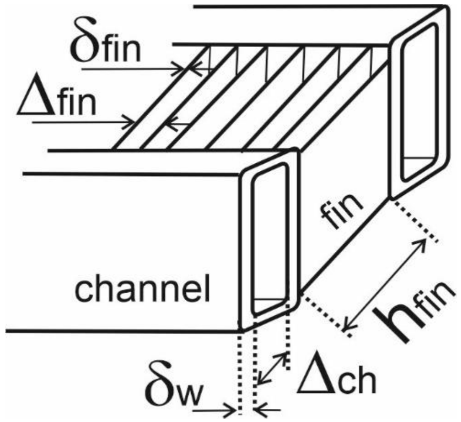


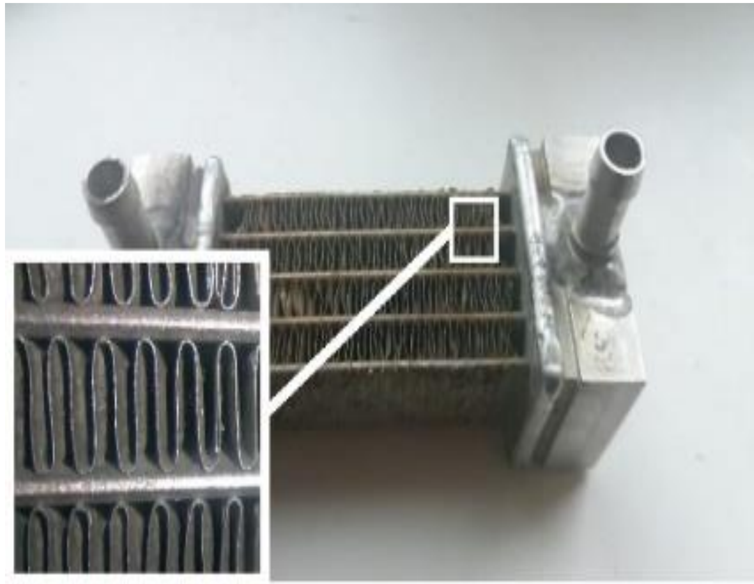
4. Heat exchanger geometry optimization

Search for the most promising FFT Hex <u>produced by industry</u>

№	d_w, µm	Δ_{ch}, mm	h_{fin}, mm	Δ_{fin}, mm	d_{fin}, µm
1	487	2,3	7,0	1,8	87
2	357	1,8	9,8	1,4	88
3	504	2,2	8,0	1,5	75
4	418	1,3	4,8	0,9	52
5	417	0,5	4,1	0,9	48
6	932	2,1	13,7	1,8	103
7	546	0,8	6,2	0,8	63
8	289	0,5	5,2	1,4	98
9	520	1,0	5,8	1,0	78

scheme





$$Q = \Delta T S_{pr}\left[\frac{1}{\alpha_1}+\frac{\delta_w}{\lambda_w}+\frac{1}{\alpha_2(1+E(k-1))}\right]^{-1} = \Delta T UA$$

UA

The higher the global heat transfer coefficient UA, the more heat will be transferred for the same temperature difference ΔT.

4. Heat exchanger geometry optimization

Search for the most promising **FFT** Hex <u>produced by industry</u>

Search for the most promising **FFT** Hex ***produced by industry***

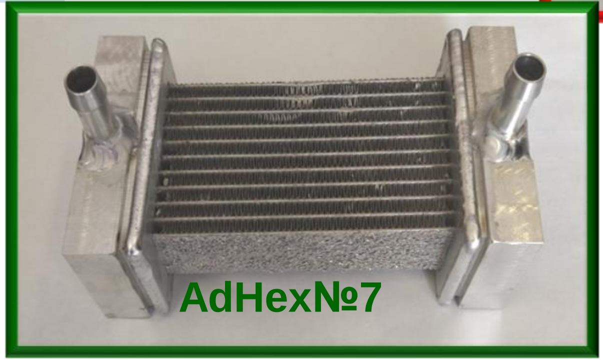
The air conditioning cycle
Tev/Tcon/Tdes = 10/35/90
f_{water} = 0,03L/s

№	d_w, µm	Δ_{ch}, mm	h_{fin}, mm	Δ_{fin}, mm	d_{fin}, µm	UA (air), W/K
1						
2						
3						
4						
5	417	0,5	4,1	0,9	48	47,3
6	932	2,1	13,7	1,8	103	12,0
7	546	0,8	6,2	0,8	63	44,6
8	289	0,5	5,2	1,4	98	26,7
9	520	1,0	5,8	1,0	78	38,5

Thus, the concepts, earlier developed for *<u>gas-to-liquid</u>* FFT HExs, can be applied for *<u>adsorbent-to-liquid</u>* Ad-HExs used for ACs, when fins transfer heat to the fixed adsorbent bed instead of the moving gas.

