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




S. Nyallang Nyamsi, Ivan Tolj & M. Lototskyy

HYPOTHESIS 2019, Foz do Iguaçu, Brazil

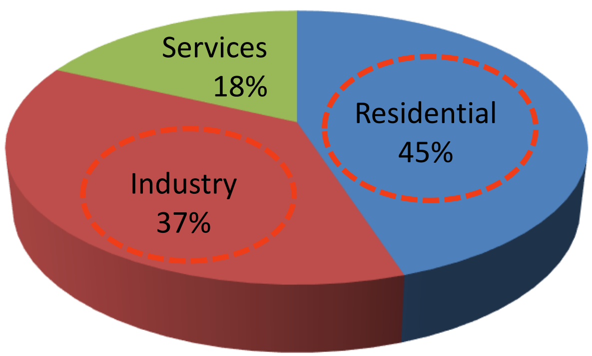
Contents

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.

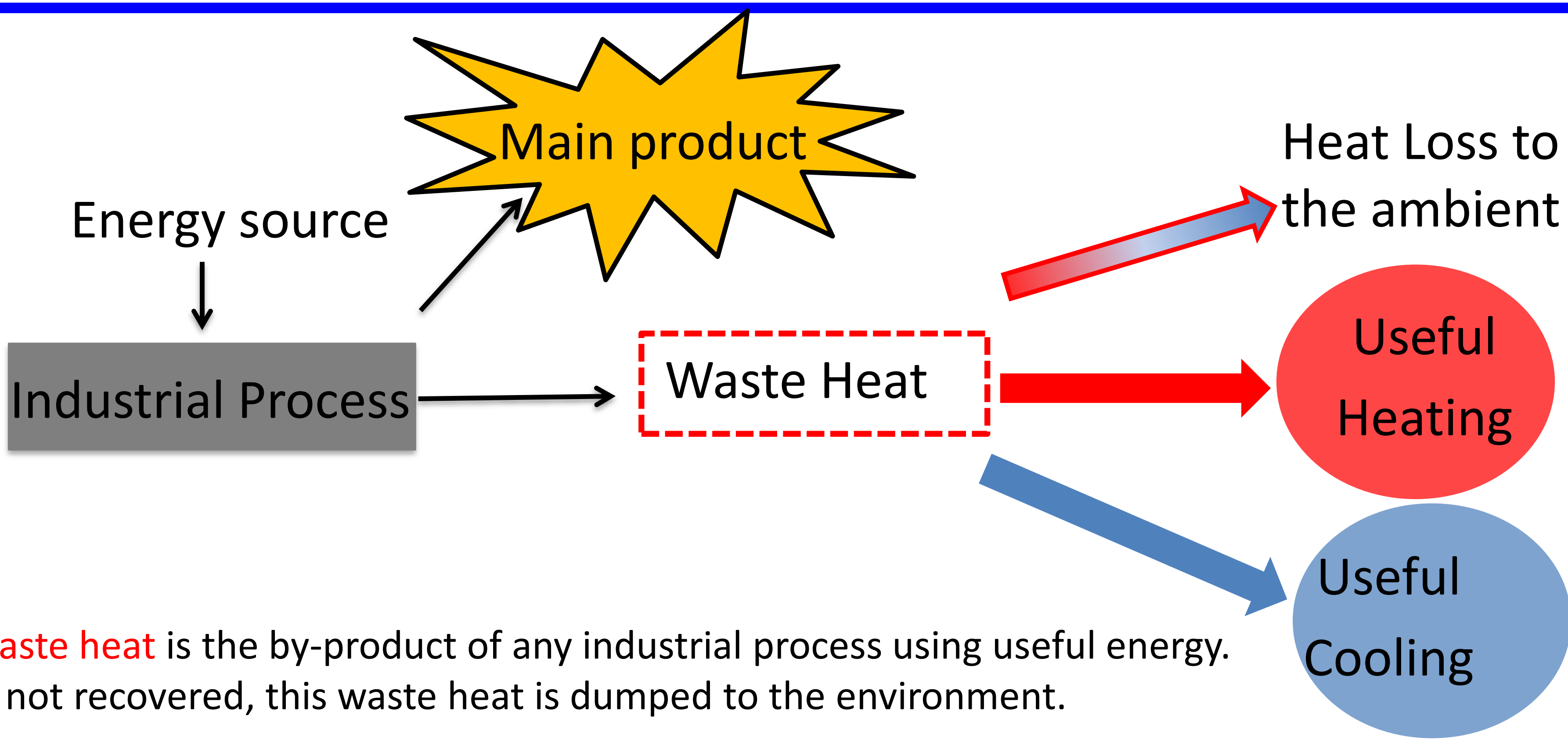


Approximate breakdown of energy consumption in heating & cooling sector

Two of the major target areas for:

