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ABSTRACTS

- Batteries & Supercapacitors
- Fuel Cells & Electrolysers
- Hydrides for Energy Storage & Conversion

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Performance simulation of combined two-tank latent and thermochemical heat storage systems for high temperature waste heat recovery

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Thermochemical heat storage materials use endo/exothermic chemical reactions to store/restore tremendous amount of heat. The past decade has witnessed a rapid growth in fundament and applied research of promising thermochemical materials, targeting high chemistry performance (high operating temperature, high heat storage density, fast kinetics, etc.). Among these materials, metal hydrides have attracted worldwide interest as an environment-friendly and reliable solid-state cadidates for energy storage applications.

Heat storage systems based on 2 tanks thermochemical heat storage are gaining momentum for their utilization in concentrated solar power plants (CSP) or industrial waste heat recovery, since they can efficiently store heat for future use[1]. However, their performance is generally limited by reactor configuration, design and optimization on the one hand and most importantly on the selection of appropriate thermochemical materials [2] on the other hand. Mg-based hydrides, although at the early stage of research and development (in heat storage applications), can offer several advantages over other thermochemical materials (salt hydrates, metal hydroxides, oxide and carbonates) such as high energy storage capacity (0.32-0.79 kWh/kg or 500-800 kWh/m^3) and power density[3,4]. In this study, we present a system that combines latent heat and thermochemical heat storage based on two-tank metal hydrides. The systems consists of two metal hydrides tanks coupled (See Figure 1).

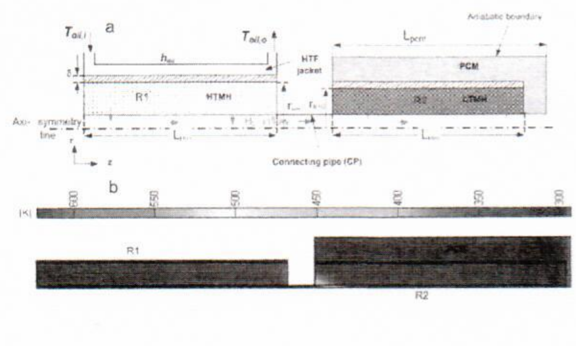

Figure 1. Concept of combined thermal energy system, a) computational model, b) Temperature distribution during the heat charging

During the heat charging the high temperature metal hydride (HTMH) desorbs hydrogen which in turn is stored in the low temperature metal hydride (LTMH). In the meantime, the heat generated from hydrogen absorption in the LTMH tank is stored as latent heat in a phase change material (PCM) jacket surrounding the LTMH tank, to be reused during the heat discharging. For simulations of this heat storage system, a metal hydrides pair based on Mg_2NiH_4 (HTMH)-$LaNi_5$ (LTMH) and Rubitherm RT(Tm) based on commercial phase change materials are selected for discussion. The preliminary results of the simulation shows that the performance indicators such as energy density, power density and storage efficiency (As seen in Figure 2) is a function of the properties of the selected phase change material, more specifically the melting temperature, Tm. The using of RT42 leads to an output energy density of 133 MJ/m^3 with specific power output of ~90 W/kg -Mg_2Ni. In addition, an optimization process will be endeavored to determine the most influencial PCM properties on the system performance.

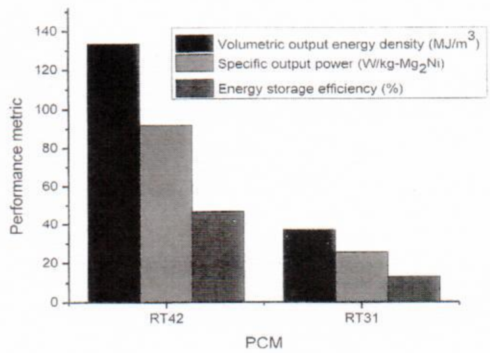

Figure 2: Performance indicator as a function of PCM melting temperature

Acknowledgements

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[1] S. Kuravi , J. Trahan et al. Prog Energy Combust Sci 39 (2013) 285

[2] S. Nyallang Nyamsi, M. Lototskyy, I. Tolj. Int J. Hydrogen Energy, 43(2018) 22568.

[3] A. Reiser, B. Bogdanovic, K. Schlichte. Int J Hydrogen Energy 25(2000) 425

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Serge Nyallang

Dr Serge Nyallang Nyamsi completed his Ph.D. degree in power engineering and engineering thermophysics from the school of Energy and Power Engineering, Xian Jiaotong University, China in 2013. He is currently a postdoctoral research at HySA Systems within the South African Institute for Advanced Materials Chemistry (SAIAMC) from the faculty of Natural science, university of the Western Cape. His research interests in energy storage technologies include design and optimization of potential metal hydrides for hydrogen storage and thermal energy storage, heat management and energy efficiency improvement. He also have interest in efficient conversion of renewable energy resources.

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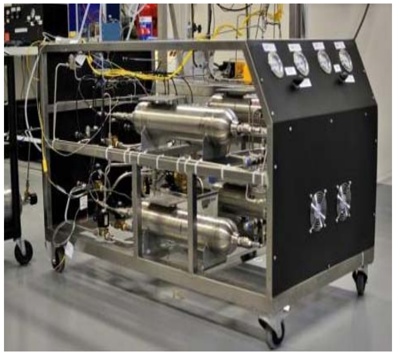


S. Nyallang Nyamsi, & M. Lototskyy (*presented by <u>M.W. Davids</u>*)

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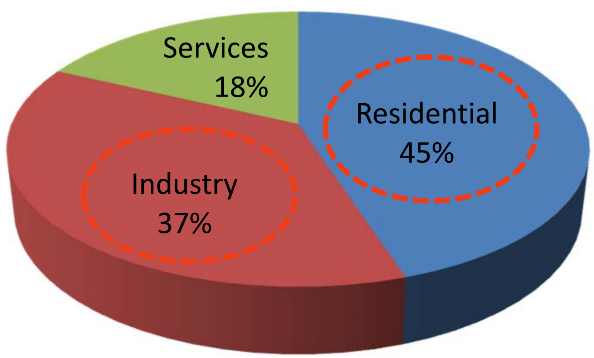
Overview of Heating and Cooling Sector

Currently, half of the EU's total energy demand is consumed by the heating and cooling sector.

- Only 18% is generated from low carbon or renewable energy sources.

Further, inefficiencies in the production, storage and utilisation of heating and cooling solutions results in a significant amount of waste along the supply chain.

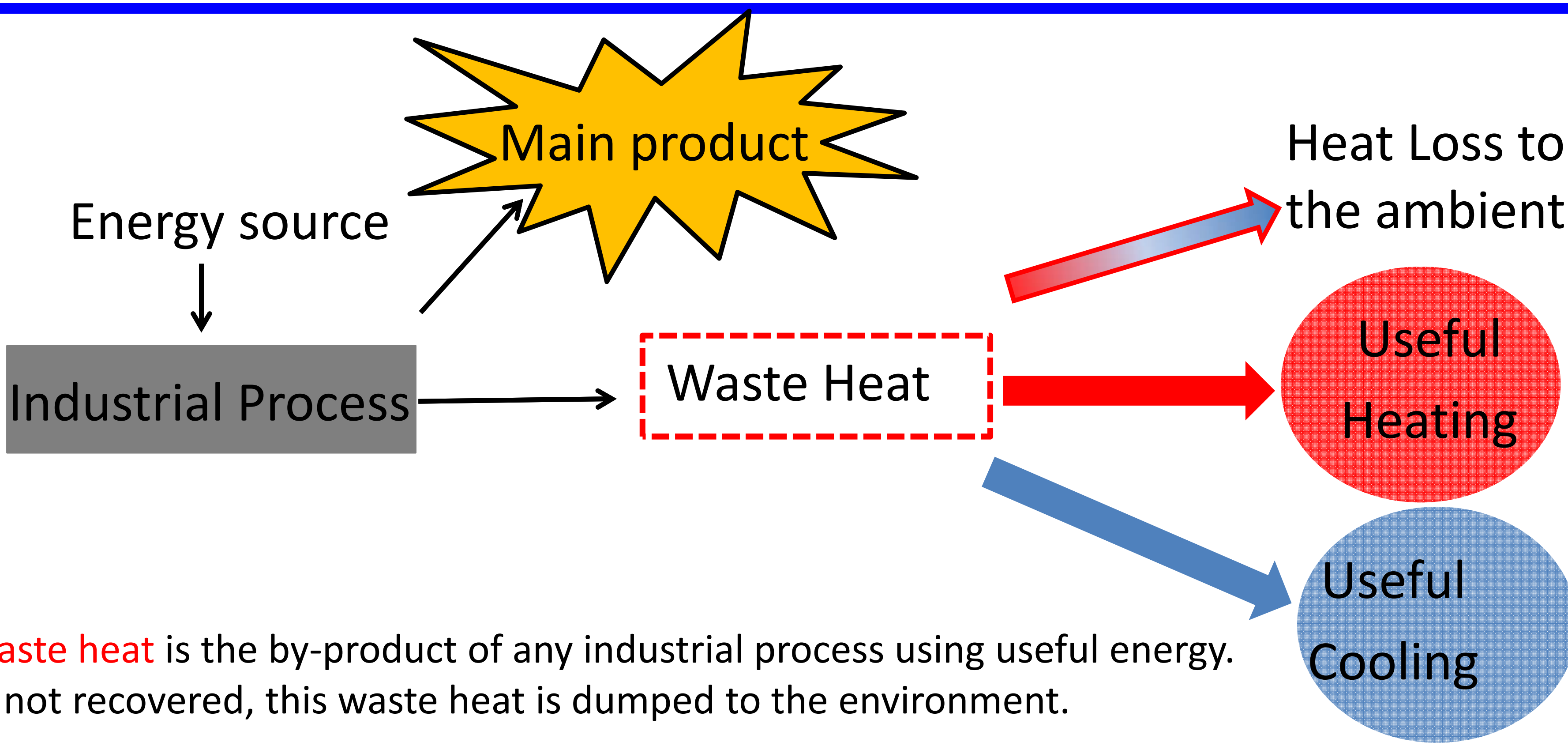


Approximate breakdown of energy consumption in heating & cooling sector

Two of the major target areas for:

- Improvements in efficiency,
- Reduction in demand,
- Shift to low carbon and renewable energy sources.