Maximum power, W

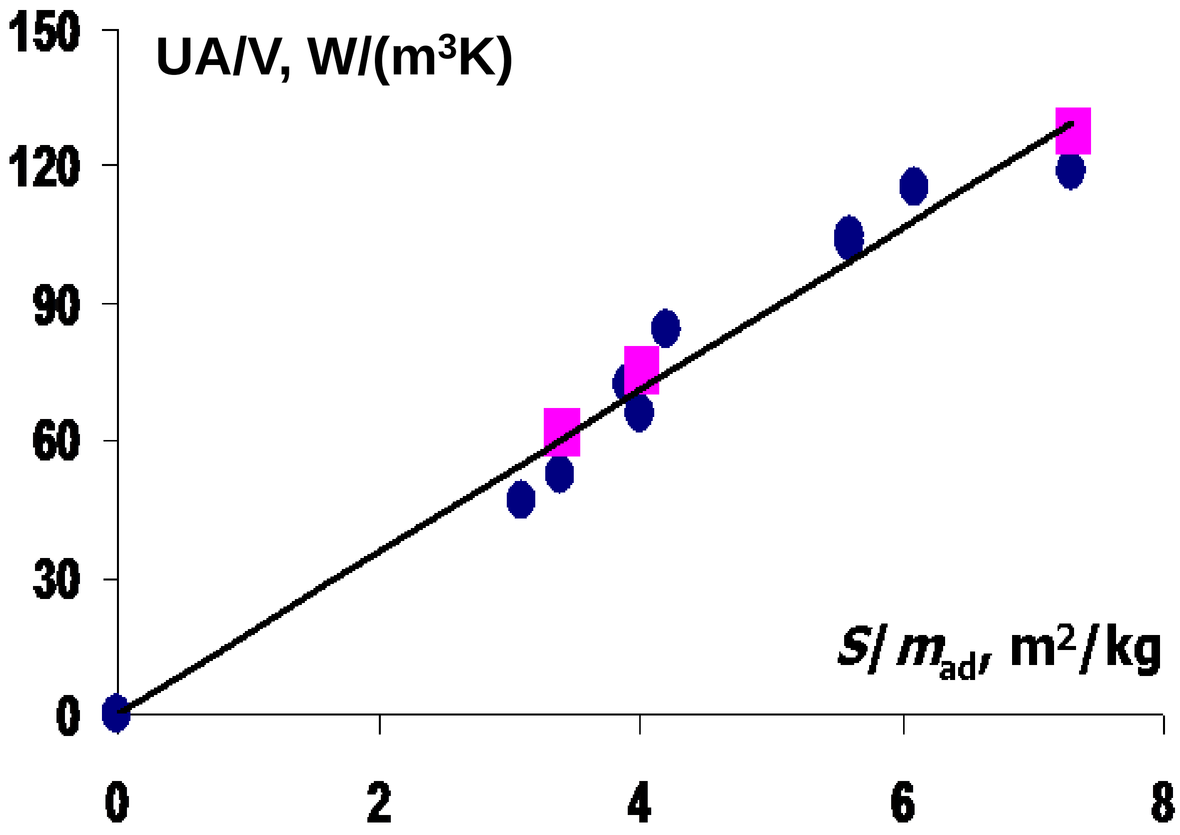
120-130



190-200

4. Heat exchanger geometry optimization

Search for the most promising **FFT** Hex <u>produced by industry</u>



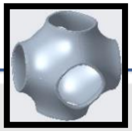
A linear relation is found between the specific global heat transfer coefficient (UA/V) HEx and the ratio (area of heat transfer surface)/(adsorbent mass), which can greatly simplify the prediction of the HEx thermal behaviour.

This approach can be recommended as an accurate and time-saving strategy for selecting commercial HExs and designing new HExs optimal for adsorption heat transformation and storage.