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

Waste heat

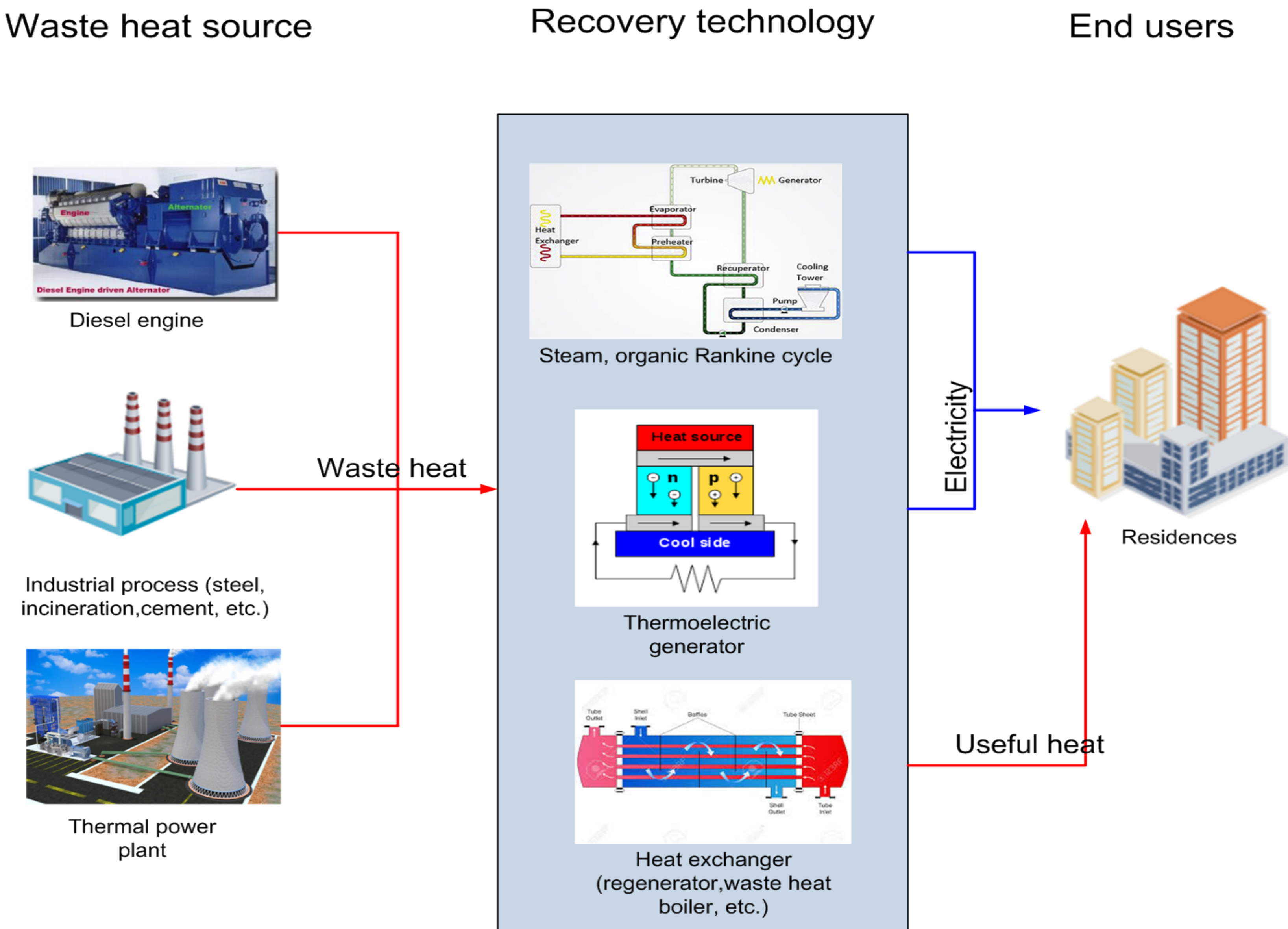


Waste heat is the by-product of any industrial process using useful energy. If not recovered, this waste heat is dumped to the environment.

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

Conventional waste heat recovery



Waste Heat source/temperature quality

Low Temperature heat source

- Internal combustion engine: 60-150 ^{o} C
- Hot processed liquids and solids: 32-232 ^{o} C
- PEM fuel cells: 30-60 ^{o} C

Medium Temperature heat source

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

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

High temperature heat source

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

UNIVERSITY *of the* WESTERN CAPE

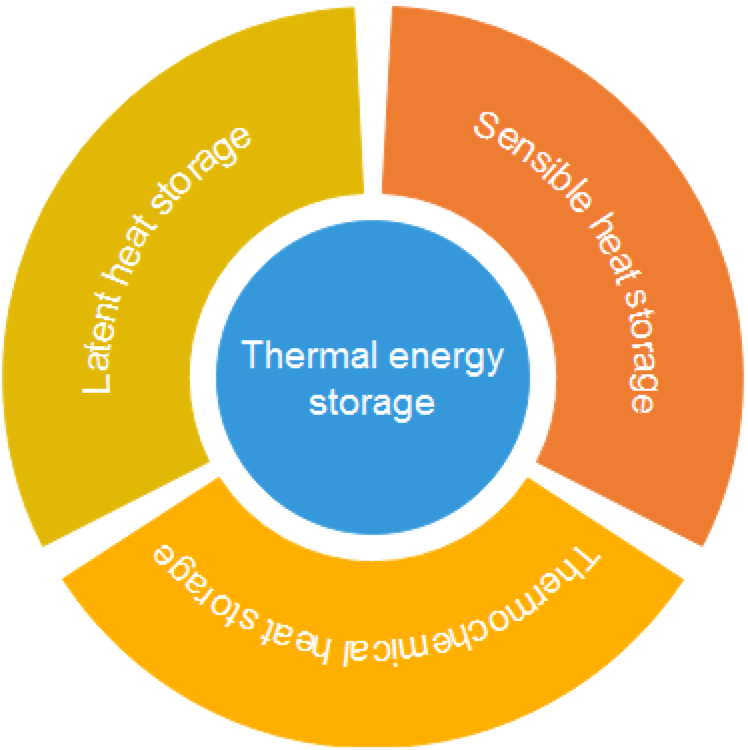
Thermal Energy Storage

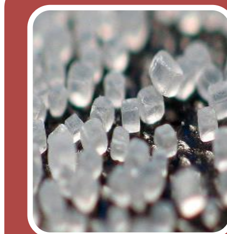
Thermal energy storage (TES) stocks thermal energy by heating or cooling a storage medium so that the stored energy can be used at a later time for heating & cooling applications, as well as power generation.

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.

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.

