

Process Integration, Chemical and Thermal Energy Storage for the Energy Transformation

743. WE-Heraeus-Seminar

**22 – 24 March 2021
Online via MeetAnyway**

**WILHELM UND ELSE
HERAEUS-STIFTUNG**



Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see <https://www.we-heraeus-stiftung.de>

Aims and scope of the 743. WE-Heraeus-Seminar:

Thermal and chemical energy storage are both necessary components for a successful transformation of the energy system towards sustainability, helping to buffer fluctuating renewable energy sources on the intermediate and long time scale. Many approaches are discussed in the literature, but neither the storage type and storage molecules or even elements, nor the assessment criteria for different storage possibilities are clear.

For thermal energy storage different temperature levels, storage sizes, materials and conversion technologies are discussed, including combinations of heat pumps and organic Rankine cycles (ORC), the combination of steam cycles or Brayton cycles etc. An open discussion of scientific and technological questions, possible efficiencies and realistic amount of storable energy is aimed.

Also, for chemical energy storage, including the formation of transportation fuels, there will not be a single way, but in order to be relevant for the energy transition, some -not yet defined- minimum criteria have to be fulfilled, which have to be quantitative. Integrated conversion of species and energy is a very rational way of using restricted resources but implies the intense collaboration and interconnection of chemical industry with energy providers, which may even reduce flexibility.

At the same time physicists, chemists, engineers and economists propose different approaches, according to the point of view of their discipline, often without considering restrictions and viewpoint from other disciplines. Within this seminar, experts in different fields, including the industrial viewpoint and the systems perspective, should discuss openly their thoughts and their research about the following topics:

- The scientific and technological state of the art and open issues of different approaches for thermal and chemical energy storage.
- General and objective criteria for the assessment of different thermal and chemical energy storage and re-usage schemes and the weighting of the importance of different criteria like efficiencies, storage power, infrastructure, availability, flexibility and ecologic impact.

Introduction

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Program

Program

Monday, 22 March 2021

08:30 – 09:00 Burak Atakan **Welcome: Let's talk about energy storage!**

09:00- 09:10 Stefan Jorda **About the Wilhelm and Else Heraeus-Foundation**

Session chair: Johannes Janicka

09:10 – 10:10 Heleen de Coninck **Limiting global warming to 1.5C: Can energy storage technology help accelerate action?**

10:10 – 11:10 André Thess **Thermochemical energy storage**

11:10 – 11:30 *COFFEE BREAK*

11:30 – 12:30 André Bardow **Power-to-What? Trade-offs in electrifying our societies**

12:30 *LUNCH BREAK*

Session chair: Uwe Riedel

13:30 – 14:30 Valentin Bertsch **Demand for and profitability of energy storage – a market perspective**

14:30 – 15:30 Fokko Mulder **Large scale energy storage using a scalable, hybrid, system approach**

15:30 – 16:00 *COFFEE BREAK*

16:00 – 17:30 **Poster session I**

17:30 – 18:45 **Discussion:**
Assessment of energy storage strategies

18:45 *END*

Program

Tuesday, 23 March 2021

Session chair: Andreas Dreizler

- | | | |
|---------------|---------------------|--|
| 09:00 – 10:00 | Walter Leitner | Smart solutions for climate protection – from power to chemicals |
| 10:00 – 11:00 | Dimos Trimis | Sulfur as energy carrier and sulfur combustion |
| 11:00 – 11:30 | <i>COFFEE BREAK</i> | |
| 11:30 – 12:30 | Francesco Contino | Hydrogen and ammonia: robust production, utilization, and systemic impact |
| 12:30 | <i>LUNCH BREAK</i> | |

Session chair: Annelies Vandersickel

- | | | |
|---------------|--------------------------|--|
| 13:30 – 14:30 | Philip de Goey | Metal energy carriers: sustainable fuels for the future |
| 14:30 – 15:30 | Sophia Haussener | High-temperature heat storage materials and devices |
| 15:30 – 16:00 | <i>COFFEE BREAK</i> | |
| 16:00 – 17:30 | Poster session II | |
| 17:30 – 18:45 | Discussion: | Research needs in thermal and chemical energy storage |
| 18:45 | <i>END</i> | |

Program

Wednesday, 24 March 2021

Session chair: Harry Hoster

09:00 – 10:00	Jutta Geldermann	Combining scenario planning, energy system analysis, and multi-criteria analysis to develop and evaluate energy scenarios
10 :00 – 11:00	Jakob Burger	Options and hurdles for implementing synthetic fuels in the transport sector
11:00 – 11:30	<i>COFFEE BREAK</i>	
11:30 – 12:30	Ralph Kleinschmidt	Smart solutions for climate protection – from power to chemicals
12:30	<i>LUNCH BREAK</i>	

Session Chair: Karsten Müller

13:30 – 14:30	Liselotte Schebeck	Assessment of energy storage technologies
14:30 – 15:30	Francesca di Mare	Turbomachines for future sustainable energy systems
15:30	Final Discussion	
	Burak Atakan Johannes Janicka	Final Remarks

End of the seminar

Posters

Posters for postsession: Monday, March 22nd

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|----|---------------------------------|---|
| 1 | Wenwen Xie | A reduced mechanism for polygeneration processes with ozone addition |
| 2 | Lukas Wehrle | Stack-scale modelling of reversible solid oxide cells (rSOCs) |
| 3 | Florian vom Lehn | Combustion property modeling in fuel design for highly efficient spark-ignition engines |
| 4 | Christian Vering | Towards a sustainable building sector: The necessity of an integrated design of heat pump systems |
| 5 | Valerius Venzik | Thermodynamic analysis of alternative working fluids for the vapour compression heat pump application: A theoretical study |
| 6 | Davide Tonelli
Xavier Rixhon | Comprehensive integration of the non-energy demand within a whole-energy system: Towards a defossilisation of the chemical industry in Belgium |
| 7 | Shkelqim Shaqiri | Experimental investigation of the influence of pressure on the oxidation of iso-octane |
| 8 | Charlotte Rudolph | Chemical exergy storage by natural gas pyrolysis in |
| 9 | Dennis Roskosch | Power-to-heat-to-storage: A technology comparison |
| 10 | Julian Quenel | Energetic and exergetic investigation of improvements for heat transfer in latent thermal storage systems |
| 11 | Erik Pohl | Environmental project portfolio selection using multi-criteria analysis |

Posters for postsession: Tuesday, 23rd March

- | | | |
|----|-------------------------------|---|
| 12 | Johannes Oehler | Sustainable heat for the process industry – high-temperature heat pumps employing a reversed brayton cycle |
| 13 | Christoph Lange | High Temperature CaO/CaCO ₃ -storage for flexible steam power plants |
| 14 | Carola Kuhn | Kinetic study of the oxidation und thermochemical reduction of iron and iron oxides |
| 15 | Josefine Koksharov | Pumped thermal electricity storage (PTES) systems based on water thermal energy storages and organic rankine cycles (ORC) |
| 16 | Dennis Kaczmarek | The influence of ozone on the homogeneous partial oxidation of natural gas mixtures |
| 17 | Dominik Goeb | Oxymethylene ether – diesel blends: Maximizing the impact of renewable fuels on vehicle fleet pollutant emissions |
| 18 | Tim Franken | Multi-objective optimization of gasoline, ethanol, and methanol in spark ignition engines |
| 19 | Andrea Düll | Potassium borohydride as hydrogen storage material for mobile applications |
| 20 | Simon Drost
Robert Schießl | RCEM Studies: Conversion of CH ₄ into unsaturated hydrocarbons and hydrogen |
| 21 | Lukas Berger | Challenges in hydrogen combustion: intrinsic instabilities in laminar & turbulent flames |
| 22 | Gesa Backofen | Thermochemical energy storage as a power-to-process-steam application in industrial energy systems |

Abstracts of Talks

(in alphabetical order)

Power-to-What?

Trade-offs in electrifying our societies

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The cost for producing electricity from wind and solar sources is rapidly declining, driving the energy transition from a fossil to a renewable basis. Electrification is therefore widely regarded as the key measure to defossilize other sectors ranging from heat and mobility to steel and chemicals. However, wide electrification based on renewable resources also leads to new challenges: The additional electricity demand from other sectors will increase the need for generation and transmission capacity. The fluctuating nature of the sun and wind requires energy storage. These additional needs will increase unwanted side-effects of the energy transition such that a targeted energy system design is required.

