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sowHat

Kinetic modelling of thermochemical
energy storage reactions for storage
of solar heat and waste heat

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Outline and Objectives

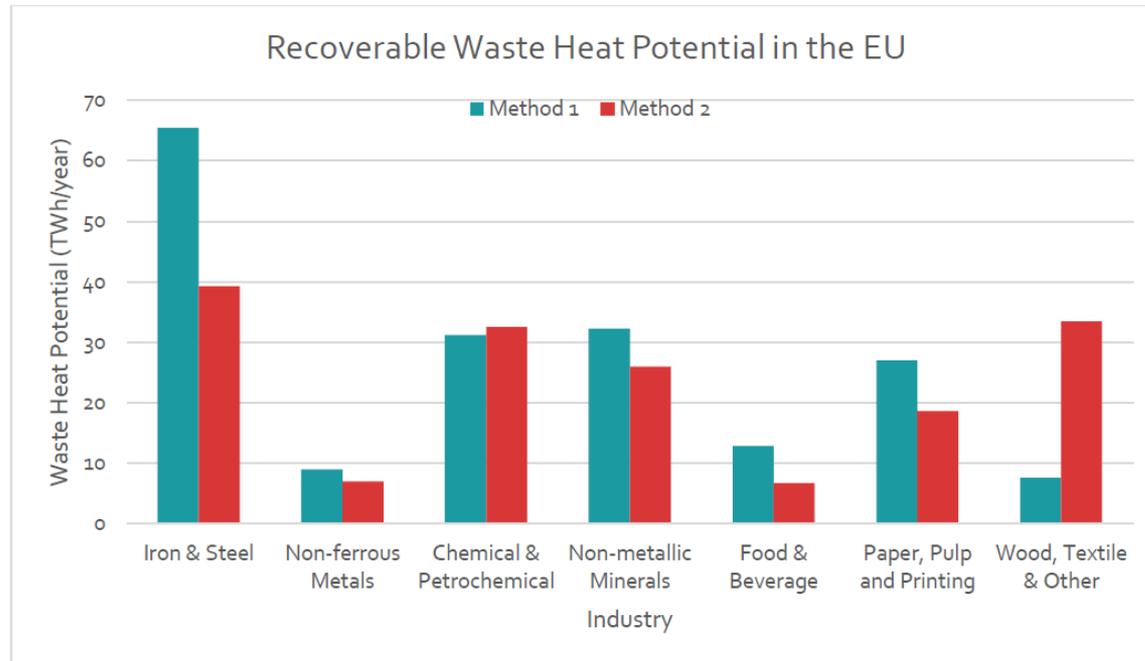


- Specific Challenge Introduce H2020 project: Supporting new opportunities for waste heat and cold valorisation toward EU decarbonisation
- Address the role waste heat recovery and thermal/thermochemical energy storage within the context of WH/C valorisation strategies
- Present selection strategy for best integration of thermal/thermochemical storage strategy to support WH/C valorisation

