Imprint

CCEM and novatlantis – Annual Activity Report 2015

Published by

Competence Center Energy and Mobility CCEM

Concept by

Urs Elber

Coordination and realization by

Agnieszka Hamburger

Editorial work, design and layout by

Peter Lutz, LUTZdocu.ch, Uster

Printed by

Paul Scherrer Institute, Villigen

Available from

Competence Center Energy and Mobility CCEM
c/o Paul Scherrer Institute
5232 Villigen PSI, Switzerland
Phone: +41 56 310 2792
Fax: +41 56 310 4416
E-Mail: ccem@psi.ch
Internet: www.ccem.ch

Copying is welcomed, provided the source is acknowledged and an archive copy sent to CCEM.

© CCEM, 2016
# Table of Contents

## Foreword

### Competence Center for Energy and Mobility – Complexity is our Business

## Mobility

<table>
<thead>
<tr>
<th>Page</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>NO\textsubscript{x} Reductions</td>
</tr>
<tr>
<td>8</td>
<td>Flex-FI-Dual</td>
</tr>
<tr>
<td>10</td>
<td>CatPor</td>
</tr>
<tr>
<td>12</td>
<td>DuraCAT</td>
</tr>
</tbody>
</table>

## Electricity

<table>
<thead>
<tr>
<th>Page</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>17</td>
<td>HITTEC</td>
</tr>
<tr>
<td>20</td>
<td>CONNECT PV</td>
</tr>
<tr>
<td>22</td>
<td>SERAN</td>
</tr>
<tr>
<td>25</td>
<td>ADMIST</td>
</tr>
<tr>
<td>28</td>
<td>TeKaF</td>
</tr>
<tr>
<td>31</td>
<td>HydroNet 2</td>
</tr>
<tr>
<td>35</td>
<td>Geotherm 2</td>
</tr>
<tr>
<td>38</td>
<td>FAMSADI</td>
</tr>
<tr>
<td>40</td>
<td>MeAwaT</td>
</tr>
<tr>
<td>43</td>
<td>SLIB</td>
</tr>
<tr>
<td>46</td>
<td>ISCHESS</td>
</tr>
</tbody>
</table>

## Heat and Buildings

<table>
<thead>
<tr>
<th>Page</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>51</td>
<td>IDEAS4cities</td>
</tr>
<tr>
<td>54</td>
<td>SECURE</td>
</tr>
</tbody>
</table>
# Table of Contents

**Fuels**

<table>
<thead>
<tr>
<th>Page</th>
<th>Project/Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>61</td>
<td>Syngas Diagnosis: Online Process Diagnostics for Performance Assessment of a Biomass Gasification Processes</td>
</tr>
<tr>
<td>65</td>
<td>ARRMAT – ARRMATplus: Attrition Resistant Fluidized-Bed Materials and Methanation Catalysts</td>
</tr>
<tr>
<td>68</td>
<td>OPTIWARES: OPTImization of the Use of Wood as a Renewable Energy Source</td>
</tr>
<tr>
<td>71</td>
<td>RENERG²: Renewable Energies in Future Energy Supply</td>
</tr>
<tr>
<td>74</td>
<td>SCHE-dual: Stable and Clean High-Efficiency Diesel and Dual-Fuel Combustion</td>
</tr>
<tr>
<td>76</td>
<td>PAWaSto: Photovoltaic Assisted Algae Production and Waste Water Treatment for Combined Heat and Power Generation and Storage</td>
</tr>
<tr>
<td>79</td>
<td>Solar Fuels: Solar Thermochemical Production of Fuels from CO₂ and H₂O Using Ceria Redox Reactions</td>
</tr>
<tr>
<td>81</td>
<td>Solar-HTG: Solar Assisted Hydrothermal Gasification Process</td>
</tr>
<tr>
<td>83</td>
<td>Hy-Form: Formic Acid – Chemical Storage of Electrical Energy and On-Site Hydrogen Production for Use in PEM Fuel Cells</td>
</tr>
<tr>
<td>86</td>
<td>HyTech: Sustainable Hydrogen Utilization</td>
</tr>
<tr>
<td>89</td>
<td>CO₂ to Methanol: Highly Efficient and Selective Catalysts and CO₂ Sorbents for the Electrochemical Production of Methanol from CO₂</td>
</tr>
<tr>
<td>90</td>
<td>GasOMeP: Gasoline Vehicle Emission Control for Organic, Metallic and Particulate Non-Legislative Pollutants</td>
</tr>
</tbody>
</table>

**novatlantis**

<table>
<thead>
<tr>
<th>Page</th>
<th>Project/Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>93</td>
<td>novatlantis: Sustainability at the ETH Domain – Promotion of Transdisciplinary Science</td>
</tr>
</tbody>
</table>

**Register**

<table>
<thead>
<tr>
<th>Page</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>105</td>
<td>List of Finalized Projects</td>
</tr>
<tr>
<td>109</td>
<td>Scientific Project Partners and Financing Institutions</td>
</tr>
</tbody>
</table>

**Appendix**

<table>
<thead>
<tr>
<th>Page</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>111</td>
<td>Presentations</td>
</tr>
<tr>
<td>119</td>
<td>Publications</td>
</tr>
<tr>
<td>127</td>
<td>Patents</td>
</tr>
</tbody>
</table>
Competence Center for Energy and Mobility
– Complexity is our Business

Since 2006 the Competence Center for Energy and Mobility CCEM has placed «Calls for Proposals» targeting joint efforts across institutional boundaries. This proved not to be an easy task at the beginning – complexity in research structures is not primarily a factor desired. But the challenges and expectations towards research grew more complex, too. Solutions could no longer be found within the traditional disciplinary research areas, more and more the key lies in transdisciplinary research.

Thanks to the foresight of the ETH-Board, CCEM was given the opportunity to orchestrate the first steps towards networked research. Compared to the beginning, most CCEM projects today are more complex, integrating more research groups of different institutions and levels, industries, city administrations, building owners, investors, public traffic planners and political institutions.

As a result, not only many relevant scientific results could be achieved. Maybe even more important, research groups have developed a most effective modus operandi characterized by a considerate way of sharing results, the incorporation of common methods and approaches, and an established way of facile initiation of cooperation.

66 funded projects (19 still ongoing) received high appreciation among our partners. Many of these projects became a base for activities in the Swiss Competence Centers for Energy Research (SCCERs).

2015, CCEM further improved the efficiency of its lean administration, which freed up 650 kCHF for 12 projects to enhance their results.

novatlantis has continued its activities for transferring knowledge and results from the ETH-domain into pilot regions, forums and presentations.

Besides accomplishing new options for our energy and mobility future, CCEMs «business» has successfully handled and reduced the complexity of networked research!

Prof. Dr. Alexander Wokaun  Urs Elber
Head of the Steering Committee  Managing Director CCEM
NOX\textsubscript{-}Reduction

In-Cylinder Emission Reduction in Large Diesel Engines

Scope of project

This collaborative effort aims at a significant technological progress towards an efficient, clean burning diesel engine that does not require exhaust gas after treatment to further reduce NO\textsubscript{X} or particulate emissions. One goal is set in the thorough comprehension of the physicochemical processes involved governing the NO\textsubscript{X} and soot formation under the combined application of Miller inlet valve timing (MT) with 2-stage turbo charging and exhaust gas recirculation (EGR), water-in-fuel emulsions and pilot injections. This understanding will yield a second key deliverable, namely a fast numerical algorithm based on phenomenological models incorporating the new technological approach and having good predictions for NO\textsubscript{X} and soot.

Status of project

During the reporting period final investigations have been performed not only related to engine testing but also in the congruent modelling predications. This leads to an overall improved understanding of the important driving mechanisms and their interactions. The results from the two engine test beds and two numerical simulation efforts successfully meet the project goals with high fidelity.