In this presentation, we review options for energy storage and electrification across sectors. For energy storage, we will analyze pumped heat energy storage (PHES) that combines a heat pump converting electricity into heat to be stored and later reconverted into electricity in a heat engine. PHES offers the theoretical potential of an ideal efficiency of 100% and the use of established technologies. To rigorously explore this potential, we present a techno-economic optimization of a PHES system employing an Organic Rankine Cycle (ORC). The techno-economic optimization is based on computer-aided molecular design (CAMD) methods to simultaneously design the working fluids for the heat pump and the ORC with the process and the required equipment. Thereby, the design space for PHES systems is efficiently explored, allowing benchmarking to alternative technologies for energy storage and also for electrification in other sectors.

For this purpose, the efficiency of energy storage and electrification will be assessed and compared across sectors. Thereby, a merit-order for electrification can be developed. For sectors with low electrification efficiency, alternative methods to mitigate greenhouse gas (GHG) emissions will be discussed such as biomass and carbon capture and storage (CCS). While mitigation of GHG emissions is a major goal of the energy transition, problem shifting to other environmental impacts should be avoided. We therefore employ life cycle assessment (LCA) to quantify potential trade-offs between environmental impacts. Considering these trade-offs in the design of future energy systems will allow us to not only mitigate climate change but to develop a more sustainable future.

Demand for and profitability of energy storage – A market perspective

V. Bertsch¹

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Germany*

Many countries worldwide have adopted policies to support the expansion of renewable energy sources (RES) aimed at reducing greenhouse gas emissions, combating climate change, and, more generally, establishing a globally sustainable energy system. As a result, energy systems around the world are undergoing a process of fundamental change and transformation. For instance, the growing share of RES leads to increasingly distributed, volatile and uncertain supply, which comes along with growing requirements for flexibility. Flexibility options include, inter alia, energy storage, demand response, sector integration or grid expansion. In this context, this talk focuses on the demand for and profitability of energy storage. Key questions from the perspective of the energy system include questions about the optimal time-phasing and choice of different storage technologies. In order to answer such questions, energy systems models have been developed and used for several decades to support different decision makers in governments and companies.

Energy systems research shows that first significant storage deployment appears at RES shares of around 70-80% [1]. On the way to carbon-neutrality and 100% RES systems, storage deployment is found to increase exponentially. From an investor's perspective, however, research shows that storage investment isn't economically viable in today's markets [2]. While revenues from system services are likely to increase in the future [3], this will not change the situation fundamentally. In this context, this talk will present a selection of findings from existing research and provide an outlook on future research needs. In particular, development needs for models and methods and requirements for multi-disciplinary collaboration are highlighted.

Acknowledgements

The research presented here draws on a variety of findings from different collaborations. In particular, I would like to thank Mel Devine, Eva Drews, Muireann Lynch, Jan Mutke, Felix Nitsch, Leonie Plaga, and Petr Spodniak.

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Options and Hurdles for Implementing Synthetic Fuels in the Transport Sector

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This presentation aims at providing a realistic, fair and optimistic view on options to produce synthetic fuels. For this presentation, synthetic fuels are hydrogen and fuels that are produced via synthesis gas, e.g. methanol, synthetic natural gas, Fischer-Tropsch fuels or oxymethylene ethers (OME). It is reasoned that there is strong future demand for fuels beyond biofuels and battery-electric vehicles.

The presentation breaks up with the narrow-minded concepts decarbonization and defossilization. Both would be individually sufficient for climate-friendly synthetic fuels but are actually not necessary. Instead, general boundary conditions for sustainable fuel production are stated. Neither specific raw materials nor specific primary energy sources are presumed. In this way, technology-open concepts for synthetic fuels are derived and compared.

The key result is a conclusive discussion of several aspects of synthetic fuels: A) Comparison and prioritization of general production routes such as Power-To-Liquid (a.k.a. E-Fuels), bio-based routes or fossil routes with carbon capture and storage (CCS). B) Carbon-free fuels vs. carbonaceous fuels. C) Fuels imitating current fuels vs. fuels with superior combustion properties. The analysis is done in quantitative terms using costs, energetic efficiencies and greenhouse gas abatement cost. Finally, potential links to the future energy storage are outlined to contribute to the discussion of the seminar.

Hydrogen and ammonia: robust production, utilization, and systemic impact

Francesco Contino¹, Xavier Rixhon¹, Gauthier Limpens¹, Kevin Verleysen^{2,3}, Diederik Coppitters^{2,3,4}, Maxime Pochet⁵, Azd Zayoud¹, Davide Tonelli¹, Charles Lhuillier^{2,3} and Hervé Jeanmart¹

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Massive storage will likely be required to match the renewable generation with the energy demand geographically and temporally. Energy storage in molecules such as hydrogen and ammonia has many advantages compared to other storage technologies. Hydrogen will be a great enabler of the renewable world, and a versatile interface between many energy- and non-energy-related sectors and uses. It is a fundamental building block for a variety of molecules and fuels. Ammonia is becoming increasingly popular as hydrogen carrier beyond its heavy use in agriculture. Together with other electro-fuels, they are expected to play a role on the path to remove fossil fuels from the energy equation [1]. Yet, their integration has many well-known challenges: production flexibility, long-term storage, or round-trip efficiency. Going from the system of today to a fully renewable one implies a paradigm shift. The introduction of such disruptive change requires a holistic approach. Our research encompasses the entire value chain—from production to robust utilization at a local scale [2] up to a regional one [3]. Moreover, we study an additional layer: the impact of those alternative energy carriers on the whole-energy system, as analyses without understanding of the global effect on our systems limits their meaning [4].

More specifically, this presentation addresses three major topics: the integrated production of hydrogen and ammonia from renewable energy [5], the utilization of ammonia and hydrogen in SI and HCCI engines [6-12], and the reduction of greenhouse gases emissions on the entire system enabled by electro-fuels [13-15]. When producing hydrogen or ammonia, we face the difficulties of flexibility and versatility—users have complex and ambiguous future demands, renewables are variable and uncertain. On the utilization side, we face the poor combustion properties of ammonia. Finally, the impact on the system is multi-scale—from regional to inter-continental—and it has multiple timescales—from hours to years.

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Limiting global warming to 1.5C: Can energy storage technology help accelerate action?

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In 2018, the Intergovernmental Panel on Climate Change (IPCC) published its Special Report on Global Warming of 1.5C (SR1.5) [1] in response to a request from the parties to the Paris Agreement. The IPCC report concludes that limiting warming to 1.5C is still possible if systems transitions in for instance energy and industry are accelerated. This requires a.o. enhanced innovation to realize the significant role of a portfolio of technologies to limit warming to 1.5C and adapt to the consequences of such warming levels and associated climate changes. The role of energy storage technologies is superficially assessed, but their significance and promise is highlighted.

This presentation will discuss how the IPCC SR1.5 came about, its main results, the need for societal embedding of innovation processes, including industrial system transitions, and the need to go even beyond multidisciplinary collaboration between physics and chemistry to advance energy storage technologies.

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Metal energy carriers: sustainable fuels for the future

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Metal powder has superior energy density compared to fossil fuels and hydrogen. Therefore, metal powders have gained interest as a material for energy storage. The main benefits of metal fuels are that they do not produce CO₂ emissions during combustion, they have the potential to be retrofitted in existing industrial processes and coal power plants and they can fit into the existing fuel transportation infrastructure. Furthermore, this enables the production of sustainable energy since metal fuels can be regenerated from metal oxides, using green hydrogen/electricity sources. In this presentation, the main characteristics of metal fuels are presented with a final focus on clean combustion. In a number of numerical and experimental studies, our fundamental understanding of the propagation, stabilization and emission formation of metal powder flames is currently enlarged. The resulting experimental tools and numerical models are subsequently used for guiding the development of practical systems. On a more practical side, a 100 KW demonstrator set-up has been developed to demonstrate clean combustion to produce steam (placed at Swinkels brewery in 2020 and the Metalot innovation centre). Projects for further scale up have been started as well. The main objective of these practical systems is the development of integrated flexible metal fuel combustion system with a capacity of 1-10 KW (TRL5). This is an essential step towards implementation of this sustainable technology. The development of this combustion system is executed by a consortium of partners which covers the entire supply chain. This includes the production of metal powder, fuel preparation, burner and combusted product handling. The industrial partners have broad experience in metal powder supply, dense energy carriers and operating coal fired power plants. Furthermore, techno-economic analyses and the assessment of retrofit potential to existing assets have been carried out. Status-quo will be presented as well.