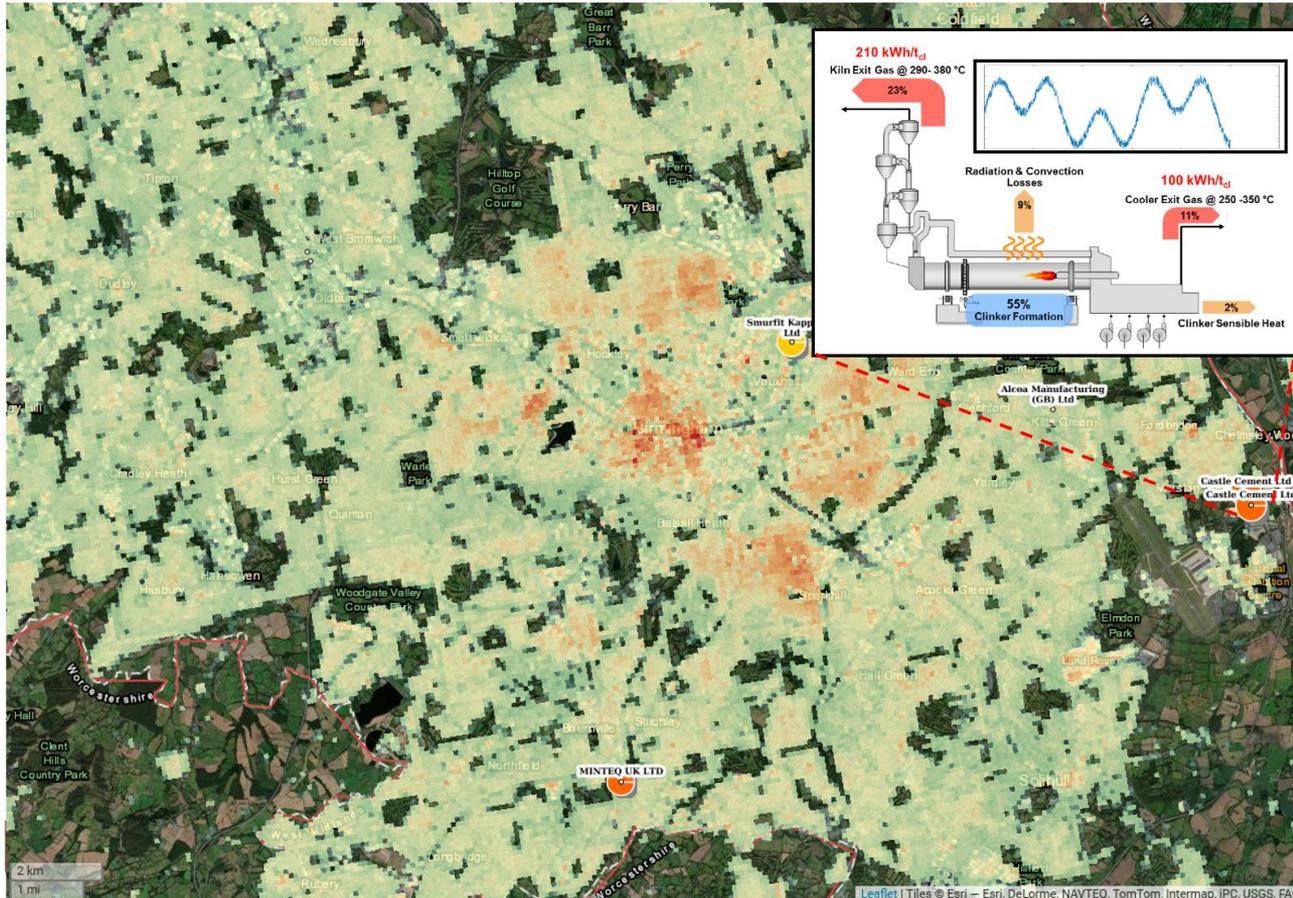


The Challenge

Current studies on the quantification of available industrial waste heat volumes showed that, in the EU, the amount of heat wasted by industries in the form of hot water or flue gases would be sufficient to cover a significant portion of EU's heating needs



From Monitoring-to-Design-to-Technologies-to-Maintenance aspects



This Project

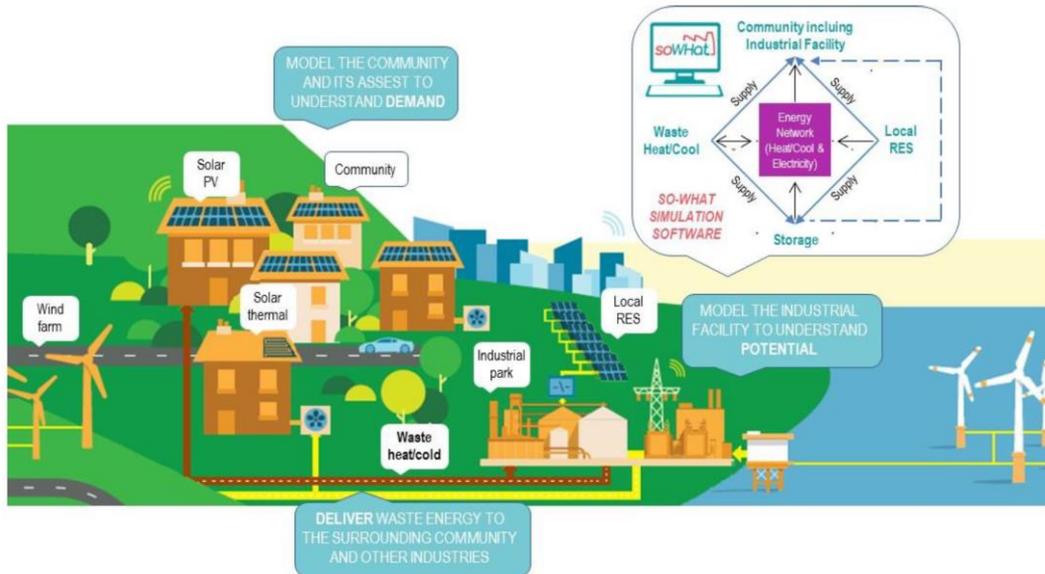
Document N. 847097



Supporting new Opportunities for Waste Heat And cold valorisation Towards EU decarbonization