Waste heat



Waste heat is the by-product of any industrial process using useful energy. If not recovered, this waste heat is dumped to the environment.

Waste heat recovery improves the overall energy efficiency

- Free energy that substitutes the purchased fuel or electricity
- Energy efficiency improvement by 10-50 %
- Reduce the thermal pollution

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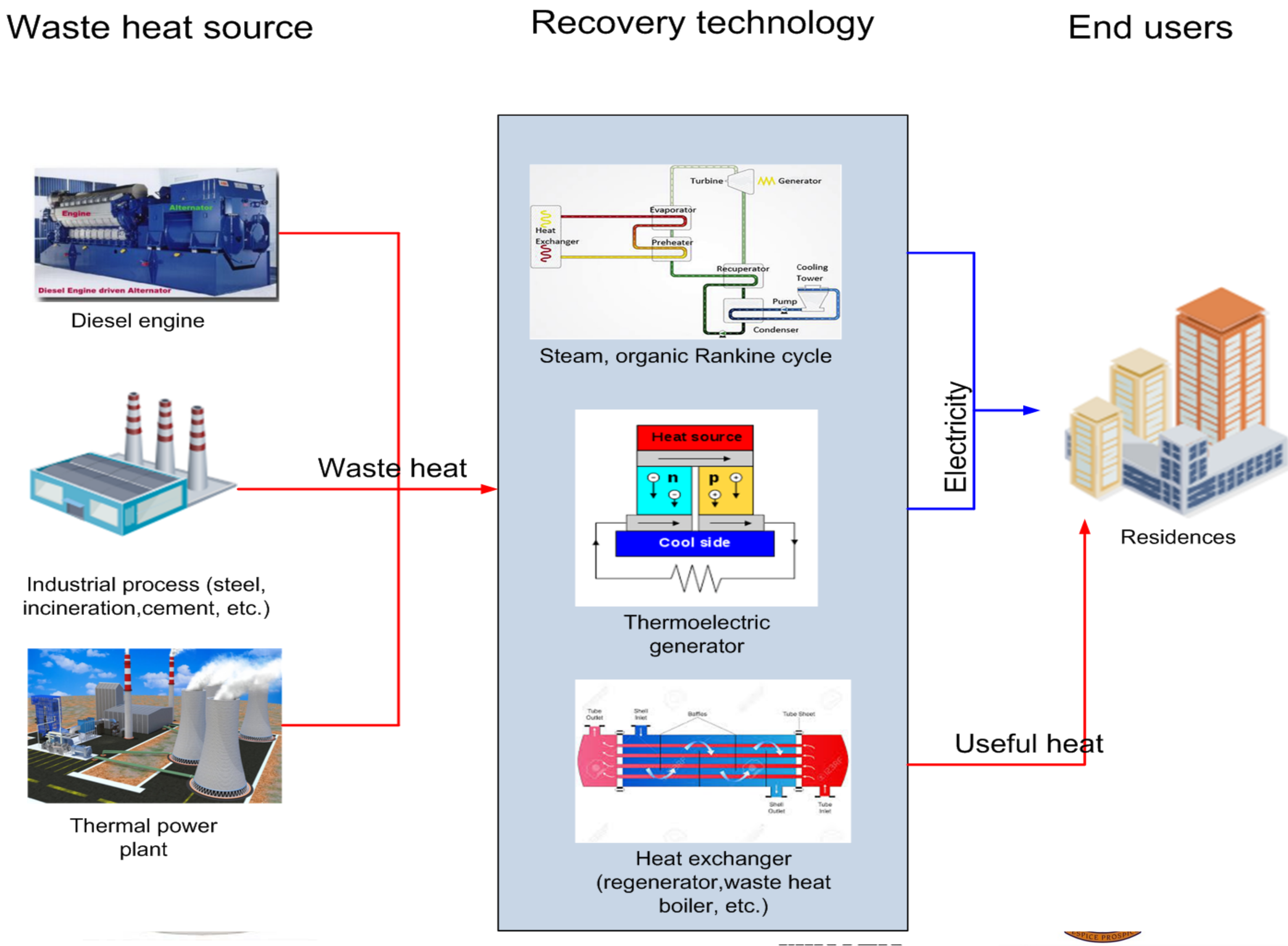
Conventional waste heat recovery



Waste Heat source/temperature quality

Low Temperature heat source

- Internal combustion engine: 60-150 °C
- Hot processed liquids and solids: 32-232 °C
- PEM fuel cells: 30-60 °C

Medium Temperature heat source

- Steam boiler exhaust : 230-480 ° C
- Gas turbine exhaust: 370-540 ° C
- Heat treatment furnace: 435-600 ° C
- Drying and baking oven: 230-600 ° C
- Reciprocating engine exhaust: 315-600 ° C

High temperature heat source

- Metal refining furnace: 650-1650 °C
- Cement kiln: 620-730 °C
- Solid waste incinerators: 650-1000 ° C
- Solid oxide fuel cell (SOFC) : 600-800 ° C

Recovering such waste heat can provide power, heat or cooling output without extra energy input

Thermal Energy Storage

Thermal energy storage (TES) stocks thermal energy by heating or cooling a storage medium so that the stored energy can be used at a later time for heating & cooling applications, as well as power generation.

Advantages of TES include:

- Bridge the gap between energy supply and demand,
- Energy savings,
- Efficient and rationale use of available resources,
- Optimum utilization of renewable energy sources (e.g. solar/PV, geothermal) and industrial waste heat.