Turbomachines for future sustainable energy systems

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Turbomachines represent the backbone of propulsion, power generation and many industrial processes. Efficient usage of renewable energy sources and the implementation of long-term energy storage solutions are the key for realising such objectives and rely strongly on novel turbomachinery concepts, capable of operating under demanding conditions whilst using a variety of working fluids. In storage plants based on high-temperature heat pumps (e.g. Carnot batteries with process temperature $\geq 400^\circ\text{C}$) for example, Brayton cycles can be conveniently adopted where supercritical CO_2 can be used as a working fluid. On the other hand, low-temperature heat sources, typical for geothermal processes, low-heating value biomass fuels and by the recovery of waste industrial heat (WHR) are ideally exploited in Organic Rankine Cycles (ORC) where compact machines and dense gases play a fundamental role. The dramatic change in the operation paradigm of modern turbomachines, (transient vs. steady operation) coupled with the need of extending the range of working conditions as well as working fluids (dense gases, supercritical fluids) poses renewed challenges for their design, optimisation and maintenance. In particular, a full virtualisation of these procedures in an industrial context requires the development of simulation tools capable of delivering a faithful and reliable description of the thermo-fluid-dynamic behaviour of machines and working fluids at acceptable computational costs. The successful development of a powerful, comprehensive DNS/LES/RANS ([1], [2] and [3]) high-performance tool, accounting for the complex thermodynamics on non-ideal fluids and encompassing efficient pre- and post-processing towards exascale computing, is demonstrated in a series of technologically relevant applications ranging from wet steam flow, compression of supercritical CO_2 , flow in a transonic ORC-turbine, to the simulation of gas turbines for flexible power generation.

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Combining scenario planning, energy system analysis, and multi-criteria analysis to develop and evaluate energy scenarios

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Energy scenarios are developed to provide decision support in the energy sector or in energy policy. In this context, scenario planning and multi-criteria decision-making can complement energy system analysis. Therefore, we propose a combination of these three methods and illustrate it in a case study that investigates the transition of the electricity sector in Lower Saxony, Germany, to energy from renewable sources. The results of our case study show that the integration of multi-criteria analysis allows for better problem structuring by focusing on relevant alternatives, external uncertainties, and evaluation criteria. The integration of scenario planning allows for a systematic investigation of external uncertainties. Thereby, the fallacy of investigating assumptions for uncertain parameters, which are not consistent with the assumptions in the scenario, can be avoided. Finally, combining the methods allows for a more balanced and objective evaluation of alternative energy systems and their development paths in terms of multiple criteria, which can be used to inform discussions among stakeholders and increase acceptance.

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High-temperature heat storage materials and devices

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High-temperature heat storage solutions can support and accelerate the transition of our current energy economy into a more sustainable energy economy. Specifically, they can help to increase the integration of stochastic, fluctuation sources of renewable energy. However, materials and devices that can efficiently store and release high-temperature ($T > 400^\circ\text{C}$) heat are sparse and – given the challenging operating conditions – are difficult to design. Rates for charging and discharging, energy density, interface and performance degradation, and cost are some of the challenges that need to be addressed before high-temperature heat storage can be employed more widely.

In this talk, I will give an overview over our research activities in the area of high-temperature heat storage. I will focus on latent heat storage approaches with encapsulated metals, given their high energy density and high thermal conductivity. I will discuss experimental and computational methods to quantify and identify the degradation mechanism in encapsulated metals, specifically focusing on the example of steel-encapsulated Al-12Si alloy [1]. Secondly, I will discuss our multi-physics modeling framework for the design of heat storage devices with tailored power and energy density, specifically focusing on identifying dominating heat transfer regimes [2,3]. Thirdly, I will show our experimental MJ-scale high-temperature heat storage testbed and share characterization results of typical charging and discharging experiments. I will end with an outlook on possible application and integration areas of such high-temperature heat storage devices.

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The objective of the Carbon2Chem® project is to link the energy, steel and chemical industries within a cross-industrial production network. To demonstrate the sectoral coupling, thyssenkrupp built a modern technical center, including 2 MW alkaline water electrolysis, pilot plant for gas cleaning and lab scale catalyst testing units.

The focus of the 2nd phase is to proof the long term stability of the methanol and ammonia synthesis catalysts under conditions of purified steel mill gases and system integration. With the completion of the 2nd phase an industrial implementation and basic engineering of the chemical complex including gas cleaning, chemical synthesis and electrolysis should be feasible. In addition to the topic long term stability, Carbon2Chem® will address other industries, such as steel production on basis of direct reduced iron, cement/lime plants, and waste incineration.

Smart Solutions for Climate Protection – From Power to Chemicals

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The industrial transformation of carbon-based raw materials into valuable products forms the basis of today's global economy and modern societies. With its products ranging from energy carriers through plastics and advanced materials to biologically active compounds, chemistry is essential to cope with the global challenges of our time. Moving towards a more sustainable future, there is an increasing need for "defossilization" of the raw material basis using non-fossil resources together with the deployment of carbon-free energy technologies.^[1] Hydrogen plays a central role as molecular relay between electrons and chemical structures for such *Power-To-X* technologies.^[2] The present contribution will discuss the opportunities and challenges of this approach highlighting the role of catalytic processes to unlock the potential as exemplified for successful technological solutions.^[3]

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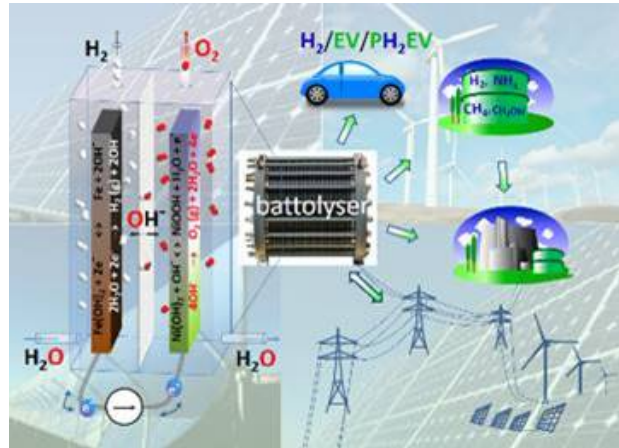
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Large scale energy storage using a scalable, hybrid, system approach

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The implementation of large scale renewable electricity generation requires electricity storage and conversion on short timescales as well as on long, seasonal, timescales.[1] Here the approach is to combine several hybrid methods based on abundantly available materials to come to an energy and feedstock system that can handle the intermittent nature of renewable energy.



The first component in the system is an

integrated nickel-iron battery and alkaline electrolyser (“battolyser”) technology that can provide both electricity storage and conversion to hydrogen when the battery electrodes are charged and more electricity is still available. [2] In the battolyser the electrodes convert from $\text{Fe}(\text{OH})_2$ and $\text{Ni}(\text{OH})_2$ to nanoporous reduced iron and NiOOH , which are good catalysts for hydrogen evolution and oxygen evolution respectively. The typical energy efficiency ranges between 80 and 90% for both functions combined, while battery capacities can still be increased further [3].

The second component in the system is the large scale storage of hydrogen in ammonia, but before that can work the Haber Bosch synthesis needs to become applicable in an intermittent fashion. For that reason an integration with battolyser electricity storage, hydrogen production and heat storage technology may be proposed to enable intermittent operation of ammonia synthesis with high peak capacity, but a low capacity factor.[4] The advantage is that then scaling up such storage and conversion relies on abundant elements Fe, Ni, K, N_2 and H_2O , which will not be limited in availability and therefore scale favorably. All other industries can then be provided with hydrogen feedstock (from ammonia cracking) and dispatchable electricity, without intermittency, and can therefore operate at high capacity factor and carbon free.