- Develop and validate, through different sector and countries real industrial test cases, an integrated software for auditing industrial process, planning and simulation of waste heat and cold (WH/C) valorisation systems towards the identification of economically viable scenarios where WH/C and renewable energy sources (RES) cooperate to match local demand



Consortium

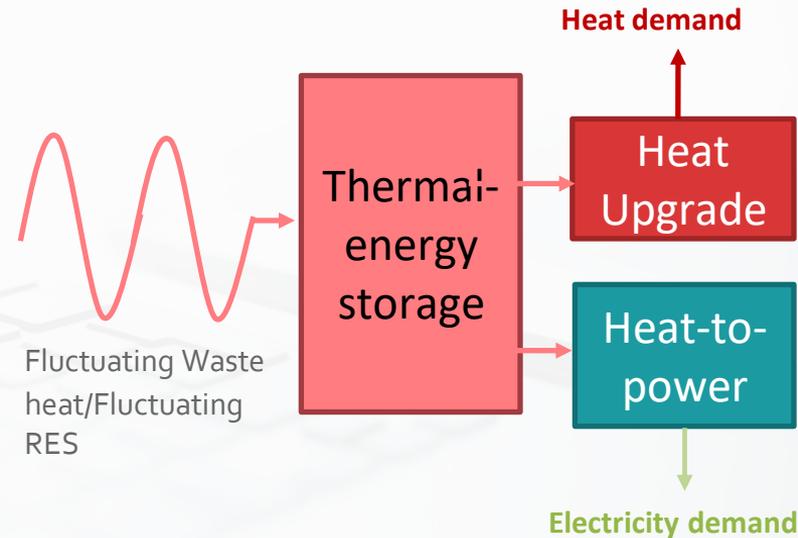


Role of WH/C and TES technologies in SO-WHAT Project



Barriers SO-WHAT aims to overcome:

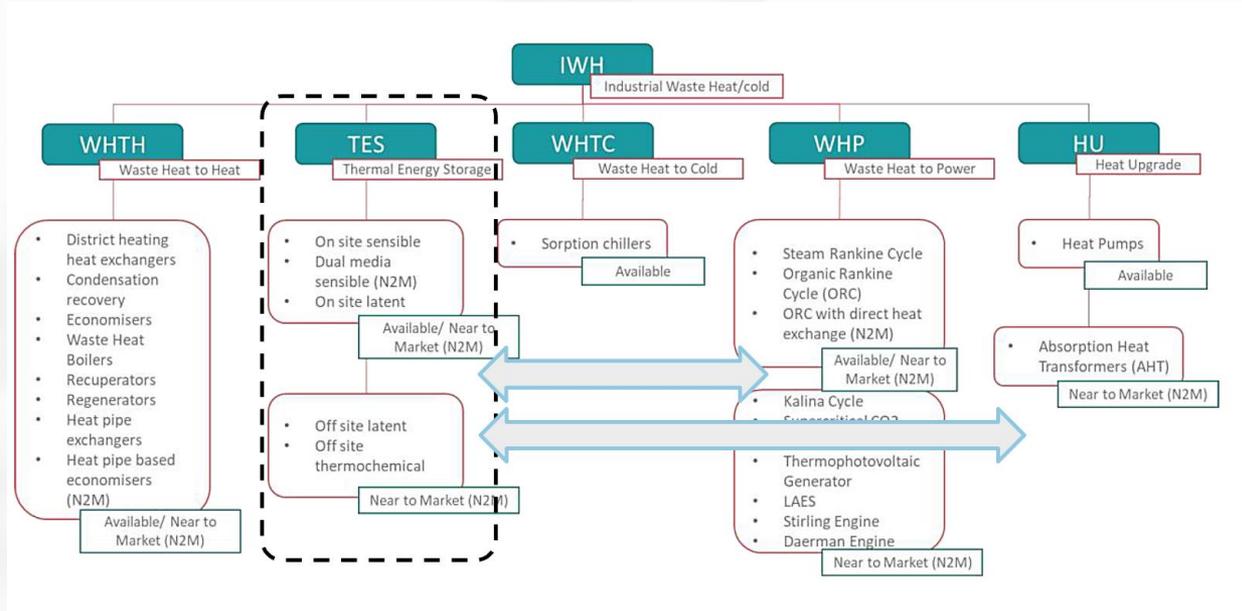
- **Uncertainties prevents investors to go ahead to realization of these WH/C investments** – a dedicated framework (technical, economic and environmental) tailored to assess and reduce such uncertainty
- **Deployment of WH/C solutions is a complex process involving a number of actors along the value chain:** industrial facilities (owner of WH/C), investors, heating providers, DH managers, tech providers, energy-companies and end users
- **Perception of technological reliability of the solutions needs to be improved, especially with reference to the WH/C capture systems with the aim of increasing the overall efficiency and the operating time system, also thanks to the Thermal Energy Storage Integration**