Main scientific results of workgroups

**ETH numerical simulation**

NO\textsubscript{X} emissions at the end of an engine cycle (MTU single cylinder) are shown in figure 1. Ignition delay increases in the direction OP1 to OP6; cases marked with (p) are with a pilot injection (e.g. OP4p is OP4 with a pilot). The values are shown relative to the baseline case OP1. The trend reversal of NO\textsubscript{X} observed in the experiment (solid green lines) in the direction of OP1 to OP6 is captured by the simulations (solid blue lines). Although the trend is captured very well, the predicted relative NO\textsubscript{X} for cases OP5 and OP6 is quantitatively much higher. The reduction in NO\textsubscript{X} by adding a post-injection (dashed blue lines) and the consequent recovery of diffusion-mode combustion is very well reproduced.

**ETH 1-D model simulation for LERF**

Studies on the improvements in the engine efficiency of the engine setup under high EGR rates were conducted using a 1-D engine model. Additional investigations of the variation of MT degree on efficiency when running with EGR were performed on the semi-short route EGR setup. The results showed that moderate MT degrees are advantageous in terms of engine efficiency due to the reduced requirements for EGR compression compared to extreme MT setups. This arises from the high scavenger pressures existing in the extreme MT cases.

Finally, an investigation on «switchability» between non-EGR and EGR operation was performed. The study showed...
that it is advantageous to use variable valve timing in order to run variable EGR rates with a constant turbine area. The use of variable valve timing (VVT) results in:

- Ability to run the engine with different EGR rates up to high loads, while respecting peak pressure levels.
- Increase in engine efficiency compared to non-VVT operation when running variable EGR rates.
- Reduction of requirements for very wide LP compressor maps, since it is possible to run the engine close to a single operating line.

**PSI LERF testing**

Besides further testing of the semi-short route EGR setup an electrically driven EGR blower was implemented. Final tests in order to determine the comparative performance of all different EGR systems applied (SSR, donor, blower; different TC setups) in terms of fuel consumption, as well as to determine the NO\(_x\) reduction potential and soot emission characteristics could be completed. In general, the measurement results showed that IMO Tier III NO\(_x\) emissions limits can be fulfilled with EGR rates around 25 % for the whole load range. However, this NO\(_x\) reduction comes with a 20-fold increase in soot emissions.

In order to abate soot, a water-fuel emulsion (WFE) prototype system, which prepares the emulsion in the fuel supply line using high pressure water injection (12 bar), providing a high degree of atomization and homogenization right upstream the common rail pump was tested on the engine. The system allows low latency variation of the water mass fraction according to demand and guarantees quick emulsified fuel burn-off after water cut-off in preparation for engine stop to protect the injectors and injection system parts from corrosion.

The use of 10 % WFE resulted in a significant improvement in the NO\(_x\)-BSFC and the NO\(_x\)-soot trade-offs (figure 2). The reduction in NO\(_x\) was determined to be from a slight prolongation of injection and the local cooling of the flame from the addition of water. The reduction in BSFC was determined through an energy loss analysis of the engine to result from significant reduction in exhaust enthalpy losses as a result of lower engine air consumption when using WFE. This effect out-weighed the high pressure efficiency loss resulting from the prolonged injection duration.

Finally, the addition of water resulted in a soot emission reduction of around 70 % with constant injection parameters. In combination with an increased injection pressure, 10 % WFE resulted in soot emissions of around 10 mg/m³ at 50 % load, which is just a 2-fold increase compared to the non-EGR setup.

**PSI HTDZ**

The fundamental experimental spray combustion studies were conducted on the high-temperature/-pressure constant volume combustion cell (HTDZ) on a Diesel model fuel (n-dodecane) varying ambient oxygen concentration, temperature and injection mode (single and multiple). Influences on spray penetration, liquid length, ignition delay, lift-off length and heat release rate have been investigated. Fuel injection pressure (1000 bar) and cell charge density (~23 kg/m³) were set constant. Overall, the following conclusions can be stated:
NO\textsubscript{x}-Reduction
In-Cylinder Emission Reduction in
Large Diesel Engines

• Spray penetration progression and quasi-steady state liquid length are not influenced by the oxygen concentration.
• Lowering oxygen content leads to an increase in lift-off length, prolonged burnout and decreased proportion of premixed combustion.
• Employing a pilot injection diminishes the ignition delay of main injection and the heat release rate maximum peak of premixed combustion mode depending on the dwell time between pilot and main injection for low ambient temperatures reflecting extreme MT.

Moreover, the influence of water-fuel emulsion (WFE) on spray combustion was investigated at the HTDZ. Applying WFE the mass flow was increased through augmented injection pressure, to attain equal energy input flux as for the unblended fuel (n-dodecane). The following main observations are made:

• The spray angle is generally larger for WFEs in regard to the pure fuel which can be attributed to elevated injection pressure and density.
• The liquid length and flame lift-off length during quasi-steady mixing limited combustion increase with ascend water content most likely due to the lower volatility of water compared to n-dodecane.
• For low amounts of water (<=5% by volume) in WFE the ignition delay is virtually unchanged. Instead, for WFE including 7.5% water by volume (WFE 7.5) the spray ignition is delayed (figure 3, left).
• The fuel conversion is enhanced and the proportion of premixed combustion rises generally for WFE spray combustion. Both might be the result of augmented spray surrounding air entrainment and mixing due to the enlarged jet momentum employing WFE.
• Lowering the charge gas oxygen concentration leads to an increase of spray liquid length and flame lift-off length for WFE 7.5. Additionally a moderate augmentation in ignition delay could be observed. Moreover, fuel conversion is slowed down leading to lower premixed combustion proportion and prolonged burnout. However, the influence of ambient oxygen availability in regard to fuel conversion is observed to be lower for WFE 7.5 than for the pure n-dodecane (figure 3).

Main achievements

• Numerical simulations capturing trend reversal of NO\textsubscript{x} for high degree of Miller valve timing.
• 1-D simulations of the variation of MT degree on engine efficiency when running with EGR as well as investigations with regard to «switchability» (non-EGR/EGR).
• Implementation of a water-fuel emulsion system at the LERF leading to improved NO\textsubscript{X}-BSFC and NO\textsubscript{X}-soot trade-offs.
• Application of an electrically driven EGR blower at the LERF.
• Fundamental spray (penetration/liquid length) and combustion (ignition delay, lift-off, HRR) investigations at the HTDZ under engine-like (e.g. EGR, WFE) operating conditions.
**Flex-FI-Dual**

Flexible Facility for the Investigation of Gas, Diesel and Dual-Fuel Combustion

**Scope of project**

The further advance of gas- and dual-fuel combustion engine technology requires test rigs that permit experimental in-depth studies of relevant in-cylinder processes at engine like conditions (mixtures, pressures, temperatures and turbulence levels). Existing test rigs like constant volume cells or the single stroke machine at LAV/ETH cannot satisfy all requirements; therefore this project aims at the development of a new test rig that combines the excellent optical access of constant volume cells with internal compression of engines and single stroke machines (to be able to work with ignitable mixtures) and the in-cylinder flow fields and turbulence levels of real engines; it is therefore especially suitable for (but not limited to) investigations into dual-fuel combustion processes.

**Status of project and main scientific results of workgroups**

The project Flex-FI-Dual initially aimed at the development of a new type of a hydraulically operated rapid compression and expansion machine. Intended as a further development of the existing single stroke machine at LAV/ETH the electronically controlled hydraulic piston drive system would enable the new machine to perform optional intake strokes before compression/expansion to provide engine like flow fields and turbulence levels if desired. However, although the emerging machine design and the accompanying simulations proved the feasibility of the concept the exorbitant costs of the necessary hydraulic piston drive system rendered this solution impossible within the (financial) scope of this project.

Therefore another solution had to be looked for that would not require a hydraulic piston drive system; it was found in a concept that uses a motored large bore Diesel engine block (including crank shaft and pistons) as basis and adds the experimentally important part, the combustion chamber, in form of specially shaped cylinder heads that provide excellent optical access.