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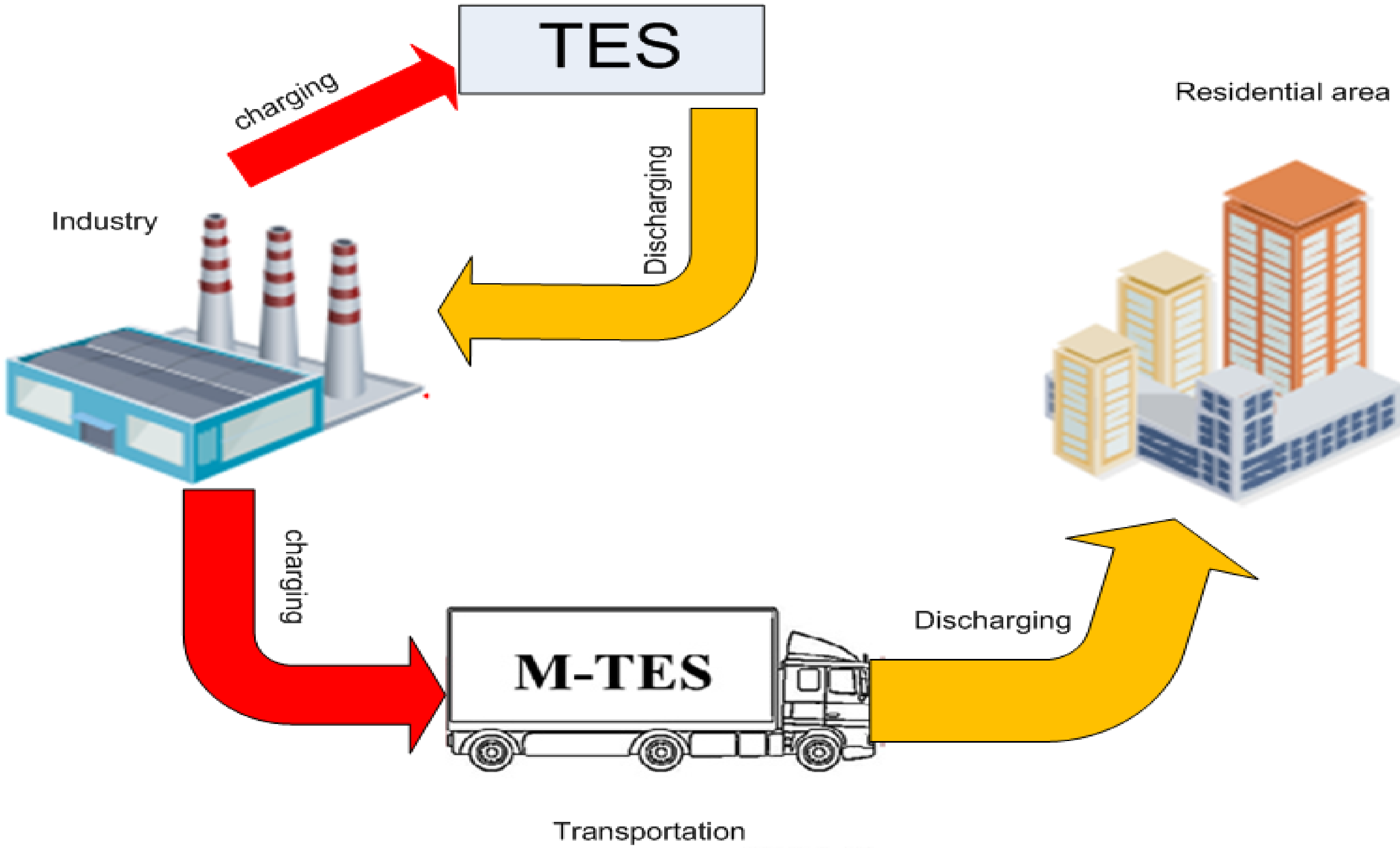
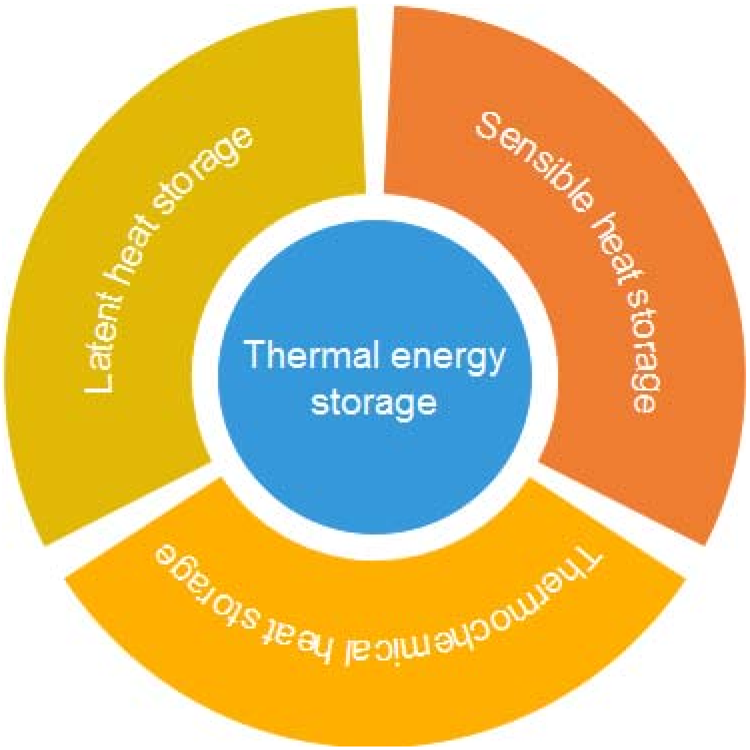
Thermal energy storage

One of the main advantages of TES over conventional waste heat recovery is its utilization both on-site and off-site waste heat resources



Thermal Energy Storage



Sensible Heat Storage

- Heating or cooling a solid or liquid storage medium.
- Examples: water, molten salts, rocks.

Latent Heat Storage

- Uses a phase change material.
- Examples: ice, paraffin, erytritol.

Thermochemical Storage

- Uses chemical reactions to store & release thermal energy
- Examples: zeolites, metal oxides, **metal hydrides.**

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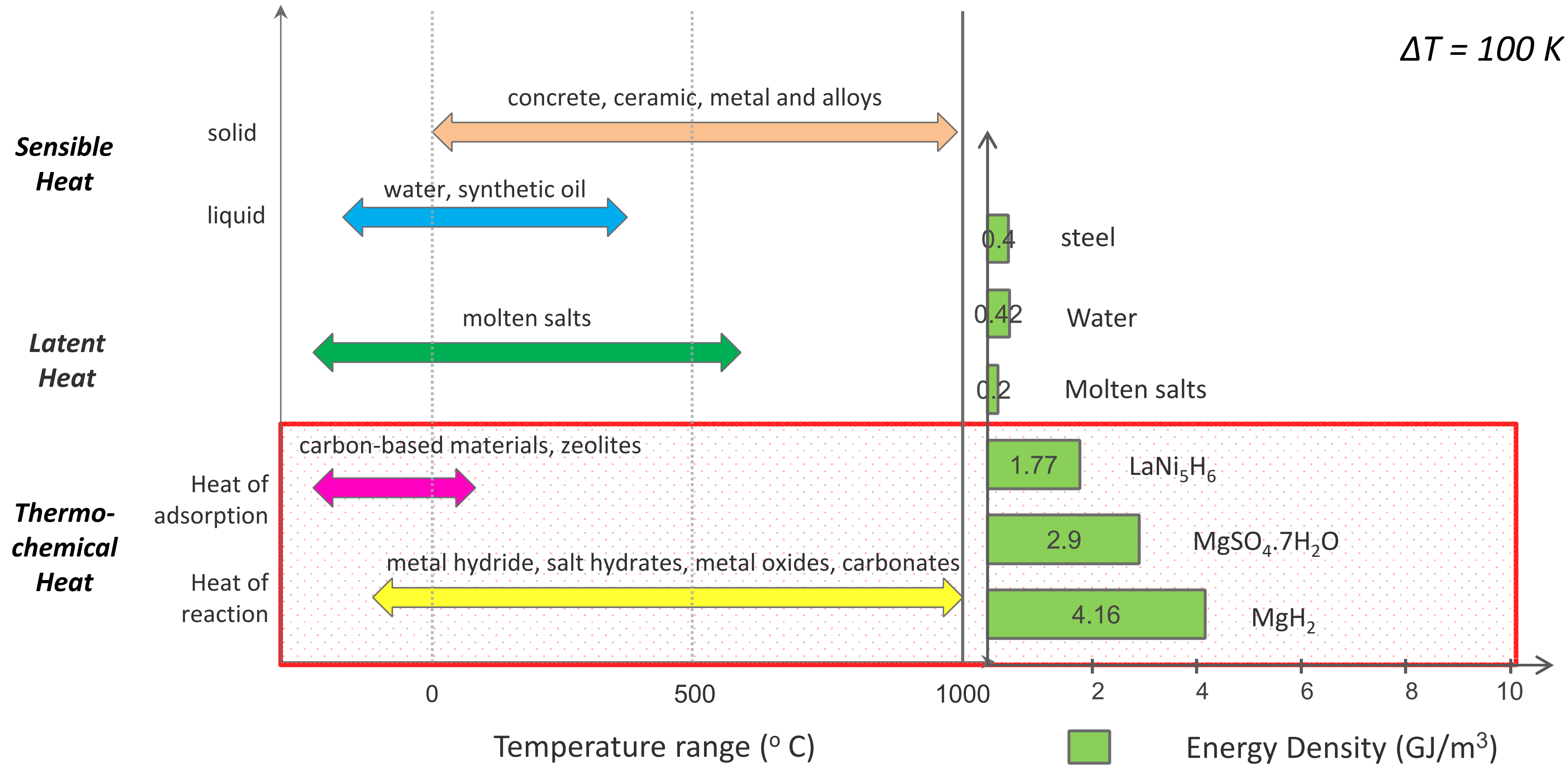
Thermal Energy Storage



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Metal Hydrides

Hydrogen storage / heat production →

$$\text{Metal} + H_2 \longleftrightarrow \text{Metal hydride} + \text{Heat}$$

← *Hydrogen discharge / heat storage*

- Safe, efficient and cost effective hydrogen storage option,
- High H_2 volumetric capacity,
- Component can be stored separately without heat loss,
- Long term heat storage,
- Wide range of operating pressures and temperatures,
- High heat storage capacity > 1 GJ/m^3.

Selecting

There are several factors to consider, including;

- Heat of reaction,
- Entropy change,
- Heat capacity,
- Temperature and pressure requirements of the overall system.

Governing Equations:

Storage Capacity: $Q_s = n\Delta H + (mc_p\Delta T)$

Heat Release Capacity: $Q_r = n\Delta H - (mc_p\Delta T)$

Overall Efficiency: $\eta = \frac{Q_r}{Q_s}$

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Selecting

There are several factors to consider for selecting a PCM, including;

- Melting temperature,
- Latent and sensible heat capacity, $Q_s = n\Delta H + \int C_p dT$
- Thermochemical stability,
- Cyclic behaviour
- Heat transfer properties (thermal conductivity, diffusivity).
- Cost,
- Corrosiveness,
- Flammability.

