MODELING THE EFFECTS OF ADDING GRAPHITE FLAKES TO FAM-Z02 IN AN ADSORBER BED

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Laboratory for Alternative Energy Conversion

Objectives

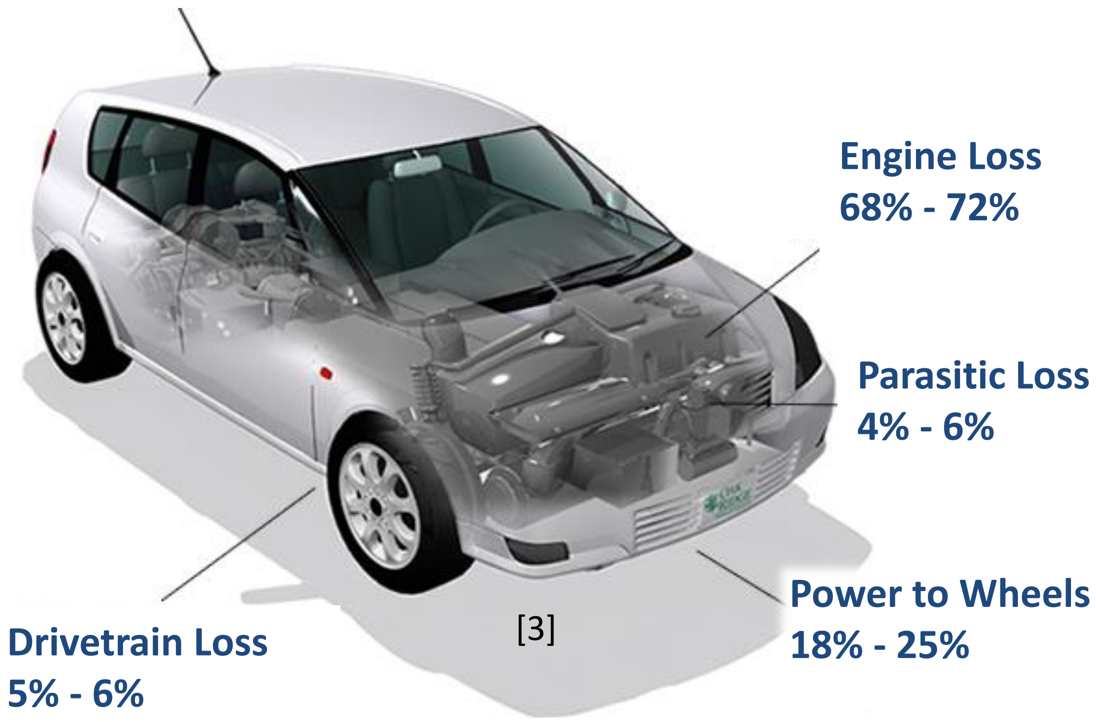
- Developing a CFD model to predict system performance under different operational conditions
- Understanding heat and mass transfer inside the adsorber bed
- Performing a comprehensive parametric study to see the effects of different parameters on the performance of the adsorption cooling system
- Studying the effects of graphite flakes additive to the adsorbent on the ACS performance
- Investigating the impact of using graphite-based heat exchangers as the adsorber bed

Motivations and Opportunities

The U.S. consumed about 140.43 billion liters of fuel a year for AC systems of light duty vehicles in 2015[1].

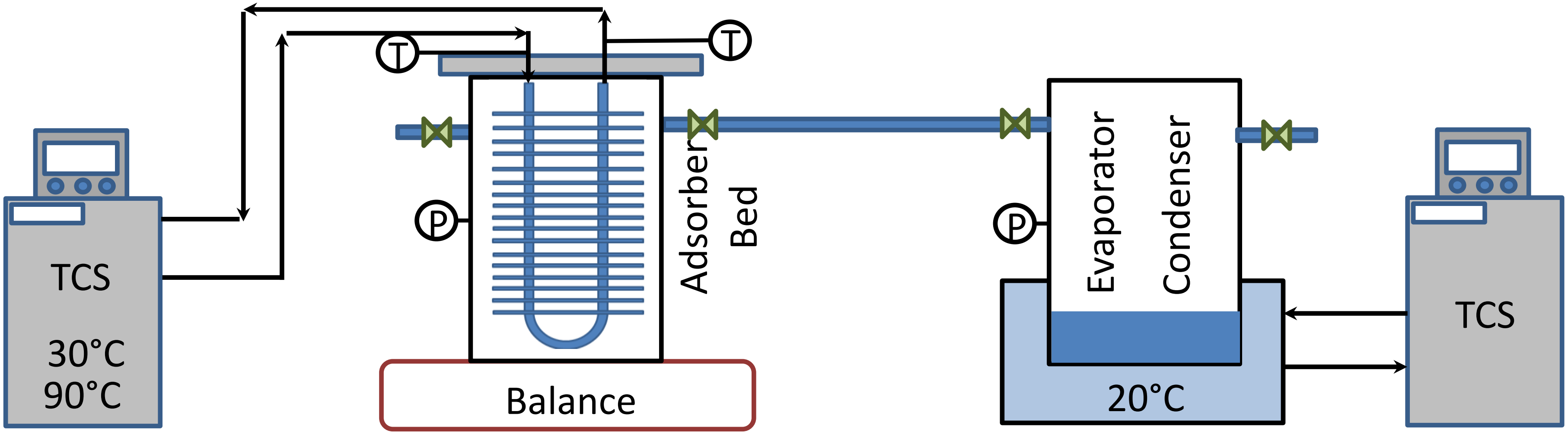
During the SFTP-SC03 driving cycle, a vapor compression refrigeration cycle of light-duty vehicle results in increasing[2]:

- CO emissions by 71%
- NOx emissions by 81%
- Non-methane hydrocarbons by 30%



[1] Independent Statistics and and Analysis, How much gasoline does the United States consume?, US Energy Information Administration (EIA), March 2016
[2] R. Farrington, J. Rugh. Impact of vehicle air-conditioning on fuel economy, tailpipe emissions, and electric vehicle range. Proceeding of the Earth Technologies Forum, Washington, D.C., October 31, 2000.
[3] US Department of Energy, Energy Efficiency and Renewable Energy, www.fueleconmy.gov

Schematic of Experimental Test Setup



TCS: Temperature control system

Parameter	Value
Working pairs	FAM Z02 – water
Heating fluid inlet temperature	90°C
Cooling fluid inlet temperature	30°C
Coolant fluid inlet temperature	20°C
Chilled water inlet temperature	20°C
Heat transfer fluid mass flow rate to adsorber bed	Not measured
Heat transfer fluid	Silicone oil

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Literature Review

Working pairs	Reference
Zeolite - Water	[1][2][3][4][5][6][7][8][9]
Silica gel – Water	[9][10][11][12][13]
Ammonia - Activated Carbon	[2]
Ethanol – Activated Carbon	[13]

Geometry	Reference
1D	[1][2][3][4][5][11]
2D	[6][7][8][9][10][12]
3D	[13][14]

Gaps in literature:

- FAM-Z02 as working pair
- Few 3D models
- No models with effects of thermal contact resistance (TCR)

[1] L.M. Sun, et al., Heat Recover. Syst. CHP. 15 (1995) 19–29.
[2] N.B. Amar, et al., Appl. Therm. Eng. 16 (1996) 405–418.
[3] L.Z. Zhang, Sol. Energy. 69 (2000) 27–35.
[4] L. Marletta, et al., Int. J. Heat Mass Transf. 45 (2002) 3321–3330.
[5] G. Restuccia, et al., Appl. Therm. Eng. 22 (2002) 619–630.
[6] K.C. Leong, Y. Liu, Int. J. Heat Mass Transf. 47 (2004) 4761–4770.
[7] K.C. Leong, Y. Liu, Appl. Therm. Eng. 24 (2004) 2359–2374.
[8] Y. Liu, K.C. Leong, Int. Commun. Heat Mass Transf. 35 (2008) 618–622.
[9] D.B. Riffel, et al., Int. J. Heat Mass Transf. 53 (2010) 1473–1482.
[10] G.G. Ilis, et al., Int. Commun. Heat Mass Transf. 38 (2011) 790–797.
[11] İ. Solmuş, et al., Int. J. Refrig. 35 (2012) 652–662.
[12] A.O. Yurtsever, et. al., Appl. Therm. Eng. 50 (2013) 401–407.
[13] H. Niazmand, I. Dabzadeh, Int. J. Refrig. 35 (2012) 581–593.
[14] H. Talebian, et al., Int. Conf. Mech. Eng. Adv. Technol., 2012: pp. 1–7

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Assumptions

Assumptions:

- Ideal gas behavior for adsorbate gas [1-14]
- Uniformly sized spherical particles [1-14]
- Constant thermo-physical properties for materials (except density of adsorbate) [1-14]
- Thermal equilibrium between particles and adsorbate [1-14]
- Thermal contact resistance

Numerical Tool:

- ANSYS Fluent was used to solve the Navier-Stokes, energy, and uptake equations
- User defined scalar (UDS) module was used in order to simulate uptake rate (ω)
- Mass generation, heat generation, and scalar generation were simulated using user defined functions (UDF)

Governing Equations

- Continuity

$$\frac{\partial\left(\varepsilon\rho_{refrigerant}\right)}{\partial t}+\nabla.\left(\rho_{refrigerant}\vec{v}\right)+\left(1-\varepsilon\right)\rho_{adsorbent}\frac{d\omega}{dt}=0$$

- Momentum

$$\frac{\partial}{\partial t}\left(\rho\vec{v}\right)+\nabla.\left(\frac{\rho\vec{v}\vec{v}}{\varepsilon}\right)=-\varepsilon\nabla p+\nabla.\left(\vec{\tau}\right)-\left(\frac{\varepsilon\mu}{K}\vec{v}+\frac{\varepsilon C_2}{2}\rho\left|\vec{v}\right|\vec{v}\right)$$

$$\bar{\bar{\tau}}=\mu\left[\left(\nabla\vec{v}+\nabla\vec{v}^T\right)-\frac{2}{3}\nabla.\vec{v}I\right]$$

- Energy

$$\left[\rho_{adsorbent}\left(\left(1-\varepsilon\right)C_{p,adsorbent}+\omega\varepsilon C_{p,refrigerant}\right)\right]\frac{\partial T}{\partial t}+\vec{\nabla}\left(\rho_{refrigerant}\vec{v}C_{p,refrigerant}T\right)=\left(1-\varepsilon\right)\rho_{adsorbent}\Delta h_{adsorption}\frac{d\omega}{dt}+\vec{\nabla}\left(k\vec{\nabla}T\right)$$

Governing Equations

- Uptake

$$\omega = \frac{mass\ of\ adsorbed\ material}{mass\ of\ adsorbent} \quad \left(\frac{kg\ of\ adsorbate}{kg\ of\ adsorbent}\right)$$

$$\frac{d\omega}{dt} = \frac{15D_{s0}}{R_p^2}\exp\left(-\frac{E_a}{R_u T_{adsorbent}}\right)\left(\omega_{eq} - \omega\right)$$ [1]

$$\omega_{eq} = f\left(T, p\right)$$

$$\omega_{eq} = \frac{1}{n_s}\frac{\sum_{j=1}^{n_s}\left(K^0\, {p}/{p^0}\right)^j \exp\left(-\frac{\Delta h_j}{RT}\right)/\left(j-1\right)!}{1+\sum_{j=1}^{n_s}\left(K^0\, {p}/{p^0}\right)^j \exp\left(-\frac{\Delta h_j}{RT}\right)/\left(j\right)!}, \quad n_s = 11$$

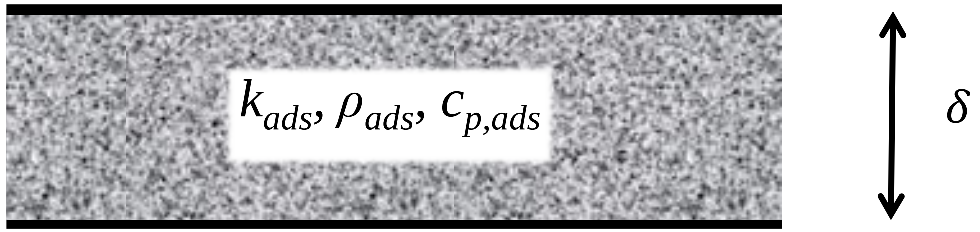
water-FAMZ02 [2]

$$\omega_{eq} = \frac{k_0 p_v \exp\left(\frac{\Delta h}{RT}\right)}{\left[1+\left(\frac{k_0 p_v \exp\left(\frac{\Delta h}{RT}\right)}{\omega_{\max}}\right)^n\right]^{1/n}}$$

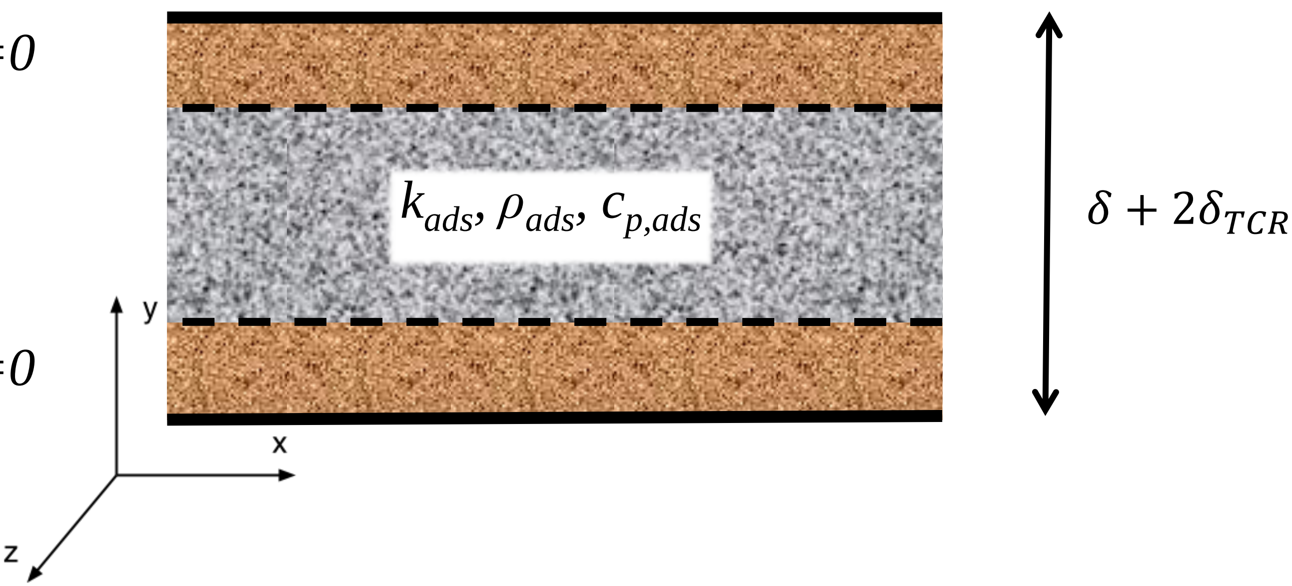
water-FAMZ02 [3]
water-silica gel [1]

[1] A. Sharafian, M. Bahrami, Renewable and Sustainable Energy Reviews, 48 (2015) 857-869.
[2] M.J. Goldsworthy, Microporous Mesoporous Material, 196 (2014) 59–67.
[3] M. Intini, M. Goldsworthy, S. White, C.M. Joppolo, Applied Thermal Engineering, 80 (2015) 20–30.

Thermal Contact Resistance (TCR)