Although the motored Diesel engine block (from a Liebherr D944 engine, donated by Liebherr SA, Bulle) does not permit pure single stroke operations it is possible to vary end of compression gas pressures and turbulence levels, in-cylinder flows and turbulence levels in the combustion chamber by varying gas intake conditions (pressure, temperature), engine speed, intake and exhaust valve timings (cycle resolved) and the timing of the injection/ignition within the firing cycle.

Several optical layouts of the combustion chamber resp. cylinder head can be envisaged as shown in figure 1. The names of the layouts are chosen to indicate the order of the observable spray resp. flame jet lengths (which in real engines is often given by the piston bowl radius). Within the scope of this project the «Car» type head version will be fully realized, the other variants are only studied regarding their feasibility and have to be fully designed once the need arises in the context of future research projects.

Figure 2 shows the CAD design of the «Car» type head in a configuration with a single axial fuel spray Diesel injector inserted from the top of the chamber. Through the two large round windows it is possible to see through the whole chamber (except for the «neck» connecting chamber and engine cylinder). Laser sheets can be brought into the chamber through two elongated windows on the sides. Although the cross section of the «neck» connecting cylinder and chamber is quite large (to optimize the flow field inside the chamber as has been shown in accompanying CFD calculations) a compression ratio ≥ 13 can be maintained to achieve maximum end of compression pressures > 100 bar and temperatures > 1000 K.

Due to space constraints in the cylinder head the four gas exchange valves cannot be as large as in a normal combustion engine; therefore the engine is supplied with a pressurized and preheated air resp. air/gas mixture. A drawing of a new intake valve is shown in figure 3. The gas exchange valve at the bottom is directly actuated by a pneumatic cylinder. The restoring force for the gas exchange valve is supplied by a gas spring instead of a normal coil spring so the
Flex-FI-Dual
Flexible Facility for the Investigation of Gas, Diesel and Dual-Fuel Combustion

restoring force can be optimized regarding the effective operating conditions. Since the gas exchange valve must open and close very quickly to maximize the gas flow in and out of the engine cylinder fast matrix type pneumatic valves are used to supply the pneumatic cylinder. The field-programmable gate array (FPGA) based valve control system allows for adjustments of opening and closing times based on cycle numbers and/or the state of the machine (for example gas pressures), so different valve timings for scavenging, filling and working (firing) cycles can be programmed to be able to cover a wide range of operating conditions (pressures, temperatures, flow field and mixture compositions) in the combustion chamber for the experiments.

By now the design of the key components, i.e. the «Car» type cylinder head and the pneumatic valves, is almost complete including dimensioning of the flywheel and the electric motor/brake. As soon as manufacturing of the key components has started the focus of the project work will shift towards the setup of the complete test rig and its environment, the control system for the engine/electric motor and the FPGA controller for the valves. Commissioning of the system is planned to start in summer 2016 so the new test rig will be ready for the first experiments before the end of 2016.

Figure 4 shows the layout of the lab where the new test rig will be set up including the main components. All the rotating parts (engine block, flywheel, shafts and electric motor/brake) are mounted rigidly on the (already existing) heavy base plate. A flywheel has been included in the drive train to minimize engine speed fluctuations during the experiments (i.e. fired cycles). The test rig can be operated safely from an adjacent control room.

Figure 4 (left): CAD drawing of the «Car» type cylinder head actuated by a pneumatic cylinder.

Figure 4: Layout of the lab with the main components of the new test rig.

Figure 1: Possible combustion chamber (cylinder head) configurations.

Figure 2: CAD drawing of the «Car» type combustion chamber in a configuration with a research type Diesel fuel injector (single axial fuel spray).
**CatPor**

**Catalysis in Porous Media for Automotive Applications**

**Scope of project**

Ceramic foams, as developed by the Empa Automotive Powertrain Technologies Laboratory, have excellent properties as catalyst substrates for automotive applications. Extensive studies, also under the support of CCEM (the completed NEADS and NADiP projects), have shown that ceramic foam based catalysts can achieve similar pollutant conversion efficiencies but with roughly a third of the precious metal amount and half of the external dimensions, compared to the state-of-the-art conventional honeycomb catalysts.

The full characterization of the catalyst behavior requires a multiscale analysis from the overall reactor dimensions and its operation time scales down to the washcoat microscale and of the chemistry time scale. Thus an experimental evaluation is extremely difficult and computational simulations are the choice for a deep investigation.

**Status of project**

The project has been completed by developing specific guidelines for the design and the manufacture of foam based catalysts. The focus was placed to the optimization of the geometrical parameters and catalysis configuration. A detailed simulation series comparing open cell structures and honeycombs provided insight on the changes required in the substitution of honeycomb with foam catalysts and on the relative advantages.

A washcoat diffusion and reaction model was developed and validated. The model was implemented and is able to handle arbitrary reaction mechanisms and geometries. The scope was to study the flow and diffusion phenomena through the submicron pores of the washcoat. Particular focus has been put on understanding their combined effect together with the chemical reaction mechanism in the overall conversion performance of catalytic reactors. The washcoat model and a mapped CO oxidation mechanism was successfully applied to a 3D Kelvin Cell (KC) structure for the analysis of cumulative emissions during warm up phases.

Small samples of both catalysts (foam and honeycomb) have been manufactured and experimental analysis has been performed in a test flow rig where flow resistance and reactivity have been measured, confirming the higher surface reactivity of the foams.

**Main scientific results of workgroups**

A direct comparison between foam and honeycomb structures (figure 1) has been performed using a computational fluid dynamics (CFD) solver to optimize the catalytic performance of foam structures and address their properties compared to the standard catalytic honeycomb. The CFD models were developed using OpenFOAM, a well-established solver.

Foam structures were idealized to a randomized structure of Kelvin cells, which are polyhedrons with 14 faces (6 quadrilateral and 8 hexagonal) and are also known as tetrakaidecahedrons. For cost reasons, the geometrical structure of honeycomb was simplified to a single channel and foams were simplified to a $2 \times 2 \times 4$ Kelvin cells structure.

The model allowed the analysis of the mass transfer properties of foam reactors (KC) and honeycomb (hc) reactors for a wide range of operative conditions ($1 \text{ m/s} < U < 10 \text{ m/s}$) (figure 2).

Conversions have been compared among different cases with and without washcoat diffusion. Conversion does not reach the limit of infinitely fast kinetics, even at the highest temperature simulated ($1000 \text{ K}$), when finite rate washcoat diffusion is considered. The difference between the actual conversion and the conversion in the limit of infinitely fast kinetics remains roughly constant above the
light-off temperature. Increasing the specific surface area of the washcoat reduces the impact of washcoat diffusion resistance above the light-off temperature. However, even with the highest specific surface area considered ($F_{cat/geo} = 500$), the washcoat diffusion resistance remains significant at all temperatures.

The washcoat diffusion resistance can be reduced by a large fraction of macropores which significantly enhance the diffusion process. Further investigation showed that a high catalytic activity ($F_{cat/geo} > 100$) combined with a large fraction of macro pores results in a difference between the infinitively fast chemistry limit and the case of finite washcoat diffusion of less than 10%.

The washcoat model was implemented in 3D-CFD simulations to investigate the cold-start transients for foam based catalytic converters with different foam properties, washcoat parameters, CO inflow mass fractions and inflow velocities (figure 3). Empirical correlations for the time to light-off were built based on non-dimensional parameters which can be generalized to all operative conditions.

Cumulative cold start emissions are investigated (figure 4) depending on inflow velocity. Although decreasing inflow velocity will delay the light-off, the cumulative emissions are minimized at an optimal inflow velocity which depends on the reactor properties. Moreover, emissions are reduced by decreasing pore size and increasing foam porosity, but increase by increasing axial conduction in the reactor. We show that doubling the inflow mass fraction of CO from 0.5% to 1% roughly triples the cumulative emissions. Doubling the active surface of the washcoat results in roughly 30% lower cumulative emissions.

Furthermore, cumulative emissions in foam reactors are compared with honeycomb. In foam reactors they are significantly lower, due mainly to the higher porosity which reduces the thermal transient phase, confirming the potential of foam based reactors in automotive applications.