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Assessment of Energy Storage Technologies: Material Cycles and Life Cycle Analysis

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Energy storage is a major issue of future energy systems: In view of the transformation to primary energy harvested to a large extent from the fluctuating energies of wind and sun, the overall performance of the energy system is crucially dependent on the effectiveness and efficiency of energy storage. As to effectiveness, beyond technological and economic issues, the contribution of energy storage to climate mitigation is the overarching goal in a systems view. Above this, storage technologies like other energy technologies may have effects on further environmental issues. Notably, functional materials based technologies like batteries require specific elements and the respective raw materials. Today, material demand of energy technologies in general and energy storage technologies in particular has been identified as one major challenge of the energy transformation [1].

In order to select most suitable technologies for a given application, but also for optimization of a technology in the course of R&D, assessment methods are helpful tools for systematic and substantiated decision making. Given the challenge of climate mitigation on one hand and material requirements on the other hand, two assessment approaches are applied most often in literature: Material flow analysis (MFA) is a method to track material flows in the full economy, in sectors and on a global scale. Life cycle assessment (LCA) is a relative method comparing indicators for global warming and other environmental impact categories on a common functional unit. Each method thus addresses specific challenges of storage technologies: while MFA gives evidence i.a. on the contribution of recycling to save primary resources, LCA quantifies net green house gases in the life cycle and possible adverse environmental impacts like toxicity of materials. In addition, so-called Consequential LCA (C-LCA) also covers systemic effects occurring from substitution of end energy or energy carriers from fossil sources.

Using the approaches of MFA and LCA, it is discussed how to structure the broad scope of existing and up-coming energy storage technologies in order to assess their impact on material flows and their systems performance as to climate mitigation.

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Thermochemical Energy Storage

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Thermochemical energy storage has the potential to store large quantities of low-carbon energy in inexpensive materials without thermal losses like calcium oxide (limestone). The lecture will provide an introduction of the basic principles of this storage technologies and sketch residential and industrial applications. It will conclude with a speculative outlook into the possibility of a global *Limestone Economy*.



Dr. Matthias Schmidt (DLR-Institute of Engineering Thermodynamics) demonstrating electrical charging of a thermochemical energy storage based on limestone.

Sulfur as energy carrier and sulfur combustion

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Recently, sulfur gained in interest as chemical energy storage material because of the possibility to use it in closed energy conversion cycles. Sulfur is a very cost-effective material and can be inexpensively transported and stored outdoor under ambient conditions for long times and in large quantities. In this talk a novel power cycle developed in the framework of the collaborative European research project PEGASUS is presented. The closed energy conversion cycle targets renewable electricity production from concentrated solar power (CSP) based on intermediate elemental sulfur storage. The basic step of this power cycle is the endothermal decomposition of sulfuric acid into SO₂, O₂, and H₂O at temperatures above 800 °C. The necessary energy is fed via a CSP receiver into the process. In a following process step, SO₂ disproportionates into S and sulfuric acid. Combustion of the separated and stored sulfur releases again the stored energy, enabling electricity generation for baseload operation. Research and development towards a high power density burner for elemental sulfur suitable for power generation in gas turbines is challenging and in focus of this talk including experimental and numerical studies as well as chemical reaction mechanisms.

Despite the fact that combustion of elemental sulfur is being performed for long time in large-scale as part of the industrial production process of sulfuric acid, little data concerning details of the combustion of sulfur is available in the literature and burners are not suitable for power generation. For the design of optimized combustion devices providing high power densities the knowledge of combustion properties such as laminar burning velocities or reaction zone structures is necessary. Prerequisites for estimating burning velocities are validated reaction mechanisms. Also the complicated rheological properties of liquid sulfur and several structure transitions (e.g. S₈-S₆-S₄-S₂-S as well as polymerization and chain formation in the liquid phase) taking place at different temperature levels make the development of high power density sulfur burners intriguing. The scope of most reaction mechanisms from literature is to describe the reactions of sulfur compounds in combination with hydrocarbon or hydrogen combustion (mostly motivated by the technically applied Claus-process). However, none of them considers the oxidation of sulfur in the absence of hydrogen or hydrocarbons. Detailed reaction mechanisms involving only sulfur and oxygen species as well as experimental data are therefore required in order to gain insight into the dynamics of heat release and flame structure of sulfur combustion.

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Abstracts of Posters

(in alphabetical order)

Thermochemical Energy Storage as a Power-to-Process-Steam Application in Industrial Energy Systems

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In the 2019 climate protection program [1], the German government defined steps for industrial plants to become more climate friendly. Short-term goals are to use resources and materials more efficiently, to reduce CO₂-emissions, and to research promising new technologies. Addressing these requirements, the TUM develops a power-to-process-heat system with integrated storage based on the reversible reaction of CaO and Ca(OH)₂. This work assesses the merits of integrating such a system in an existing industrial power plant, as a first step towards large scale deployment of power-to-process-heat. The reaction takes place in a continuously operated fluidized bed reactor which is connected to two separate storage silos. During charging, Ca(OH)₂ decomposes into CaO and steam. The heat for this endothermic reaction can be supplied to the reactor by electric heaters. The steam can be utilized as low-pressure process steam in a connected energy system. During discharge, the CaO recombines with steam. The heat from this reversible exothermic reaction can then be used to create high-pressure process steam at approx. 480 °C.

The storage system is integrated into an industrial energy system with 31 bar, 16 bar, and 6 bar process-steam demand, which is currently met by a gas fired CHP unit and additional gas boilers. The storage is charged at low electricity prices when selling electricity from the CHP unit is not profitable. Discharging the storage to supply the process steam demand at high electricity prices increases profits by operating the CHP at an overall higher electrical efficiency. It also reduces the CO₂-emissions of the overall electricity production by displacing generation from coal fired plants from the grid. The potential savings in gas consumption, CO₂-emissions and expenses are calculated with MILP using the optimization solver Gurobi and the simulation software TOP-Energy. Simulations show a promising profitability with increasing natural gas prices.

Keywords: Thermochemical energy storage, industrial CHP, energy system simulation, MILP, CaO/Ca(OH)₂

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Challenges in Hydrogen Combustion: Intrinsic Instabilities in Laminar & Turbulent Flames

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The recent rise of electricity production from renewable energy sources has increased the need for appropriate energy storage, thus promoting the use of hydrogen as a carbon-free energy carrier. One way to integrate hydrogen into the existing energy infrastructure is its thermochemical energy conversion. However, several problems arise for combustion processes that involve hydrogen. The combustion behavior of lean premixed hydrogen flames is significantly affected by intrinsic instabilities, which substantially change flame dynamics, heat release rates, and flame speed. These aspects are particularly relevant for safety considerations to avoid flash backs, but can be also exploited to increase thermal efficiencies.

In this work, the impact of intrinsic instabilities on the flame propagation is discussed for laminar and turbulent lean premixed hydrogen flames. For the laminar flames, simulations of initially planar flames are performed and due to the intrinsic instabilities, cellular structures are formed along the flame front and a strong flame front wrinkling is observed. A parametric variation of the unburned conditions shows that an increase of pressure, a decrease of equivalence ratio, or a decrease of unburned temperature lead to an enhancement of the instabilities and flame speed. For the turbulent flames, a large-scale Direct Numerical Simulation (DNS) of a turbulent lean premixed hydrogen flame at a jet Reynolds number of 11,000 has been performed in a slot burner configuration to study interactions of flame intrinsic instabilities and turbulence. Since the flame intrinsic instabilities result from the high diffusivity of the hydrogen molecule with respect to the other species, an additional reference DNS at the same Reynolds and Karlovitz number, with diffusivities of all species equal to the thermal diffusivity, was conducted to artificially suppress the instability mechanism. For the DNS with realistic diffusivities, the profiles of heat release and temperature clearly show the characteristic behavior of the flame intrinsic instabilities with local flame extinction, temperature overshoots in the burned gas, and an enhanced flame speed; on the contrary, these effects are not seen in the reference DNS. Thus, intrinsic instabilities are capable to significantly affect the flame evolution in laminar and turbulent flames, which needs to be considered for the design of combustion devices using hydrogen as a fuel.

RCEM Studies: Conversion of CH₄ into unsaturated hydrocarbons and hydrogen

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We study the conversion of small alkanes (CH₄, C₂H₆, C₃H₈) into unsaturated hydrocarbons, notably C₂H₂, C₂H₄ and hydrogen, in a Rapid Compression/Expansion Machine (RCEM). The newly formed molecules can have a higher value in terms of economic use, handling, or in terms of further utilization in a chemical process. By the conversion, also chemical energy is stored, because the unsaturated products feature larger standard enthalpies of formation compared to the initial substances.