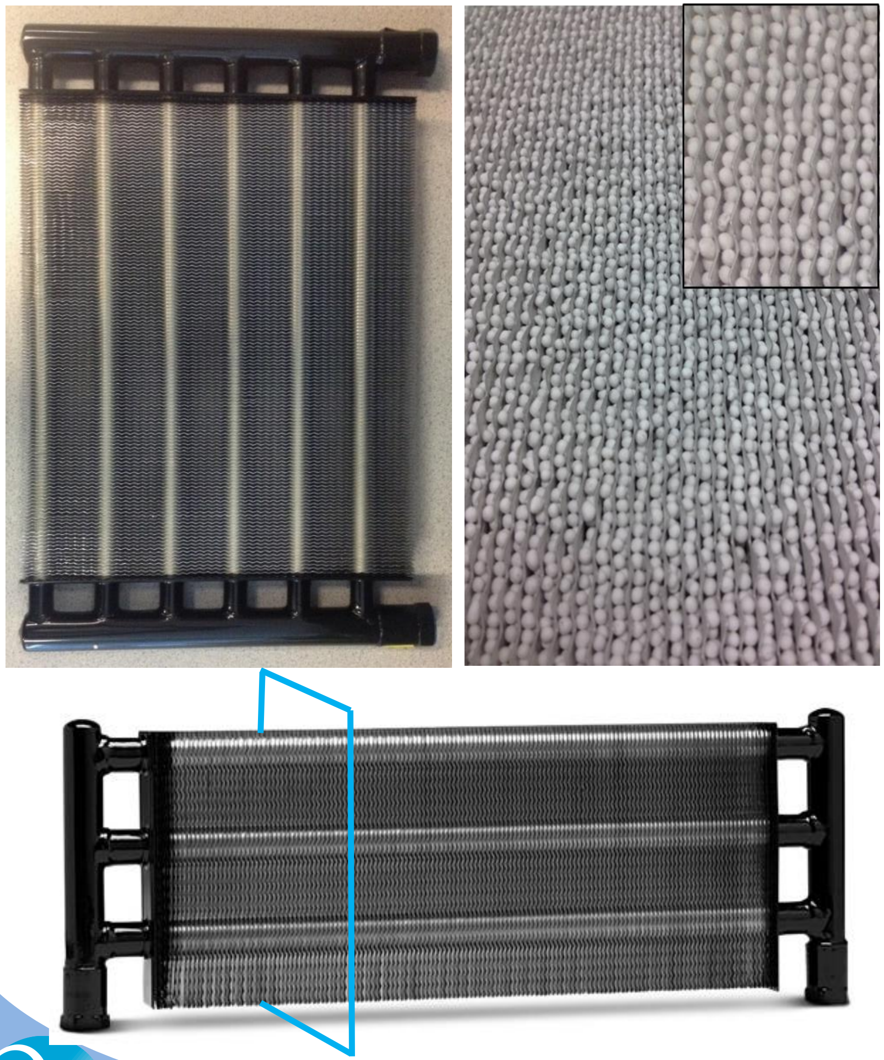


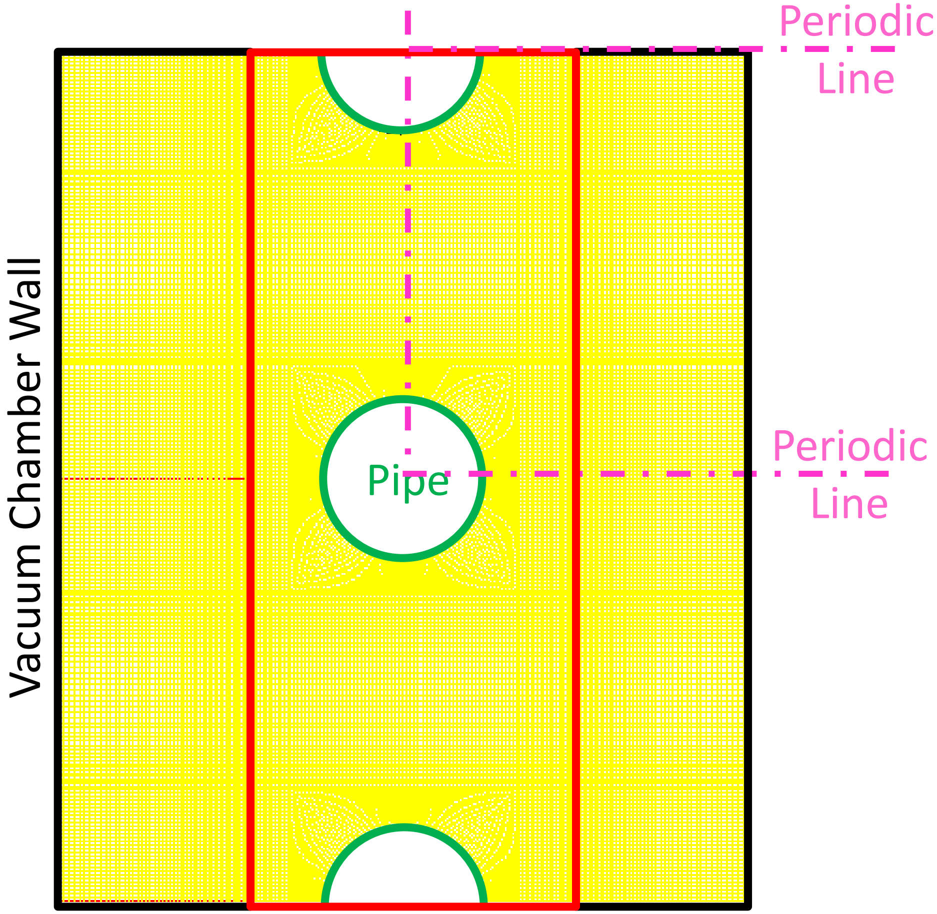
$k_{yy}=k_{ads}$
$k_{xx}= k_{zz}=0$
$\rho=c_p=0$



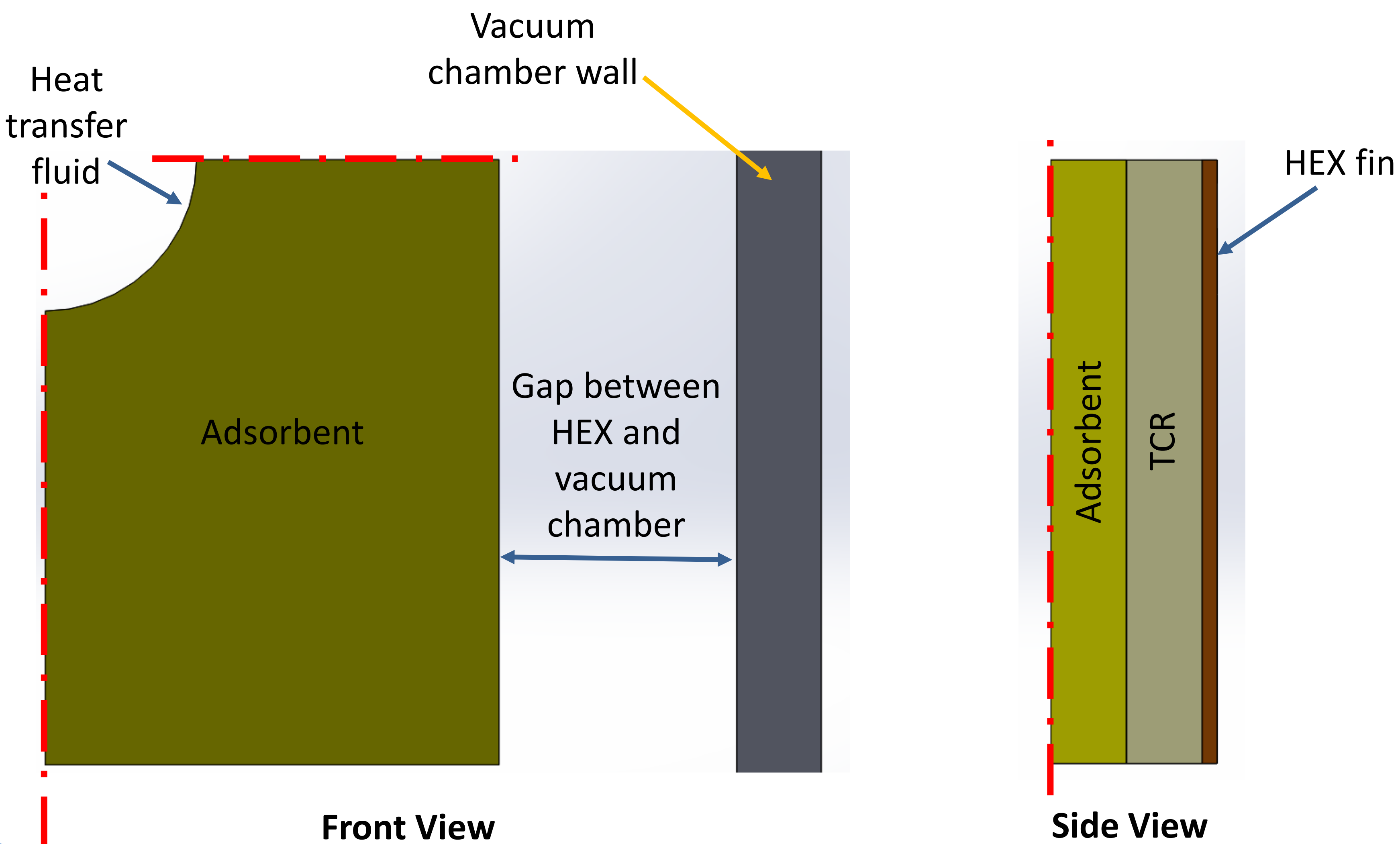
$k_{yy}=k_{ads}$
$k_{xx}= k_{zz}=0$
$\rho=c_p=0$

Geometry




Symmetry Line
Periodic Line
Vacuum Chamber Wall
Pipe
Periodic Line

HEX and Vacuum Chamber Arrangement

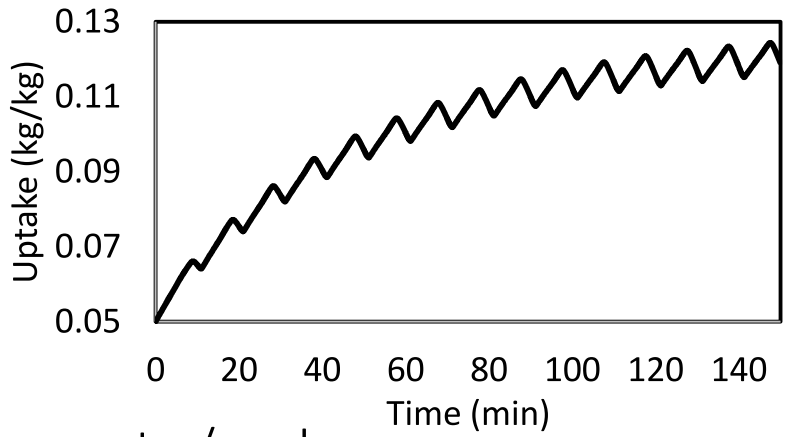


Initial and Boundary Conditions

Initial Conditions:

- The final solution does not depend on initial conditions due to cyclic operation of ACSs.

- Incorrect initial conditions can result in divergence (esp. for pressure)



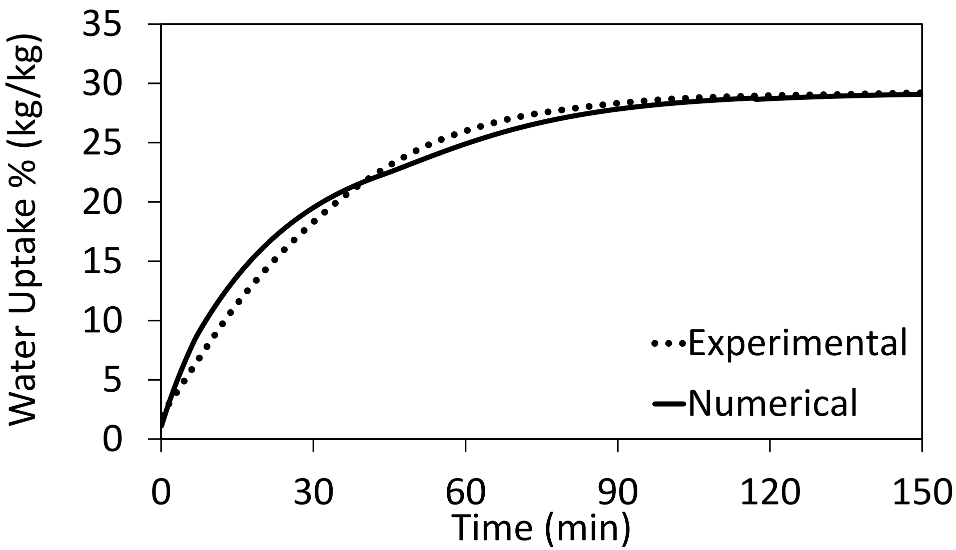
Boundary Conditions:

- Pressure at outlet / inlet → Represents pressure at evaporator / condenser

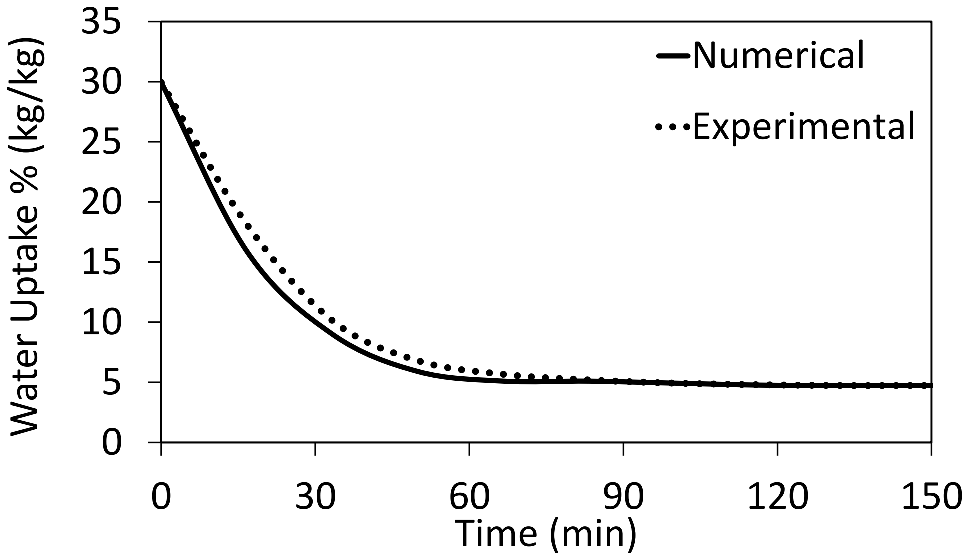
- Temperature at outlet / inlet → Representative for temperature of vapor coming from (or going to) at evaporator (condenser)

- Temperature at heat exchanger walls → Represents temperature of heating/cooling fluid

Results – Equilibrium Uptake



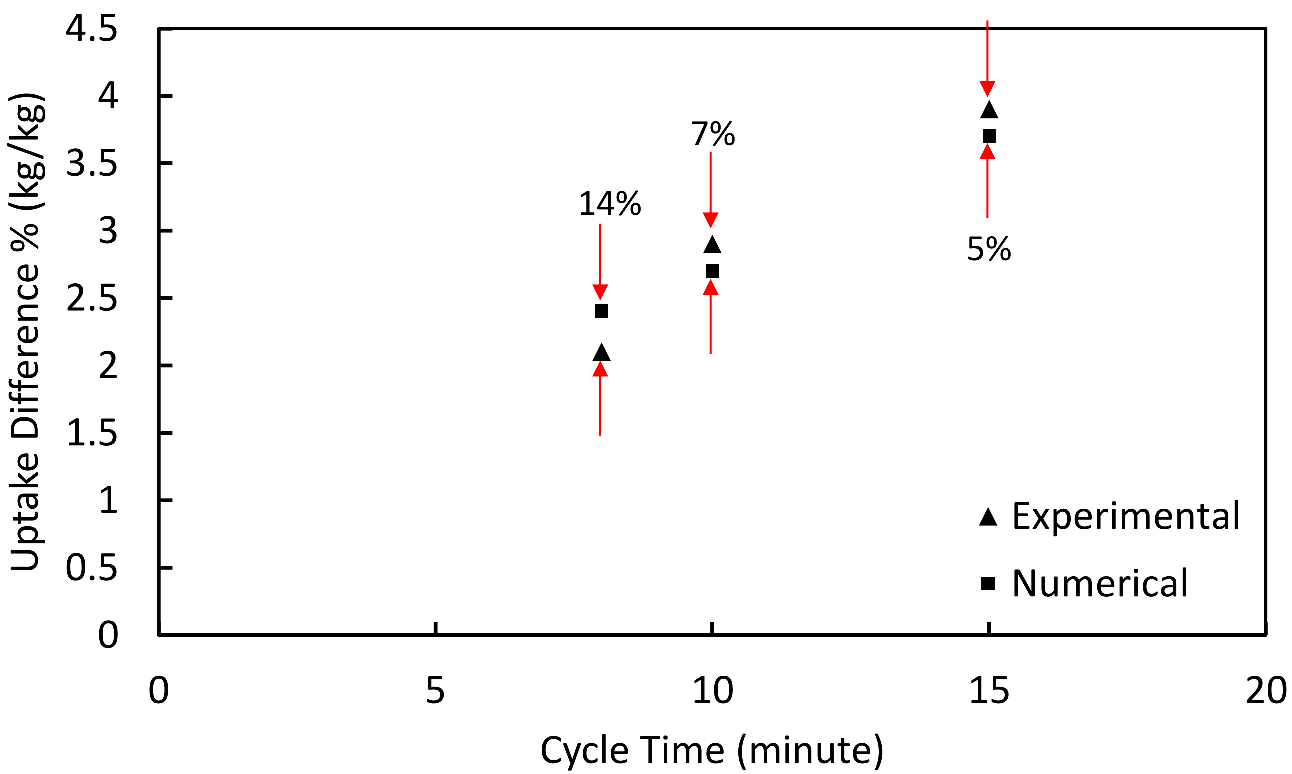
Adsorption



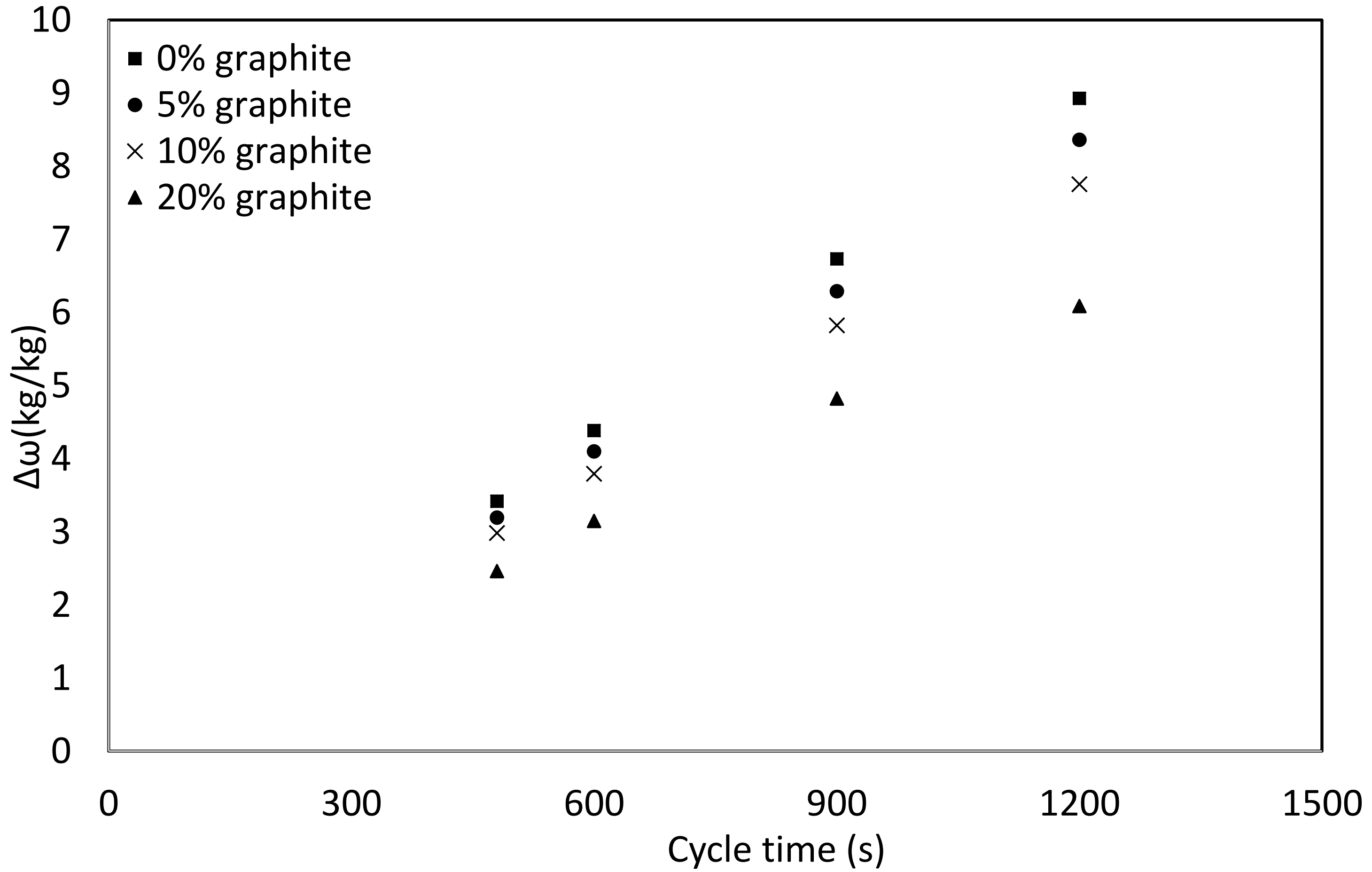
Desorption

Results – Cyclic Operation

Δω: the difference between the maximum and the minimum values of the uptake



Graphite Doped Adsorbent



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Conclusions and Future Works

Conclusions

- A full three-dimensional finite volume based computational fluid dynamic model was developed.
- It was shown that if thermal conductivity improvement is performed by adding some non-adsorptive material like graphite, it could decrease the adsorption performance of the adsorber bed

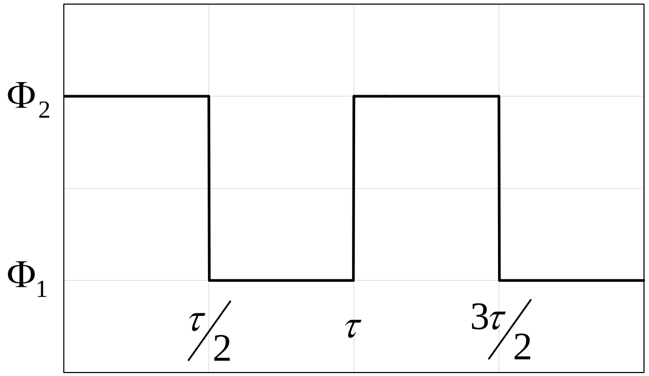
Future Works

- Adding the effects of uptake value on thermo-physical properties of an adsorbent.
- Studying the effects of the ideal evaporator and condenser.