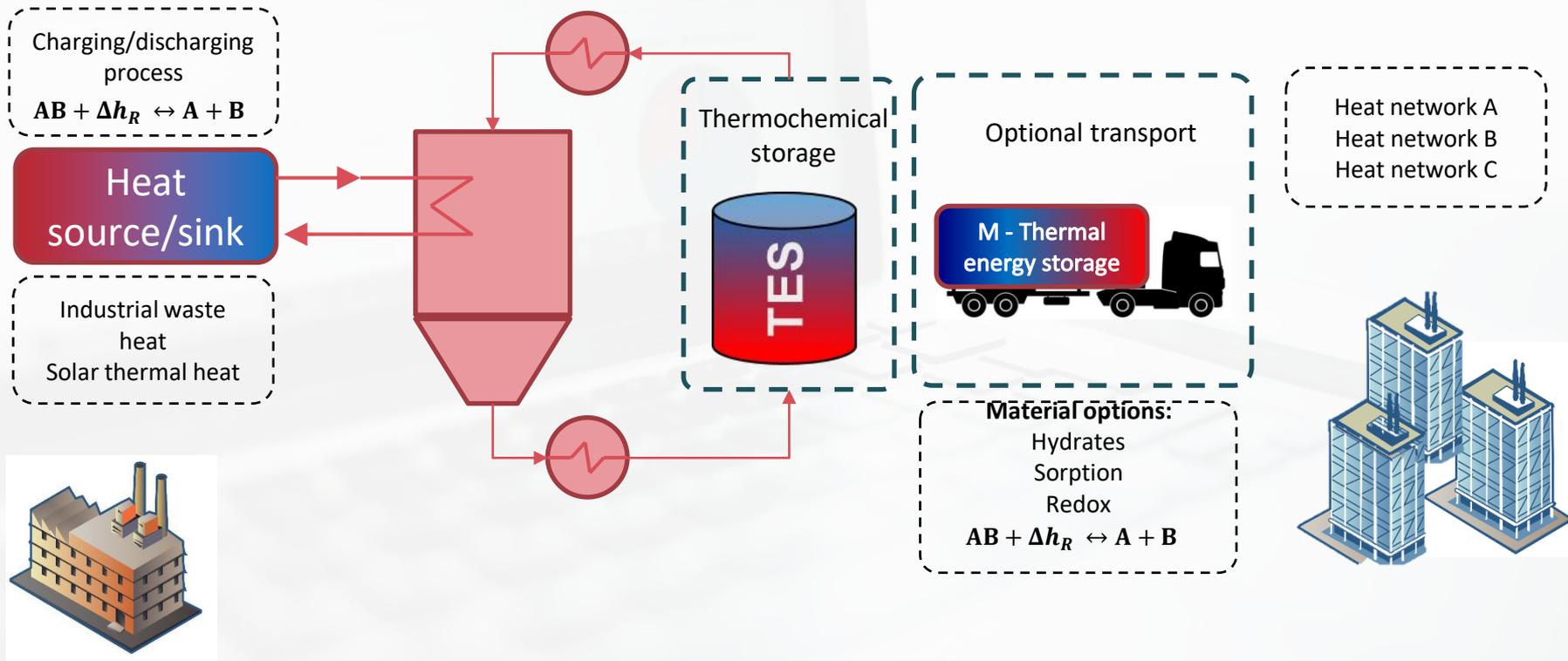
Role of WH/C and TES technologies in SO-WHAT Project



Perception of technological reliability of the solutions needs to be improved, especially with reference to the WH/C capture systems with the aim of increasing the overall efficiency and the operating time system, also thanks to the Thermal Energy Storage Integration



Role of Thermochemical energy storage



SO-WHAT selection and Integration strategy for TcES



1 - Calculation of heat available from WH/C sources or RES sources

2 - Selection of functional parameters of TES (operational envelop)