Main achievements / outreach

In conclusion the main achievements are:

- A parametric CFD analysis and characterization of open cell foam structures has been performed determining mass and momentum transfer properties of open cell foam reactors.
- A direct and rigorous comparison between Kelvin cell and honeycomb structures was performed showing the potential of foam catalysts to reduce the size and the catalytic surface compared to commercially available reactors.
- Foam porosity was identified as the main parameter effecting conversion over pressure drop efficiency in foam catalysts.
- Experimental tests of sample reactors have been started, and first results confirmed a higher activity per unit of catalyst surface of the foam reactors.
- Internal washcoat diffusion resistances have been evaluated by low dimensions analysis combined with detailed chemistry kinetics.
- Cold-start transients for foam based catalytic converters are simulated and cumulative emissions are analyzed as a function of all main parameters characterizing the catalytic reactors.

Figure 2 (left): Volumetric mass transfer coefficient of Open Cell structures (KC) with two different porosities ($\varepsilon = 0.80$ and $\varepsilon = 0.90$) and an honeycomb (hc) with a standard commercial porosity ($\varepsilon = 0.73$).

Figure 2 (right): Cumulative emissions ($Ecum$) per unit cross section area versus the inflow velocity. A reference case (ref) is compared to cases with higher porosity, lower cell size ($L_{Kelvin}$) and lower thermal conductivity.

Figure 3: Temperature and CO mass fraction during light-off transient. The slice shows the CO mass fraction on the upper half and the temperature on the lower half. The foam surface temperature is also shown.
**DuraCAT**

**Highly Durable Oxide-based Catalysts for Polymer Electrolyte Fuel Cells**

**Scope of project**

For a sustainable economic growth, many efforts have been directed in the last few decades towards the development of efficient energy conversion systems using environmental friendly, renewable energy resources. In this scenario, particularly for automotive applications, the development of polymer electrolyte fuel cells (PEFCs) plays a critical role in the development of a sustainable hydrogen-based-economy. State-of-the-art PEFC cathodes are based on Pt nanoparticles supported on high surface area carbons. Despite the good performance, Pt-based catalysts supported on high surface area carbons suffer from corrosion stability which is at present one of the main issues hindering PEFC widespread market penetration. Therefore, alternative support materials to carbons showing adequate stability under typical PEFC operative conditions are needed to meet the durability requirements for practical applications. Besides being resistant to corrosion at high potentials, support materials for PEFCs must also be chemically stable under acidic conditions, good electronic conductors, and low cost and high surface area materials. The DuraCAT project aims at developing stable cathodes for PEFCs using a multi-level approach towards the understanding and the development of high durable cathode catalysts based on doped metal oxide supports.

**Status of project and main scientific results of workgroups**

One of the main goals of the project is to develop a fundamental understanding of the main structural, morphological, chemical and electrochemical properties of stable oxide materials under typical PEFC operating conditions (at the positive electrode). For this reason model electrodes have been first developed and investigated. Producing oxide thin films by physical deposition techniques, important physicochemical properties, such as composition, microstructure and surface termination can be controlled and studied in detail. Among binary oxides which are known to be stable in acidic environment, we have selected SnO2 compounds as potential catalyst supports. Therefore, SnO2-based thin-films were studied experimentally and from First Principles.

SnO2 thin films have been prepared by reactive magnetron sputtering using a metallic tin target and O2 as reactive gas. Doping of SnO2 thin films has been achieved by modifying the tin target with Niobium, Tungsten, Platinum, Antimony or Tantalum chips. Doped SnO2 films showed electrical conductivities 2–3 orders of magnitude higher than those of undoped SnO2 films. The highest conductivities of approximately 700 Scm⁻¹ have been achieved for Nb and Ta doped SnO2 films with dopant concentration of 2 and 1 at%, respectively. Successively, platinum catalysts have been deposited by magnetron sputtering on the SnO2 film electrodes, with a fixed loading of 2 μg/cm². The oxygen reduction reaction (ORR) activity of Pt catalysts supported on glassy carbon (GC), undoped and doped SnO2 has been evaluated by rotating ring disc (RDE) measurements performed inside a three electrode glass cell in 0.1 M HClO4.

Figure 1 shows that ORR activities similar to Pt/GC can be achieved by having as support doped SnO2 with Ta, Sb or Pt.
Two times higher activities of the Pt catalysts were observed when supported on W or Nb doped SnO$_2$. No direct correlation between the support conductivity and activity of the catalysts could be observed in the present study. These observations are proofing that the SnO$_2$ dopant and the dopant concentration can drastically influence the ORR activity of the supported Pt catalyst. Dopant-induced modifications of the SnO$_2$ films can affect the electronic properties of the supported catalyst which seems to have a direct influence on the catalyst activity.

Computational materials design, based on hybrid Density-Functional-Theory (DFT) was successfully integrated with the experimental synthesis and characterization program. Experimental findings were rationalized from First Principles, distilling general design guides and synthesis strategies from the focused experimental program.

Electronic interactions between metallic Pt nano-particles supported on SnO$_2$ were investigated using large-scale DFT calculations. As the work function of nano-particulate Pt and the support differ, bringing them into contact will lead to charge transfer across the interface to equilibrate the respective Fermi levels. We find that the reduction of the (110) surface of SnO$_2$ leads to a large change of the work function of the surface from around 6 eV for the fully oxidized (110) surface to about 3.5 eV for reduced surfaces. As the work function of nano-particulate Pt is of the order of 5.5 eV, this results in a change of direction for the charge transfer, as shown in figure 2, impacting the electrostatic properties of the electrocatalysts with implications for activity towards oxygen reduction.

Our modelling work indicates that these effects become more pronounced for low Pt loadings and are sensitive towards support chemistry and surface treatments, providing simple and novel routes to improve activity of the precious metal electrocatalyst whilst retaining or even improving stability. Our calculations indicate that at least a two-fold increase in oxygen reduction activity of Pt supported on reduced SnO$_2$ relative to oxidized SnO$_2$ can be attributed to electronic metal-support interactions.

Parallel to the fundamental understanding of novel Pt/oxide catalyst systems, improvements of the corrosion resistant, benchmark cathode catalyst Pt/IrO$_2$-TiO$_2$ (Umicore®) have been explored. IrO$_2$-TiO$_2$ support with reduced Ir content, high surface area, and relatively high conductivity was successfully synthesized by an Adams method route. Transmission electron microscopy (TEM) images of pure TiO$_2$ and IrO$_2$ show particles with approximate diameters of 5 and 1 nm respectively. Measuring electrical conductivity of these materials shows an approximately exponential increase in conductivity with Ir content, which was modelled using percolation theory. Sufficient conductivity for fuel cell applications (>$0.1 \, S\,cm^{-1}$) is achieved at 40 molM% Ir. To test the influence of TiO$_2$ on electrical conductivity, IrO$_2$-SnO$_2$ and IrO$_2$-NbO$_2$ materials were also prepared by an identical Adams method route with 40 molM% Ir. Surface area...
Highly Durable Oxide-based Catalysts for Polymer Electrolyte Fuel Cells

determinations show that all samples have high surface areas, although that of IrO$_2$-SnO$_2$ is lower. Although HAADF-STEM images show similar morphology for the three samples (figure 3), the electrical conductivities of IrO$_2$-SnO$_2$ and IrO$_2$-Nb$_2$O$_5$ are considerably reduced in comparison to IrO$_2$-TiO$_2$. This reduction in conductivity may be due to the coverage of IrO$_2$ surfaces by SnO$_2$ or Nb$_2$O$_5$, which would be expected to hinder conductivity due to the low electrical conductivity of these oxides.

The Umicore® benchmark catalyst, Pt/IrO$_2$-TiO$_2$, has been assessed in terms of performance and stability under operating conditions in a PEFC. Once the optimization the membrane electrode assembly (MEA) based on the benchmark catalyst was achieved, the stability of the new system was tested in real fuel cell operation regime. These results were compared with MEAs based on Pt/Carbon (EC10E50E TKK) state-of-the-art catalyst.