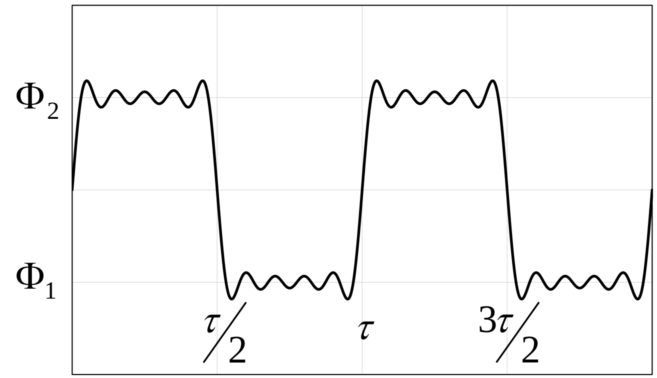
THANK YOU!

Q&A

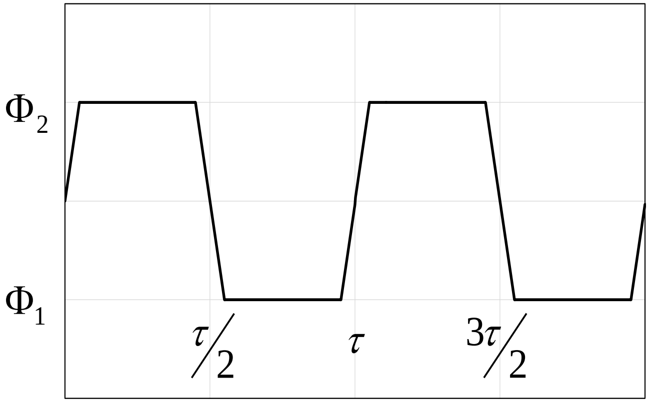
Boundary Conditions



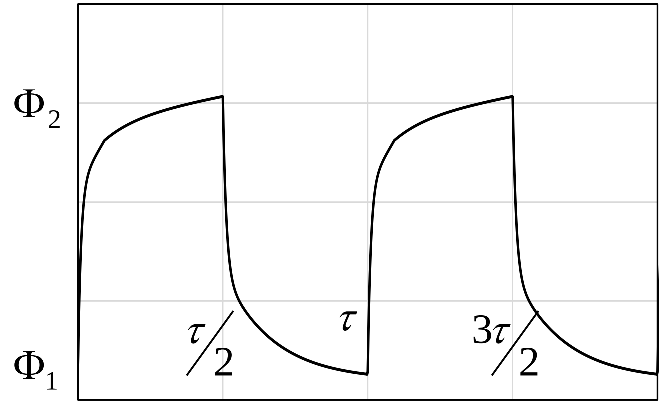
Rectangular Wave
(Ideal Case)



Fourier Series of
Rectangular Wave

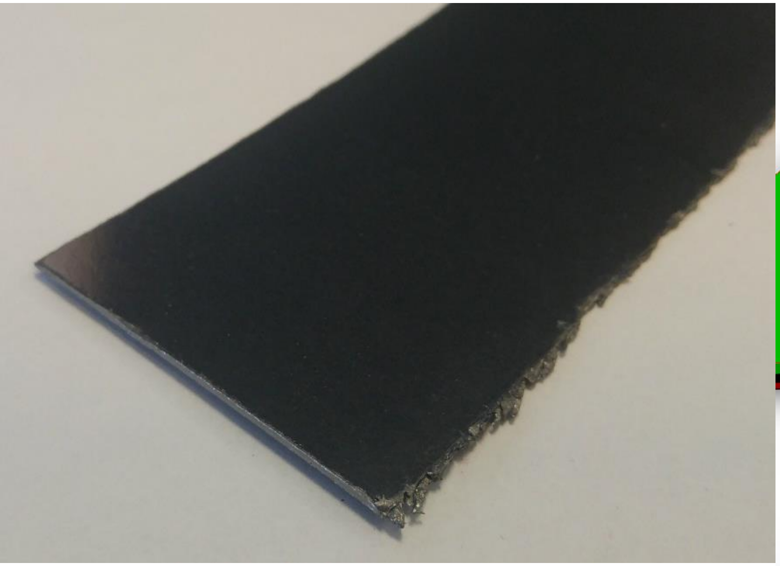


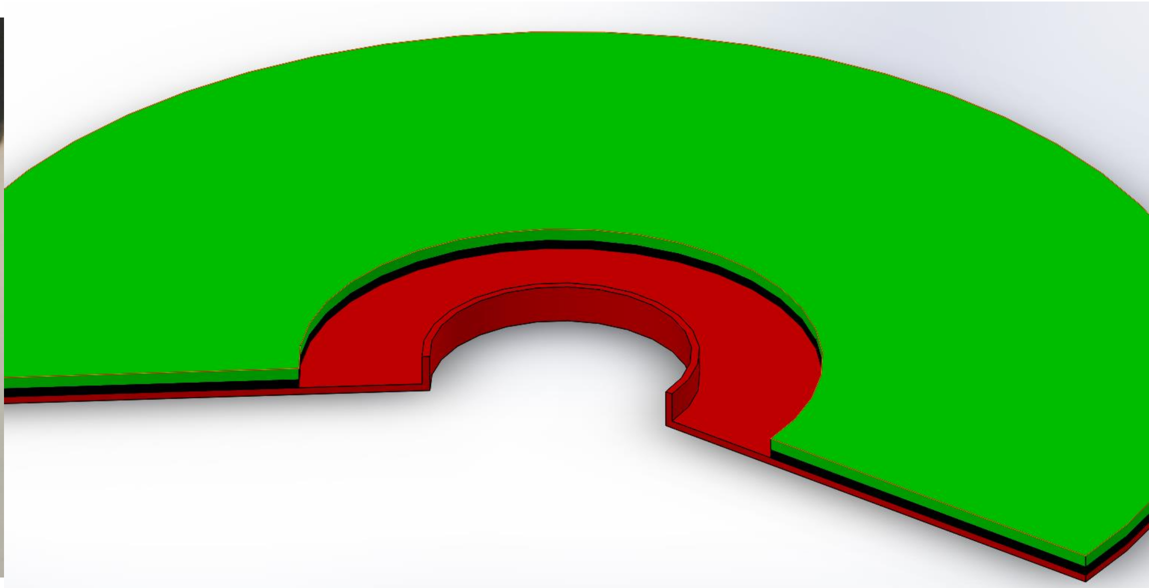
Trapezoidal Wave

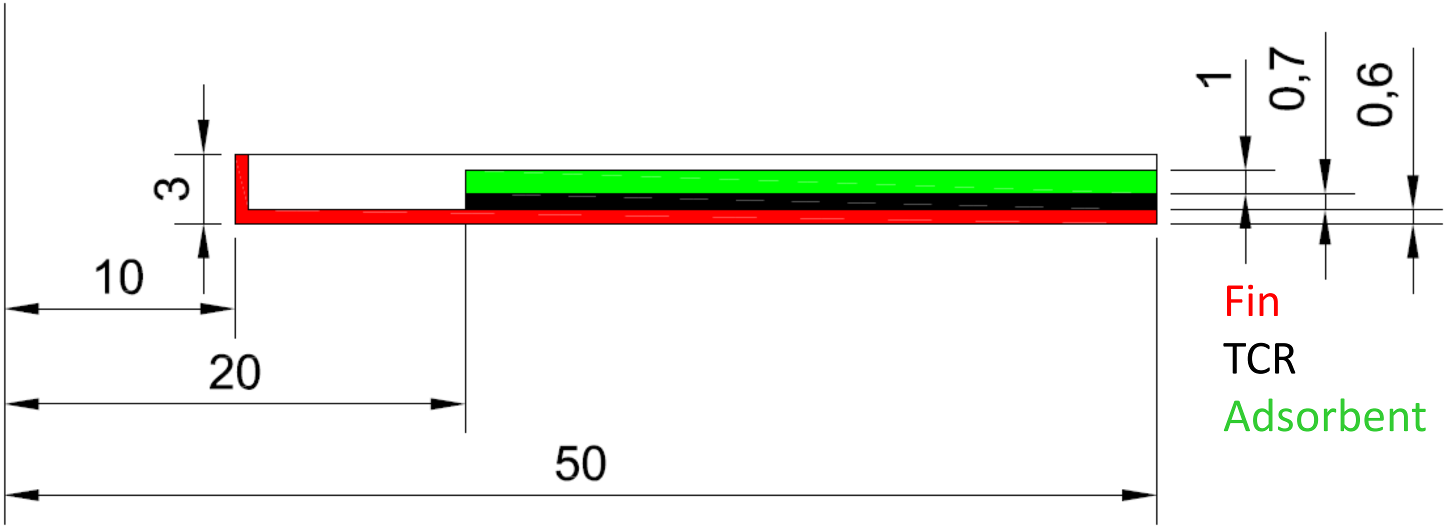


Actual Case

Graphite HEX vs. Aluminum HEX







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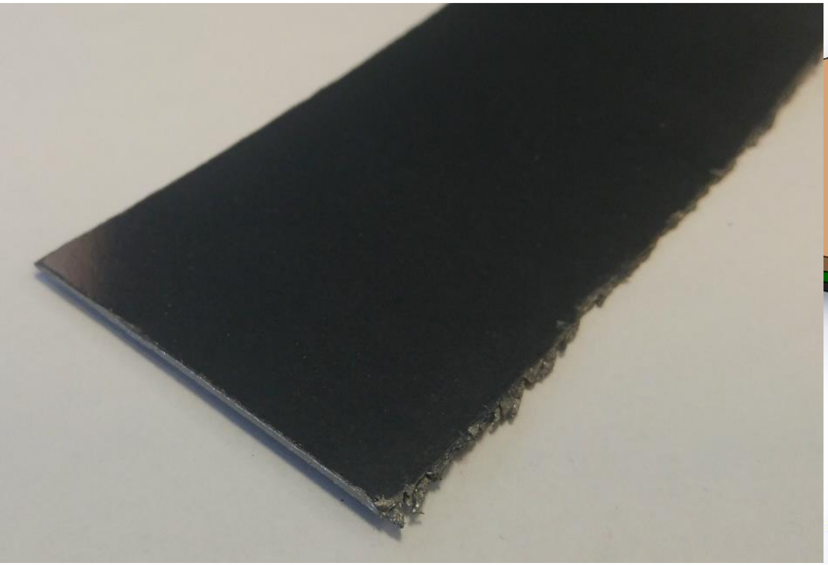
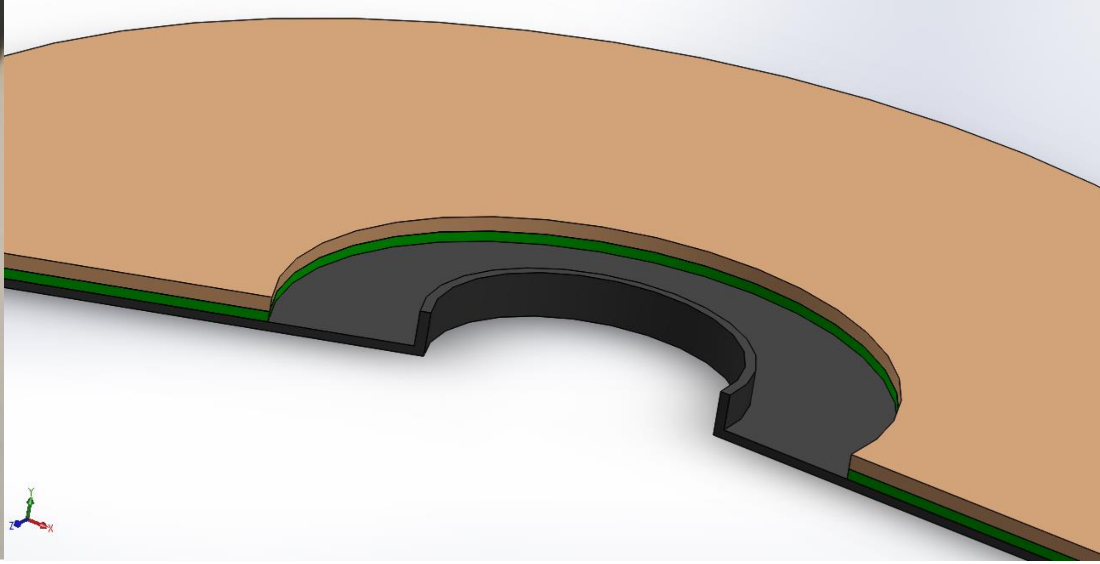
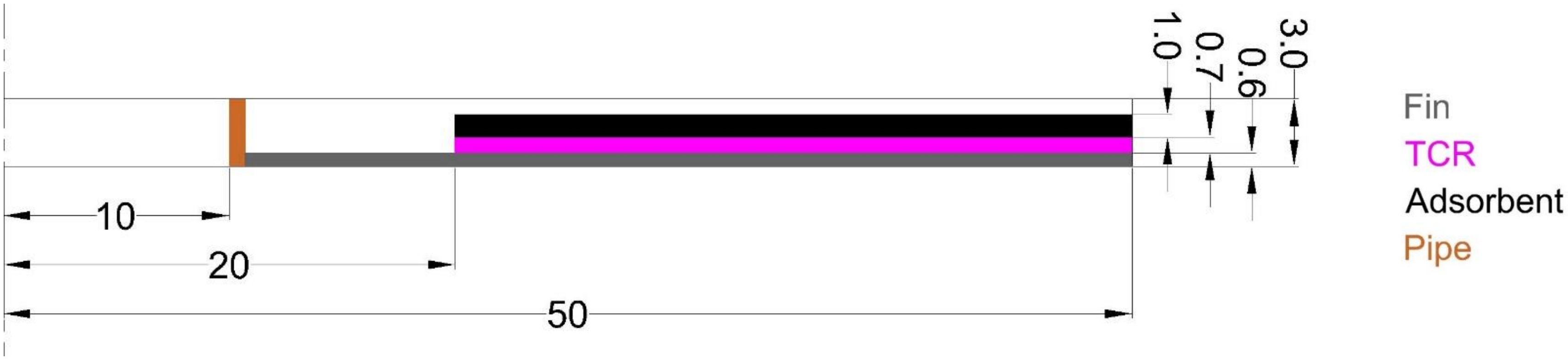
Graphite HEX vs. Aluminum HEX