In the experiments, the conversion (defined as amount of consumed initial reactant relative to initial amount) levels between 15 to 38 %. The dependence of the conversion on compression temperature, pressure and dilution by monatomic gas was investigated. The temperature was found to be the most important factor, followed by the dilution. However, these variables in respect to the mentioned pyrolysis process have physical and practical limitations (e.g. soot formation or a gas separation process) to increase the conversion further.

A limiting factor in conversion is also the duration time which the gas mixture resides in a high temperature environment. During one cycle, this time is limited because wall heat losses and endothermal reactions cause the temperature to drop to a point where chemical reactions practically stop. We study how multiple consecutive compression and expansion cycles can achieve longer effective residence times in the high temperature environments, and thus increased conversion and yield. It was found that both the conversion and the yield can be increased significantly by a factor of 2 to 4 by multiple compressions.

Acknowledgements

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Potassium borohydride as hydrogen storage material for mobile applications

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Hydrogen could play a vital role as a carbon-free energy carrier in future mobility solutions. However, due to its low density under normal conditions, the storage of hydrogen onboard fuel cell electric vehicles poses a major challenge [1].

In recent years, a wide variety of hydrogen storage technologies have been developed. The material-based storage in metal borohydrides has been identified as a promising option for mobile applications as the chemically bound hydrogen can be released via hydrolysis under relatively mild conditions. Sodium borohydride (NaBH_4) has received particular attention, its successful implementation in technical systems is, however, complicated by the limited solubility of the hydrolysis byproduct sodium metaborate (NaBO_2) in aqueous media [2].

In this context, the onboard and offboard performance of potassium borohydride (KBH_4) as an alternative hydrogen carrier material is theoretically evaluated in this contribution.

It is shown that, in comparison to NaBH_4 , higher gravimetric storage capacities are practically achievable with the heavier carrier material (KBH_4) over a relatively wide temperature range. This is due to the hydrolysis byproduct's (KBO_2) higher solubility in aqueous media and the consequently lower excess of water necessary for avoiding byproduct crystallization.

A special emphasis is given to the energetic and ecological analysis of a full KBH_4 -based hydrogen storage cycle, which includes the costly regeneration of the hydrolysis byproduct (KBO_2). The latter is usually re-hydrogenated in the presence of magnesium as an auxiliary material, which is oxidized in the course of the regeneration process. The subsequent reduction of the generated magnesium oxide is identified as the critical -however rarely considered- process step in the overall storage cycle, as it significantly increases the energy demand and greenhouse gas emissions linked to the carrier regeneration.

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Multi-objective Optimization of Gasoline, Ethanol, and Methanol in Spark Ignition Engines

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In this study, an engine and fuel co-optimization is performed to improve the efficiency and emissions of a spark ignition engine utilizing detailed reaction mechanisms and stochastic combustion modelling. The reaction mechanism for gasoline surrogates [1], ethanol, and methanol [2] is validated for experiments at different thermodynamic conditions. Liquid thermophysical properties of the RON95E10 surrogate (iso-octane, n-heptane, toluene, and ethanol mixture), ethanol, and methanol are determined using the NIST standard reference database [3] and Yaw's database [4]. The combustion chemistry, laminar flame speed, and thermophysical data are pre-compiled in look-up tables to speed up the simulations (tabulated chemistry).

The auto-ignition in the stochastic reactor model is predicted by the detailed chemistry and subsequently evaluated using the Bradley Detonation Diagram [5 - 7], which assigns two dimensionless parameters (ξ and ε). According to the defined developing detonation limits, the auto-ignition is either in deflagration, sub-sonic auto-ignition, or developing detonation mode. Ethanol and methanol show a knock-reducing characteristic, which is mainly due to the high heat of vaporization.

The multi-objective optimization process includes mathematical algorithms for design space exploration with Uniform Latin Hypercube, pareto front convergence with Non-dominated Sorting Genetic Algorithm II (NSGA-II), and multi-criteria decision making [8, 9]. The optimization input parameter ranges are selected according to the previous sensitivity analysis, and the objectives are to minimize specific CO₂ and specific CO and maximize indicated efficiency. The performance study of different optimization algorithms shows that the incorporation of metamodels is beneficial to improve the design space exploration, while keeping the optimization duration low. The comparison of different reaction mechanisms, which are applied in the optimization process, shows a strong impact on the pareto front solutions. This is due to differences in the emission formation and auto-ignition between the different reaction schemes. Overall, the engine efficiency is increased by 3.5 % points, and specific CO₂ emissions are reduced by 99 g/kWh for ethanol and 142 g/kWh for methanol combustion compared to the base case. This is achieved by advanced spark timing, lean combustion, and reduced C:H ratio of ethanol and methanol in relation to RON95E10.

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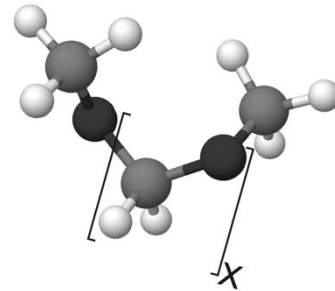
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Oxymethylene ether – diesel blends: Maximizing the impact of renewable fuels on vehicle fleet pollutant emissions

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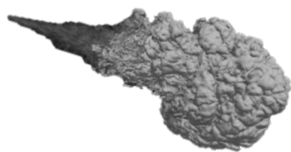
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During the upcoming transition period towards battery-electric vehicles and fully renewable fuels, the optimal utilization of available renewable power for e-fuel production becomes of key importance in terms of maximizing the impact on transportation CO₂ reduction, but also in terms of other goals such as minimizing pollutant emissions. Oxymethylene ethers



(CH₃O(CH₂O)_xCH₃, short OME_x) are a well-known group of oxygenated e-fuels for compression ignition engines, which allow simultaneously for both very low engine-out NO_x and soot emissions, even when blended with conventional fossil diesel fuel. As only around 35 vol-% of OME_x in diesel fuel are necessary to achieve near-zero soot emissions [1], its utilization can maximize the impact of the available amount of green fuel on the total vehicle fleet pollutant emissions. A larger number of vehicles can be reached within a short period of time compared to more disruptive technologies such as hydrogen engines or fuel cells.

In this work, we review production and life cycle assessment, as well as opportunities and challenges in introducing OME_x into the market. Our own research focusses on the application side and is presented in more detail, discussing the mixture formation and combustion behavior of blends of OME₁ with *n*-dodecane, a common surrogate fuel for fossil diesel [2]. We establish that, despite significantly altered fuel properties, commonly used spray and combustion models are able to deliver predictive results for these fuels. We investigated the impact of the liquid fuel properties on mixture formation and ignition and present a combination of experimental and numerical results. Finally, the most dominant cause for the strongly super-linear reduction of soot precursor production in a blend of OME₁ and *n*-dodecane is shown to be the shift of fuel-air stoichiometry due to the fuel oxygen content – a result that likely holds also for other oxygenated fuels.



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The influence of ozone on the homogeneous partial oxidation of natural gas mixtures

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The future energy system requires flexible energy conversion technologies to overcome the fluctuating nature of renewable energies. One option could be fuel-rich operated homogeneous charge compression ignition (HCCI) engines, fueled with methane (CH₄). Such an engine could be used to supply electricity and heat when there is not enough renewable energy available, or to produce synthesis gas and thus store excess energy when there is a sufficient supply of renewable energy. Because methane is relatively stable, high temperatures and pressures are required for its conversion. Alternatively, small amounts of additives can be introduced into the mixture to form radicals at relatively low temperatures and initiate CH₄ conversion. Carbon-based additives tend to preferentially consume the available oxygen and radicals so that the conversion of methane remains low. The addition of ozone could be a viable way to overcome these challenges by providing O radicals at very low temperatures that can react with the fuel. In this study, the ozone-assisted partial oxidation of diluted CH₄ and CH₄/C₂H₆/C₃H₈ mixtures is investigated in a plug-flow reactor at temperatures between 373 and 973 K, a pressure of 4 bar, and an equivalence ratio of 2. The product spectra are analyzed by time-of-flight mass spectrometry and compared to kinetic simulations performed with literature reaction mechanisms.