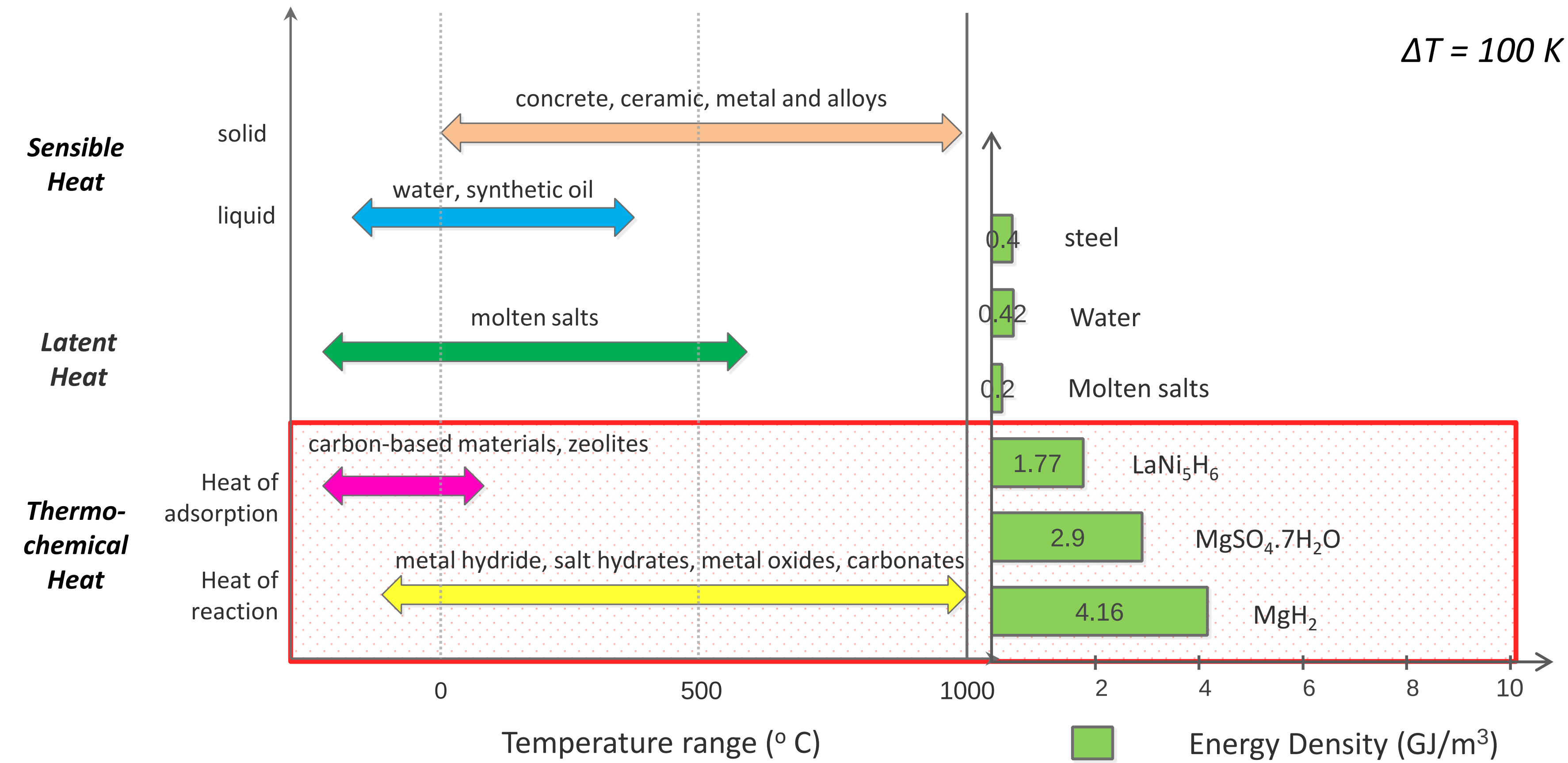
Thermochemical Storage

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

HySA Systems Hydrogen South Africa

UNIVERSITY *of the* WESTERN CAPE

Thermal Energy Storage



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: $\eta = \dfrac{Q_r}{Q_s}$

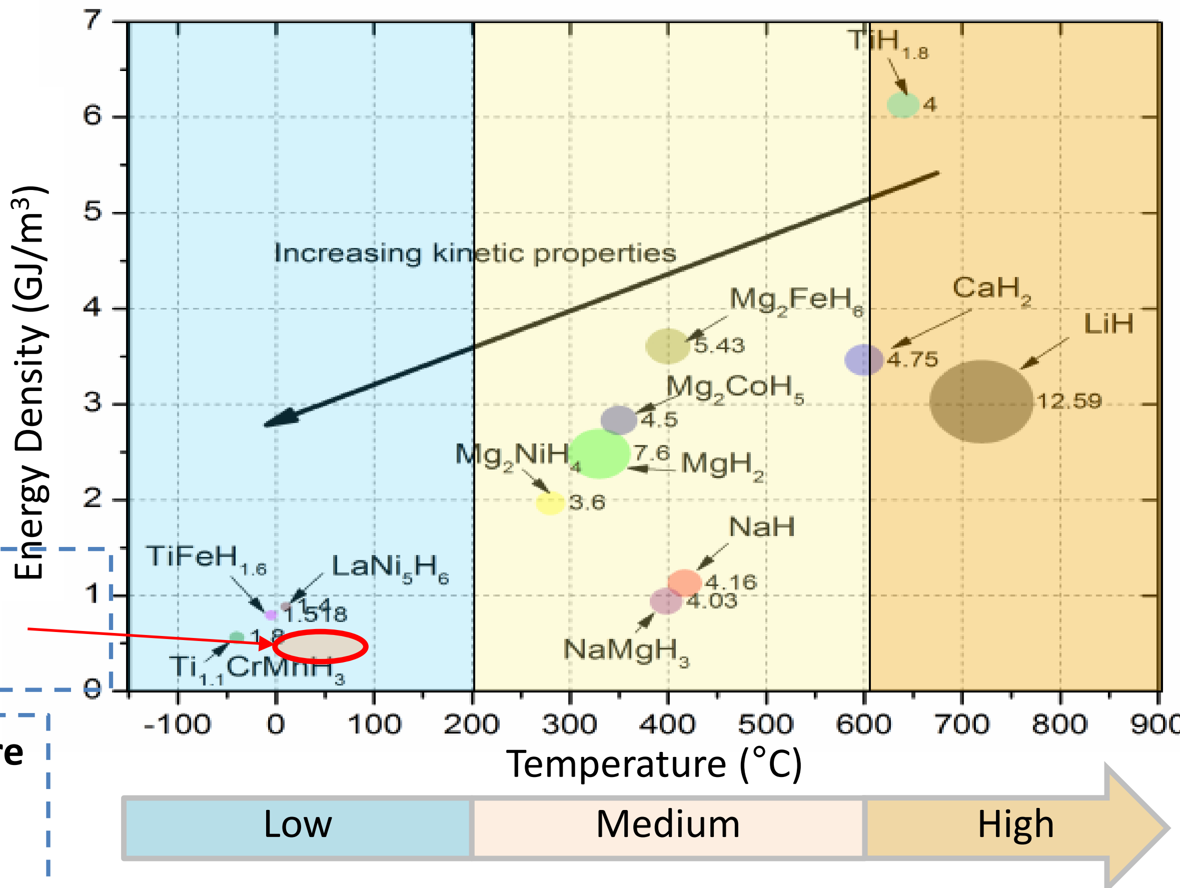
Selecting

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.