MEA stability was tested using specific accelerated stress test (AST) protocols developed by the US Department of Energy’s (DOE) fuel cell program. For catalyst stability evaluation, i.e. platinum nanoparticles stability, a first AST protocol was applied. In a standard manner a triangular potential cycling at 50 mV/s between 0.6 and 1 V vs RHE (16 seconds per cycle) was applied to the cathode. For the evaluation of support stability another AST protocol (start-stop protocol) was used. The air electrode (cathode) potential was cycled between 1 and 1.5 V vs RHE with a scan rate of 500 mV/s (2 seconds per cycle). 10,000 cycles were recorded on a fresh MEA at 80 °C, 100 % relative humidity (RH) and atmospheric pressure.

Figure 4 (A) shows the comparison of the fuel cell performances of both catalysts at the beginning and end of AST protocol (BOT and EOT, respectively). The iR-corrected initial performances are comparable in both cases. These results show that when using a conductive oxide support with a good MEA design, similar performances can be obtained. The voltage losses at 0.8 A/cm$^2$ are around 100 mV for both MEAs. The EOT data suggest that the corrosion resistance of platinum phase is not improved by the alternative support when compared to the carbon-supported catalyst.

Figure 4 (B) shows the polarization curves obtained on MEAs based on the two catalysts studied here, before and after exposure to the start-stop AST protocol. The Pt/C-based MEA revealed a significant loss in performances, whereas the Pt/IrO$_2$-TiO$_2$-based MEA showed a minimal loss in performances after exposure to 10,000 cycles. The loss in cell voltage at 0.8 A/cm$^2$ was only about 25 mV for Pt/IrO$_2$-TiO$_2$, whereas for Pt/C, the loss was too high to maintain operation at this current density. These observations can be attributed to the stability of the IrO$_2$-TiO$_2$ catalyst support.
Electricity
HITTEC
High Temperature Thermoelectric Converter for Electricity Generation in a SOFC System

Scope of project
A continuously rising energy and especially electricity demand on the one hand, but limited resources and reduction of environmental impact in terms of CO₂ emissions on the other hand make it necessary to implement energy technologies for an efficient energy production. New approaches in materials research, modelling and engineering are pursued here to succeed with the project aim: a novel SOFC-TEC hybrid system.

The here presented HITTEC project is co-funded by CCEM and SFOE and is focusing on the development of a novel high temperature thermoelectric converter (TEC) module, to be applied as integrated device, e.g. in a solid oxide fuel cell system (SOFC) at temperatures as high as 1200 K. Waste heat, usually used to prepare domestic hot water should then be directly converted into additional valuable electricity. The goal of the interdisciplinary HITTEC consortium is the development of such an oxide based thermoelectric module, operated in environmental air up to 1200 K. The «cold side» of the TEC module has to be established by an available preheated air flow with a temperature of about 900K, which is used as oxygen source for the SOFC. It is aimed for a specific power output of 75 mW/cm² for the TEC module, what would correspond to an overall power output of about 100 W per SOFC system.

Status of project
The elaborated HITTEC modules performed very well and reached a power density of 640 mW/cm² at ideal conditions (ΔT = 800 K). But also under conditions that are more realistic for an application in a solid oxide fuel cell the HITTEC modules outperformed the projects goals: 100 mW/cm² and even 180 mW/cm² can be achieved with a temperature gradient of 400 and 500 K, respectively. The intended 100 W would have been reached with 12 modules, integrated in the SOFC.

However, although the module was operated for more than 500 hours without any degradation at the high operation temperature, which is unique in this research field, it turned out that the heat transfer from the TEC module to the «cold air stream» of the SOFC system is insufficient to realize the prerequisite temperature gradient. Due to constructive limitations of the SOFC system, it was not possible to implement cooling fins on the TEC for an optimized heat transfer and measured TEC power output resulted in a value which was far below the power output reached under laboratory conditions. It can be concluded, that materials and methodologies for a high temperature application of TECs are made available by this project, but heat transfer, especially on the cold side is crucial for a successful implementation of this technology.

Main scientific results of workgroups
Development of a high temperature TEC
After an initial selection of materials this work package (WP) focussed on perovskite-type oxides (ABO₃) as thermoelectric materials for both, n- & p-type materials. Integration of titania-based materials, which showed very promising thermoelectric results, were not considered, due to their substantially different reactivity during the TEC module manufacturing process. Especially their combination with the contacting materials would make it necessary to come up with a new procedure yet to be developed.

Therefore, misfit layered Calcium Cobalt Oxide Ca₃Co₃.9O₉.3-δ and the perovskite-like Calcium Manganite phase CaMn₀.97W₀.03O₉.6 emerged as the best performing materials for the construction of all-oxide thermoelectric converters for the application in SOFCs (figure 1).

For the p-type material Ca₃Co₃.9O₉.3-δ a reduction of 50 % for the electrical resistivity was achieved by compaction of powders by SPS technology. For the n-type CaMn₀.97W₀.03O₉.6 material it turned out, that standard SPS is not a suitable approach: Stress due to reduction of the oxide caused massive cracks and a significant in-
crease of resistivity compared to classically sintered samples. A revised classical sintering procedure starting from nanopowders was developed, which provides crack-free and easy to process samples. In a joint project with our cooperation partner Advanced Industrial Science & Technology (Japan) thermoelectric all-oxide converters were developed using these materials. Such hot-pressed modules exhibit excellent contact resistance and outperform the brazed modules by a doubling of the generated current.

Temperature dependent oxygen loss and structural phase transitions have a strong impact on the transport as well as on the mechanical properties of n-type Ca$_{1-x}$A$_{x}$Mn$_{1-y}$B$_{y}$O$_{3-δ}$ materials. The oxygen loss creates additional charge carriers and causes additional lattice extension. The phase transition from an orthorhombic to a cubic crystal structure results in a strong increase of the thermal conductivity and the lattice extension increases by almost three.

In particular, different expansion coefficients are problematic for all-oxide converters. In order to shift these events to higher temperatures a series of A-site (Dy$^{3+}$, Yb$^{3+}$) and B-site substituents (pentavalent Nb$^{5+}$ or Ta$^{5+}$ and hexavalent Mo$^{6+}$ or W$^{6+}$) were synthesized. The onset of the reduction predominantly depends on the number of additional electrons introduced by substitution. At high temperatures this results in an equalization of the nominal concentration of Mn$^{3+}$. Therefore, differences in the Seebeck coefficient diminish with increasing temperatures and almost vanish at temperatures exceeding $T=1200$ K. The structural phase transition is not directly linked to a critical oxygen deficiency, but correlates strongly with orthorhombic distortion of the initial crystal structure.

Modelling of TEC properties & design guidelines

During the HITTEC project ZHAW-ICP developed a software tool for the simulation of a high-temperature TEC module (figure 2). The model for the TEC module takes into account the temperature dependence of material constants, the contact resistances between the TEC legs and the contacting material, and the lateral heat transfer among the module. The geometry of the legs can be modified quite easily in the software. For the modelling of the electrical potential and temperature within the TEC legs thermoelectric equations are solved and these equations are coupled to a 2D model for the lateral heat and current transport between the legs. This allows taking into account the non-constant temperature distribution delivered to the TEC module by the HEXIS SOFC. This (2+1)D approach has been compared to full 2D simulations using the software Comsol in order to verify its accuracy. The developed software tool is written in Mathematica and is also suitable for the optimization of TEC modules geometry.

In conclusion the simulations of the TEC modules performed in this project indicate that the power which can be extracted from a TEC module installed within the HEXIS SOFC is too...
HITTEC
High Temperature Thermoelectric Converter for Electricity Generation in a SOFC System

low to contribute significantly to an enhancement of the electrical efficiency of the SOFC. The reason is mainly due to a relatively low temperature gradient. But simulations also showed that the developed high-temperature TEC modules can be beneficially used in such applications where high temperature gradients can be constantly maintained on the cold side.