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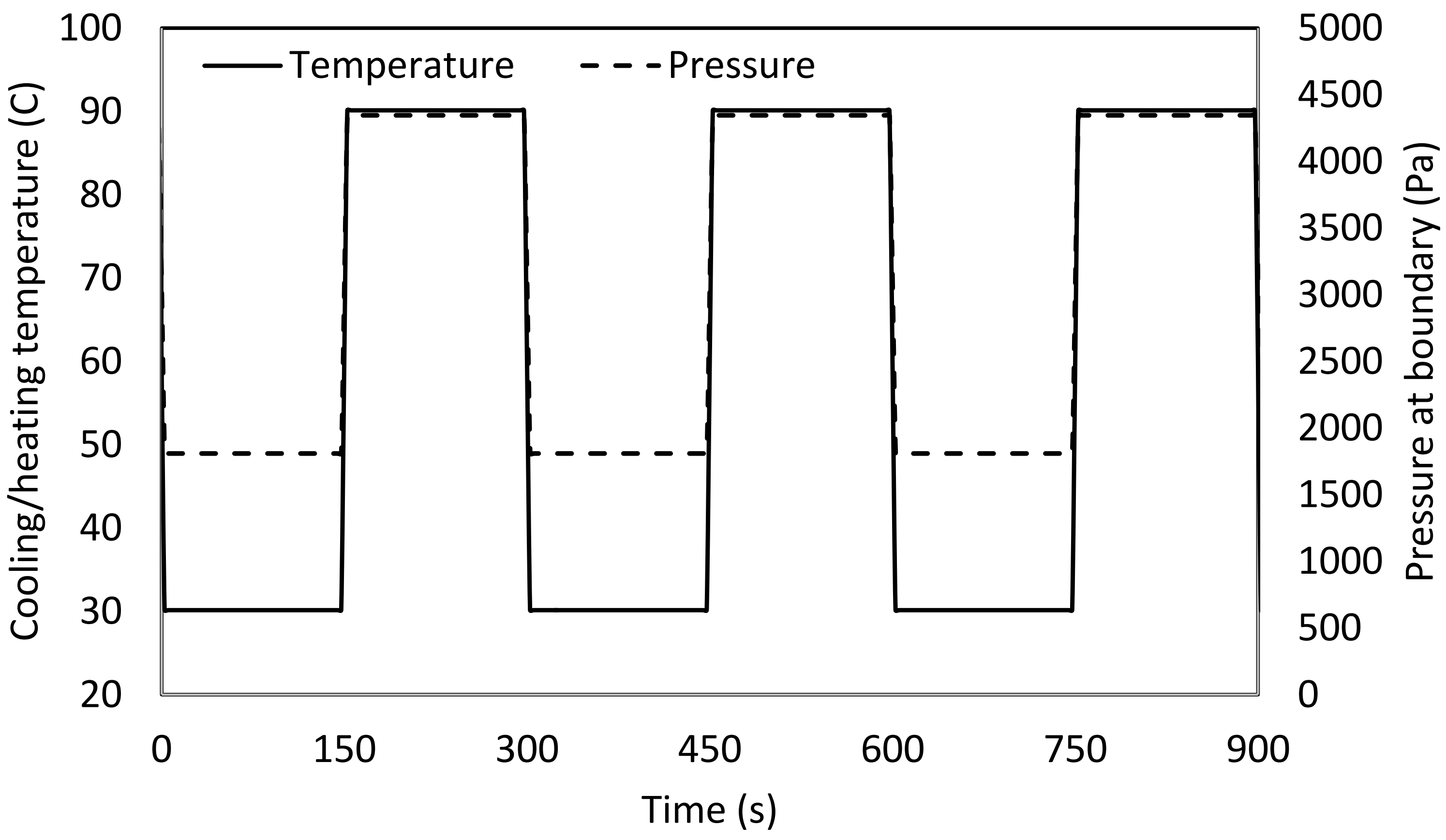
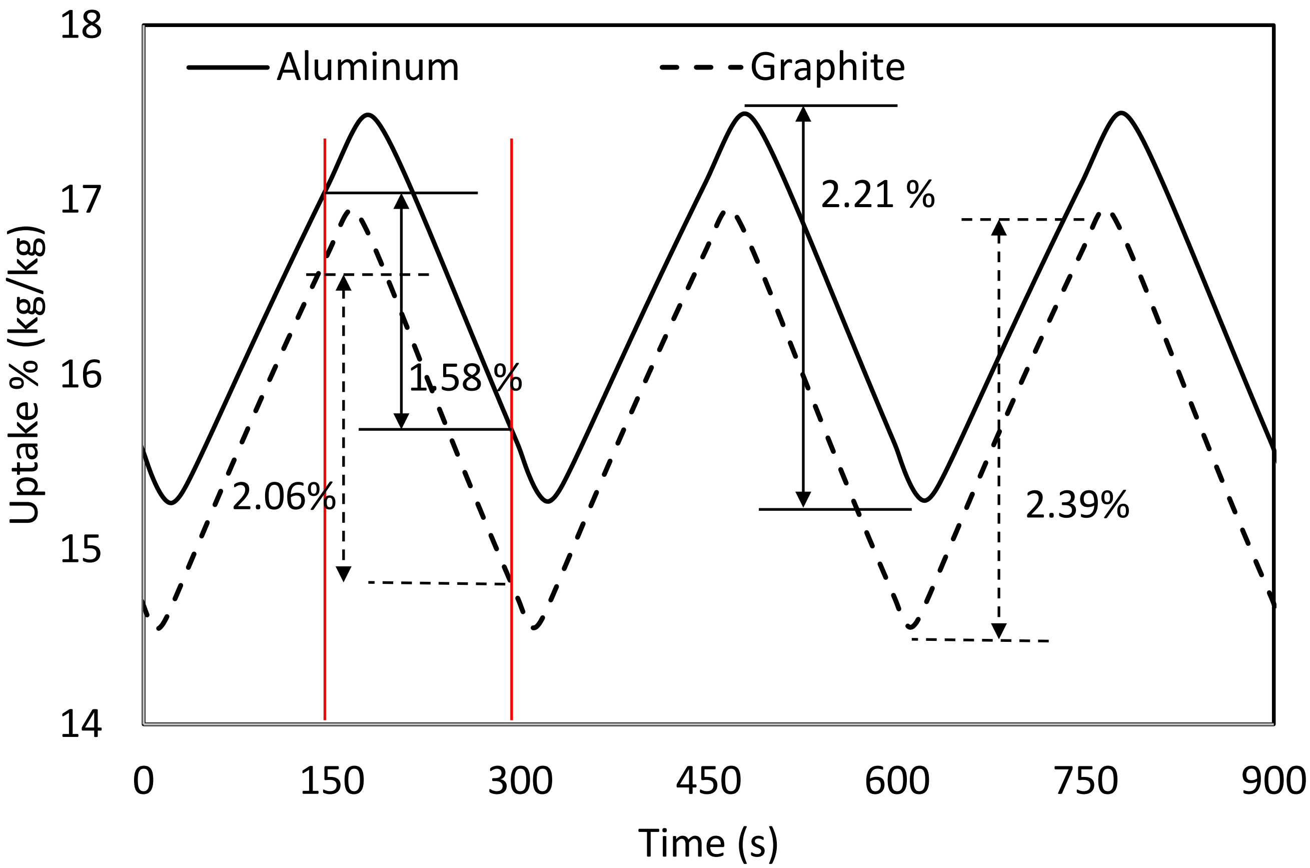
Boundary Conditions



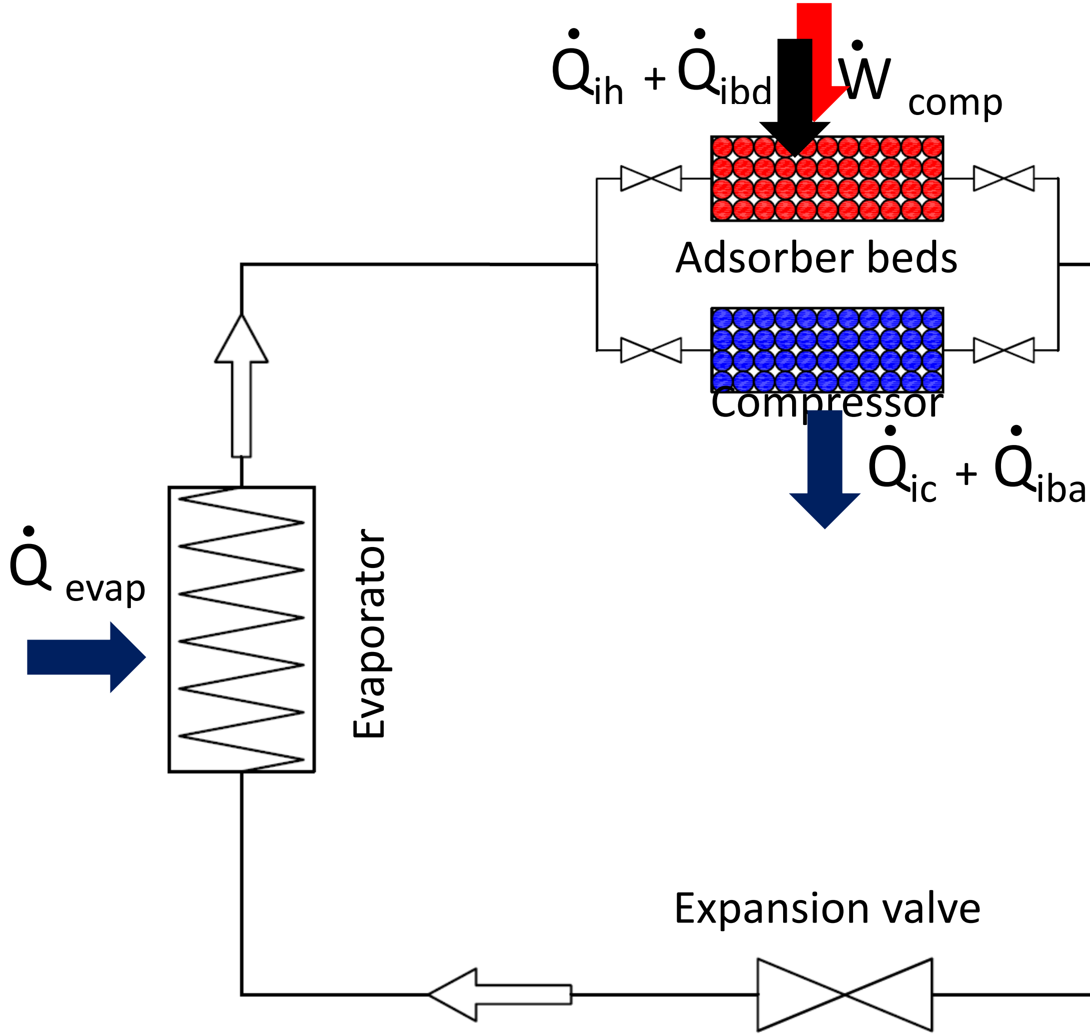
Results - Graphite HEX vs. Aluminum HEX



Results - Graphite HEX vs. Aluminum HEX

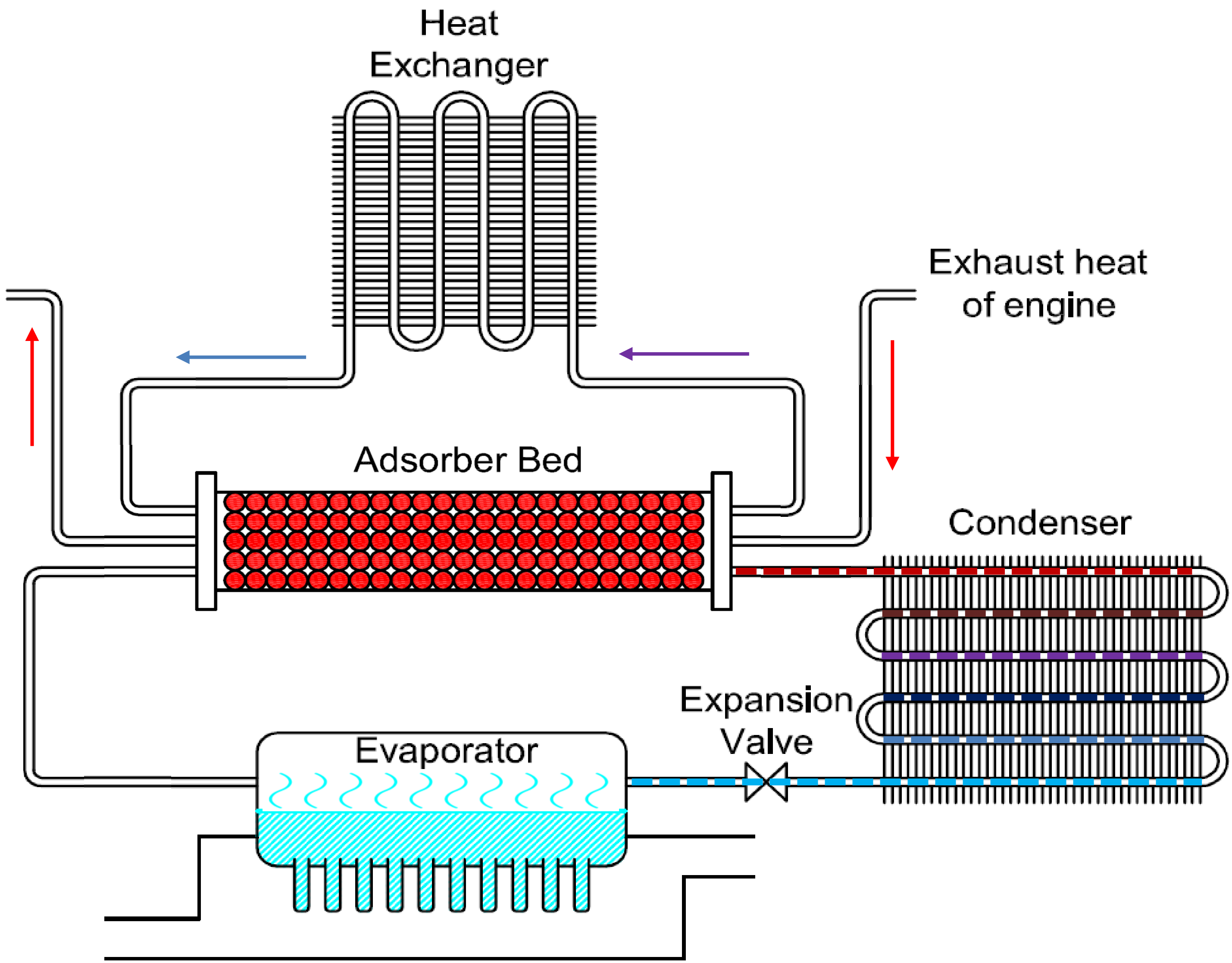
Cycle Time (s)	Δω with Aluminum HEX (SCP)	Δω with Graphite HEX (SCP)	Enhancement of Δω
300	1.58 % (132)	2.02 % (168)	31 %
480	3.11 % (161)	3.56 % (185)	15.7 %
600	4.12 % (171)	4.62 % (192)	12.1 %
900	6.57 % (154)	7.05 % (175)	7.3 %

Vapor Compression Refrigeration (VCR) vs. Adsorption Cooling System (ACS)



ih: isosteric heating
ibd: isobaric desorption
ic: isosteric cooling
iba: isobaric adsorption

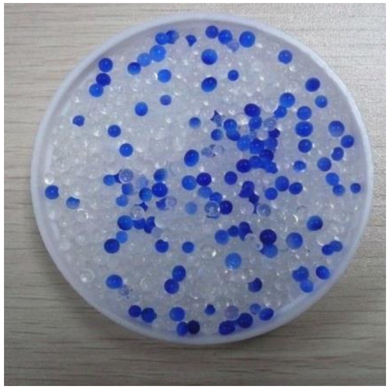
Adsorption Refrigeration Cycle



ACS Working Pairs

ACS sorbent material (adsorbent):

Activated carbon [6]



Silica gel [7]

Zeolite [8]

ACS refrigerant (adsorbate):

- Water
- Methanol
- Ethanol
- Ammonia

LDF model: $$\frac{\partial \omega}{\partial t} = K(\omega_{eq} - \omega)$$

$$\omega_{eq} = F(T, P)$$

[6] http://www.ucicarbons.com/medical-benefits-activated-carbon/
[7] http://www.weiku.com/products/15374902/_gt_All_kinds_of_desiccant_Desiccant_pack_moisture_absorber_.html
[8] http://www.rwlwater.com/zeolite-holds-key-to-waste-heat-use/

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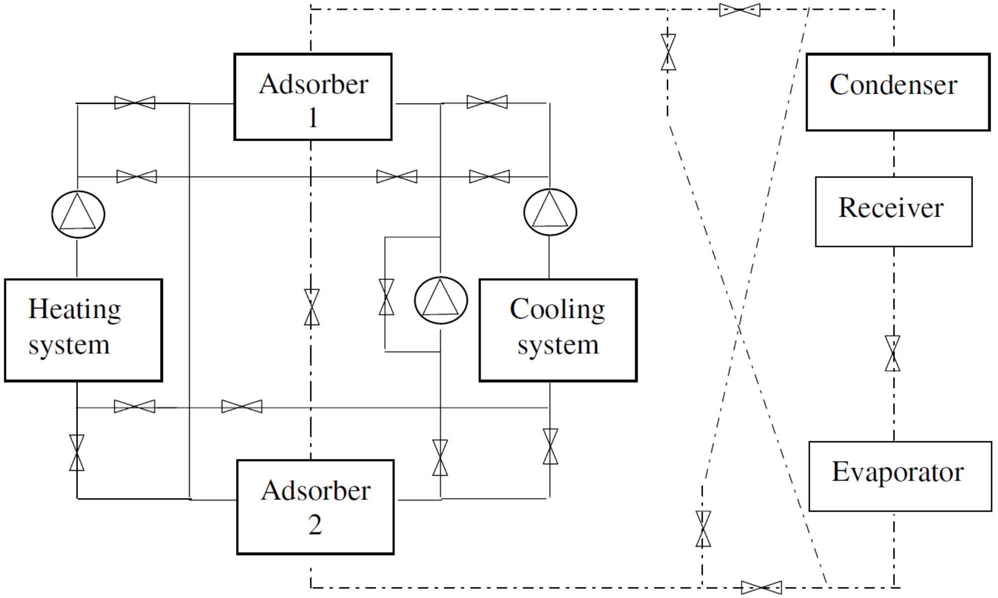
How to improve adsorption cycle

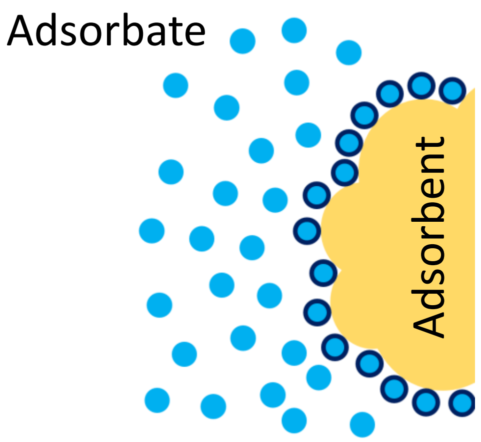
- Adsorbate/Adsorbent Pair
  - Material
  - Physical shape (consolidated, powder, pelletized particles)
- Heat Exchanger Design
  - Dimensions
  - Weight
  - Mass transfer resistance
- Thermodynamic cycle
  - Heat Recovery
  - Mass Recovery
  - Heat and Mass Recovery
  - Temperature range
    - Heat source (Exhaust gas, Coolant)
    - Refrigerant



Adsorption Concepts

Adsorption is the adhesion of atoms, ions, or molecules of gas, liquid, or dissolved solids to a solid surface

Adsorbents	Adsorbates
silica gel zeolite activated carbon FAM-Z02	water methanol/ethanol ammonia



Two main processes:

- Cooling → Adsorption → Evaporation at evaporator (Adsorption: Exothermic Process)
- Heating → Desorption → Condensation at condenser (Desorption: Endothermic Process)

Uptake: $\omega = \dfrac{mass\,of\ adsorbed\ material}{mass\,of\ adsorbent} \left(\dfrac{kg\,of\ adsorbate}{kg\,of\ adsorbent}\right)$

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Advantages and Disadvantages

Advantages of ACS [1,2]:

- Utilization of waste heat
- Few moving parts (valves) ⇨ less maintenance is required
- Non toxic materials
- Environmental friendly refrigerants

Major challenges facing commercialization of ACS [2,3]:

- Low working pressure in many cases (1 kPa – 7kPa for the case of water)
- Small specific cooling power values

$$SCP = \frac{Q_{evap}}{m_{ads}\tau_{cyc}}$$ 10<typ.<270

- Small COP values

$$COP = \frac{Q_{evap}}{Q_{ih} + Q_{ibd}}$$ 0.02<typ.<0.6

- Bulky and heavy systems

[1] M. O. Abdullaha, I. A. W. Tana, L. S. Limb., Renewable and Sustainable Energy Reviews (2011); 15: 2061–2072.
[2] H. Demir, M. Mobedi, S. Ulku., Renewable and Sustainable Energy Reviews (2008); 12: 2381–2403.
[3] R.Z. Wang, J.Y. Wu, Y.X. Xu, W. Wang., Energy Conversion and Management (2001); 42: 233–249.