The addition of 380 ppm ozone shifts the reaction onset from 823 K to very low temperatures of 448 K and 423 K in the case of neat CH₄ and the CH₄/C₂H₆/C₃H₈ mixture, respectively. Because the reactivity is still low at these temperatures, the formation of oxygenated species such as methanol and formaldehyde is favored. Also, the conversion of methane and the formation of other valuable chemicals such as synthesis gas is significantly increased in the investigated temperature range. The results show that ozone is a promising reaction enhancer for a polygeneration process using HCCI engines.

Pumped Thermal Electricity Storage (PTES) systems based on water thermal energy storages and Organic Rankine Cycles (ORC)

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In 2019 the share of renewable energy sources in gross power generation was 42% in Germany. The federal government aims at expanding this share further to 45% in 2025 and to 65% in 2030 [1]. The increasing share of renewable energy sources leads to a strong fluctuating production of electrical energy, and storage systems are required because of the mismatch between supply and demand. Pumped Thermal Electricity Storage (PTES) systems are a technology for solving these problems.

Here, two concepts for PTES systems based on Organic Rankine cycles at different storage temperatures are presented and analyzed. In order to store thermal energy, in the first concept (A) an atmospheric water storage tank is used while the other concept (B) contains a pressurized water tank. The atmospheric storage tank consists of two zones. This enables a pressureless storage at temperature above 100°C. The maximum storage temperatures are limited to 115°C for concept A and to 140°C for concept B. Both PTES systems are implemented in detail and calculated stationary applying the software Epsilon Professional. The supplied electrical power is 5 MW in each case. The two PTES concepts are compared with regard to the exergetic efficiency of components, subsystems and the entire PTES systems, the levelized costs of electricity (LCOE) and the technology readiness level (TRL). For the application of the LCOE the purchase equipment costs (PEC) are calculated using cost functions. In addition, a simplified sensitivity analysis is employed to assess the influence of the uncertainties of the economic parameter on the LCOE results.

Concept B achieves a better round trip efficiency (43.91%) and a lower LCOE (55 €cent/ kWh) than concept A. However, concept A reaches a higher TRL level of the charging.

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Kinetic study of the oxidation und thermochemical reduction of iron and iron oxides

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The energy sector is responsible for a high amount of the released greenhouse gases and thus driving climate change. Major challenges regarding the generation of electricity from renewable resources, e.g. solar and wind, are the long-time storage and transportation of energy.

One promising technology solving these problems is the chemical storage of energy in metal fuels. Energy is released by the direct combustion of metal powders with air under the formation of metal oxides. The obtained metal oxides can be recycled by reduction with green energy and thus leading to a closed CO₂-free cycle. Iron with its high energy density and high occurrence in the earth's crust is a possible candidate for this technology.

Beside the oxidation the reduction plays a major role for the efficiency of the process. The thermochemical reduction with green hydrogen is a possible route and is the subject of future work. The aim is to contribute to the detailed understanding of the oxidation as well as the reduction kinetics.

The reduction of iron oxide (Fe₂O₃) is highly complex as it is a multistep reaction over different intermediates (Fe₃O₄, FeO) and depending on several parameters e.g. reaction temperature, reductant concentration or particle size. Additionally, the reduction with hydrogen is a heterogeneous reaction, thus several phases and phase boundaries need to be considered. The same applies for the oxidation process with oxygen.

Thermogravimetric analysis coupled with IR-spectroscopy and mass spectrometry will be conducted under variation of the experimental conditions. Based on the experimental results a detailed kinetic model will be developed to describe the chemical conversion in the different phases and at the phase boundaries. The developed reaction mechanism will be integrated in numerical simulations to verify established models with experimental results. Validated simulation results are important for reactor upscaling and the further development of the technology.

High Temperature CaO/CaCO₃-Storage for Flexible Steam Power Plants

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The need for more flexible steam power plants brings high temperature carbonate storage in focus. Carbonate storage offers high storage and heat flux density allowing for dynamical charge & discharge and small storage volume compared to power output and storage capacity. To make use of the enormous power density, our concept uses sodium heat pipes with optimal heat transfer capacities in stationary fluidised beds to efficiently transport heat of reaction. This allows an almost isothermal reactor temperature profile for outstanding heat flux densities compared to conventional fixed bed storage.

Charging of storage happens through calcination of CaCO₃ to CaO+CO₂. During discharge, CO₂ re-enters the reactor and carbonates CaO to release heat ($\Delta h_R^0 = 179$ kJ/mol) at up to 850°C. Varying CO₂ partial pressure can quickly change equilibrium as needed and allows for dynamic variation of power output. An integrated steam generator produces steam suitable for steam turbines.

Applications scenarios include the use of renewable surplus electricity to charge the storage in times of negative residual load gradients or negative electricity prices. Discharge through carbonation is especially valuable when high residual load gradients and load peaks in the grid can only be supplied by fossil power plants. Furthermore, discharge at night time could supply zero emission electricity from stored renewable power to the grid. High carbonation temperatures above 800 °C allow for substitution of fossil-fueled steam in steam turbines, not only in existing thermal power plants but also as a stand-alone power plant of the future.

We present results of cyclical CaO conversion capacity for CO₂-capture under real operating conditions in a lab-scale fluidised bed carbonate storage compared to own and literature TGA data. As sintering reduces pore volume and limits reaction surface, we try to find optimised operating conditions for cyclical fluidised bed carbonation and calcination through variation of temperature and CO₂ partial pressure.

Sustainable Heat for the Process Industry – High-Temperature Heat Pumps Employing a Reversed Brayton Cycle

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Climate change has been recognized as one of the most difficult challenges for humankind. Despite agreed climate targets, global emissions of greenhouse gases have actually increased over the last three decades [1]. Especially in the energy-intensive industrial sector, there is still great potential for CO₂-reduction, which has not yet been exploited. The Institute of Low-Carbon Industrial Processes of the German Aerospace Center (DLR) dedicates its research efforts to drastically cutting down on these emissions and pave the way for net-zero emissions by 2050 [2]. The Institute's scope is the total of heating and cooling requirements which amounts to 50 % of Europe's final energy consumption [3]. The poster sheds light on the most recent and upcoming research topics for reducing or eliminating fossil energy sources as well as process-related CO₂-emissions caused by industrial production.

A first high-temperature heat pump prototype was developed and is currently being built at a pilot scale. This prototype will operate employing the reversed Brayton cycle and air as the working medium. This pilot project goes far beyond temperature levels of current high-temperature heat pumps and will provide process heat at above 250 °C and deliver up to 200 kW of thermal energy.

Based on the novel concept for the control and operation system of the pilot heat pump the part-load behavior and capability of a high-temperature heat pump is studied. The thermal output can be adjusted by variation of compressor shaft speed, use of internal recuperation and additionally by variation of the fluid inventory. The latter allows operation of our prototype within a broad part load range down to 25 % of the nominal power at nearly constant efficiencies and output temperatures. Brayton cycle heat pumps can therefore be adapted to a wide range of industrial processes and enable highly efficient thermal energy storage systems to balance grid fluctuations.

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Environmental project portfolio selection using multi-criteria analysis

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Due to legal regulations and social responsibility, environmental protection, energy and resource efficiency are central topics in production and logistics. In most cases, there is a variety of potential options to reduce the future environmental impact of a system, but each with a limited impact. A combination of several individual options can yield the required reduction. The problem is to select options that both significantly reduce environmental impact and make the best possible use of financial resources. Thus, the options must be evaluated and then combined into portfolios. Both the evaluation of the individual options and of the portfolio should take into account several criteria and the given preferences e.g., of company's decision-makers. PROMETHEE (Preference Ranking Organization Method for Enrichment of Evaluations) [1] is an outranking method to treat multi-criteria problems with a discrete set of available alternatives and has been widely applied in environmental decision-making [2].

This poster presentation shows a new approach to determine a portfolio of options based on their PROMETHEE ranking while considering various constraints [3]. We illustrate this approach with a case study on energy saving and emission reduction options in a container terminal [4]. The underlying mathematical problem requires determining a set or portfolio of alternatives regarding goals and constraints, i.e., find a subset of good alternatives maximizing the PROMETHEE net flow under different constraints considering dependencies among alternatives.