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.

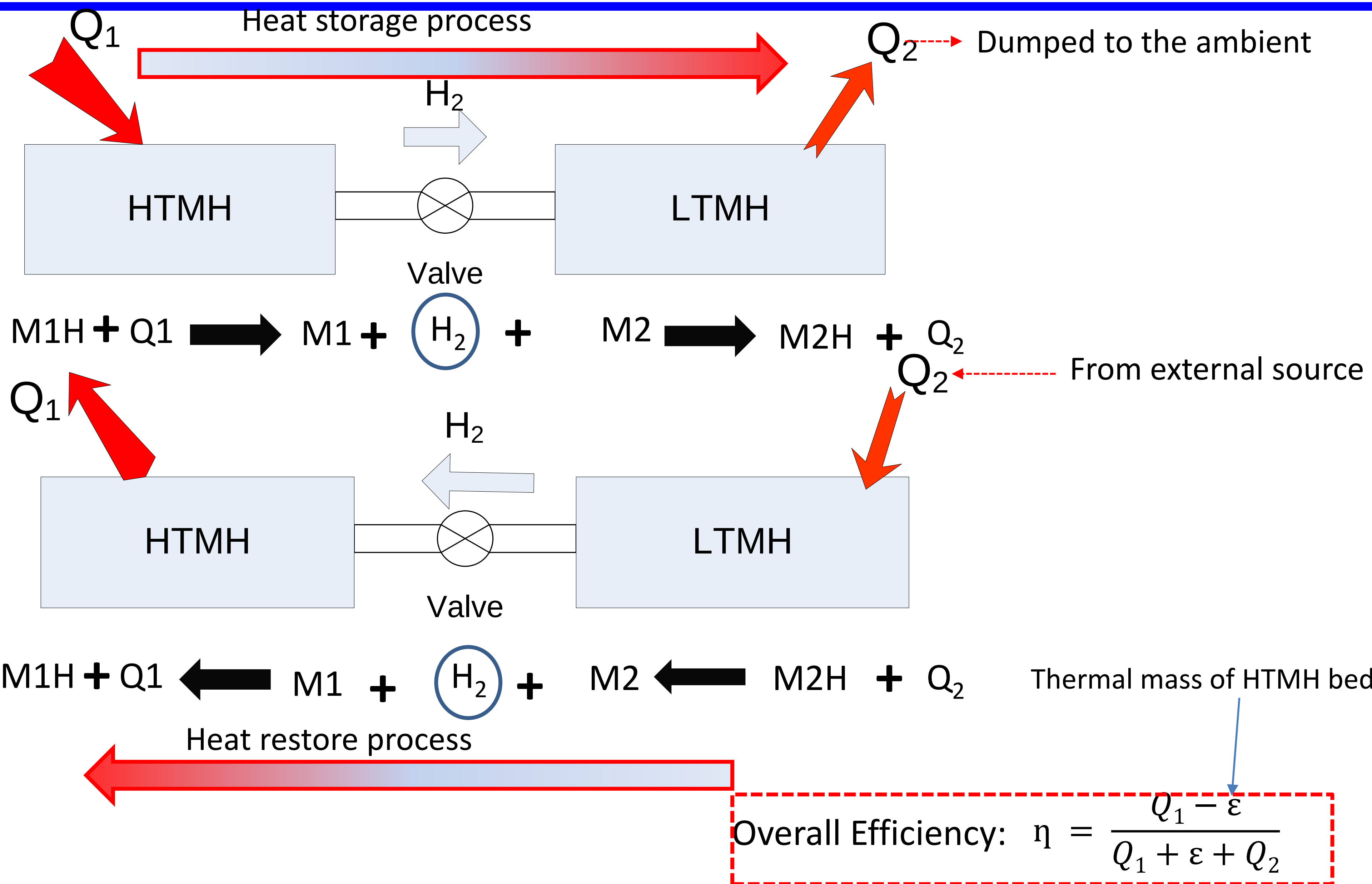
Objectives

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

Sub-objectives:

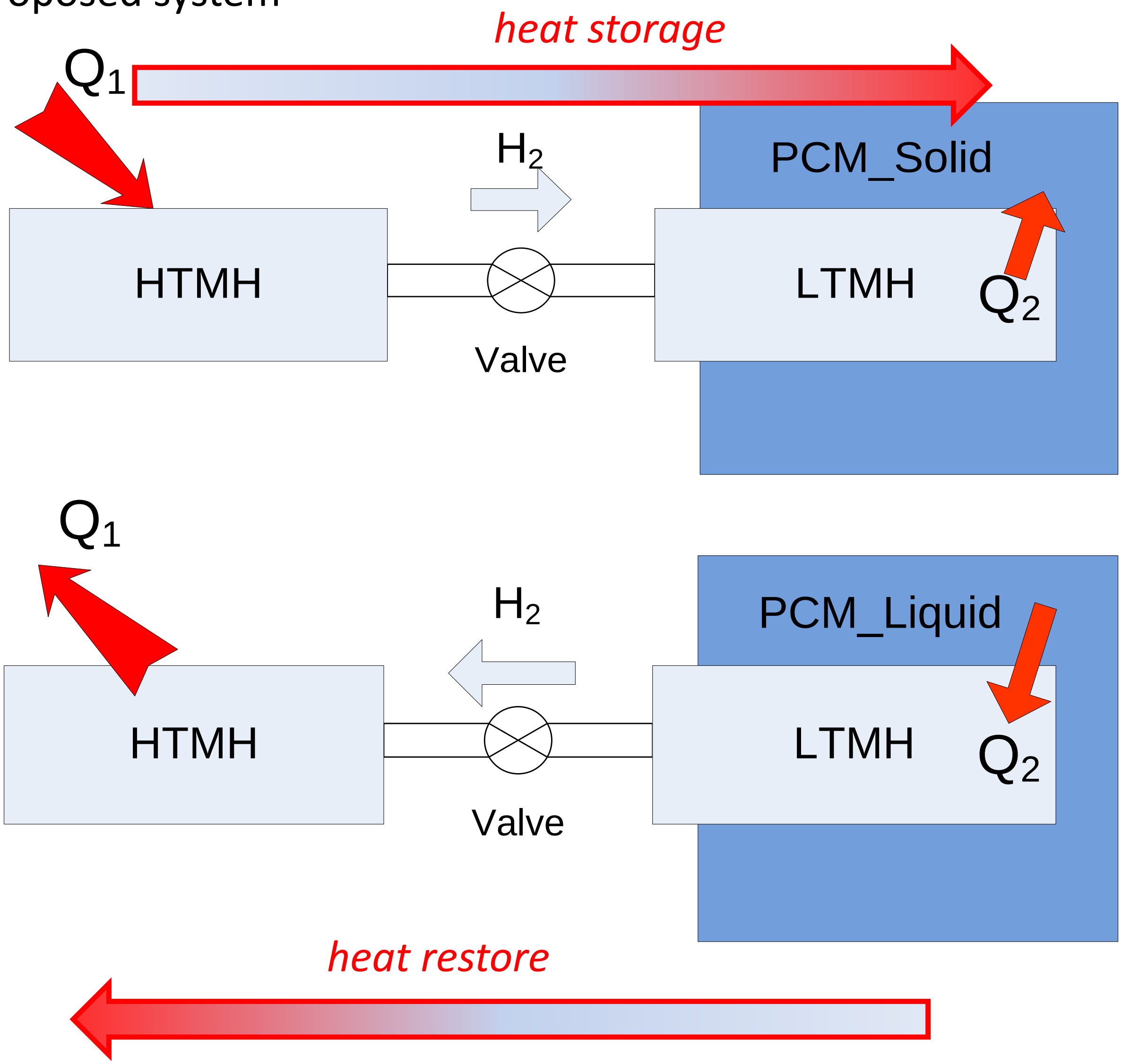
- Proposal of an energy storage system consisting of PCM encapsulated in a two-bed metal hydride heat storage
- Selection of PCM and metal hydride pairs with optimized properties
- Investigating by numerical simulation the overall performance of the storage system.
- Investigating the effect of PCM properties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