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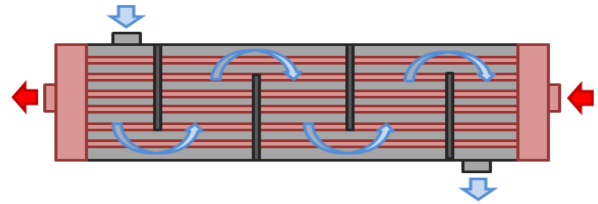
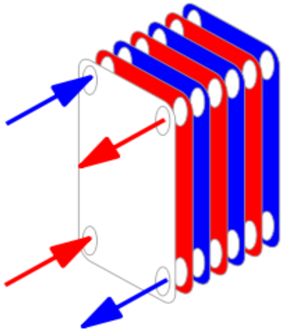
Adsorber Bed Designs

Spiral plate

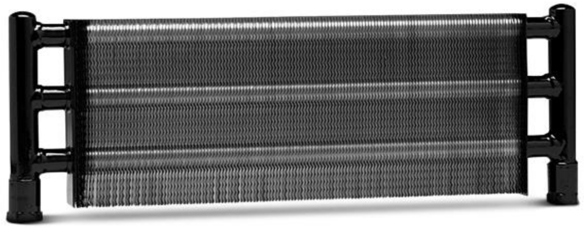


Shell and tube

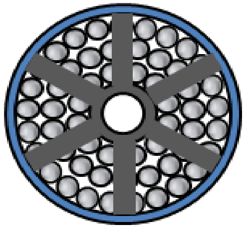
Hairpin



Plate



Finned tube



Annulus tube

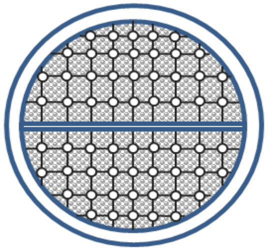
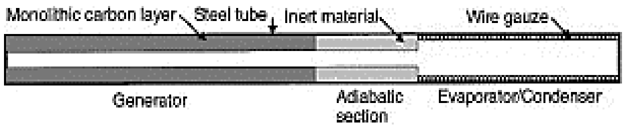


Plate-tube



Tube

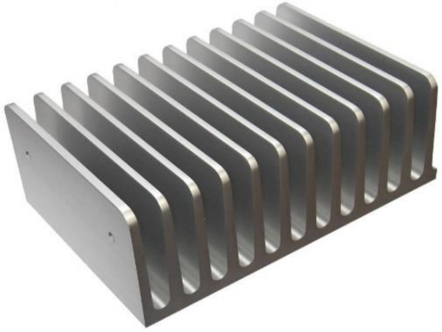


Plate fin

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Literature Review on Mass Measurement

Mass of adsorbent	Reference	Working pair
Less than 1 g	[1] [2][3][4][5][6] [7][1] [8] [9]	silica gel - water silica gel + $CaCl_2$ (SWS-1L)-water FAM-Z02-water zeolite-water activated carbon-methanol
1 g < mass of adsorbent < 100 g	[10] [10] [11][8][12][13] [9][14]	silica gel-water silica gel + $CaCl_2$ (SWS-1L)-water zeolite-water SAPO 34-water
100 g < mass of adsorbent < 1 kg	[15] [16]	zeolite 13X-water FAM-Z02-water
1 kg < mass of adsorbent	[17] [17] [16]	silica gel-water zeolite-water FAM-Z02-water

[1] Glaznev I, et al., Heat Transf Eng 2010;31:924–30.
[3] Aristov YI, et al, . Int J Heat Mass Transf 2008;51:4966–72.
[5] Okunev BN, et al. Int J Heat Mass Transf 2010;53:1283–9.
[7] Dawoud B. J Chem Eng Japan 2007;40:1298–306.
[9] Freni A, et al., Appl Therm Eng 2015;82:1–7.
[11] Dawoud B, et al., Int J Heat Mass Transf 2007;50:2190–9.
[13] Santamaria S, et al., Appl Energy 2014;134:11–9.
[15] Storch G, et al., Adsorption 2008;14:275–81.
[2] Aristov YI, et. al.,. Chem Eng Sci 2006;61:1453–8.
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[16] Dawoud B. Appl Therm Eng 2013;50:1645–51.
[17] Riffel DB, et al., Int J Heat Mass Transf 2010;53:1473–82.

Adsorber Bed Design – 3 fin per inch – Design I

Design Parameters

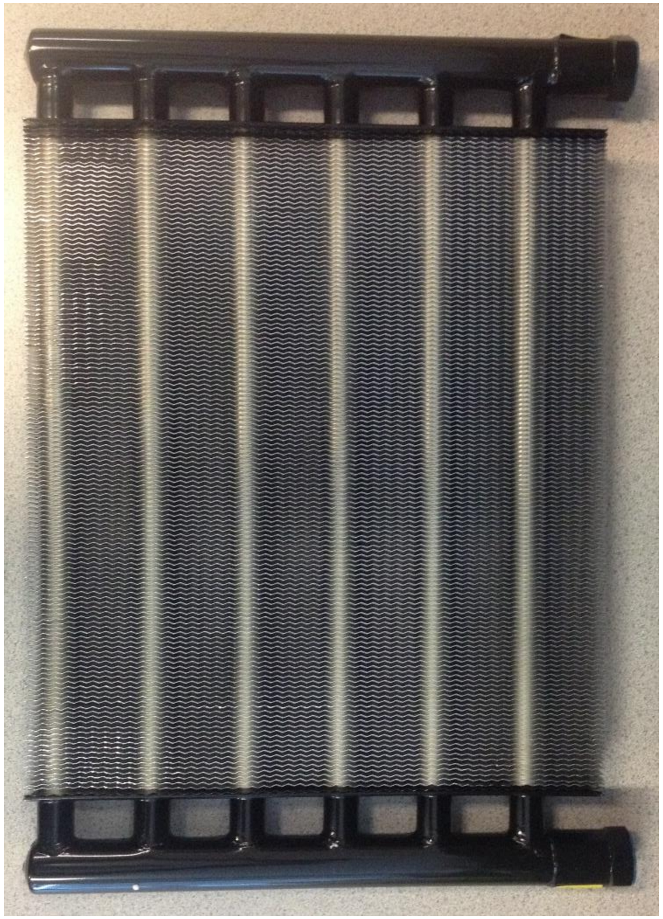
Parameter	Value
No. of supply pipes	1
Supply pipes size	1/2 in
No. of return pipes	6
Return pipes size	3/8 in
No. of fins	17
Fin spacing	9 mm
Fin diameter	6 in
Fin thickness	1/16 in
Fin material	Copper

Working Parameters

Parameter	Value
Cycle time	60 – 90 – 120 – 180 min
Mass of adsorbent	0.620 kg

SFU

Adsorber Bed Design – 10 fin per inch – Design II



Design Parameters

Parameter	Value
No. of passes	1
Branch pipes size	½ in
Fitting Size	¾ in
No. of return pipes	6
Fin spacing	10 fpi
Overall Size	12 ¾ x 18 x 1 ½ in
Fin width	1 ½ in
Fin thickness	0.2 mm
Fin material	Aluminum

Working Parameters

Parameter	Value
Cycle time	8 – 10 – 20 – 30 – 60 – 90 – 120 min
Mass of adsorbent	1.5 kg

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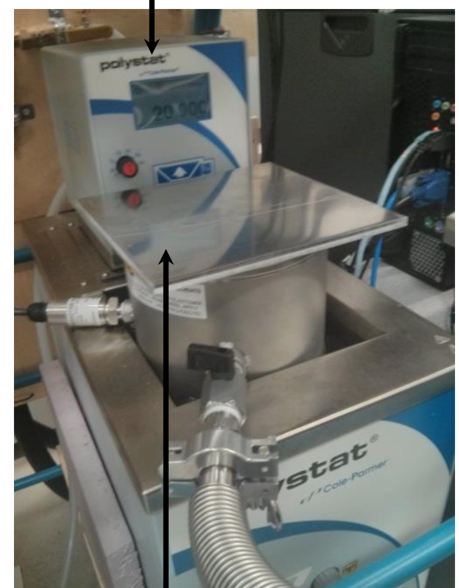
In-situ Uptake Measurement Setup – Design I

Pressure transducers

Heat transfer fluid (at 30 and 90°C)

Adsorber bed

Chiller



Evaporator/ Condenser (at 20°C)

Hosing

Scale

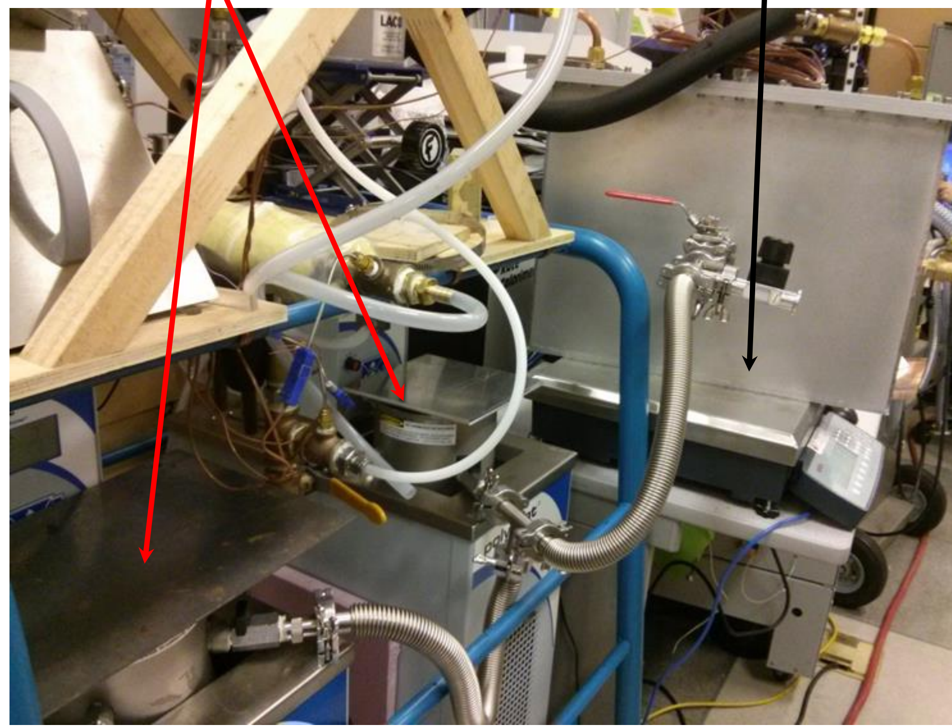
Aluminum lid

In-situ Uptake Measurement Setup – Design II

FAM Z02 in new adsorber bed

Evaporators 1 and 2

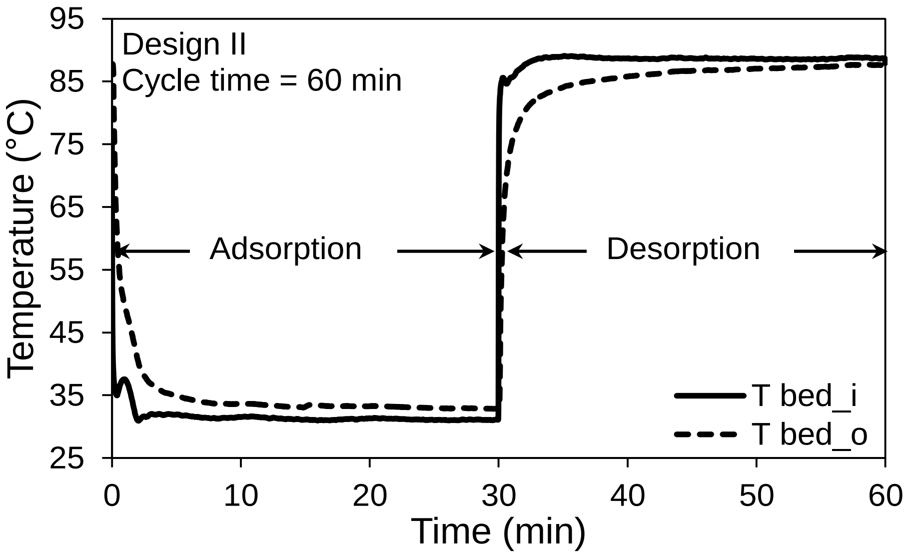
Adsorber bed

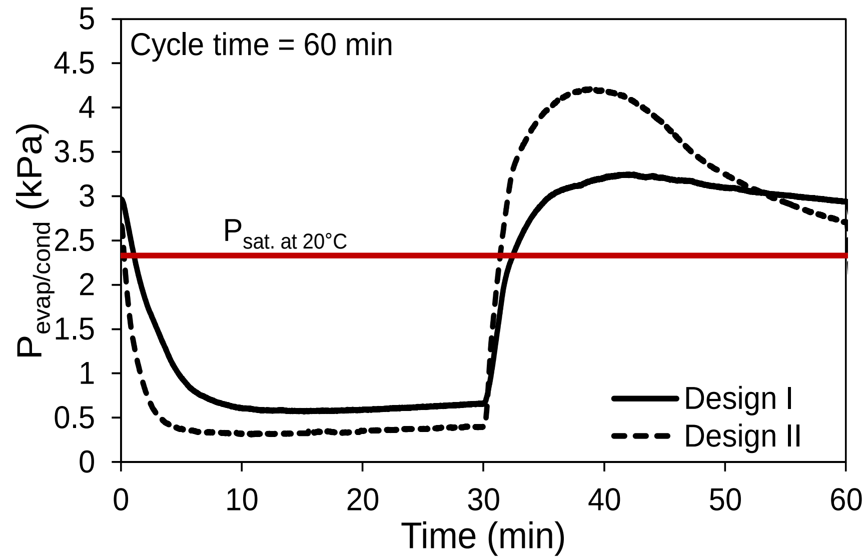


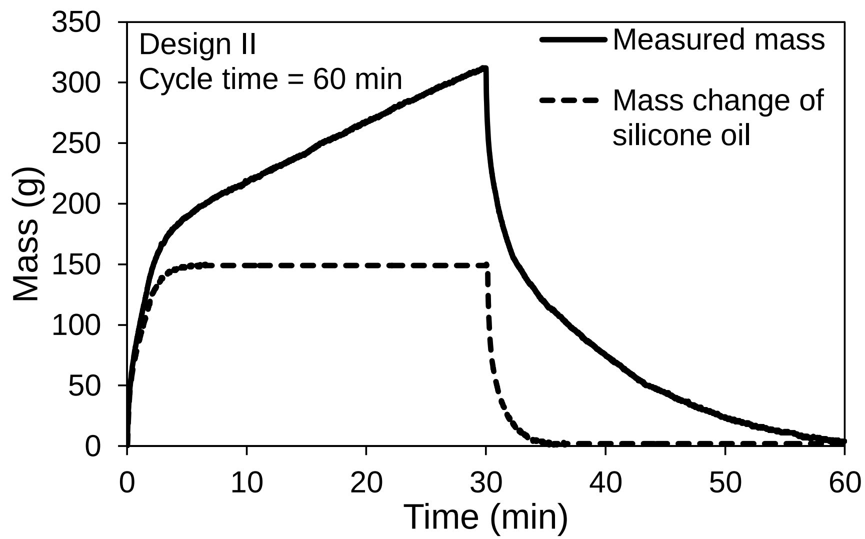
Challenges

- Low working pressure of adsorption system (1 kPa – 7 kPa)
  - Designing vacuum chamber
  - Leaking (Helium leak detector)
- Changes of the density of the heat transfer fluid (silicone oil) with temperature
- Changes of hosing stiffness with temperature