3 - Shortlisting TES material options on the basis of MCDA

4 - Techno-economic sizing and costing

5 - Simulated in-operando performance

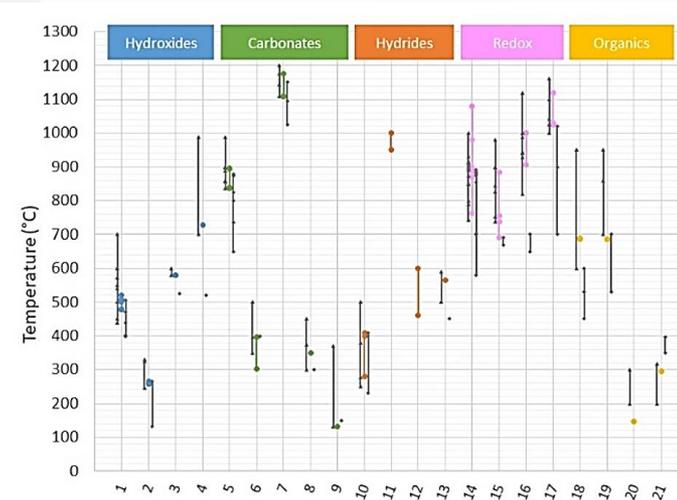
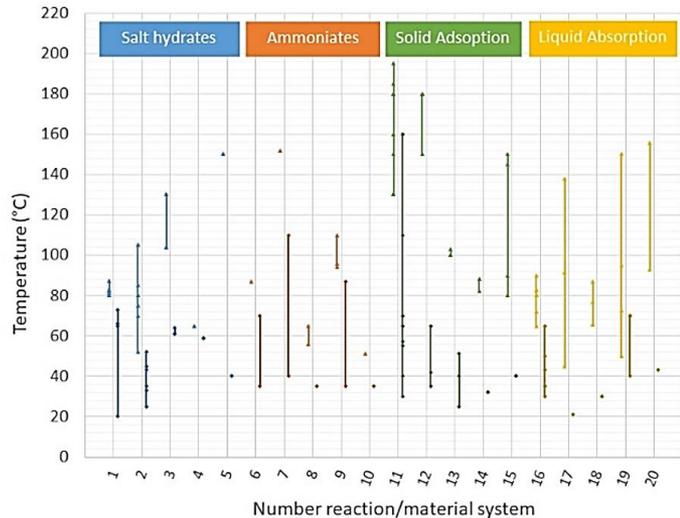
Experimental data on materials



Shortlisting of TcES material options

Systematic screening of TcES options and devices suitable for the WHTP and HU sink/sources at multiple temperatures:

- 50 candidates from 100+ studies
- TRL <5-6 in the vast majority the cases although potentially attractive for WH/C recovery



Charge/discharge temperature of selected TcES: left) Low-temperature; right) Medium-High Temperature

Shortlisting of TcES material options

- TcES options have been identified by comparing the operating temperature envelope of other WH/C technologies
- Example 1 - Only a few LT TCMS and/or favorable operating conditions can drive a LT-ORC. E.g. discharging temperatures higher than 90°C were reported only for zeolite 13X
- Example 2 - the temperature mismatch between charging and discharging discloses a variety of opportunities for LT TCES integration with VCHP