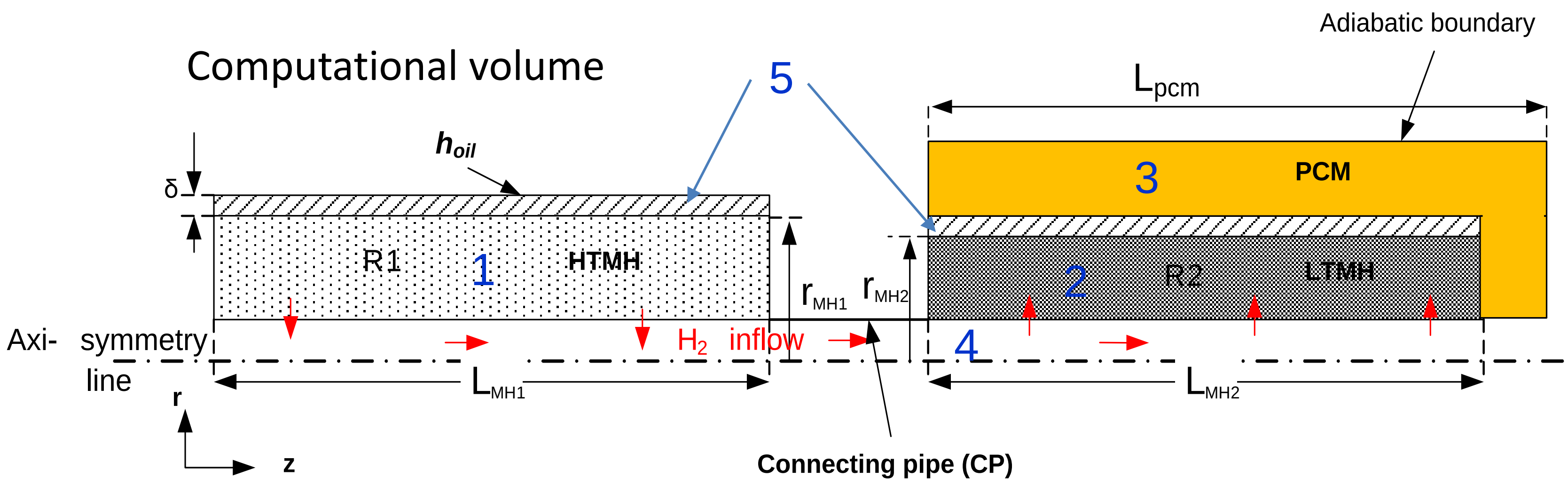
$$\eta = \frac{Q_1 - \varepsilon}{Q_1 + \varepsilon}$$

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 :

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

$$\frac{d\alpha}{dt} = k_{a,d}exp\left(\frac{E_{a,d}}{RT}\right)f_{a,d}(p)\,g_{a,d}(\alpha)$$

$$f_{a,d}(p) = \begin{cases} ln\left(\frac{p}{p_{eq}}\right) \\ \left(\frac{p-p_{eq}}{p_{eq}}\right) \end{cases}$$