Measured Parameters







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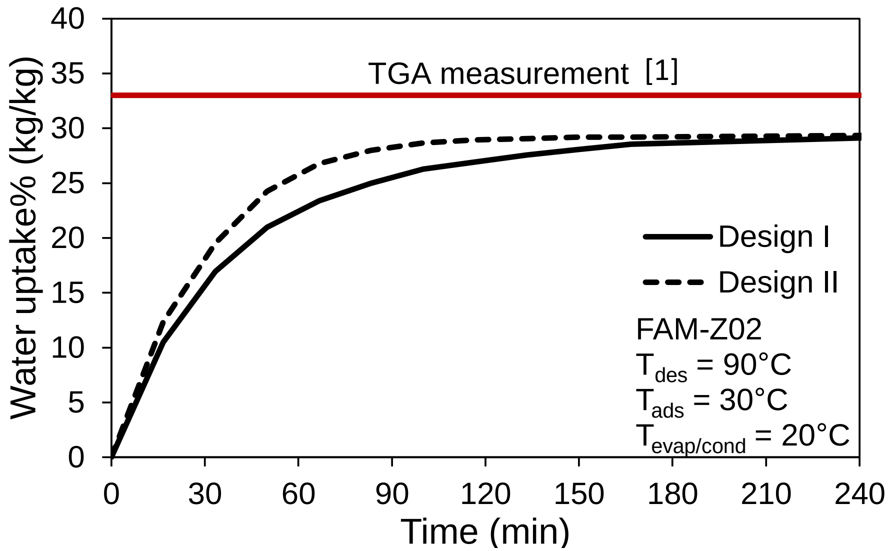
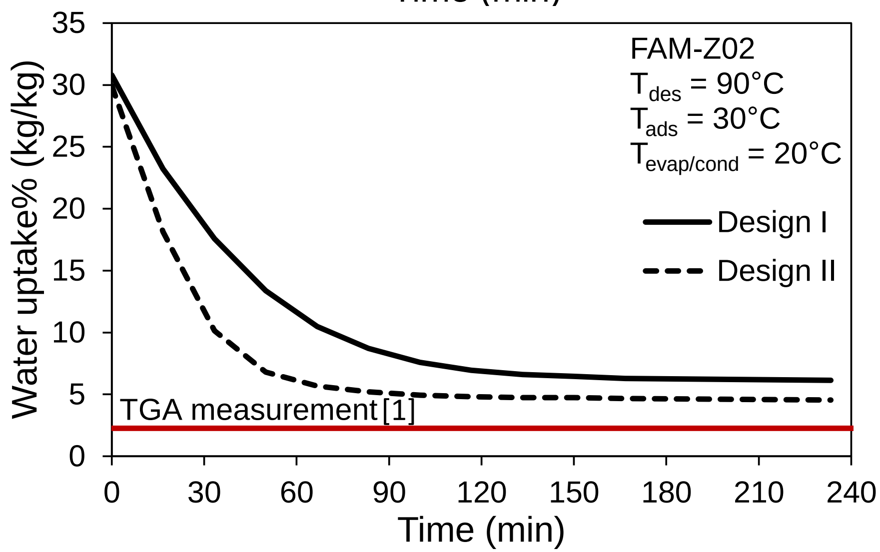
FAM Z02- Equilibrium Uptake



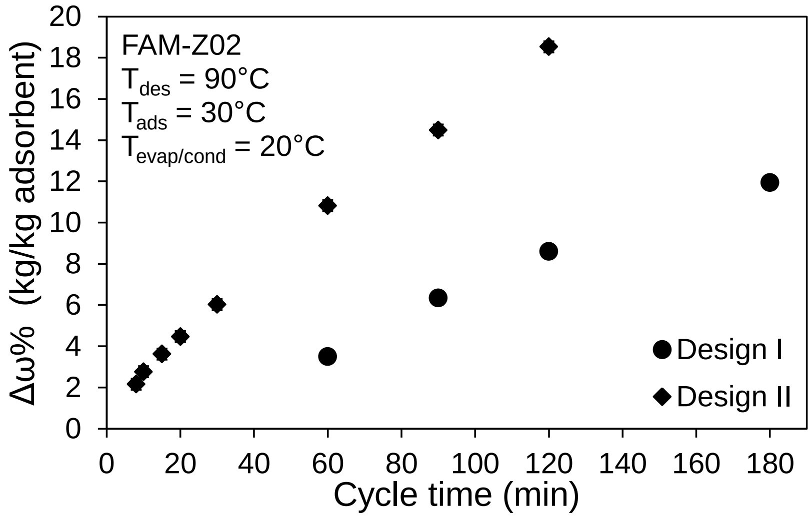
Adsorption

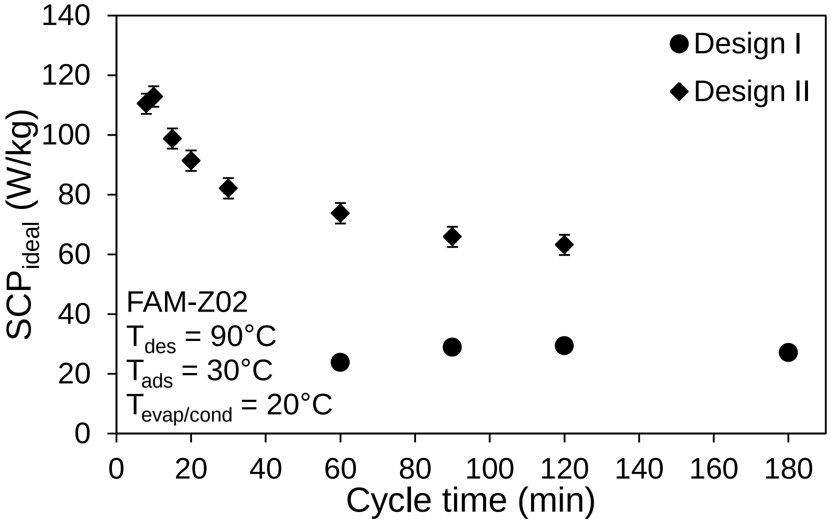


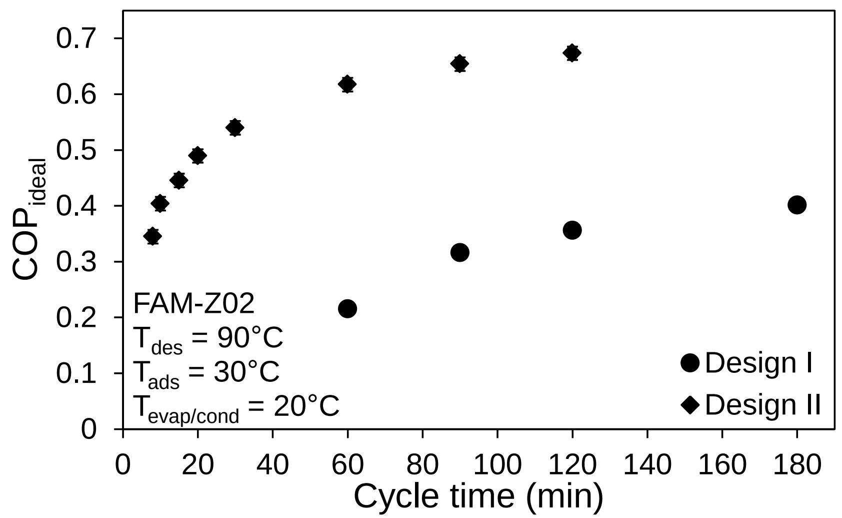
Desorption

[1] Okamoto K, et. al., Int. Symp. Innov. Mater. Process. Energy Syst., Singapore, 2010.

FAM Z02- Cyclic Operation







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Ideal SCP vs. Actual SCP

$$SCP_{\text{Ideal}} = \frac{\Delta\omega \times h_{fg}}{\tau_{cycle}} = \frac{\Delta m_{ref} \times h_{fg}}{m_{ads} \times \tau_{cycle}} \quad \begin{cases} Numerical\ Modeling \\ Mass\ Measurement \end{cases}$$

$$SCP_{\text{Actual}} = \frac{Q_{evap}}{m_{ads} \times \tau_{cycle}} \quad \{Cooling\ Effect\ at\ Evaporator$$

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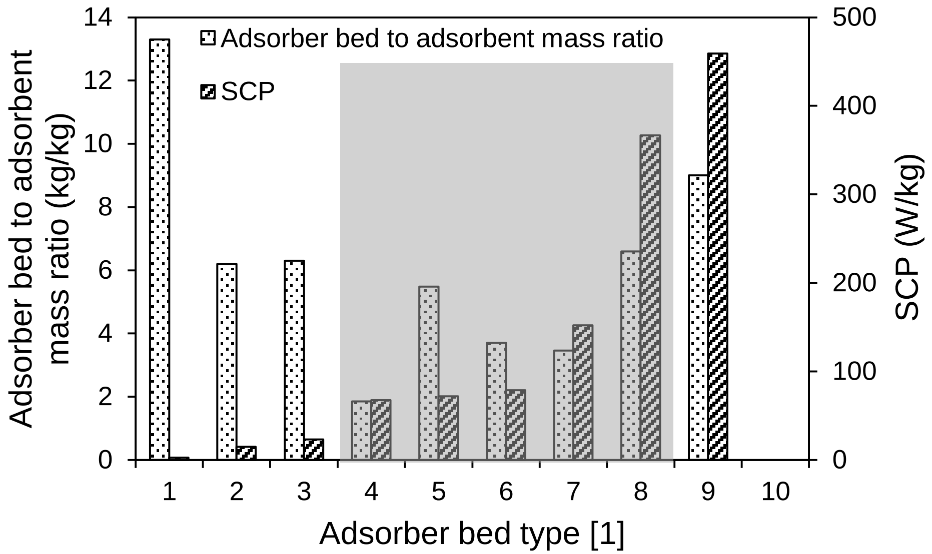
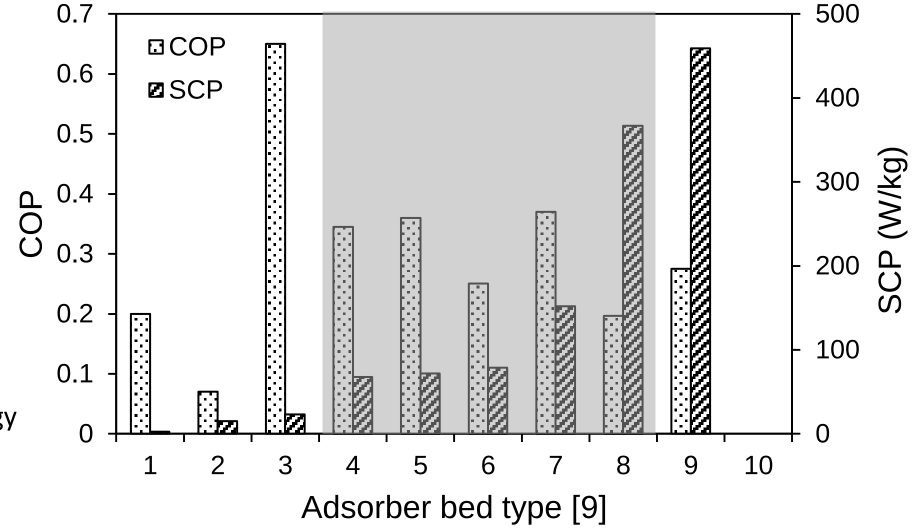
Performance of Different Adsorber Bed Designs

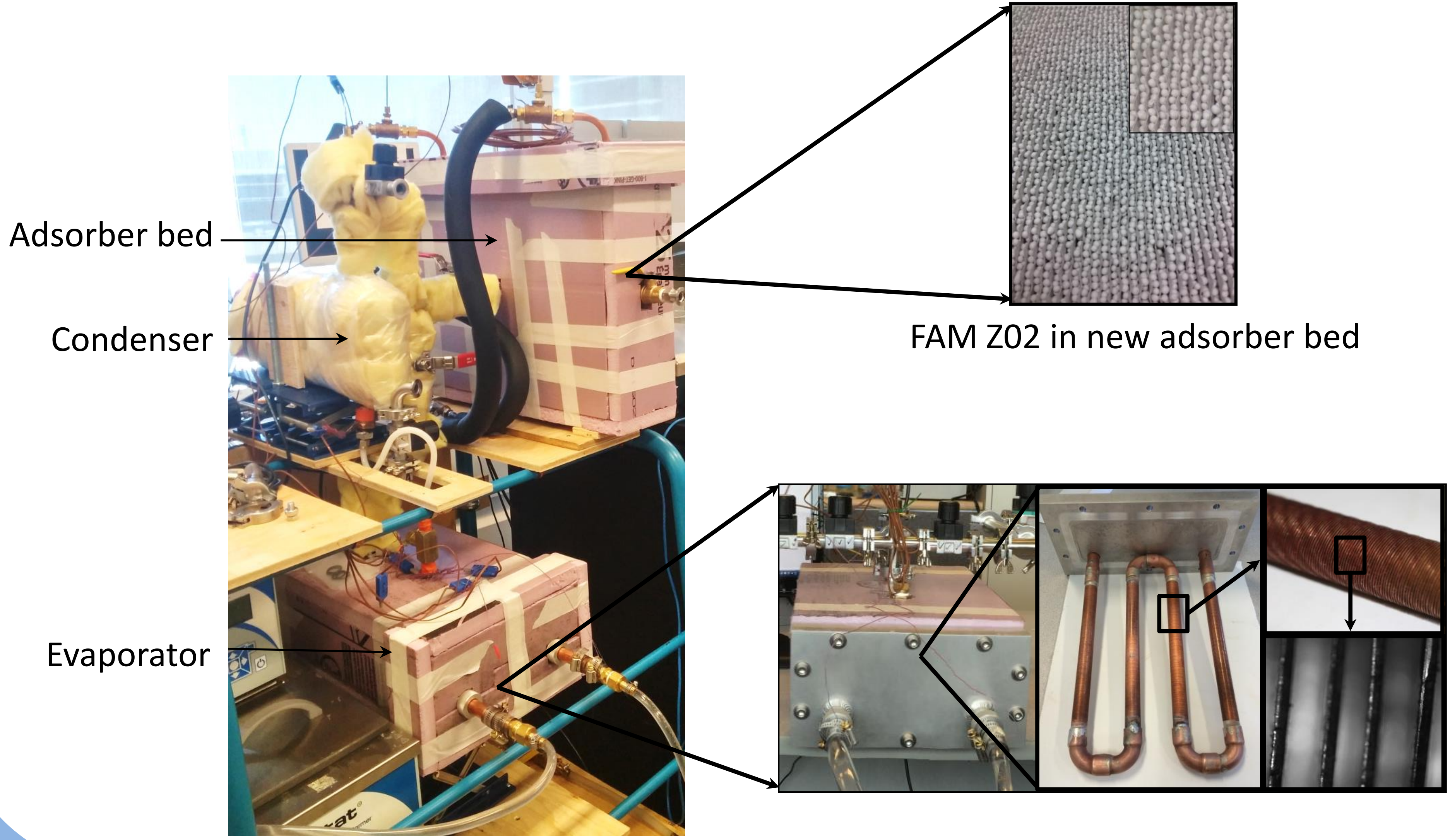
1. Spiral plate
2. Shell and tube
3. Hairpin
4. Annulus tube
5. Plate fin
6. Finned tube
7. Plate-tube
8. Simple tube
9. Plate





[9] A. Sharafian, M. Bahrami. Renewable and Sustainable Energy Reviews. 30 (2014) 440–451.