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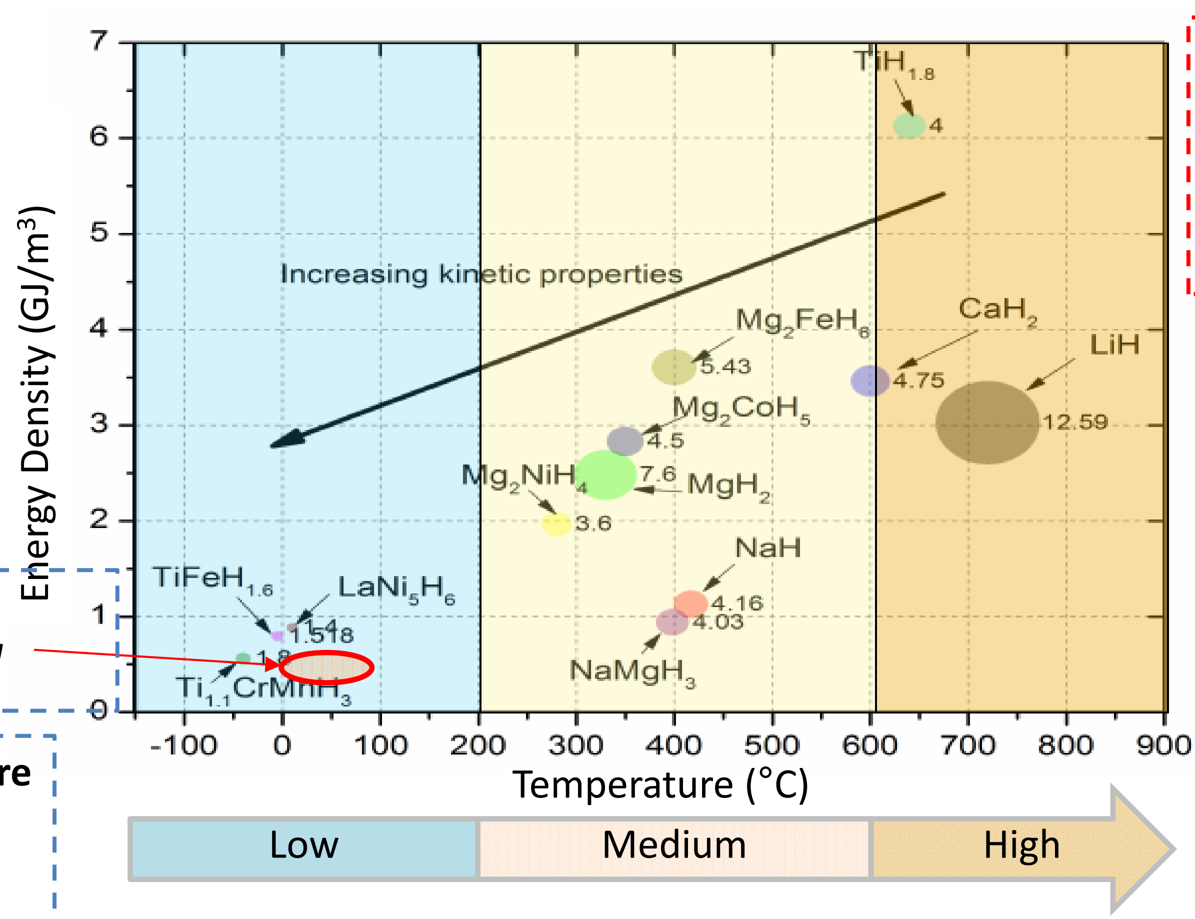
Intrinsic Volumetric Energy Density vs. Operating Temperature

High temperature metal hydrides (HTMH): *high energy density and slow kinetics*



Low energy density PCM

Low temperature metal hydrides (LTMH): *low energy density and fast kinetics*

Sandrock G., Thomas G., The IEA/DOE/SNL on-line hydride databases, Applied physics A, 72,153-155 (2001).

David R. Lide "Standard thermodynamic properties of chemical substances", in *CRC Handbook of Chemistry and Physics,* 2005.

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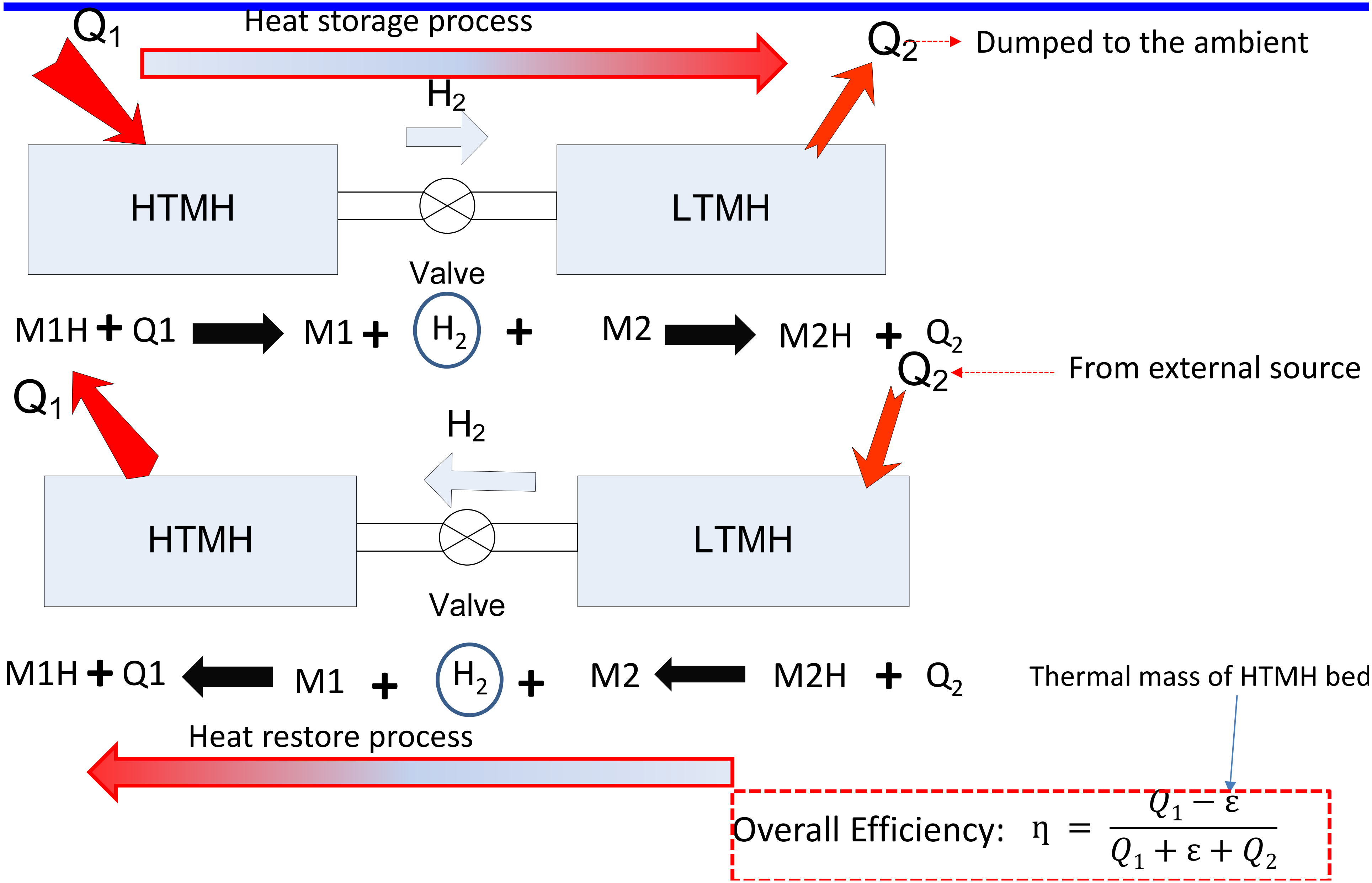
Objectives

Main objective: Design and optimize a combined latent and thermochemical heat storage for medium-high temperature waste heat recovery.

Sub-objectives:

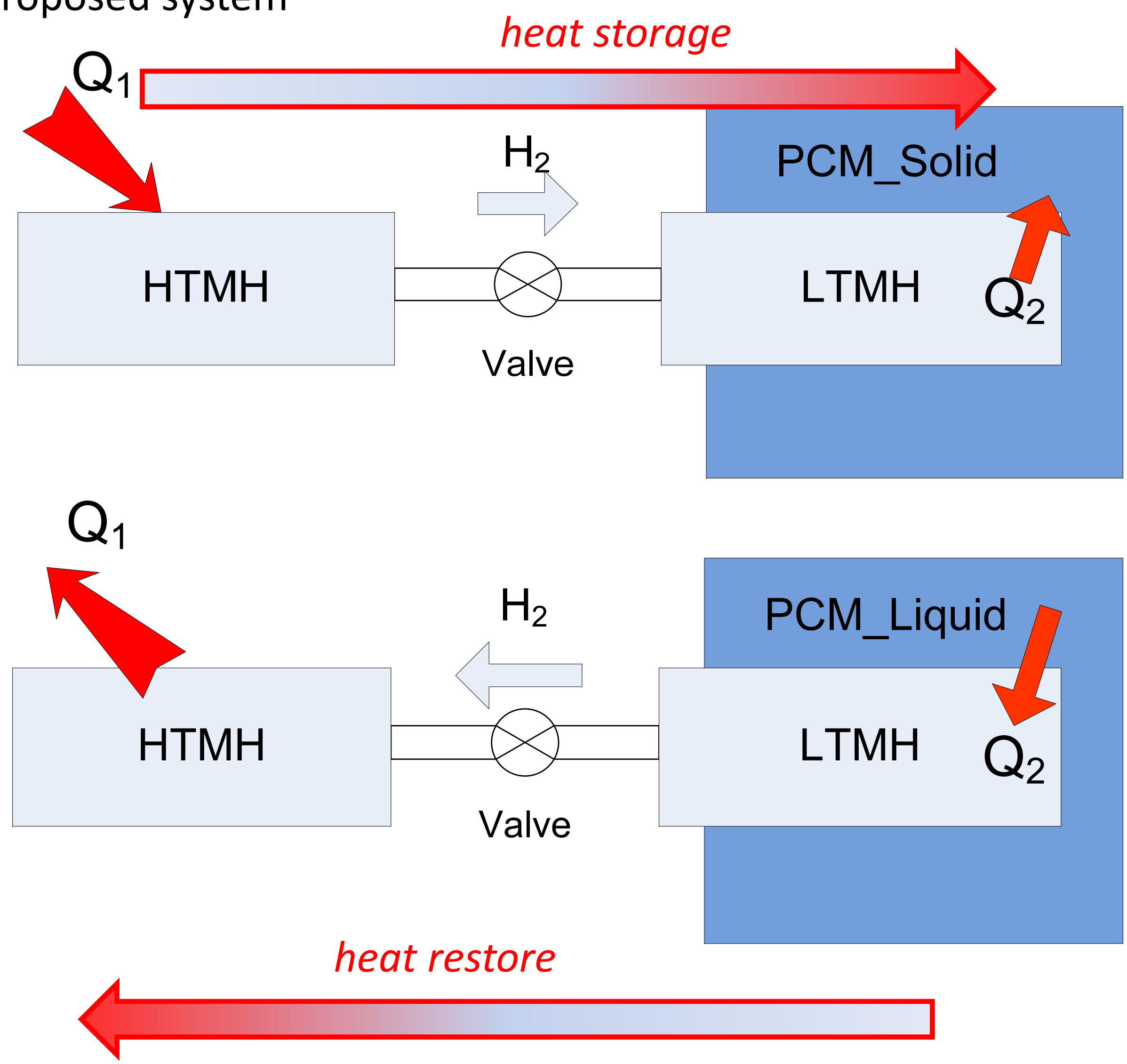
- Proposal of an energy storage system consisting of PCM encapsulated in a two-bed metal hydride heat storage
- Selection of PCM and metal hydride pairs with optimized properties
- Investigating by numerical simulation the overall performance of the storage system.
- Investigating the effect of PCM properties on the performance of the heat storage system

Conventional two-beds heat storage systems



Proposed concept of waste heat recovery, cont..

Proposed system



Overall Efficiency:

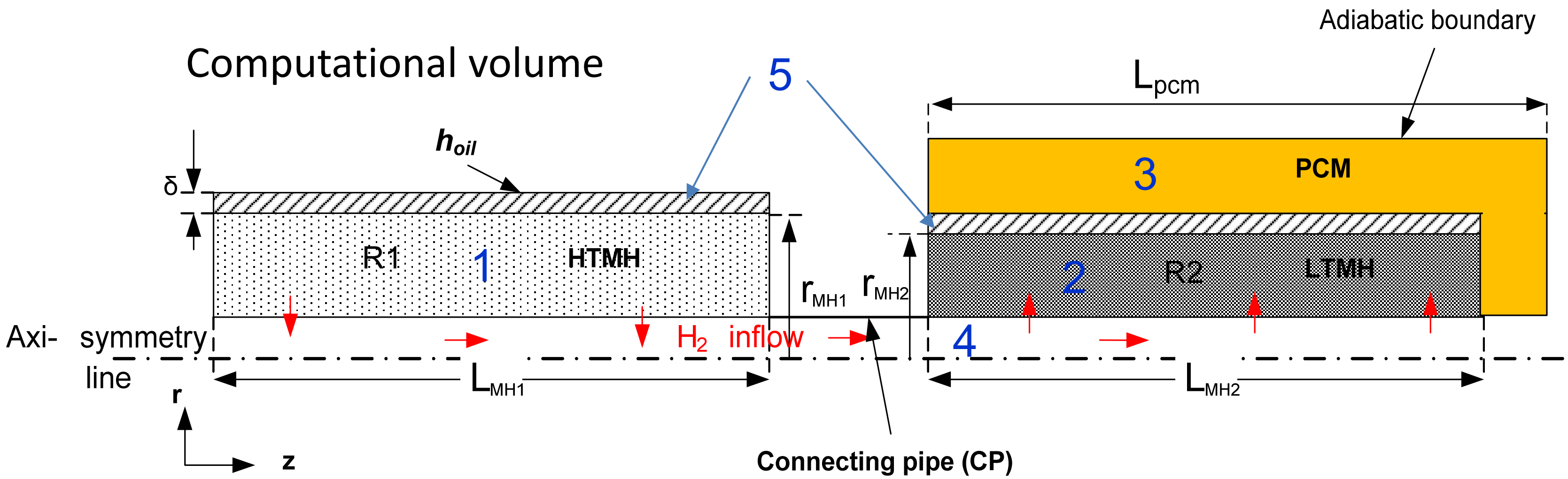
$$\eta = \frac{Q_1 - \varepsilon}{Q_1 + \varepsilon}$$

Alloy/PCM Selection

Parameter	Interstitial Hydrides		Complex Hydrides	
	AB_5	AB_2	MgH_2	Mg_2NiH_4
Heat of reaction (J/mol)	30000	18463	75000	64000
Entropy change	108	78.1	135	134.35
Reversible capacity (wt%)	1.3	1.5	7	3.5
Packing density (kg/m^3)	4200	3100	860	1600
Heat capacity (J/mol. K)	419	500	1545	1414
Max. Energy density (GJ/m^3)	0.81	0.43	2.26	1.8
	LTMH			HTMH

PCM	Melting Temperature/ o C	Density, Solid/liquid/ $kg \cdot m^{-3}$	Thermal conductivity/ $W \cdot m^{-1} \cdot K^{-1}$	Specific heat, Cp/ $J \cdot kg^{-1} \cdot K^{-1}$	Latent Heat of fusion/ $kJ \cdot kg^{-1}$	Volumetric heat capacity/ $MJ \cdot m^{-3}$
RT31	31	880/760	0.2	2000	165	145
RT42	42	880/760	0.2	2000	165	145

Numerical model



Basic assumptions:

- The thermo-physical properties of hydride are constant with regard to temperature and concentration.
- The thermal equilibrium between the gas and solid is established
- The jacket is perfectly insulated (adiabatic wall)
- The radiative heat transfer is neglected; this is the consequence of the previous one
- The hydrogen gas pressure inside the reaction bed is constant.
- The hysteresis in the equilibrium pressure is negligible for any material under study

Governing equations

Energy balance:

Domain 1,2: $$(\rho C_p)_{eff}\frac{\partial T}{\partial t} + \nabla\cdot\left(\rho_g C_{pg}\vec{V}T\right) = \lambda_{eff}\nabla^2 T + \frac{(1-\varepsilon)}{M_g}\rho_{MH} wt\frac{d\alpha}{dt}\Delta H$$

Domain 3: $$\rho_{mix}C_p(T_{pcm})\frac{\partial T_{pcm}}{\partial t} = \lambda_{mix}\nabla^2 T_{pcm}$$

Domain 4: $$(\rho C_p)_{wall}\frac{\partial T_{wall}}{\partial t} = \lambda_{wall}\nabla^2 T_{wall}$$

Momentum balance:

Darcy's law in domains 1 and 2: $$\vec{V} = -\frac{K_{eff}}{\mu_g}\nabla p$$

Navier-Stokes in domain 4: $$\frac{\partial}{\partial t}\cdot\left(\rho_g\vec{V}\right) + \nabla\cdot\left(\rho_g\vec{V}\cdot\vec{V}\right) = -\nabla p + \mu_g\nabla^2\vec{V}$$

Reaction kinetics domains 1 and 2 :

$$\varepsilon\frac{\partial\rho_g}{\partial t} + \nabla\cdot\left(\rho_g\vec{V}\right) = -(1-\varepsilon)\rho_{MH} wt\frac{d\alpha}{dt}$$

$$\frac{d\alpha}{dt} = k_{a,d}exp\left(\frac{E_{a,d}}{RT}\right)f_{a,d}(p)\,g_{a,d}(\alpha) \rightarrow \begin{cases} f_{a,d}(p) = \begin{cases} ln\left(\frac{p}{p_{eq}}\right) \\ \left(\frac{p-p_{eq}}{p_{eq}}\right) \end{cases} \\ g_{a,d}(\alpha) = \begin{cases} 1-\alpha \\ \alpha \end{cases} \end{cases}$$

$$\ln\left(\frac{p_{eq}}{p_0}\right) = \frac{\Delta H}{RT} - \frac{\Delta S}{R}$$