Contacting & module testing

Further geometric and material improvements (e.g. one piece AlN heat pile with integrated heater) lead to a reduction of thermal resistances, which is crucial for testing and reaching high temperatures at the hot side of the thermoelectric modules. Additionally the test setup now allows hot side temperatures of 920 °C, which is unique.

After the decision on optimized p-type (Ca₃Co₄O₉) and n-type material (substituted CaMnO₃), an adapted contacting material for long term operation of the generators was developed in collaboration with the National Institute of Advanced Industrial Science & Technology in Japan. For a reduced contact resistance and an increased lifetime of the silver contacts 6 weight-% Ca₃Co₄O₉ powder were added and mixed with the silver paste. For CaMn₀.₉ₓWₓO₃ a contact resistivity of ρₚ = 0.04 mΩcm² was found for soldering done in the same way as for the modules. In contrast, for the Ag-Ca₃Co₄O₉ contacts the contact resistivity is too small for a reliable estimate, but for soldering without pressure for the Ag-Ca₂.₉₇Bi₁₀.₃Co₄O₉ interface a contact resistivity of ρₚ = 0.025 mΩcm² was found.

Implementation & demonstration of the TEC module in a Galileo 1000 N

A four-leg converter performed for more than 120 h under laboratory conditions without any signs of degradation. It was proven that these results are representative for the modules implemented into the SOFC system. It was shown that the additional power output exceeds the required 50 W provided that temperature gradients can be reached which meet the initial expectations of the project (about 400–500 K). Nevertheless, the additional power generation has an exponential dependency on the temperature gradient. Therefore, the framework conditions hugely influence the performance.

The converters manufactured by TES NewEnergy were implemented into the Hexis SOFC system (figure 4). The converters sustained the harsh and oxidizing conditions in the pre-heating zone of the SOFC for more than 500 hours without any signs of degradation. The performance of the SOFC system was not negatively influenced by the implementation of the TECs. Power generation under such demanding conditions was not shown in literature before. Nevertheless, the power output was much smaller than expected (180 mW per module, which corresponds to additional 2.2 W per SOFC equipped with 12 TECs). This can be explained by a significantly smaller temperature gradient across ceramic cover and therefore across the TEC module.
**CONNECT PV**

Conductive Transparent Electrodes: a Competence Cluster for Highly Efficient Thin Film Photovoltaics

### Scope of project

The objectives are focused towards the development of highly conductive and transparent interface materials and their application in thin film solar cells. The two overall objectives are 1) to develop new materials that compete or outperform the commonly used transparent contacts in terms of costs, transparency, electrical resistance and resistance to cracking when bent and 2) to develop processes that thin films of such materials can be deposited at low temperatures by large-area compatible coating methods on flexible substrates.

### Status of project

After the first year of the project, multiple advancements in transparent contact (TC) quality, as well as in the implementation of the same, have been made in the consortium. New and improved transparent conducting oxides (TCOs) are leading to improved spectral response in the solar cells produced by the project partners.

With new TC emerging in the different groups, a healthy exchange of samples and cells was established between the project members. Several cross-group collaborations are in progress to harness the specific expertise of all project partners for the benefit of all investigated photovoltaics (PV) technologies.

### Main scientific results of workgroups

#### Solution based TCO

The Aluminum doped Zinc Oxide (AZO) deposited by chemical bath deposition (CBD) at Empa-TFPV is now implemented into the different solar cell technologies represented in the consortium. Beside the Copper Indium Gallium di-Selenide (CIGS) technology from Empa-TFPV, it is also applied as rear TCO for Si heterojunction (SHJ) solar cells from EPFL-PVLab and as front TCO in flexible organic PV cells from Empa-FP.

#### Vacuum based TCO

High mobility TCOs have been developed in both EPFL-PVLab and Empa-TFPV. Figure 1 shows the improvement in near infrared (NIR) transmission for Hydrogenated Indium Oxide (IO:H) in comparison to state-of-the-art AZO.

Further investigations regarding annealing and environmental stability of these TCOs are under way.

At the same time, EPFL-PVLab has developed an AZO/SiO₂ co-sputtering process, aimed on reducing the refractive index of the TCO. As a result, the optical dissipation losses in the rear contact could be decreased, leading to an improvement of the photocurrent density of 0.5 mA/cm² (figure 2).

#### Metallic wire based TC

Organic solar cells with a laminated back contact utilizing metallic meshes have been produced by CSEM and Empa-FP. The resulting solar cell stack shows comparable fill factor (FF) and open circuit voltage (VOC) to a reference with evaporated silver electrode. The short circuit current density (JSC) is reduced due to the semi-transparent nature of the mesh.

Good progress has also been made in the development of WO₃ ink, giving a possible al-
CONNECT PV
Conductive Transparent Electrodes: a Competence Cluster for Highly Efficient Thin Film Photovoltaics

Alternative to PEDOT:PSS as hole extraction layer in these devices.

New scaffold materials

The search for new scaffold materials pursued by EPFL-LPI lead to perovskite solar cells (PSC) with photon conversion efficiency (PCE) above 19%, using a surface modified TiO₂. While these scaffolds normally require temperatures over 200 °C during production, low temperature scaffolds of TiO₂ and Alumina have also been produced with comparable PCE to the state of the art technology.

Further, a low temperature process to produce planar PSC with efficiency over 18% has been developed. In order to achieve this result, the TiO₂ electron selective layer has been replaced by low temperature processed SnO₂. Better band alignment between SnO₂ and perovskite material allows for an efficient extraction of charges. In those devices, the hysteresis behavior normally observed in planar perovskite devices is not observed anymore (figure 3/table 1).

Device modelling

Simulations with regard to light management based on surface structures have been performed at ZAHW. Improvements of approximately 8% in absorption could be expected when applying an external texture on the sun exposed side of organic photovoltaic cells.

In a second task, a model for designing large area modules, considering the coupled influence of TCO thickness, conductivity, and parasitic absorption was developed.

Main achievements / outreach

The implementation of new transparent contacts within this report period shows the feasibility of the investigated approaches for real devices. Contacts deposited by vacuum as well as non-vacuum processes show promising results for further improvements in solar cell properties.

The developed low temperature scaffold materials and electron selective layers for perovskite devices are an important milestone on the road to flexible devices in a cost effective production process.

---

**Table 1:**

<table>
<thead>
<tr>
<th>Material</th>
<th>Scan direction</th>
<th>( J_{sc} ) (mA cm⁻²)</th>
<th>( V_{oc} ) (V)</th>
<th>FF</th>
<th>PCE (%)</th>
<th>Light Intensity (mW cm⁻²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SnO₂</td>
<td>backward</td>
<td>21.3</td>
<td>1.14</td>
<td>0.74</td>
<td>18.4</td>
<td>98.4</td>
</tr>
<tr>
<td>SnO₂</td>
<td>forward</td>
<td>21.2</td>
<td>1.13</td>
<td>0.75</td>
<td>18.1</td>
<td></td>
</tr>
</tbody>
</table>

Figure 2:
- a) Geometry for synthesizing the ZnO:Al-SiO₂ mixture,
- b) Cross section SEM elemental map of different elements in the SHJ device,
- c) EQE enhancement and d) J-V curve of the optimal device.

Figure 3:
- J-V characteristics of planar perovskite solar cells fabricated with SnO₂ and TiO₂ electron selective layers.
Self-Regenerating Anodes: Durability Improvement of SOFC Technology by Novel Smart Materials with Sulfur Tolerance

Scope of project

SERAN focuses on the development and demonstration of the next generation catalyst for the anode compartment in solid oxide fuel cell (SOFC) systems and tries to overcome the drawbacks of currently used conventional catalysts. Nickel cermet as state-of-the-art anode material in SOFCs lacks of microstructural stability against high temperature, humidity, varying oxygen partial pressures as well as of sulfur tolerance. Especially sulfur, used as odorant in natural gas but also present in large amounts in biogenic fuels, is well known as a catalyst poison and causes significant performance degradation.