4. Heat exchanger geometry optimization

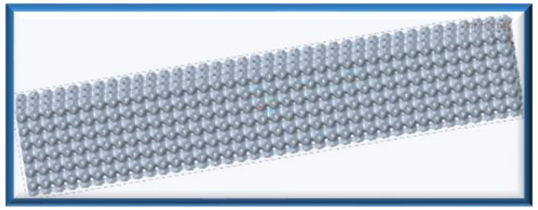
Search for new optimal FFT Hex geometry

The HExs with replaceable secondary heat-transfer elements were considered. Global heat transfer coefficient UA was calculated for 17 various geometries of these elements.



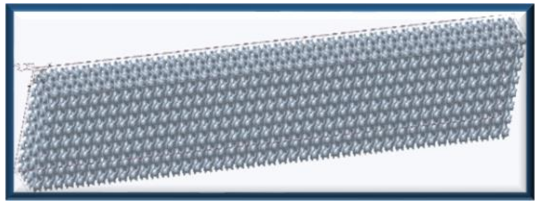
P-surface, primitive

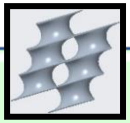
$$\cos\frac{x}{a}+\cos\frac{y}{b}+\cos\frac{z}{c}=0$$



P, D-surface, gyroid

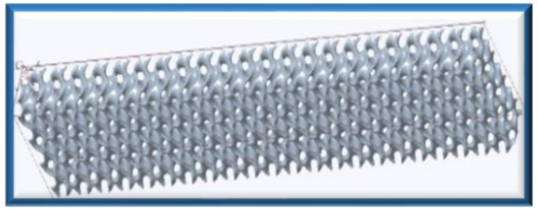
$$\sin\frac{x}{a}\cos\frac{y}{b}+\sin\frac{y}{b}\cos\frac{z}{c}+\sin\frac{z}{c}\cos\frac{x}{a}=0$$



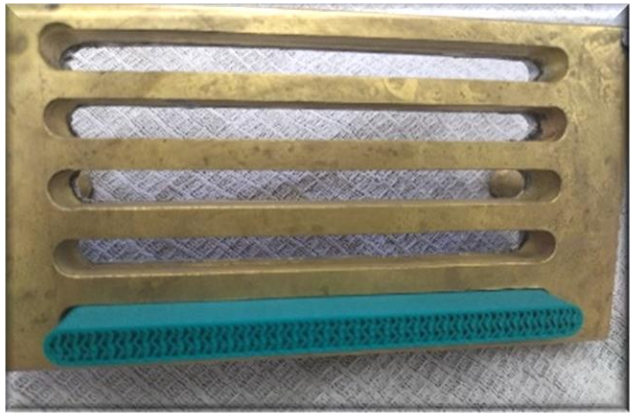


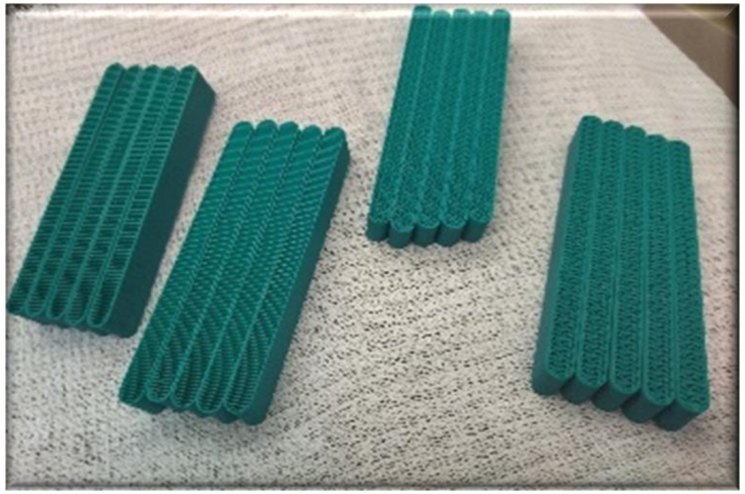
D-surface, rhomboid

$$\sin\frac{x}{a}\sin\frac{y}{b}\sin\frac{z}{c}+\sin\frac{x}{a}\cos\frac{y}{b}\cos\frac{z}{c}+\cos\frac{x}{a}\sin\frac{y}{b}\cos\frac{z}{c}+\cos\frac{x}{a}\cos\frac{y}{b}\sin\frac{z}{c}=0$$