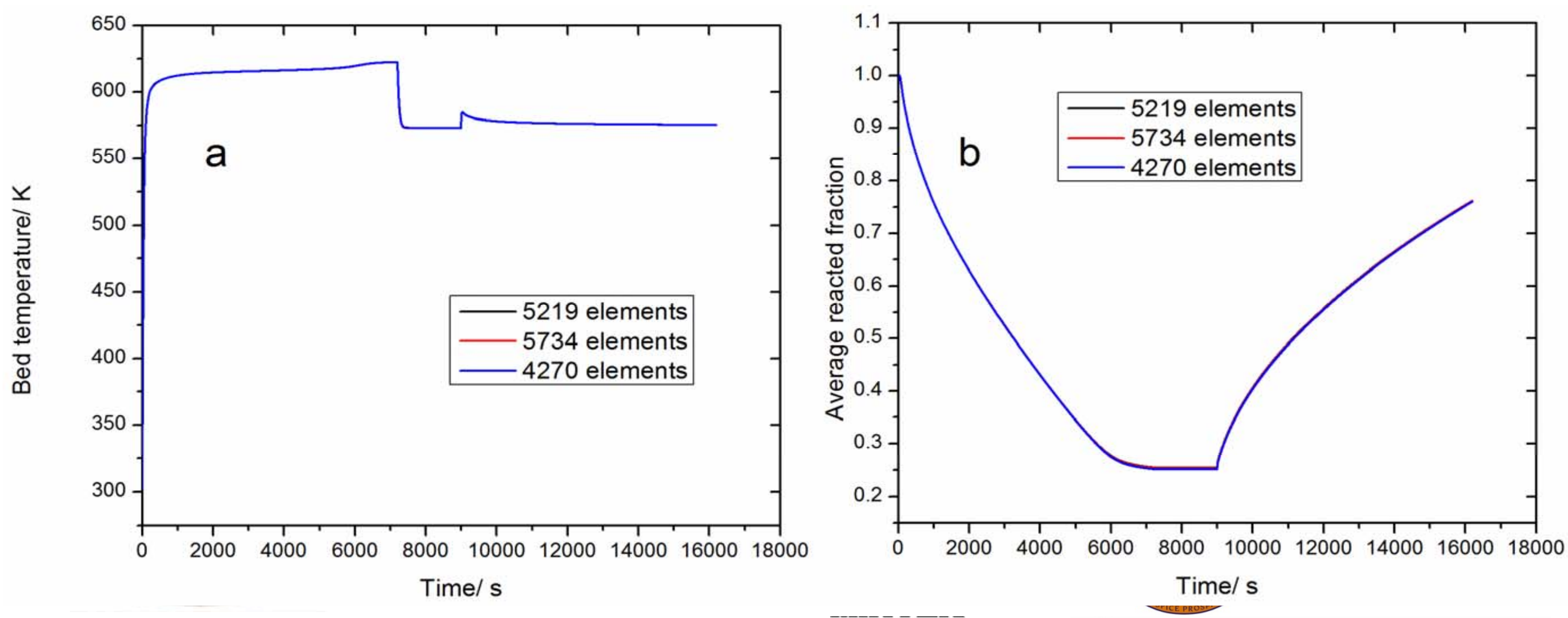
Parameters used in the simulation

	Mg_2Ni	$LaNi_5$
Enthalpy of formation / $kJ \cdot mol^{-1}$	64.5	30.5
Entropy of formation/ $J \cdot mol^{-1} K^{-1}$	122.2	108
Activation energy, abs-des/ $kJ \cdot mol^{-1}$	52.20/63.46	21.17/16.47
Rate constant abs-des/ s^{-1}	175/5452.2	59.18/9.57
Density/ $kg \cdot m^{-3}$	3200	8400
Specific heat, M-MH/ $J \cdot kg^{-1} \cdot K^{-1}$	697	419
Hydrogen capacity/ wt%	3.6	1.39
Porosity	0.5	0.5
Permeability/ m^2	1.3×10^{-12}	1.3×10^{-12}
Reactor radius/ m	0.018	0.018
H_2 filter radius, r_0 / m	0.003	0.003

Grid dependence

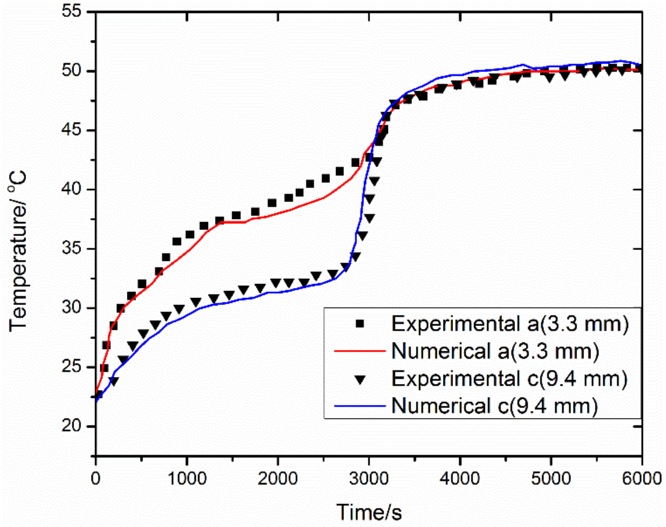
Parameter	4270	5219	5734
Energy density (MJ/m^3)	286.56	286.14	286.33
Power output ($W/kg\text{-}Mg_2Ni$)	91.95	91.84	91.94
Storage efficiency (%)	46.64	46.65	46.69

The absolute error is within 0.03%, therefore a mesh of 5219 elements is used for the simulation.



Model validation

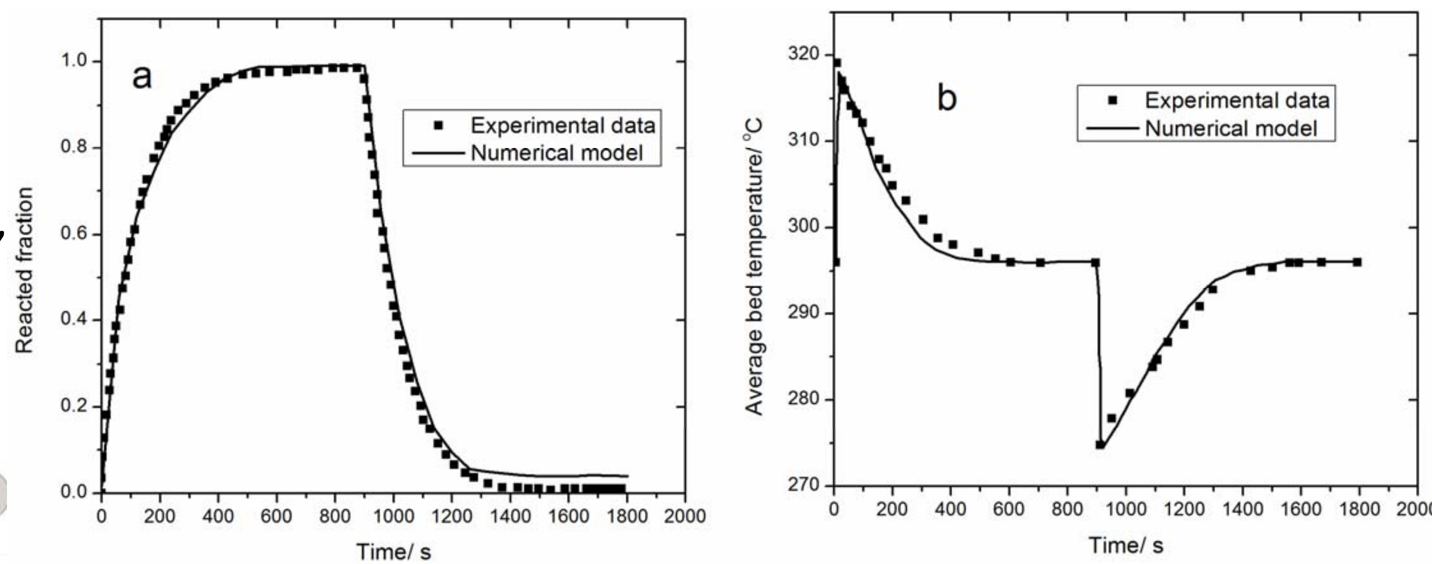
Heat storage using PCM, numerical validation



Longeon et al. Experimental and numerical study of annular PCM storage in the presence of natural convection. Applied Energy 2013; 112: 175-184

Laurencelle, goyette. Simulation of heat transfer in a metal hydride reactor with aluminum foam. Int J Hydrogen Energy 2007;32:2957-2964.