N.	Chemical reaction / Material	Category	HTP/HU Technology														
			LT-ORC		LT-KC		VCHP		HT/VHT-VCHP		AHP			AHT			
			so	si	so	si	so	si	so	si	so1	so2	si	so	si		
1	$\text{Na}_2\text{S}\cdot 5\text{H}_2\text{O} \leftrightarrow \text{Na}_2\text{S}\cdot 0.5\text{H}_2\text{O}$	SALT HYDRATES															
2	$\text{SrBr}_2\cdot 6\text{H}_2\text{O} \leftrightarrow \text{SrBr}_2\cdot 1\text{H}_2\text{O}$																
3	$\text{MgCl}_2\cdot 6\text{H}_2\text{O} \leftrightarrow \text{MgCl}_2\cdot 2\text{H}_2\text{O}$																
4	$\text{K}_2\text{CO}_3\cdot 1.5\text{H}_2\text{O} \leftrightarrow \text{K}_2\text{CO}_3$																
5	$\text{MgSO}_4\cdot 6\text{H}_2\text{O} \leftrightarrow \text{MgSO}_4$																
6	$\text{CaCl}_2\cdot 8\text{NH}_3 \leftrightarrow \text{CaCl}_2\cdot 4\text{NH}_3$	AMMONIATES															
7	$\text{MnCl}_2\cdot 6\text{NH}_3 \leftrightarrow \text{MnCl}_2\cdot 2\text{NH}_3$																
8	$\text{BaCl}_2\cdot 8\text{NH}_3 \leftrightarrow \text{BaCl}_2$																
9	$\text{SrCl}_2\cdot 8\text{NH}_3 \leftrightarrow \text{SrCl}_2\cdot \text{NH}_3$																
10	$\text{NaBr}\cdot 5.25\text{NH}_3 \leftrightarrow \text{NaBr}$																
11	Zeolite 13X/H ₂ O	SOLID ADSORPTION															
12	Zeolite 4A/H ₂ O																
13	Zeolite 5A/H ₂ O																
14	Microporous silica gel/H ₂ O																
15	Composite with CaCl ₂ /H ₂ O	LIQUID ABSORPTION															
16	LiBr(solution)/H ₂ O																
17	CaCl ₂ (solution)/H ₂ O																
18	LiCl(solution)/H ₂ O																
19	NaOH(solution)/H ₂ O																
20	H ₂ O/NH ₃																

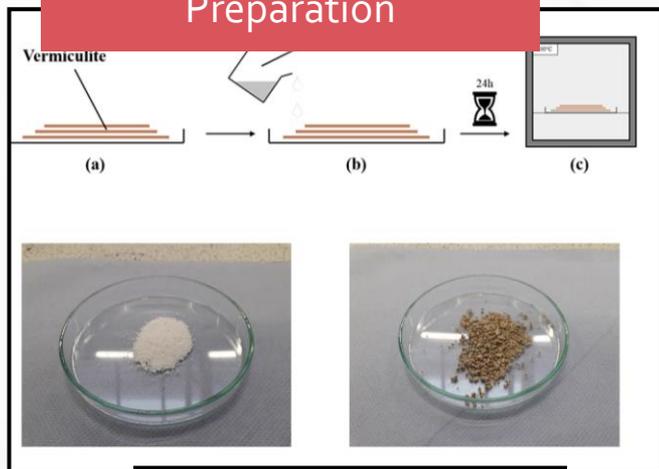
Temperature legend LT TCES (Table 3)

	T < 20°C
	20 < T < 40°C
	40 < T < 100°C
	100 < T < 150°C
	150 < T < 200°C

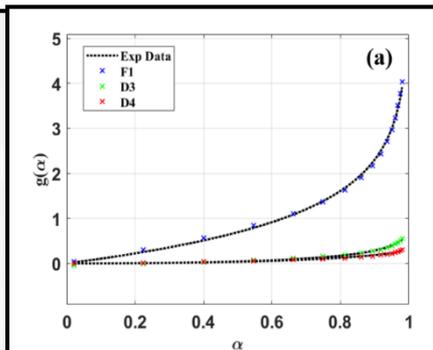
The diagonal in a cell means that the temperature range extends to two intervals