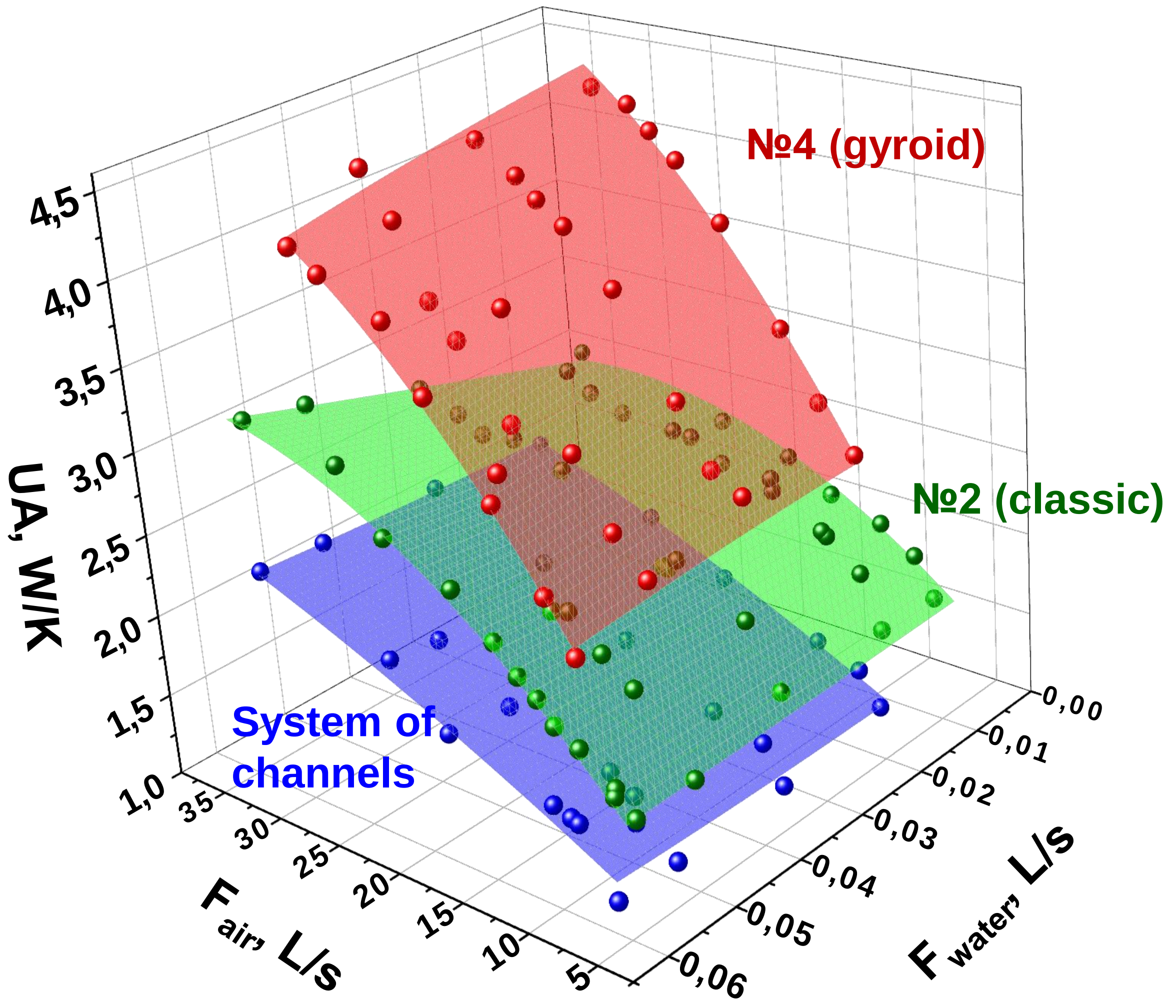
where x,y,z are coordinates, a,b,c are unit cell parameters





The HExs with replaceable secondary heat transfer elements were made of ABS plastic by 3D printing, and UA-coefficients were measured.

4. Heat exchanger geometry optimization



It is shown that the sample with the "gyroid" geometry actually exceeds the UA coefficient of the TO with the "classical geometry" by 30%-40% depending on the experimental conditions.

Symbols are experimental points, surfaces are the result of approximation by the 2nd order equation

Global heat transfer coefficient

Thank you for your kind attention!