To overcome these major degradation effects, a new material-based strategy is applied to develop and demonstrate a novel type of catalyst as active anode material in SOFCs. On the one hand, it has to withstand common sulfur contamination levels, while state-of-the-art nickel catalysts in Ni/YSZ anodes suffer from instantaneous and additionally irreversible degradation if operated on a long-term level. On the other hand degradation of the microstructure caused by harsh temperatures and transient dynamic operating conditions need to be limited. Such catalysts are developed and examined with respect to their conversion performance under SOFC anode operation conditions under sulfur load.

Status of project and main scientific results of workgroups

Catalytic activity and structural reversibility

A key point of WP 1 is studying the effect of A- and B-site variation of LSTN on the reoxidation temperature at which segregated Ni is reincorporated into the oxide lattice (Trev). Temperature programmed reduction (TPR) has shown to be a powerful tool to assess the state of Ni before and after redox treatments of the sample to determine Trev. The effect of increasing Ni B-site concentration, increasing La/Sr ratios and the effect of partial substitution of Sr by Ca on structural reversibility were studied by TPR. This was supported by further characterization with respect to X-ray diffractometry, morphology, specific surface area and water gas shift (WGS) activity at a SOFC relevant temperature of 800 °C.

Increasing Ti substitution by smaller Ni causes contraction of the lattice. Upon reoxidation the movement of Ni back into the lattice can be regarded as sterically hindered and high temperatures are needed for complete reincorporation (figure 1 a–c). This effect can also be seen for LSCT samples (figure 1 d). Ca2+ shows a smaller ionic radius than Sr2+ which also leads to a contraction of the lattice and an increase of Trev. When changing La3+ to Sr2+ ratios the overall charge on the A-site was kept constant. Facilitated structural reversibility is observed despite the increase in concentration of the smaller La3+ as well as A-site sub-stoichiometry. The effect of different degrees of charge disproportionation could not be assessed individually during these experiments and is subject of further research.

Materials design, synthesis, and characterization of self-regeneration concept

ZHAW-IMPE is focusing on the development and characterization of new catalytic materials with a self-regeneration effect which are applied as anode in a SOFC. Particular attention is paid to Ni doped LST (LSTN) and the evaluation of the self-regeneration concept, in which a repetitive exsolution and re-integration of the Ni catalyst phase is applied. New material compositions with additional elemental substitutions for A-site was kept constant. Facilitated structural reversibility is observed despite the increase in concentration of the smaller La3+ as well as A-site sub-stoichiometry. The effect of different degrees of charge disproportionation could not be assessed individually during these experiments and is subject of further research.

Characterization of the materials under repetitive redox cycles has been carried out by X-ray diffractometry (XRD), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), thermogravimetry (TG), and scanning transmission electron microscopy (STEM). Exsolution and subsequent reintegration of the metallic Ni phase from
the perovskite structure has been proven at IMPE and confirmed the self-regeneration mechanism on a microstructural level (figure 2). Several compositions have shown suitable phase purity, depending on their A-site stoichiometry. Interestingly, a certain LSTN stoichiometry showed morphological anomalies: where Ni is reintegrated into the host structure, small holes appeared at the Ni particle substrate interface. Currently, larger powder amounts were prepared to process them into porous anodes microstructures for an advanced electrochemical testing.

**Electrochemical evaluation of S tolerant anode microstructures**

Activities of the FUELMAT Group at EPFL is focussing on electrochemical testing, including cell characterization, and sulfur poisoning of cells. Cells were characterized at different temperatures and current densities. Initially, the cell was operated at open circuit voltage (OCV) and 850 °C for 24 h under 96 % H₂ and 4 % N₂ to stabilize the performance.

Since first and non-optimized anode microstructures of LSCT showed a large polarization resistance of about ~40 Ωcm in electrochemical impedance spectroscopy (EIS) measurements, those microstructures were subjected to an impregnation step with a Ni composite. The derived sample with 5 wt% NiO showed a very much improved cell performance.

Finally, samples were evaluated with respect to the water gas shift reaction (WGSR), redox cycling and poisoning with H₂S to investigate recovery behavior by a subsequent redox cycle. Results showed that the cell can withstand a redox cycle and performance even became more stable after performing the redox cycle. Finally and most promisingly, the redox cycle could recover the sample which was exposed to H₂S (figure 3).

![Figure 1: TPR thermograms after re-oxidation at increasing Tox (700 °C ≤ Tox ≤ 1000 °C) for 20 vol% O₂/2 h: a (LST), -2 % Ni, b (LST), -5 % Ni, c (LST), -10 % Ni, d LSCT-5 % Ni, e (LST), -5 % Ni, f (LST), -5 % Ni. Thermograms that show identical features to the ones obtained for calcined materials are marked in green indicating full Ni re-incorporation at the corresponding Tox.](image1)

![Figure 2: Comparison of samples subjected to 5 redox cycles, indicating the reversibility of the Ni exsolution subsequent reincorporation (top & middle). Remaining nanostructured «holes» at Ni-particle LSTN-substrate interface (bottom).](image2)

![Figure 3: Redox cycle measurement of LSCT exposed to H₂S: at time = 0 h sample is exposed to 1 ppm H₂S, at time = 2 h H₂S is stopped and redox cycled, at time = 3 h sample is reduced, at time = 3.5 h sample is operated again, polarization at 0.05 A/cm².](image3)
Quantitative microstructure analysis and FE-modelling

A stochastic model was developed from ZAHW-ICP and University of Ulm (Germany) to produce virtual 3D-microstructures, that have properties close to real anodes microstructures. This model is currently used to create systematic variations of 3D-microstructures by varying the ratio of an ionic conductive phase with LSTN. These virtual 3D structures (figure 4) are also used as input for numerical transport simulation, which provides the corresponding effective conductivities. Using a statistical error minimization we obtain a quantitative relationship between effective conductivity ($\sigma_{\text{eff}}$) and microstructure parameters [volume fraction ($\epsilon$), constrictivity ($\beta$), geodesic tortuosity ($\tau$)], as follows:

$$\sigma_{\text{eff}} = \epsilon^{1.15}\beta^{0.37}\tau^{-4.39}$$

This relationship is of generic meaning for all diffusive and conductive processes, e.g. it describes microstructure-property relationships of ionic conductivity in CGO, electric conductivity in LST (and CGO), but also diffusivity in the pores. The structure of the catalyst, i.e. LST substrate with Ni nanoparticles, is investigated with STEM-EDX. Based on this know-how the nanoparticle structure can be superimposed onto the composite of an ionic conductor and LST, again in a modelling approach. In this way a variation of composition (i.e. CGO/LST-ratio, Ni-content) can be realized. From these virtual microstructures effective transport properties, catalyst surface area, and TPB-lengths are extracted to compute the electrode performance as function of the microstructure. By this a design guideline for anodes with optimized microstructure and composition can be given to the industry partner.
ADMIST
Advanced Understanding of Micro Structures in Fuel Cells and Batteries through X-ray Imaging

Scope of project

The ADMIST project aims at improving the durability and performance of high (HT) and low (LT) temperature polymer electrolyte fuel cells (PEFC) and Li-ion batteries (LIB). The lifetime and the performance of these three technologies is largely determined by the microstructure of the constituents, the temporal changes to the microstructure, and the related mass transport properties in the micro-porous domains. X-ray imaging, in particular in-situ X-ray tomographic microscopy (XTM) offers a powerful method to visualize the relevant structures in low and high temperature PEFCs and advanced LiB. In particular X-ray tomography has proven to be an extremely powerful method to reveal the relevant micro-structural details for in- and ex-situ research questions. The aim of ADMIST is to further develop by X-ray imaging for all three applications, leading to a profound understanding and thus the basis of significant improvements for the complex materials.