Metal hydride reactors, numerical validation



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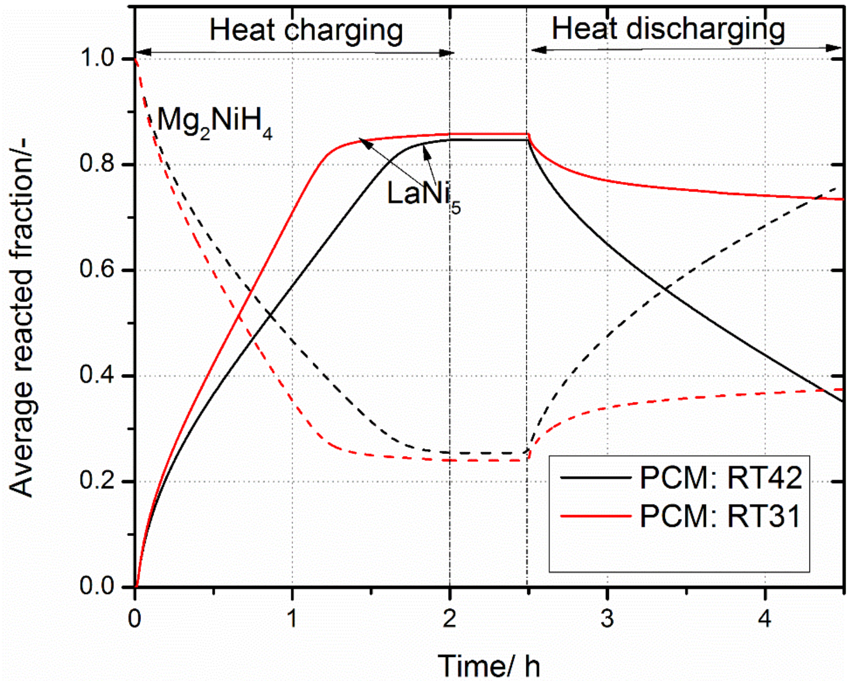
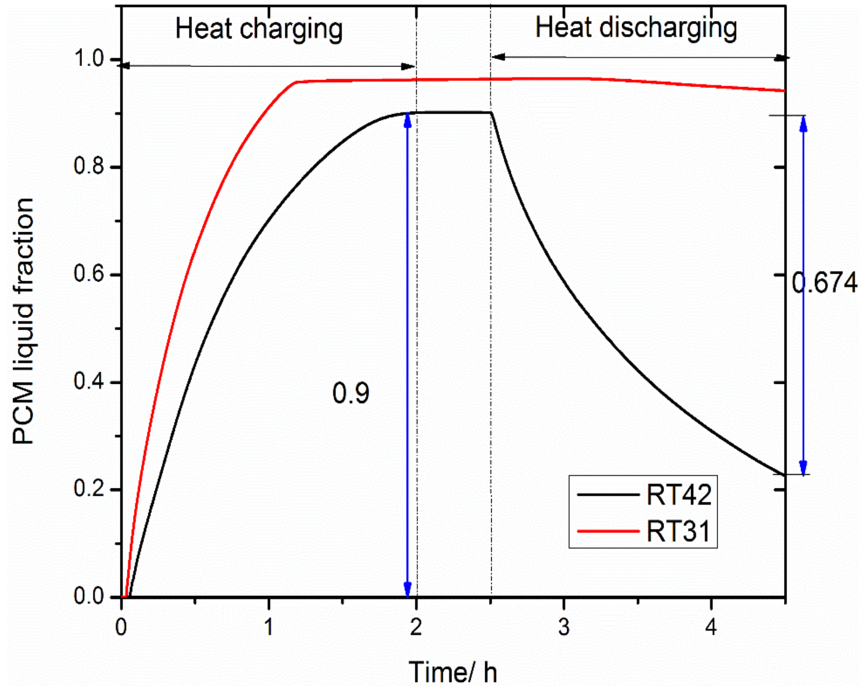
Results and discussion