$$g_{a,d}(\alpha) = \begin{cases} 1-\alpha \\ \alpha \end{cases}$$

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

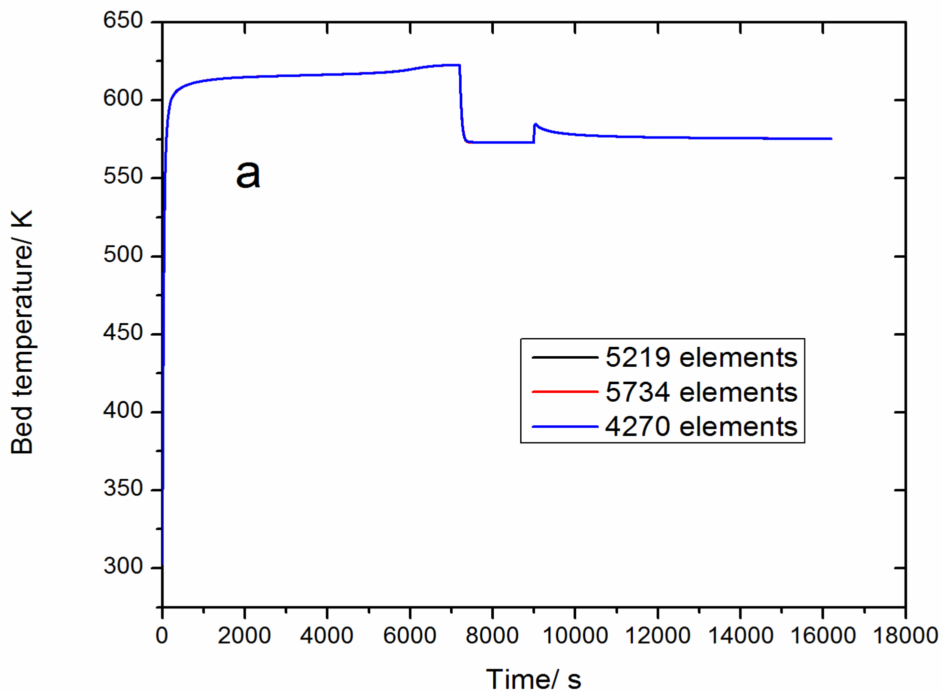
Parameters used in the simulation

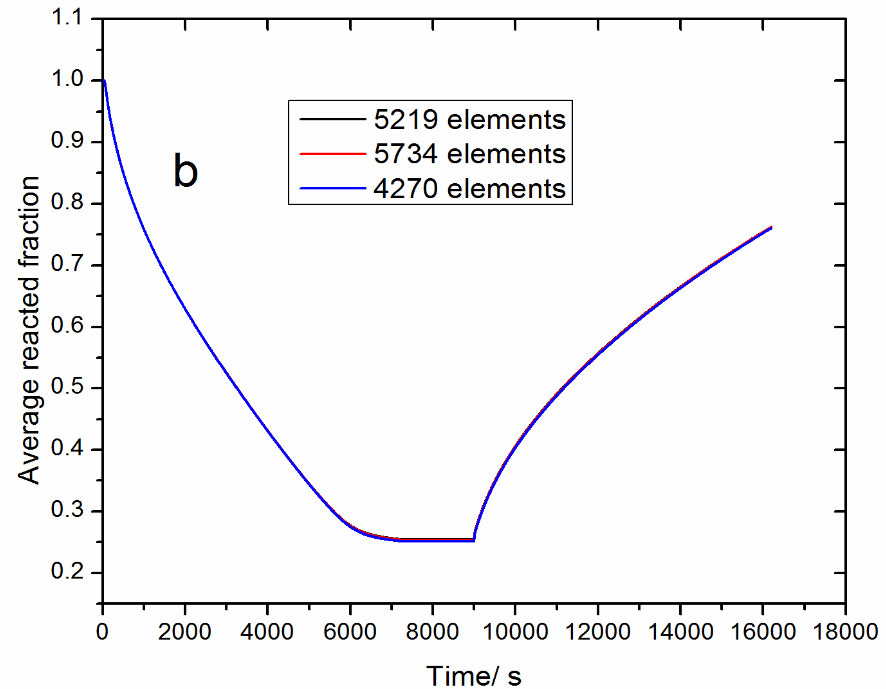
	Mg_2Ni	$LaNi_5$
Enthalpy of formation / $kJ{\cdot}mol^{-1}$	64.5	30.5
Entropy of formation/ $J{\cdot}mol^{-1}K^{-1}$	122.2	108
Activation energy, abs-des/ $kJ{\cdot}mol^{-1}$	52.20/63.46	21.17/16.47
Rate constant abs-des/ s^{-1}	175/5452.2	59.18/9.57
Density/ $kg{\cdot}m^{-3}$	3200	8400
Specific heat, 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-Mg_2Ni)	91.95	91.84	91.94
Storage efficiency (%)	46.64	46.65	46.69

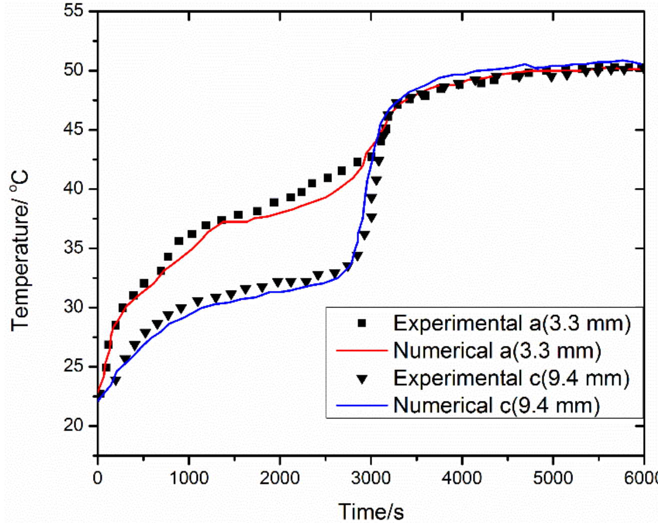
The absolute error is within 0.03%, therefore a mesh of 5219 elements is used for the simulation.





Model validation

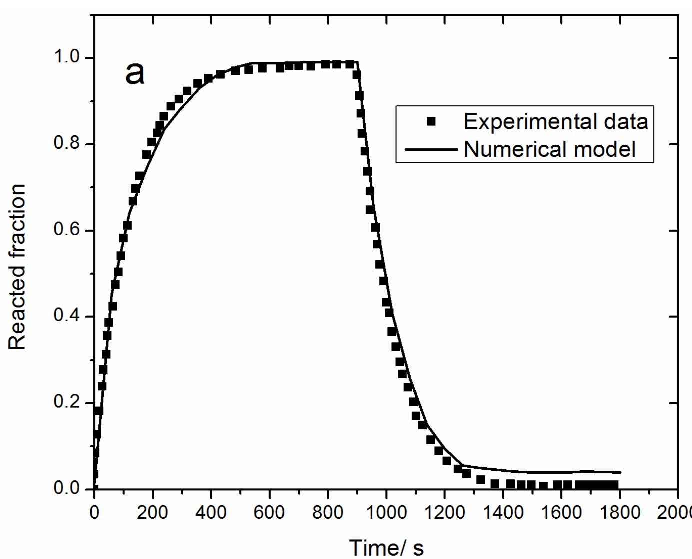
Heat storage using PCM, numerical validation