Single-Bed ACS Equipped with Capillary-Assisted Evaporator



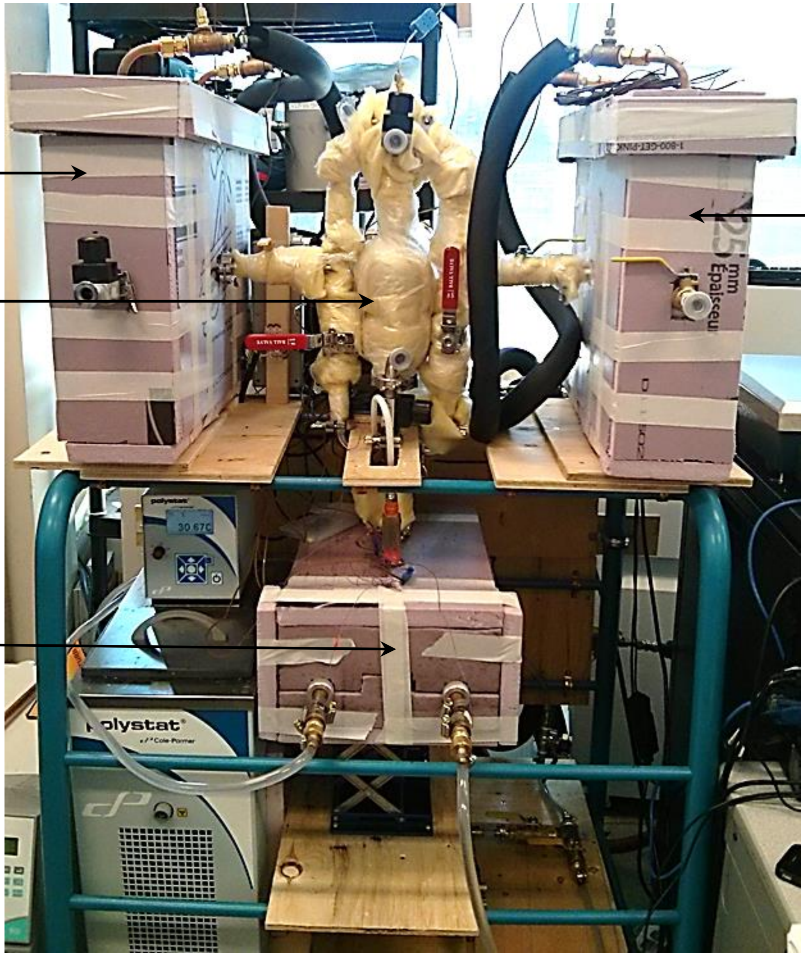
Two-Adsorber Bed FAM-Z02-Water ACS

Adsorber bed 1

Adsorber bed 2

Condenser

Evaporator



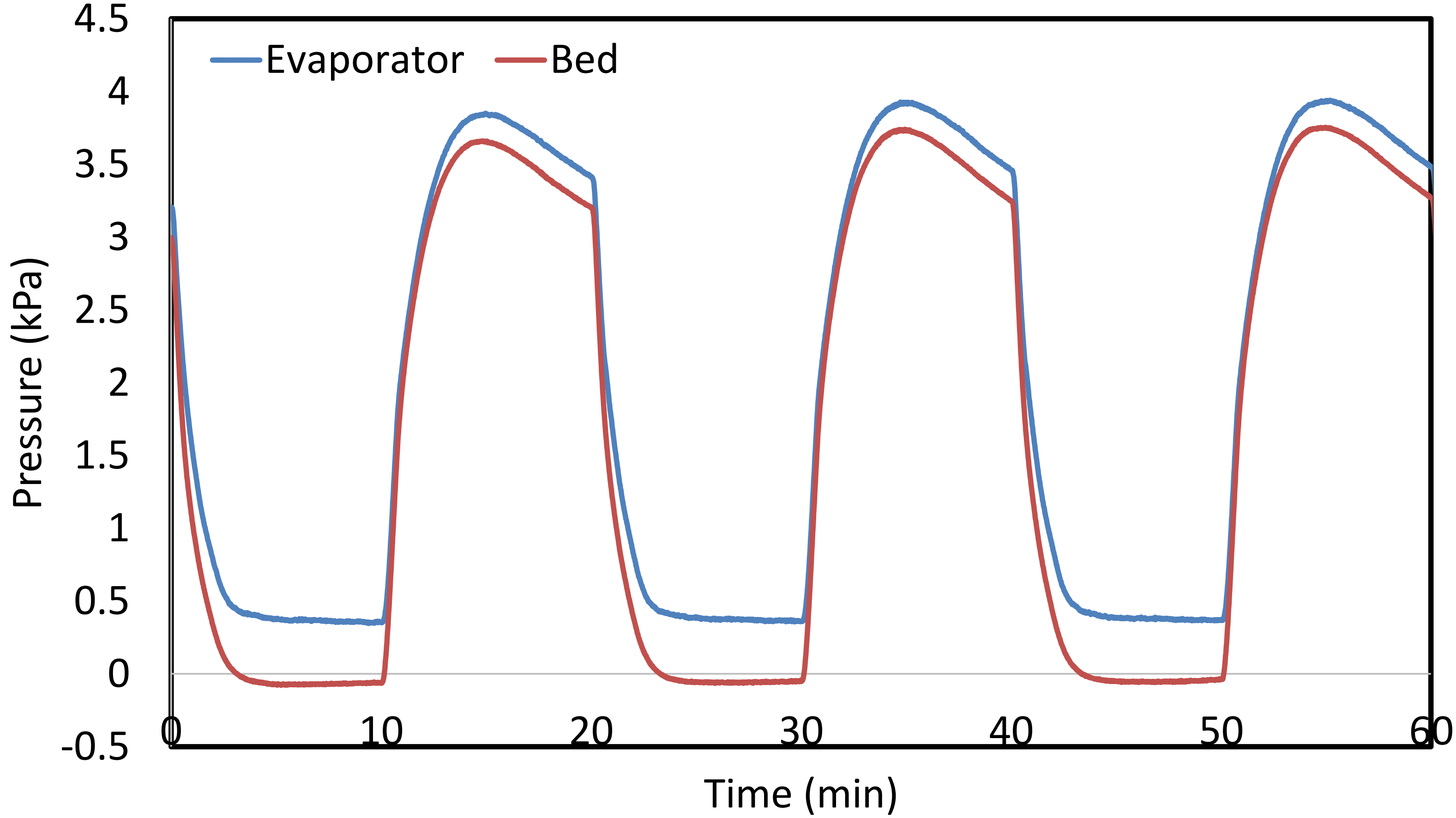
Modified Test Setup

- Heat transfer fluid flow rate ≈ 4 lit/min
- Evaporator flow rate ≈ 3 lit/min

Adsorber Bed Designs

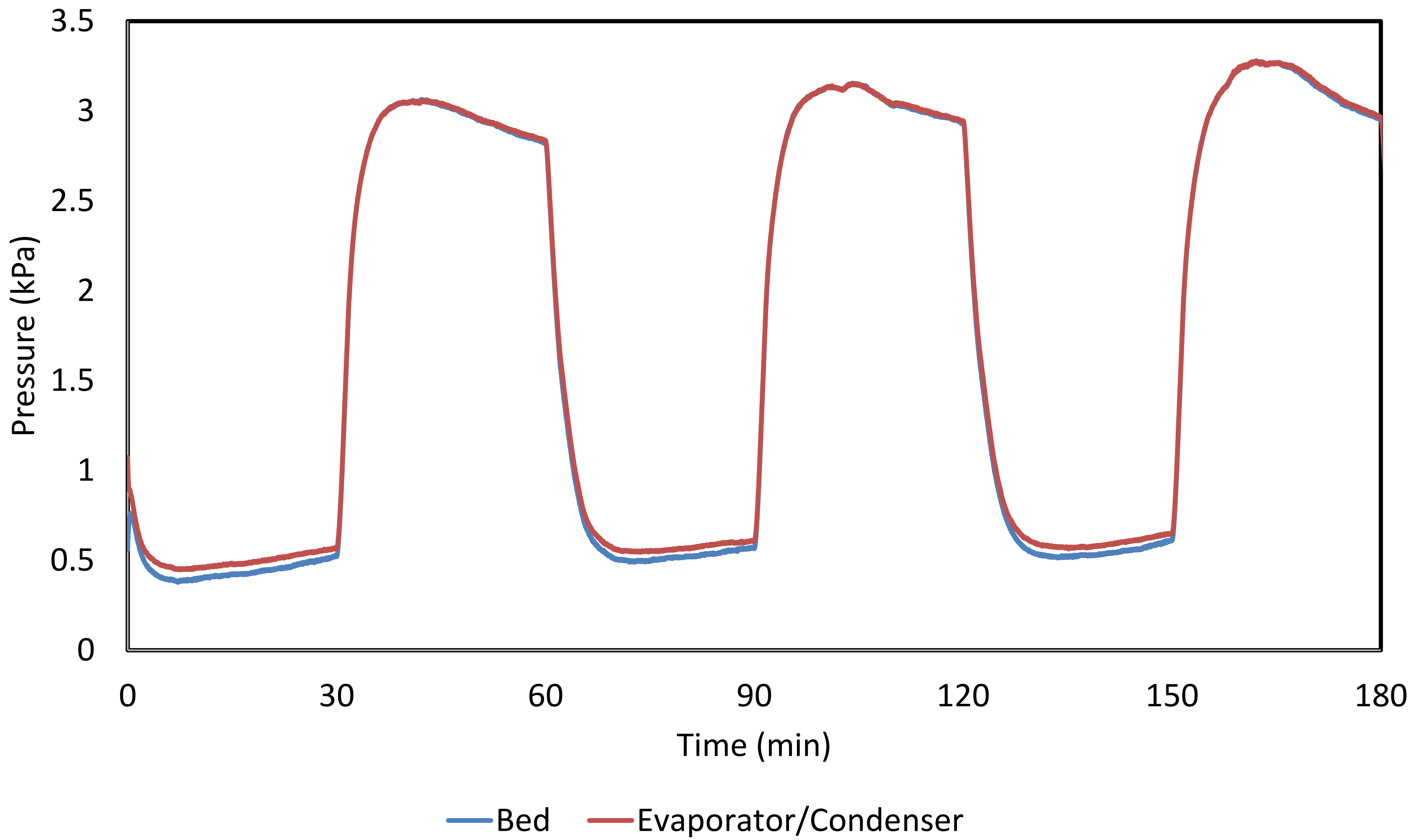
Parameter	Design I	Design II
Working pairs	AQSOA FAM-Z02/water	
Adsorbent particles diameter (m)	0.002	
Mass of adsorbent (kg)	0.62	1.50
Metal mass of adsorber bed (kg)	2.80	2.87
Adsorber bed heat transfer surface area, A_{bed}, (m^2)	0.235	2.80
Fin spacing (mm)	6.47 (3.5 fins per inch)	2.34 (10 fins per inch)
Fin dimensions	12.7 cm (5”) diameter	43.18×30.48 cm (17”×12”)
Heating fluid mass flow rate to adsorber bed (kg/s)	0.058 (4.1 L/min of silicone oil)	
Cooling fluid mass flow rate to adsorber bed (kg/s)	0.062 (4.1 L/min of silicone oil)	
Heat capacity of silicone oil (kJ/kgK)	1.8	
Heating fluid inlet temperature (°C)	90	
Cooling fluid inlet temperature (°C)	30	
Evaporation/condensation temperature (°C)	20	

Pressure – 10 fpi, 1500gr



SFU

Pressure - 3 fpi, 620 gr – Cycle time 60 min



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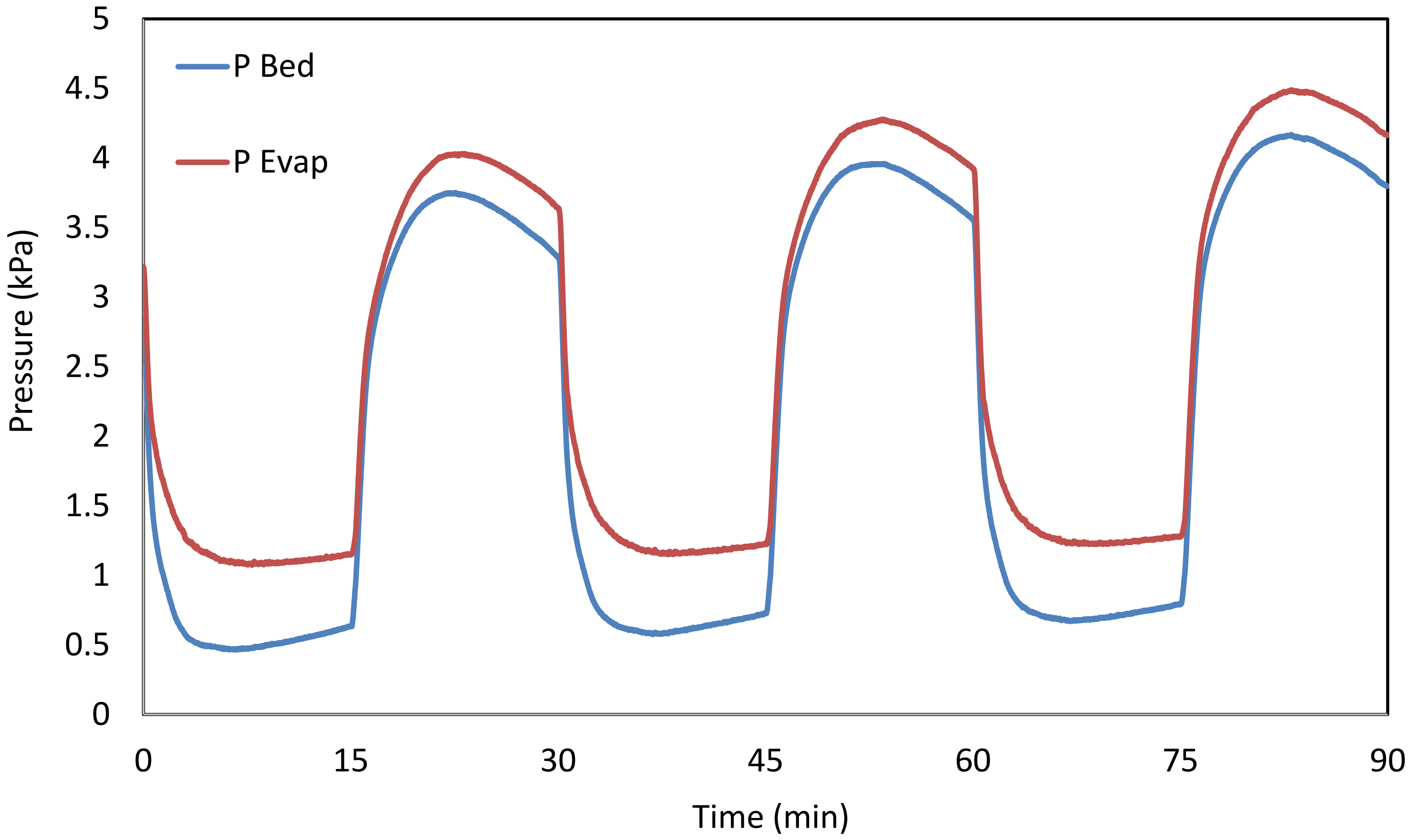
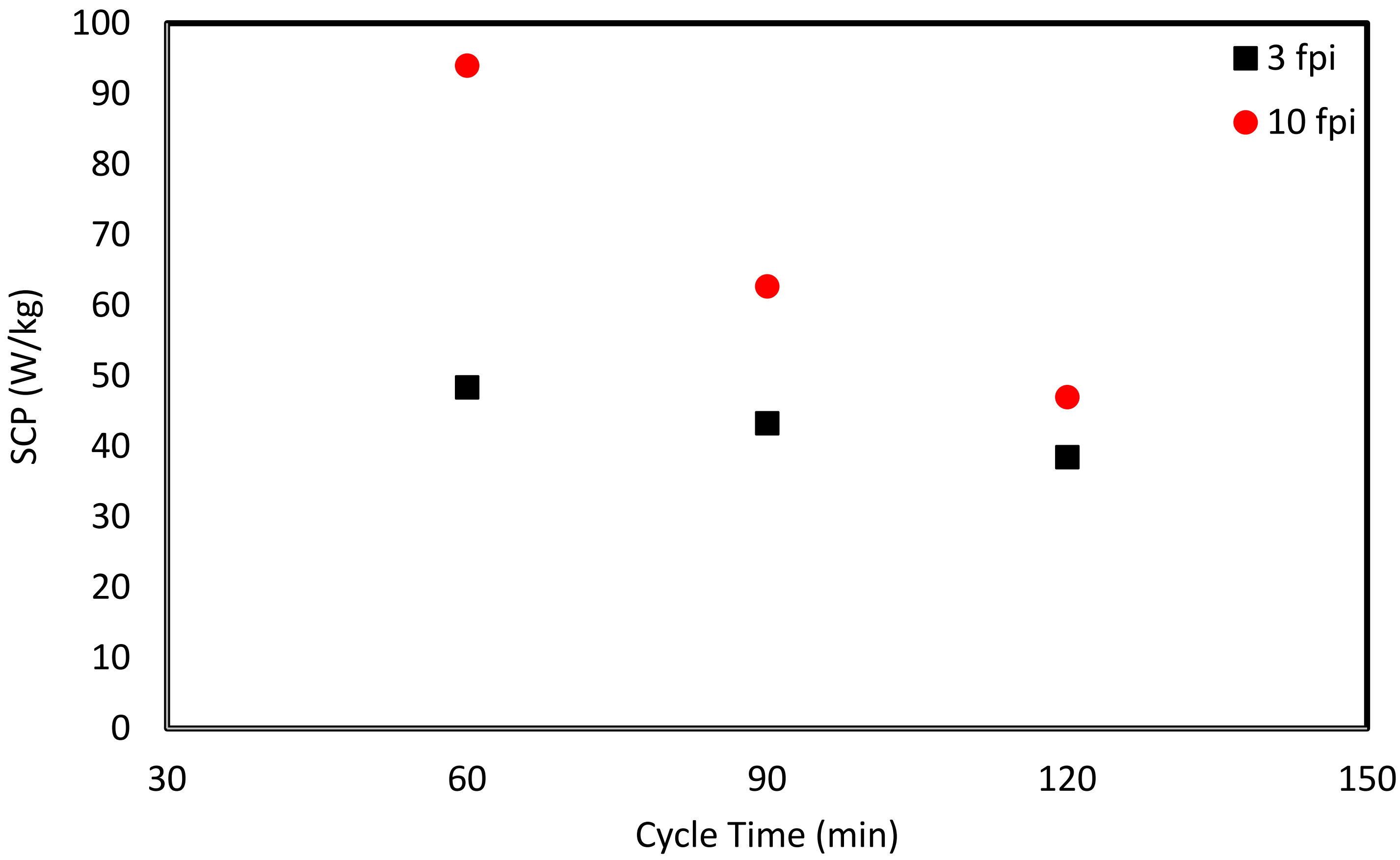
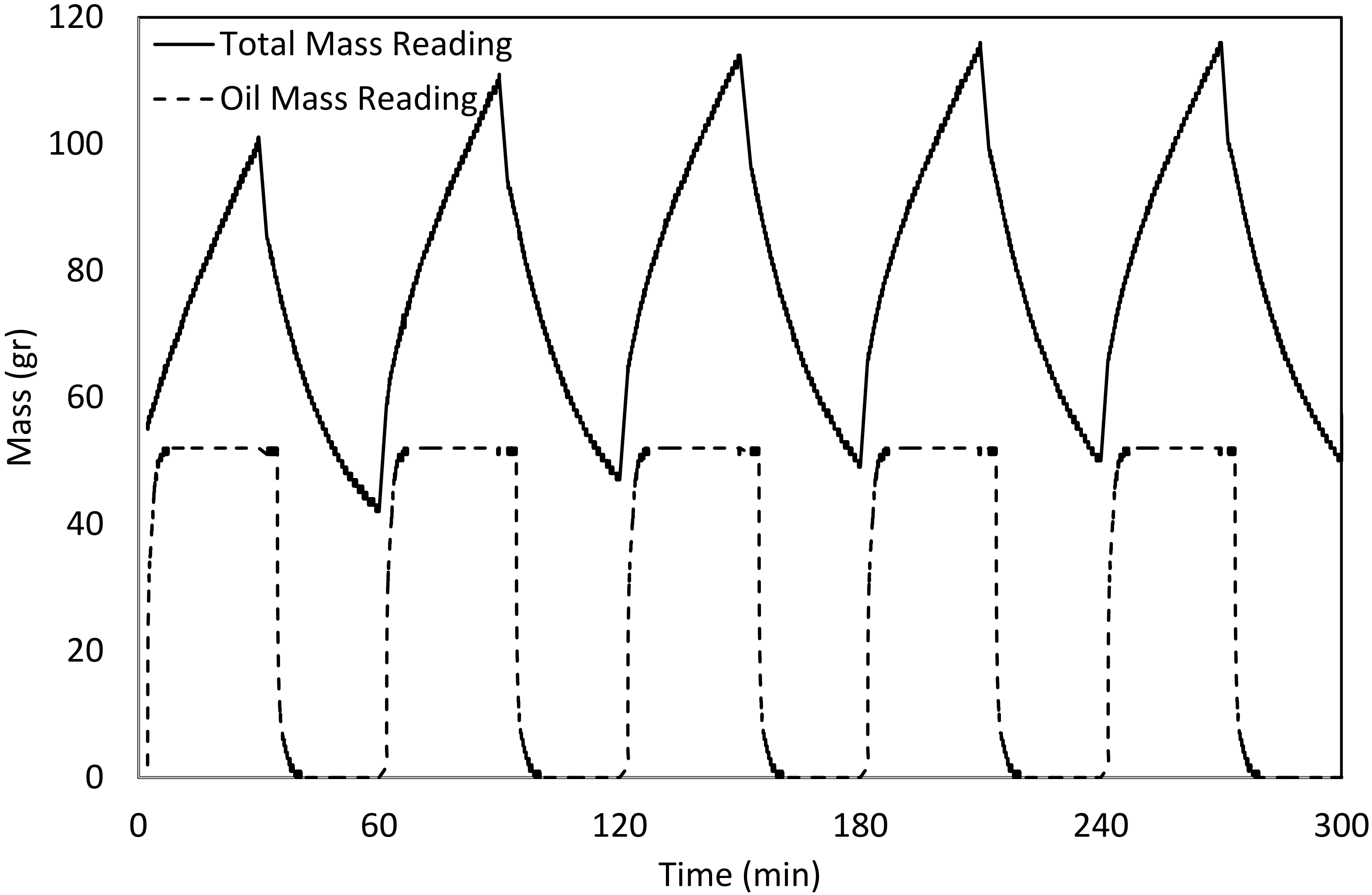
Pressure within Bed and Evaporator – Design II Modified