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Energetic and exergetic investigation of improvements for heat transfer in latent thermal storage systems

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Energy storages offer the possibility to reduce the temporal discrepancy between demand and supply of energy. In times of the climate change it is necessary to compensate the natural fluctuation of renewable energy resources such as sun and wind. Thermal energy storages represent a good opportunity due to their cost-effectiveness and high flexibility because of the use of heat.

Latent thermal energy storages use the phase change of a storage material to store a large amount of energy in a small temperature interval. The materials for this type of storage often have low thermal conductivity, which makes quick charging and discharging difficult. For this reason, various methods are used to improve heat transfer, such as built-in metal fins or better conducting particles that are mixed into the storage material.

Based on the geometry of a rectangular storage tank with fins, the discharge of an latent thermal energy storage was investigated with a simulation in Python by using the FiPy module under idealized boundary conditions. The influence of the volume fraction of the fins with simple geometry and the increase of the thermal conductivity of the storage material on the achieved heat flux density, the heat transfer and the storage discharge time is discussed. Also, a variation of the temperature of the secondary fluid to discharge the storage tank and exergetic considerations are presented. The used storage material is a paraffin as a phase change material with a low phase transition temperature of 317.15 K

It was shown that higher fin areas lead to higher heat flux densities, but with increasing fin volume the increment of heat flux density decrease. The impact of higher temperature difference was greater than higher conductivity of the phase change material or more fin volume fraction. Furthermore, the impact on the discharge time reduction and the heat flux density with increased thermal conductivity of the storage material is higher with less fin area. The investigated exergy loss was higher with decreasing discharge temperature. When the temperature of the secondary fluid was lowered, the exergy loss was initially less than the reduction in discharge time. If the temperature difference to the discharge was too high, the exergy loss was shown to be greater than the reduction in time to discharge.

Comprehensive integration of the non-energy demand within a whole-energy system: Towards a defossilisation of the chemical industry in Belgium

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Today, non-energy use (e.g. production of plastics or fertilizers) represents about 10% of the final energy consumed worldwide and is dominated by petroleum products, natural gas and coal. However, due to complex flows of materials and ambiguities between net and gross energy in non-energy data sets, this sector is generally misunderstood. The defossilisation of this sector requires to properly define the lever of actions: can we use renewable alternatives to the currently used fossil fuels as direct inputs to this sector? Can the use of these alternatives in the non-energy demand be more efficient and lead to synergies with the other energy sectors (i.e. electricity, heat and mobility)? This paper focuses on the case-study of Belgium and its non-energy demand, mostly from chemical and petrochemical industries (20% of Belgium final energy consumption). It investigates the required molecules of the end-use demand, i.e. High-Value Chemicals (HVC), methanol, and ammonia, as well as the related mature conversion technologies. A transition is analysed to switch the production of the final molecules from fossil fuels to renewable resources as feedstock (e.g. HVC from naphtha-cracking to biomass gasification or methanol-to-olefins). To fully assess the role of these energy carriers, we used and customised Energy Scope TD, a whole-energy system model which optimises the design and hourly operation of an energy system to minimise its costs and emissions. With the aim of carbon-neutrality, this work emphasises the major role of biomass and methanol as the cornerstones to defossilise the non-energy demand, mostly for HVC. To do so, when reaching high global warming potential reductions, biomass is preferably converted into methanol and, subsequently, into HVC. Finally, given the limited availability of local renewables in Belgium, this study highlights the predominant impact of imports like ammonia and methanol.

Power-to-Heat-to-Storage: A Technology Comparison

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The transition to renewable energy sources, such as wind power, photovoltaics, or hydropower, results in a stronger focus on electricity also for heat generation. This focus increases the need for efficient power-to-heat processes, in particular in industry. However, the time-dependent heat demand is often in conflict with the fluctuating electricity supply from renewable sources. This problem can be solved by the integration of thermal energy storage. However, the efficient integration of thermal energy storage and highly efficient power-to-heat processes, such as heat pumps, is still an open question, in particular, for high-temperature applications.

This work compares three power-to-heat processes: electrical heater, vapor-compression heat pump, and inverse-Brayton heat pump, and their combination with various storage technologies. The analysis is based on thermodynamic process modeling. Assessment criteria are typical thermodynamic parameters such as exergetic efficiency, but also technological aspects. The technological aspects include technical limits and challenges in the combination of power-to-heat processes and thermal storage. At this, typical challenges stem from realizing an efficient heat transfer from power-to-heat process to storage. Key factors are, e.g., whether additional heat transfers to and from secondary fluids are necessary as well as the number and types of phases of the fluids/materials involved.

Our study shows the highest power-to-heat exergetic efficiencies for the vapor-compression heat pump. However, the vapor-compression heat pump is also subject to the most severe limitations that are due to the working fluid. Also, integration with thermal storage is more challenging for vapor-compression heat pumps than for other power-to-heat processes. Combining a vapor-compression heat pump and thermal storage usually requires an additional heat transfer that produces further exergy losses and decreases the power-to-heat-to-storage exergetic efficiency. Thus, the most efficient power-to-heat-to-storage technology is case-specific and can be identified by the presented analysis method based on fundamental thermodynamic and technological aspects.

Chemical exergy storage by natural gas pyrolysis in piston engines

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Environmental changes due to the combustion of fossil fuels lead to an increased use of renewable energies. Chemical energy storage systems are needed to compensate for the discrepancies between energy supply and demand, especially if a high energy density or long-term storage is required. The use of piston engines as chemical reactors for polygeneration processes has proven to be feasible. In the present work the pyrolysis of natural gas to produce higher exergy hydrocarbons in a piston engine is investigated theoretically. The required energy to initiate the endothermal reaction is provided by the compression stroke. The thermal decomposition of methane has a high activation energy so that high temperatures are needed for its conversion. To reach high temperatures at the end of the compression stroke the mixture is diluted with argon, reducing its heat capacity. During the expansion stroke reactions are quenched, so even some reactive products remain. The main products are hydrogen, acetylene, ethylene, and benzene. Also the production of a high amount of larger PAHs and soot is predicted.

The piston engine is modeled in Cantera [1] within Python using a time-dependent four-stroke single-zone model with detailed chemical kinetics. The elementary reaction mechanism from Zhou et al. [2] is used to simulate the chemical kinetics. A thermodynamic and kinetic analysis is performed to analyze the process. Investigated parameters include the intake temperature and intake pressure, and the intake argon mole fraction.

The maximum stored exergy and exergetic efficiency are 1.5 kW and 52%, respectively, for $T_0 = 423$ K and $x_{AR} = 0.96$. An intake pressure of 2 bar is chosen since lower intake pressures lead to outlet pressures below 1 atm. Here, 74% of the natural gas is converted and achievable yields for target species like hydrogen, acetylene, ethylene, and benzene are 54%, 13%, 8%, and 9%, respectively. But, besides usable chemicals, 30% of the carbon remains in soot precursors.

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Experimental investigation of the influence of pressure on the oxidation of iso-octane

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Iso-octane is frequently used as a surrogate fuel or as a component in primary reference fuel blends when low temperature combustion strategies in engines are investigated. To develop control strategies for these engines, the reaction kinetics of iso-octane must be known starting from the low temperatures and intermediate pressures before ignition to high temperatures and pressures of combustion. This work adds new experimental data sets to the validation data for reaction mechanism development by investigating the oxidation of iso-octane in stoichiometric mixtures in a flow reactor at pressures of $p = 1, 5, 10, 15,$ and 20 bar and $523 \text{ K} \leq T \leq 973 \text{ K}$. The experimental data are compared to simulations with recent reaction mechanisms by Atef et al. [1], Bagheri et al. [2], Cai et al. [3] and Fang et al. [4]. The comparison between experimental and simulated mole fractions as function of temperature show reasonable agreement for all investigated pressures. In particular, the experimentally observed shift of the NTC region of iso-octane oxidation with increasing pressure to lower temperatures and the acceleration of the high temperature chemistry is captured well in the simulations. Deviations between experimental and simulated results are discussed in detail for the NTC behavior of iso-octane and some key intermediates such as 2,2,4,4-tetramethyl-tetrahydrofuran, iso-butene and acetone. Furthermore, chemical kinetic model of iso-octane is developed.