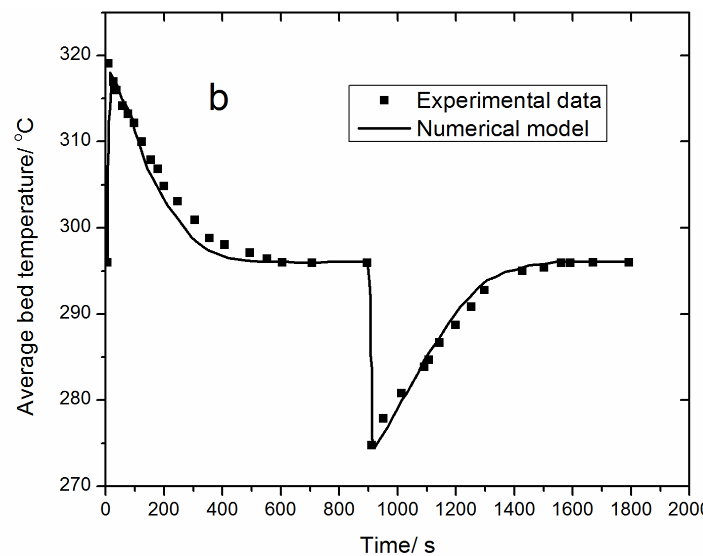


Longeon et al. Experimental and numerical study of annular PCM storage in the presence of natural convection. Applied Energy 2013; 112: 175-184

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

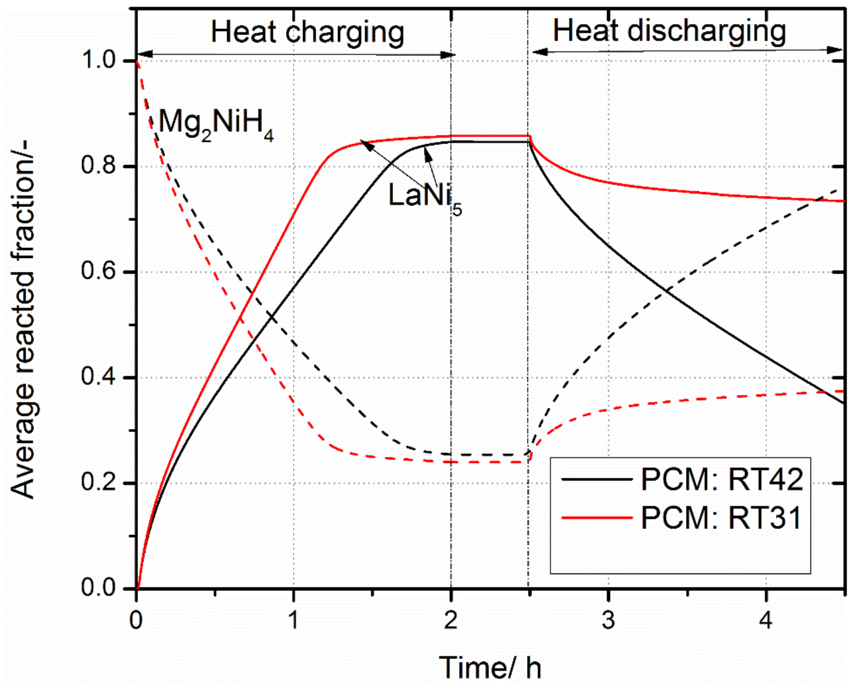
Metal hydride reactors, numerical validation