SCP – Two different Design Comparison

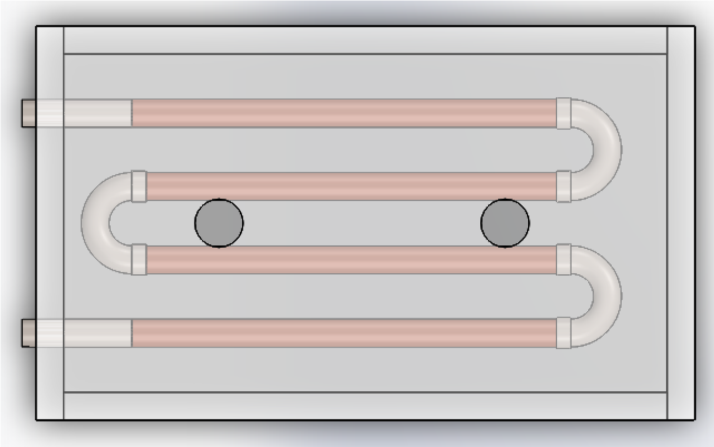


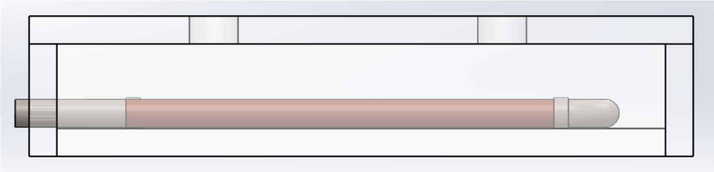
Results – effects of silicon oil density change



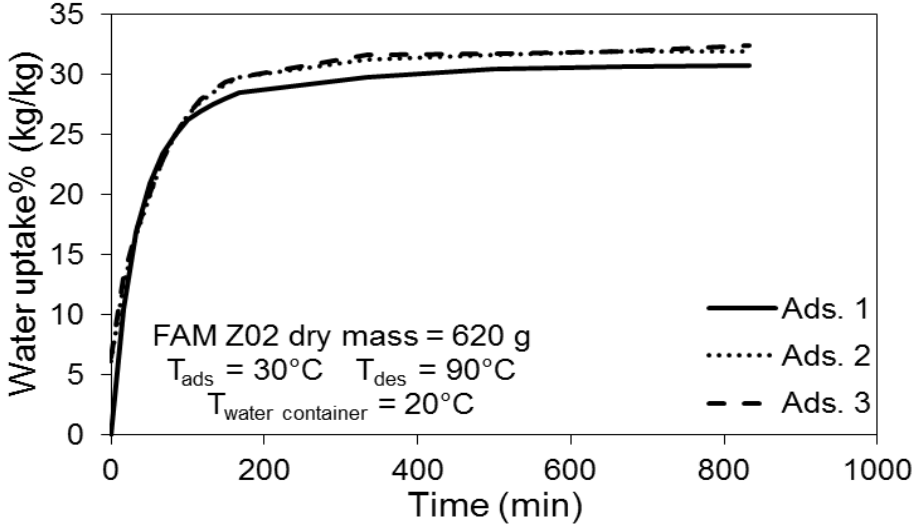
Low Pressure Evaporator

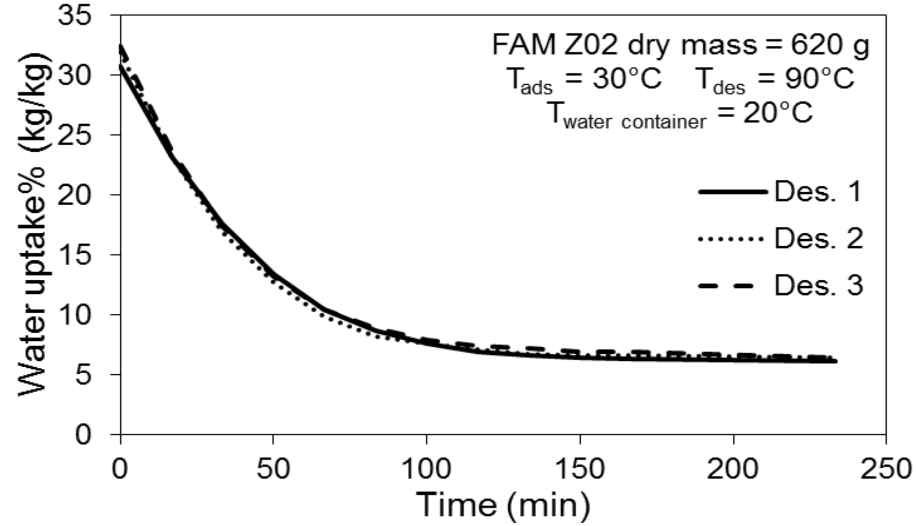
- Using the new evaporator (capillary assisted)
- Decreasing cycle time to reach the maximum SCP

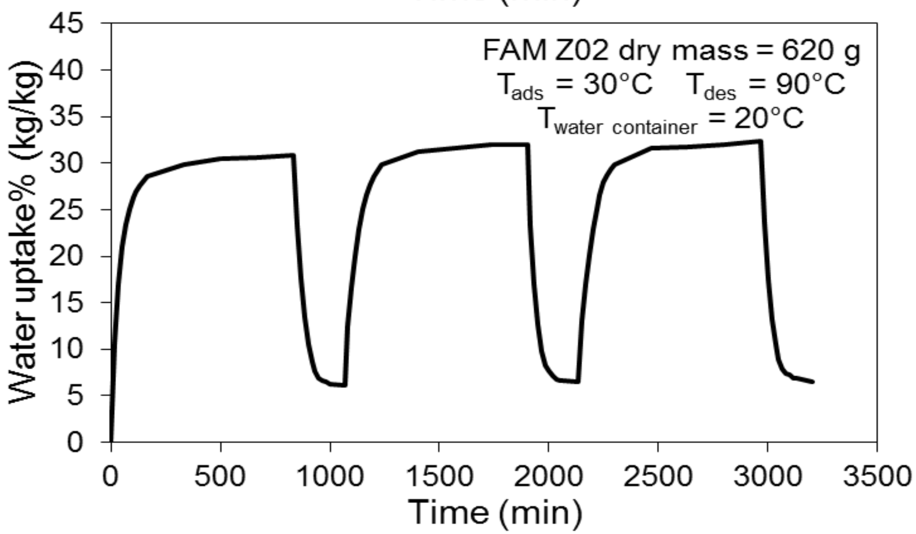


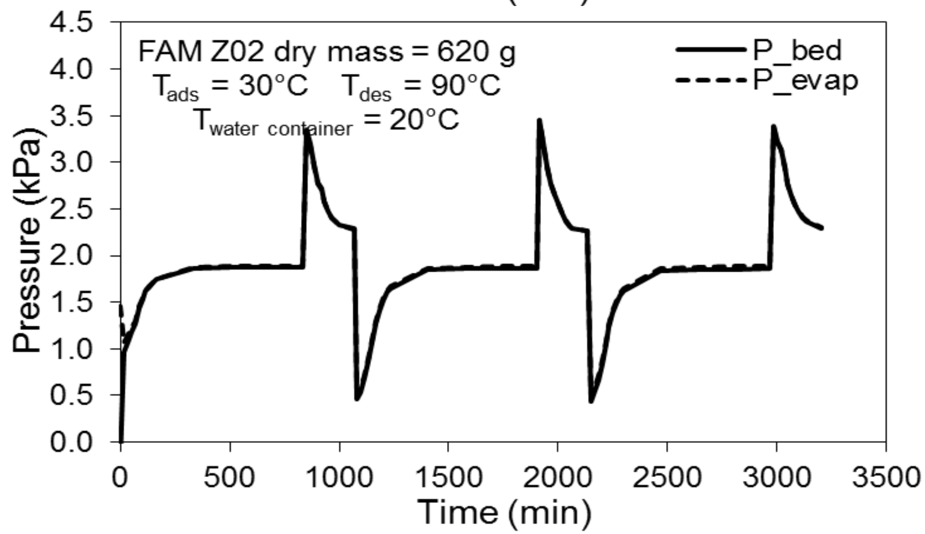


FAM Z02- Equilibrium Uptake

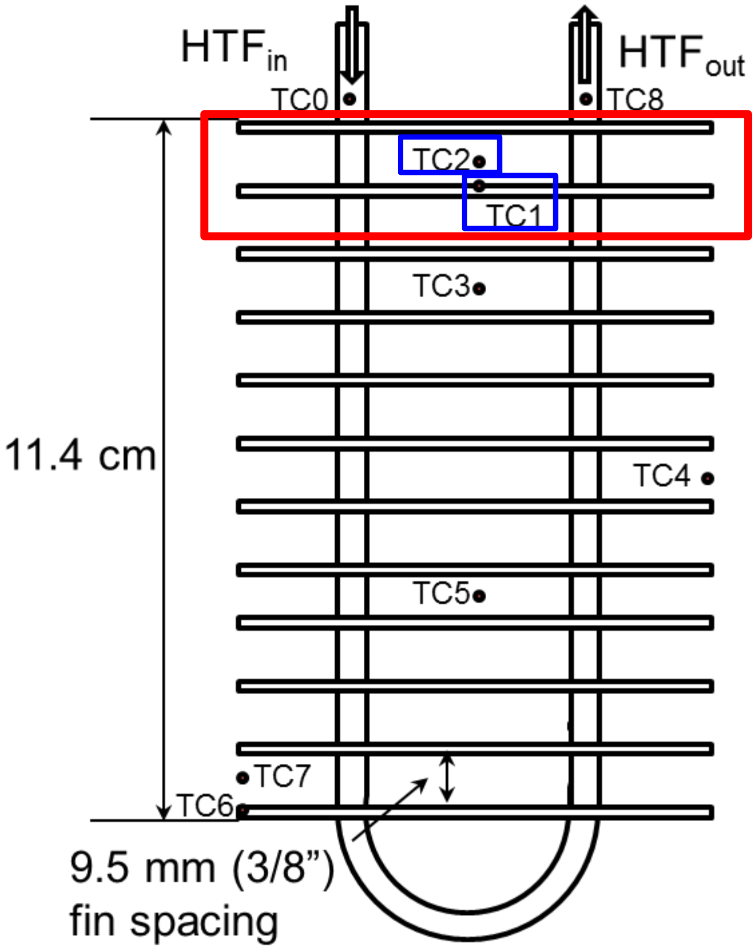


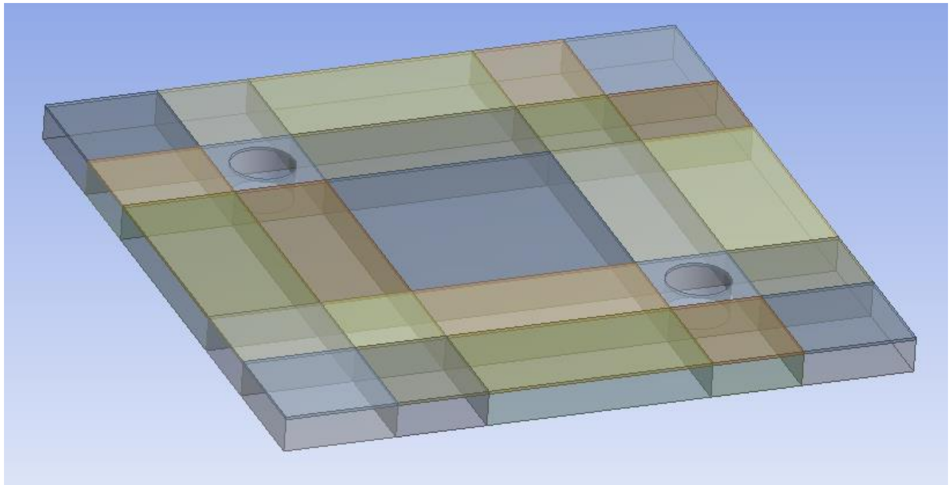


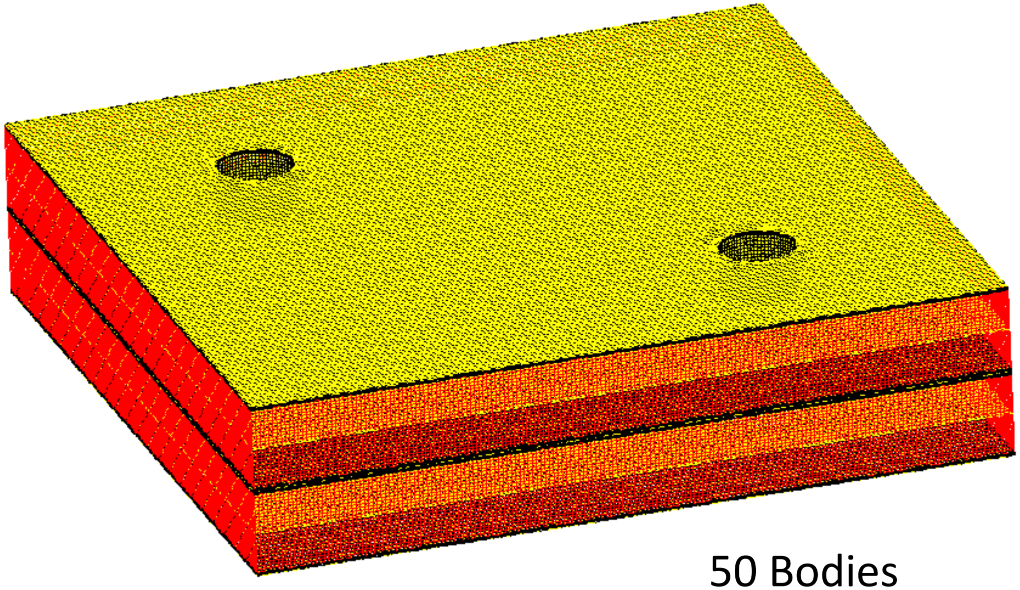




The First Generation

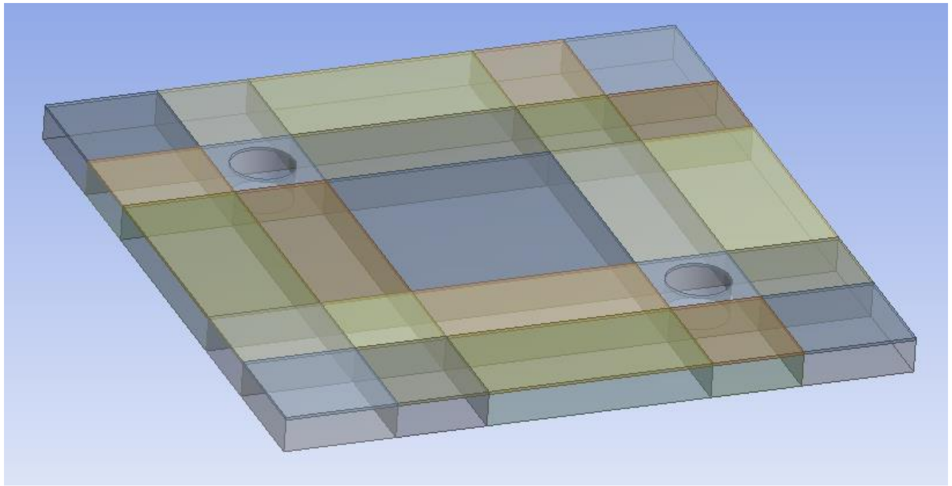


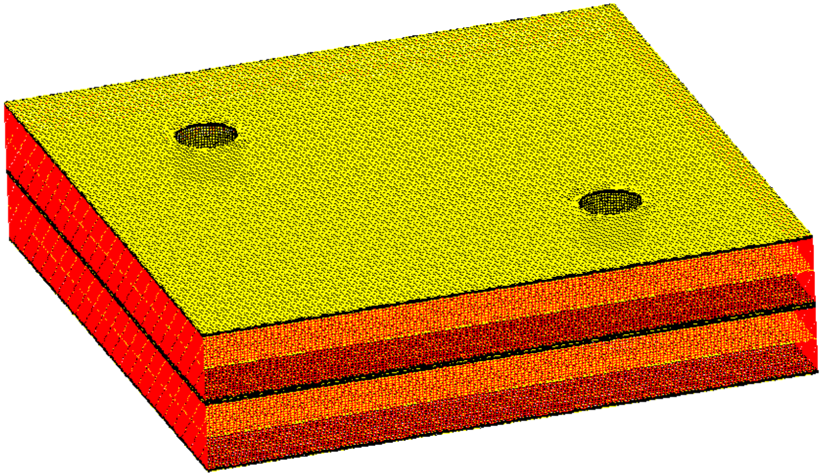




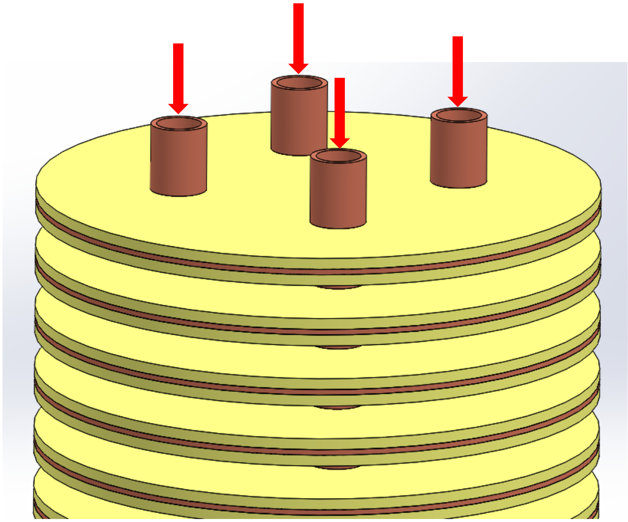
50 Bodies
511,000 Cell

Geometries





Flow in



Flow in