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Thermodynamic analysis of alternative working fluids for the vapour compression heat pump application: A theoretical study

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Vapour-compression cycles offer a highly efficient solution to provide both heating and cooling. The working fluid, however, is subject to increasingly strict regulations regarding its properties. Thereby, a low global warming potential and a zero ozone depletion potential are required while keeping a high overall cycle efficiency. According to the current state of research, the usage of zeotropic mixtures in vapour-compression cycles is considered particularly promising. Based on basic thermodynamic considerations, the temperature glide characteristic of zeotropic mixtures leads to reduced exergy losses in the heat exchangers and thus to an increase in the coefficient of performance. Besides the heat exchangers, however, the other components (compressor and expansion valve) are influenced also. Within this work, we investigated the improvement potential of the binary mixture propane/isobutene. Firstly, a theoretical study is conducted. Secondly, the theoretical results are compared with experimental investigations. Similar to the experimental set-up, the heat pump model consists of an evaporator, compressor, condenser and an expansion valve. For the theoretical cycle evaluation, two different compressor modeling approaches are used to analyze the effects of the compressor on the overall cycle efficiency as well as the influence of adjusted mixture compositions on the isentropic compressor efficiency. According to the state of the art, the first model uses a fluid independent isentropic efficiency (constant isentropic efficiency of 0.7). For an extended analysis, a semi-physical compressor model is used which evaluates the compressor efficiency based on the fluid and the operating point. The fluids are evaluated for both compressor models using the operating point A2/W65 and a defined temperature difference of the heat source and heat of 5 K. With respect to the *COP*, we found that the usage of both compressor model approaches lead to strong deviations. The optimal mixture composition for a constant isentropic compressor efficiency is located at 20 mol-% propane and 80 mol-% isobutane, while the fluid dependent isentropic compressor efficiency results in an optimal composition of 90 mol-% propane and 10 mol-% isobutane. The high deviations result from the shifts in isentropic efficiency. By using the semi-physical compressor model propane achieves the highest (0.67) and isobutane (0.54) the lowest isentropic efficiency. In this context, experimental results show equal results. Therefore, the authors conclude that precise models for the heat exchangers as well as for the compressor are necessary when different working fluids are studied and compared.

Towards a sustainable building sector: The necessity of an integrated design of heat pump systems

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Heat pump systems are a key technology to replace conventional heating technologies such as gas-fired boilers towards a sustainable building sector. Especially in existing buildings, heat pump systems commonly consist of an air-source heat pump, an auxiliary heater and thermal energy storages. Compared to an almost constant energy efficiency of boilers, the energy efficiency of heat pump systems is highly dependent on various factors such as operating condition, vapour compression flowsheet and refrigerant choice. To operate this system in the most efficient and thus sustainable way, there is a need for an integrated design of all system levels and consideration of the operation during the system's life time.

In this contribution, we utilize process intensification to systematically describe the design process with its constraints and objectives. As the major constraint, we model the thermal comfort of users. Attributing to ecological and economic sustainability dimensions, we minimize annualized costs and emissions simultaneously. We solve the resulting mixed integer non-linear problem in a two-stage optimization framework. According to an annual building performance simulation, the system design is optimized in the first stage. A surrogate-based optimization procedure solves the problem efficiently. In the second stage, a genetic algorithm optimizes the system operation on a daily basis.

The method is successfully implemented in Python using Modelica models and optimizes simultaneously heat pump system design and operation, which decreases costs by about 10 % and emissions up to 20 % for different buildings. Depending on the intensification scenario, different refrigerants and flowsheets are chosen, which outperform all other configurations. Compared to normative design according to DIN EN 15450, our findings indicate the necessity for an integrated design approach to exploit the full potential of heat pump systems. In future research, we plan to extend the control strategy towards model predictive control to further leverage the potential of the thermal energy storage in design and operation of heat pump systems. To capture validity checks within on framework, we will also include experiments for verification or falsification of our assumptions.

Combustion property modeling in fuel design for highly efficient spark-ignition engines

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The large variety of hydrocarbon and oxygenated hydrocarbon molecules, which could potentially serve as future transport energy carriers to replace petroleum fuel and improve engine efficiencies, necessitates streamlined fuel design for identification of the most promising candidates. One approach for finding high-priority candidate fuels lies in the generation of a large pool of molecules in form of a fuel database, based on which the most promising ones can be selected by applying property limits and ranking criteria. This requires the ability to predict key fuel combustion properties rapidly without the necessity for resource consuming experiments or detailed modeling. In the present work, quantitative structure-property relationship models are developed to predict such combustion properties, including research octane number, octane sensitivity, and laminar burning velocity. High values of these properties will enable high engine efficiencies through both knock resistance and fast flame propagation. The developed models are based on artificial neural networks and only require sets of basic molecular descriptors as input parameters [1]. In the laminar burning velocity model, pressure, temperature, and fuel/air equivalence ratio serve as additional inputs. Detailed functional group analyses subsequently identify those molecular features whose presence or absence in the molecule structure leads to beneficial fuel combustion properties. This allows to formulate guidelines for the design of future high-performance fuels. The practical selection of high-priority fuels for spark-ignition engines is finally demonstrated by compiling a large database of more than 600 fuel compounds [2], with properties predicted by the developed models, and ranking them according to the efficiency merit value proposed recently in the literature [3].

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Stack-Scale Modelling of Reversible Solid Oxide Cells (rSOCs)

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The envisioned transformation to a clean and distributed energy system based on renewable energy sources (RES) can only be realized by integrating energy storage concepts. This is due to the strongly fluctuating power supply produced by RES, which requires balancing the electricity demand and supply. While batteries suffer from capacity limitations and pumped hydro storage from geological constraints, chemical storage concepts are attractive due to long-term storage options and high energy density carriers, e.g. on the basis of H₂, CH₄ or CO. The reversible solid oxide cell (rSOC) is a high-temperature device that is capable to operate in “fuel cell mode” (SOFC) producing electrical power, and in “electrolysis mode” (SOEC) producing fuel that is stored in tanks for later usage. In this way, the momentary load profile of the electric grid can be followed by the rSOC, by switching between both operation modes. In contrast to the more established low temperature fuel cells like polymer-electrolyte membrane cells (PEMs), rSOCs operate in the range of 600-900 °C. This enables very high roundtrip efficiencies and fuel flexibility, but it is evident that operation at such elevated temperatures comes along with major obstacles that need to be solved. In this work, we focus on the dynamic process of mode switching. Firstly, a 1-D+1-D model of a single planar repeating unit is calibrated and validated against published experimental polarization data at various temperatures and fuel compositions in both operation modes. After, a scale-up to the stack level is performed. By applying a transient multi-physics 3D simulation tool [1], the impact of mode switching on the thermal behavior of the rSOC-stack is illustrated. Additionally, strategies to lower temperature gradients during the mode switch are discussed. Temperature control strategies include variation of the excess air supply, and the variation of the load gradient that the stack is exposed to during the switch.

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A reduced mechanism for polygeneration processes with ozone addition

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Combustion devices such as piston engines are considered to be promising reactors for polygeneration processes at ultra-rich reaction conditions. Combined with its conventional function of power generation, internal combustion engines have the potential for flexible change from work production to chemical synthesis and energy storage, which would be meaningful for coping with fluctuations in electricity supply and the demand for achieving low-carbon emissions. Detailed reaction mechanisms describing the oxidation and pyrolysis of fuel-rich methane/dimethyl ether (DME)/air mixtures have been reported in previous studies. To facilitate a faster conversion of methane, ozone at a concentration of up to 380 ppm is added to the system as a reaction accelerator. An updated detailed mechanism for polygeneration considering the impact of ozone addition, namely PolyMech 3.0, which consists of 133 species and 762 elementary reactions is used in this work. The large number of species and reactions, as well as the broad range of timescales involved, makes it computational cost demanding when applied to realistic three-dimensional simulations. To this end, this work aims at developing a reduced mechanism based on the Global Quasi-Linearisation (GQL) concept [1,2]. The construction of GQL matrices is investigated. It is found that the dimension of fast dimension is higher if high-temperature chemistry is the only target. To obtain a reduced description for certain ranges of operating conditions, sample points have better to cover the whole range. As a preliminary result, a GQL matrix having 31 fast modes is reported, which still has a problem predicting autoignition processes at some other initial conditions though. We will improve algorithms for the calculation of eigenvalues and eigenvectors in future, and develop an automatic method to determine the optimal GQL matrix.

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