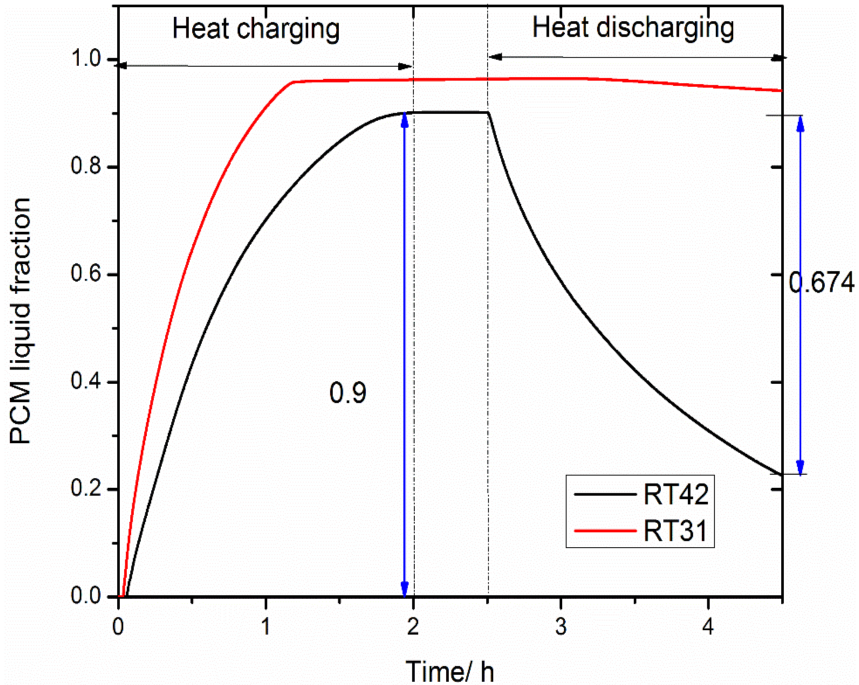


Results and discussion

Heat storage cycling

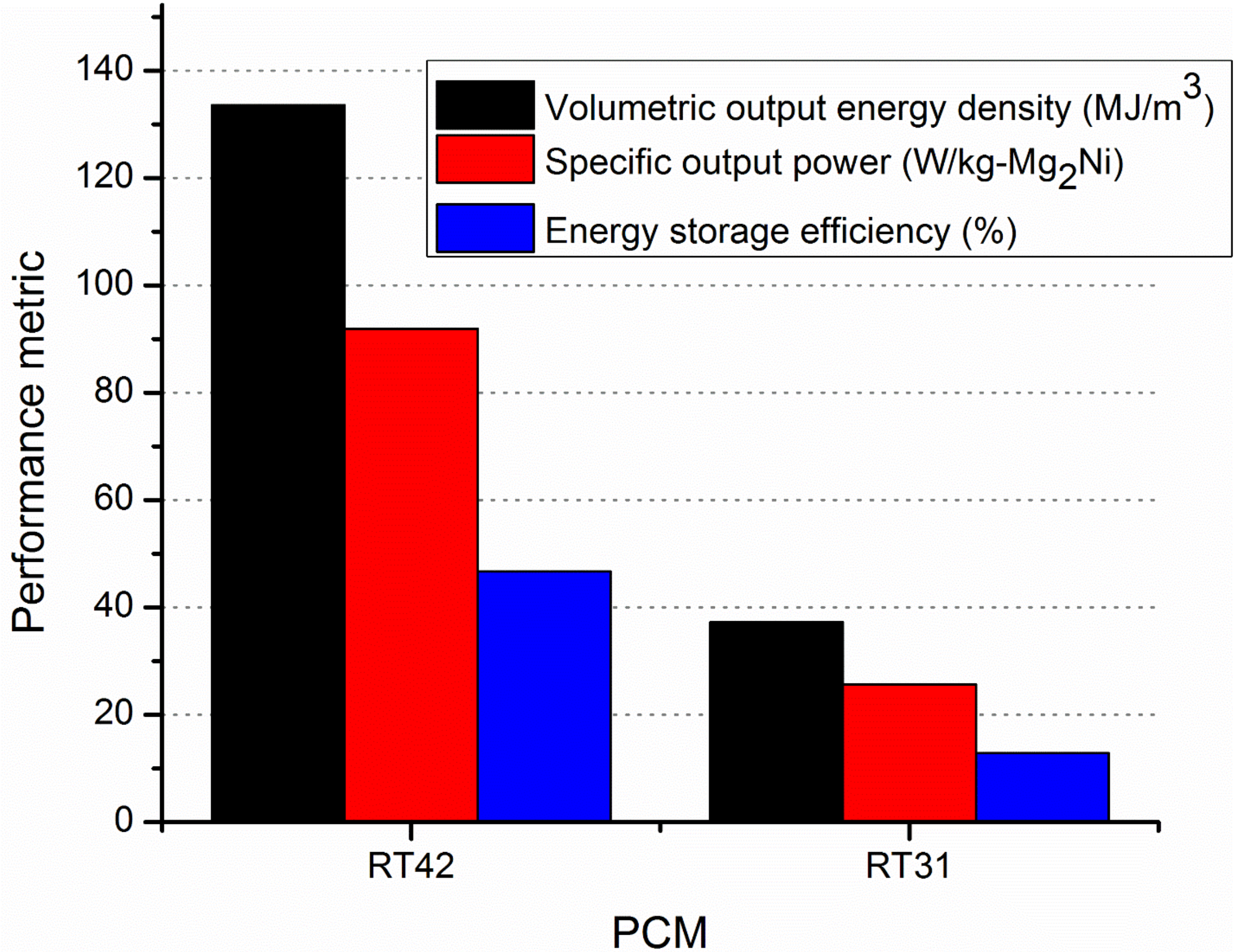


Temporal profile of PCM liquid fraction



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.

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

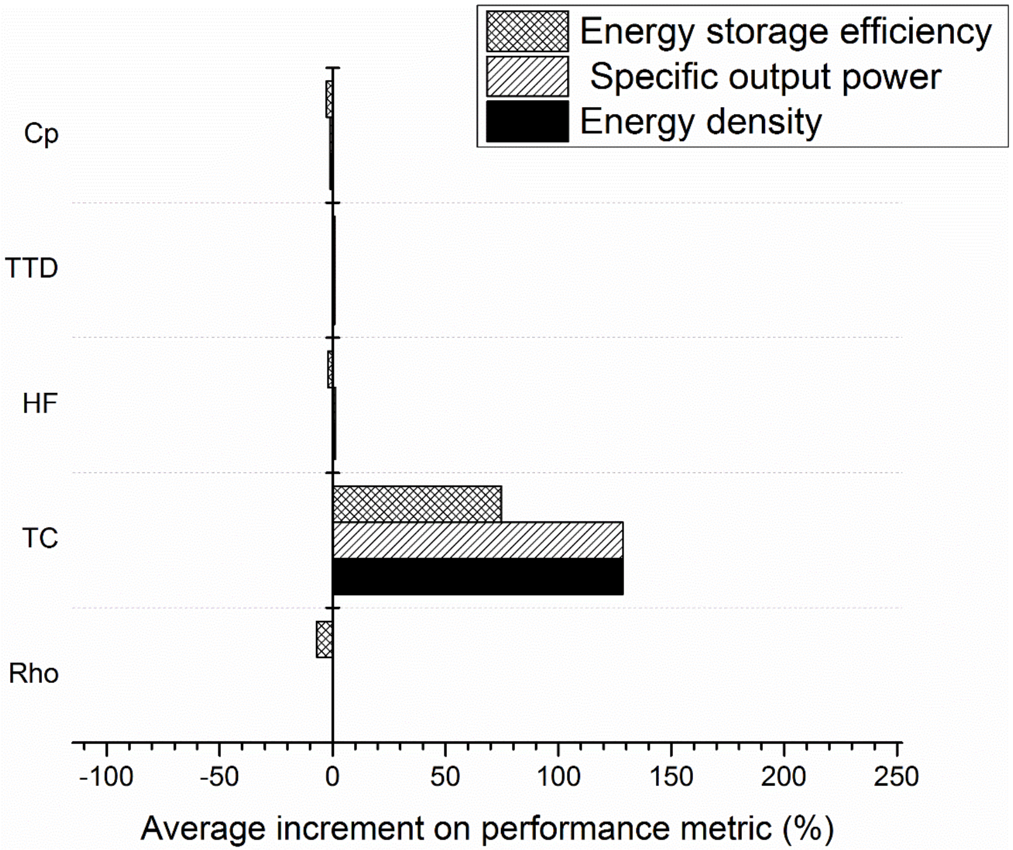
Sensitivity analysis

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.

Contributors & Acknowledgements

I wish to thank the following people who contributed to this presentation:

- Serge Nyallang Nyamsi
- Mykhaylo Lototskyy

Acknowledgements

This project was supported by the FP7 program ERAfrica, project RE-037 Advanced Hydrogen Energy Systems ‘HENERGY’ and HORIZON2020 – RISE 2017 project ‘HYDRIDE4MOBILITY’ project number 778307.

Thank you for listening!

Any questions?

www.hysasystems.com