MgCl₂ as a case study

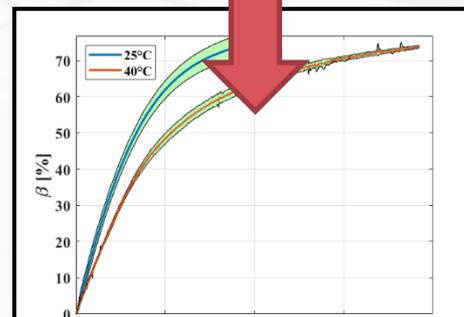
Preparation



Thermo-physical characterization

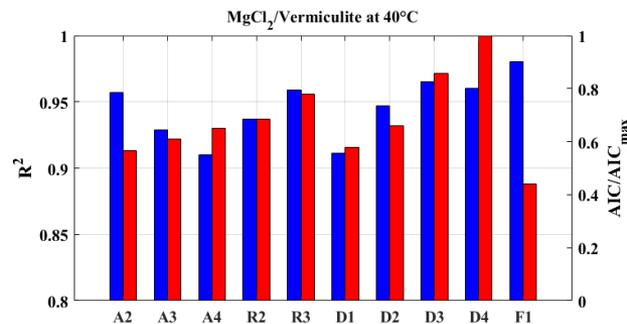
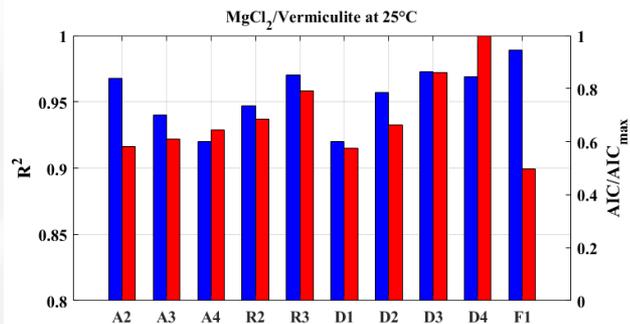
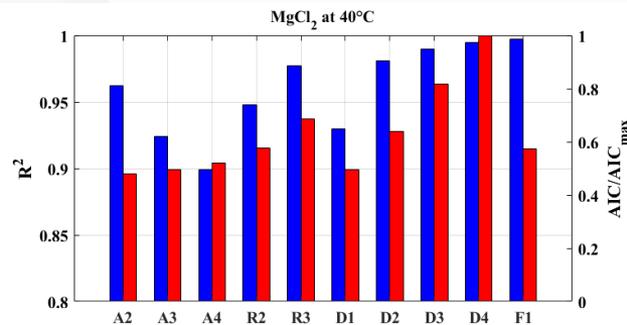
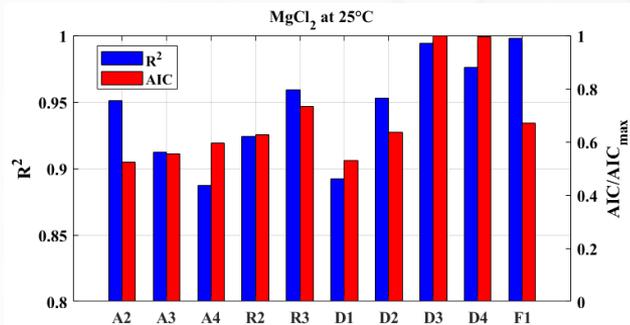


Reconstructed kinetics for assessment



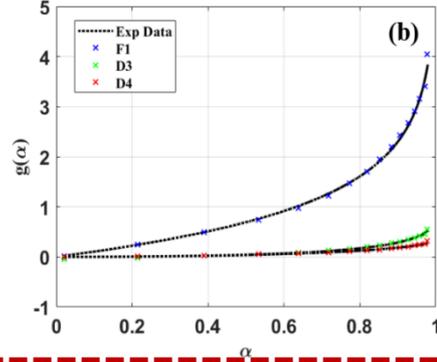
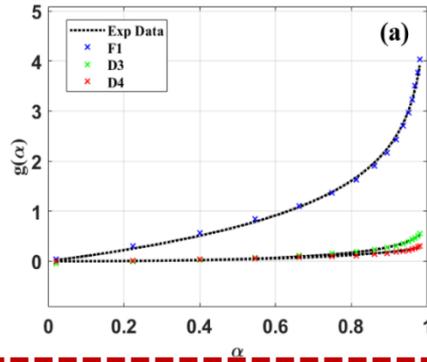
Experimental data

Shortlisting of TcES material options



Quality of reconstructed kinetics measured by statistical indicators

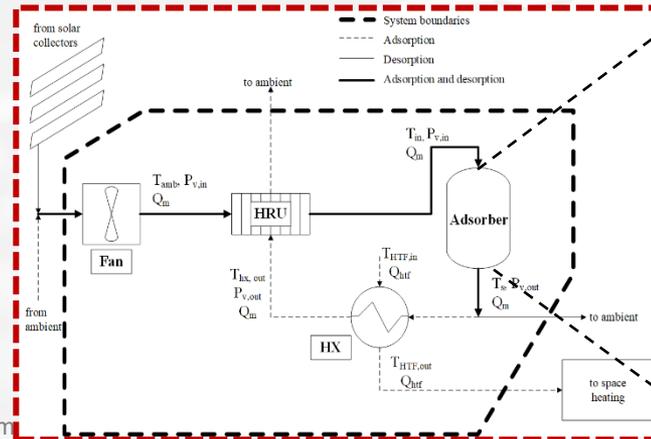
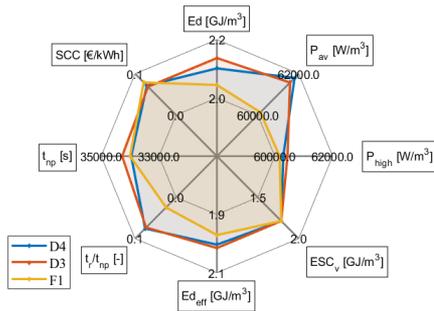
MgCl₂ as a case study: kinetics to UXI