Heat storage cycling

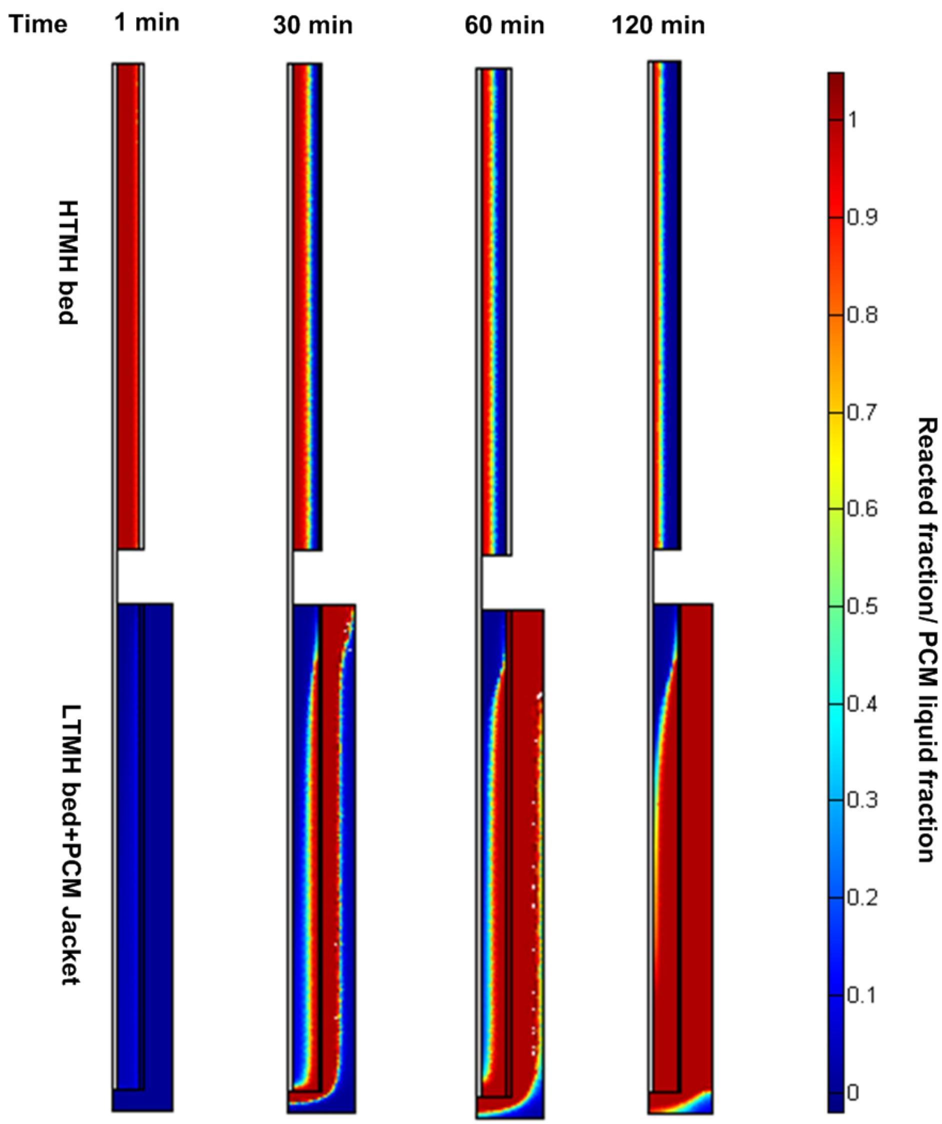


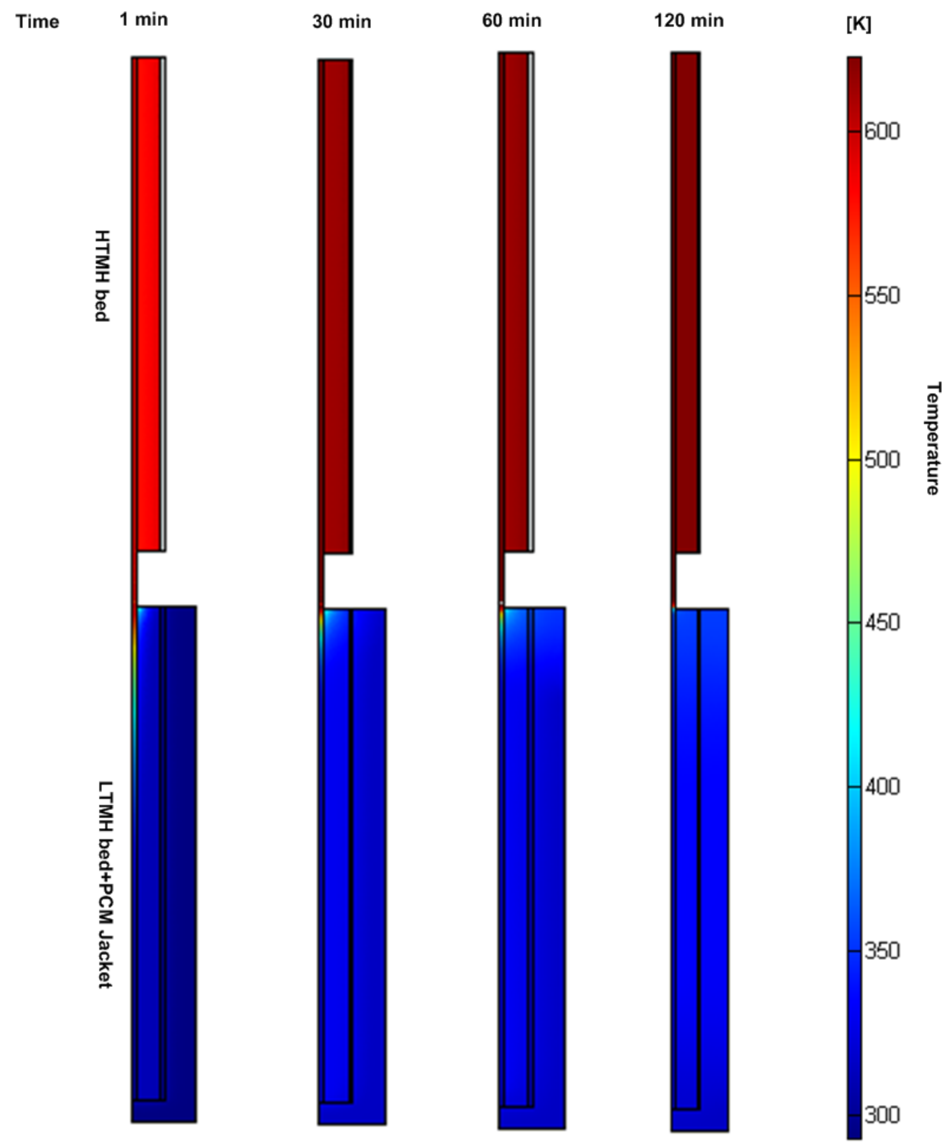
Temporal profile of PCM liquid fraction



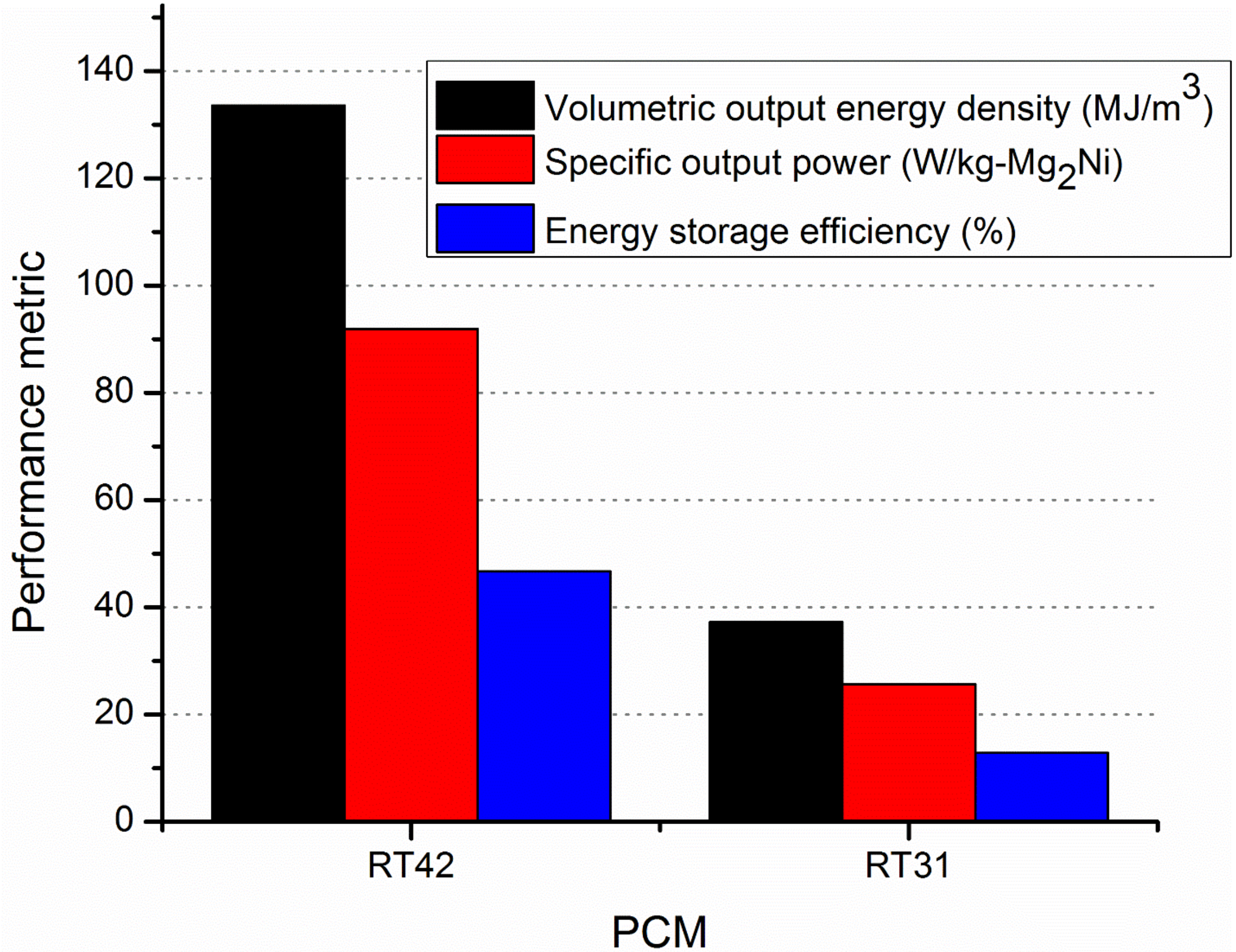
These figures shows how important is the selection of PCM melting temperature : as can be seen using RT42, 90 % of PCM liquefies during the heat charging while 67.4 % solidifies during the heat discharging process.

Bed temperature, reacted fraction, PCM liquid fraction distribution





Performance comparison



This Figure displays the performance of the heat storage system:
Using RT42 results in 133.57 MJ/m^3 energy density, 91.88 W/kg-Mg_2Ni of power output.

The waste heat recovery efficiency is 57 % giving a theoretical energy density of 234.3 MJ/m^3

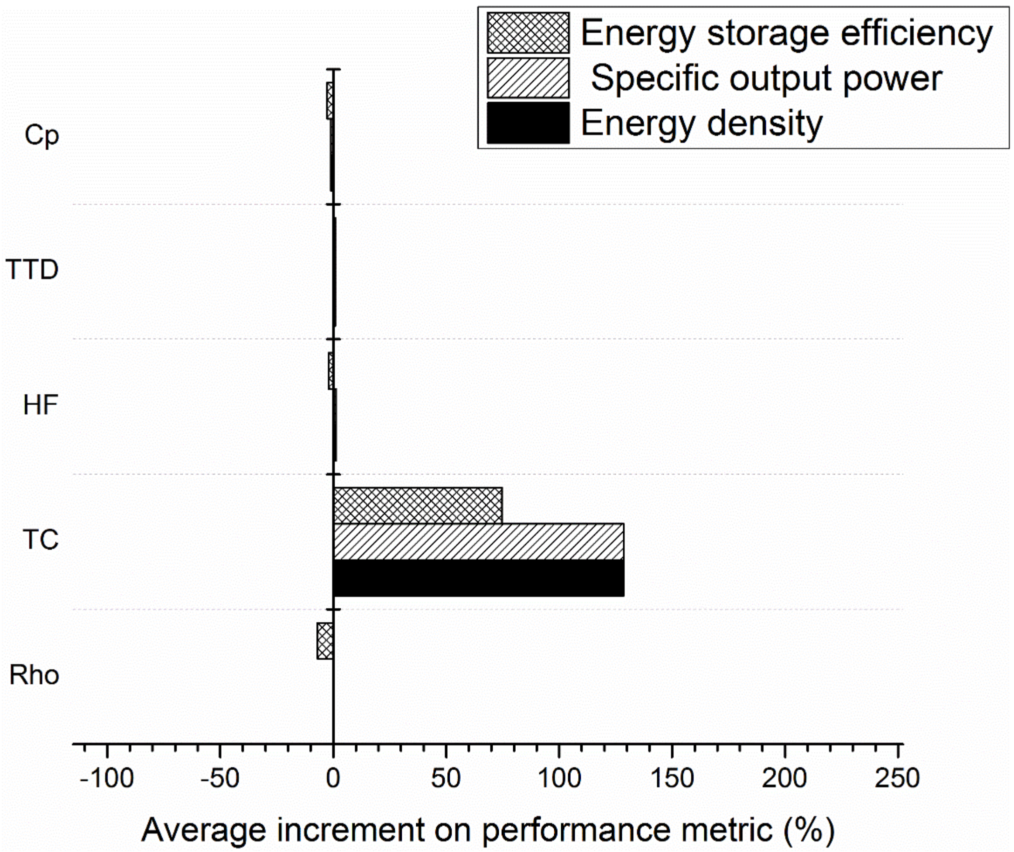
Sensitivity analysis

Aim: to detect the most influential factors on the performance metrics

Parameter	Range
PCM density (Rho)	780-2000 kg m^{-3}
Thermal conductivity (TC)	0.2-5 W m^{-1} K^{-1}
Latent heat of fusion(HF)	140-200 kJ kg^{-1}
Mushy region (phase transition) (TTD)	0.6-5 K
Heat capacity(Cp)	1800-2800 J kg^{-1} K^{-1}

The parametric study is done by varying one factor and fixing the others to the baseline parameters (RT42).

Sensitivity analysis



- As the heat capacity increases, the specific power ,energy density and energy storage efficiency decrease by (1.14) and 2.74 % ,
- As the transition temperature difference (TTD) increases, the power density, energy density and energy efficiency increase by no more than a percent (0.96 %)
- The increase of PCM heat of fusion leads to 1.29 % increasing in power and energy density at a cost of energy efficiency (-2 %)
- The increase of the PCM thermal conductivity brings about 128.6 % augmentation of energy storage density and 74.65 % in energy storage efficiency improvement.
- The increase of the PCM density reduces the energy storage efficiency by 6.88 %

Conclusions

- TES is imperative to make waste heat recovery (and other renewable energy sources) more reliable and competitive.
- Further research into latent and thermochemical TES materials can improve the efficiency of waste heat recovery.
- Metal hydrides are a viable option as TES materials. Further, Mg-based hydrides can be used in waste-heat related energy storage with an storage efficiency higher than 50%.
- Future work will involve modelling of different MH materials (in particular those based on Mg) to identify alloys with favourable thermodynamic and kinetic behaviour.

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- Mykhaylo Lototskyy

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Thank you for listening!

Any questions?

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