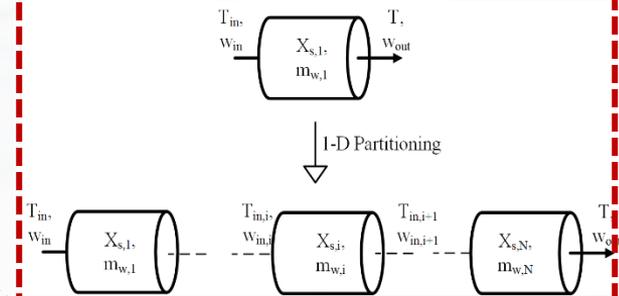
- Reconstructed kinetics for MgCl₂ hydration at 25°C and (b) 40°C with best fitting models

$k(T), f(\alpha)$

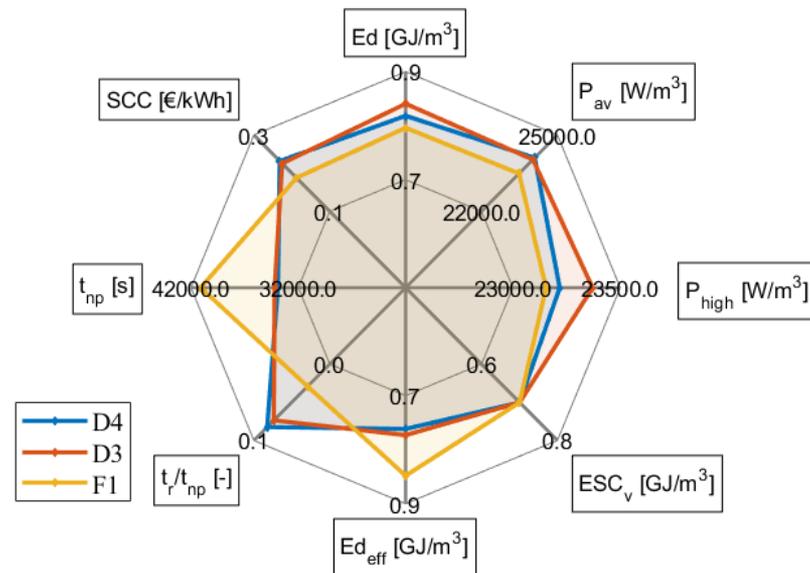
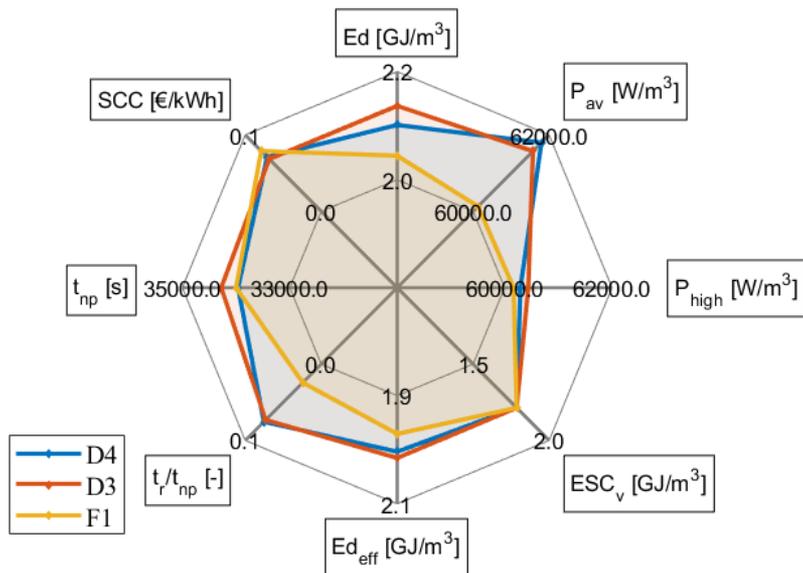
UXI for assessment



sample scale kinetic parameters into reactor model



MgCl₂ as a case study: Final assessment stage



- A rigorous framework for assessing the role of TcES in storing and valorizing fluctuating heat (solar, waste heat) has been introduced
- A six step procedure to guide the user/stakeholder has been developed to support decision making, including the effect of kinetic behaviour and kinetic models
- Generalization of the procedure has been implemented to cover 50+ TcES materials and devices



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THANK YOU FOR YOUR ATTENTION

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