Status of project

In the second year of the ADMIST project the installation of the laboratory tomographic CT scanner and the verification of it’s imaging capabilities provide the basement for the achievement of the scientific goals of the project. The low and high temperature PEFC in-situ/operando setups were adapted to the geometrical requirements of the laboratory CT machine and the expected image quality could be verified.

Structural analysis of ex-situ GDL samples revealed an anisotropy of the pore geometry and explains the preferential direction of the liquid-water invasion front in LT-PEFC systems. Additional synchrotron operando XTM measurements with the HT-PEFC setup were used to broaden the understanding of phosphoric acid migration during load cycling for different membrane compositions and it’s influence on HT-PEFC performance degradation.

The inhomogeneity of different negative electrodes of lithium ion batteries was quantified on different length scales and linked to battery performance by 3D electrochemical simulations. Degradation of LIBs was addressed by exploiting XTM to depict lithium metal dendrite growth and lithium metal plating.

Main scientific results of workgroups

WP 1: CT Scanner Installation

The micro CT scanner «nannotom M» from General Electric was installed in February 2015 and set into operation until end of March 2015. It features a 7.2 Mpixel flat panel detector and a 180 kV nano-focus X-ray tube with a spot size diameter down to about 800 nm. The imaging capabilities were verified using X-ray transmission line chart samples. As specified from the manufacturer, periodic line patterns with line and gap width down to 0.8 µm could be identified. Figure 1 shows, that even finer structures can be detected.

Figure 1: Line detectability test with a JIMA RT RC-04 X-ray transmission sample for different feature sizes (1.5 µm (left), 0.8 µm (middle) and 0.7 µm (right)); the averaged transmission profiles (bottom) are evaluated in the yellow domains (top) and reveal the features of the Tungsten structures for all pattern sizes.

List of abbreviations

GDL Gas Diffusion Layer
HT High Temperature
LIB Lithium Ion Battery
LT Low Temperature
PEFC Polymer Electrolyte Fuel Cell
XTM X-ray Tomographic Microscopy
WP Work Package

Main Investigators
Felix Büchi, PSI
Vanessa Wood, ETHZ

Project Partners
PSI
ETHZ
BASF SE
swisselectric research
BFE

Time frame of Project
2014–2017

Part of SCCER
Mobility
Thematic Relationship to SCCER
HaE (Energy Storage)

Major partners in the ETH domain
- PSI – Electrochemistry Laboratory (ECL)
- ETHZ – Laboratory for Nanoelectronics (LNE)
**WP 2: HT-PEFC**

Movement and redistribution of phosphoric acid within the porous components (catalyst layer, micro-porous and gas diffusion layers) of a HT-PEFC cell are expected to play a significant role for fuel cell performance and durability. The rearrangement of the phosphoric acid is depicted by operando X-ray micro tomography in a dedicated imaging HT-PEFC. Since the lab CT scanner relies on the principle of geometrical magnification, the positioning of the sample between X-ray source and detector is different than at a synchrotron CT beamline. The sample has to be placed close to the head of the X-ray tube and far from the flat panel detector to achieve high magnification.

The present HT-PEFC XTM cell was designed to match with the X-ray microscope at the TOMCAT beamline of the Swiss Light Source, but it does not allow to exploit the best possible magnification for the sample diameter of 6 mm, as the sample can not be located close enough to the head of the X-ray tube in the nanotom (see figure 2a). The cell housing was elongated and fixture of cell components was modified such that the sampling position of the cell can be placed at the required distance to the head of the X-ray tube (see figure 2b). Thereby, the voxel size reduced from 3.5 µm to 2.2 µm and will allow a precise representation of the GDL fine structures that are based on carbon fibers with diameters of only about 7 µm (see figure 2c).

Parallel to the modification of the cell design, operando XTM measurements at the TOMCAT beamline were implemented to broaden the understanding of phosphoric acid migration during load cycling for different membrane compositions. It was found that the migration of phosphoric acid towards the anode flow field during high current operation is dependent on the doping level and synthesis process of the membrane. As the migration process seems to be dominated by capillary forces on the phosphoric acid in GDL micro-structure, well engineered GDL materials could help to mitigate the process and lower the phosphoric acid losses at high current density operation.

The results were presented including a conference paper awarded with a student travel award for Sebastian Eberhardt at the 228th ECS conference.

**WP 3: LT-PEFC**

The accumulation of the liquid water in the void space of the porous materials is regarded as a major limitation for high power density operation of LT-PEFC systems for the use in automotive power trains. Within the ADMIST project an in-situ saturation - capillary pressure XTM imaging setup is used to study the percolation processes during liquid water invasion in the GDL with a setup that is derived from the same design as the HT-PEFC XTM cell. Synergistic effects could be achieved as it was redesigned together with the HT-PEFC such that now also this setup can benefit from smallest possible voxel size for 6 mm sample diameter. It could be shown that the percolation front is stable during the scan times of 1 to 2 hours, but also shorter scan times are in reach. The segmentation procedures are currently adapted to handle CT data with a lower signal to noise ratio.

Additional, structural analysis of ex-situ GDL samples revealed an anisotropy of the pore geometry and explains the preferential direction of the liquid-water invasion front in LT-PEFC systems. The bottlenecks that define break-
through position of the percolation paths from the catalyst layer towards the flowfield could be located in the mixed region of the macroporous substrate and the microporous layer coating of the GDL (see figure 3).

**WP 4: Lithium ion battery**

In the first 18 months of the project, we successfully worked to quantify electrode microstructure and inhomogeneity over multiple length scales. Using X-ray tomographic microscopy, we obtained three-dimensional reconstructions of carbon-based negative electrodes from four different lithium ion battery manufacturers (figure 4). The inhomogeneity of each electrode has statistically been quantified over multiple length scales and electrochemical simulations have been performed on the digitalized microstructures to isolate and understand the influence of inhomogeneity of different microstructural parameters on battery performance. We demonstrated that the extent of heterogeneity can be assessed by examining the spread in particle surface area, particle size, and effective transport values (figure 5), and quantified how inhomogeneity of electrode microstructure plays an important role in limiting battery performance by lowering accessible capacity and increasing the risk of degradation from non-uniform current distributions.

The findings suggest that manufacturers aiming to improve electrode homogeneity should prioritize selection of monodisperse particles, since a heterogeneous particle size distribution not only lowers the accessible capacity but also leads to a non-uniform effective transport parameter, increasing the risk of lithium concentrations in the electrolyte that locally exceed the solubility limit during fast discharge. The mean particle size must be selected based on known side reactions, the solid-state diffusion coefficient, and the desired operating conditions. This work has been written up for publication and is currently waiting for approval from the industrial partners, who provided the samples. Simon Müller won the Zuger Wissenschaft Prize for this work. It will be extended to cathodes. Currently, we are exploring different ways to investigate degradation in lithium ion batteries. The use of X-ray tomography to identify lithium plating and lithium metal dendrite growth is very promising. The protocol that is being developed is as follows:

A battery is cycled and then disassembled in an Argon-filled glovebox. Lithium metal (in the form of plated or dendritic lithium) can then be stained slowly with OsO₄ at low temperatures (to counteract the exothermic nature of the reaction), which results in LiO₂ and OsO₂ (as well as associated compounds). This results in samples with high-contrast between the osmium-stained lithium and the polymer separator matrix that can be imaged by X-ray tomography. Following identification of places with plating or dendritic growth, finer resolution images can be obtained with FIB-SEM tomography.
**TeKaF**

**Temperature Dependent Ampacity Limit Modelling of Overhead Power Lines**

**Scope of project**

The goal of the project is to deliver the necessary know-how that allows the grid operator to better estimate the remaining capacity (current) of each single line. The information needed is the maximum possible steady-state current value (or the maximum operating time for a given overcurrent), corresponding to the actual weather situation. The calculation of the maximum current value also takes into account the long-term behaviour (conductor lengthening and loss of mechanical strength) of the line. The focus is on all aluminium alloy conductors (AAAC, Aldrey) as this is the main material used in Switzerland and not enough information is available for this type of conductor. To apply the results of the conductor limits in the context of network operation, dynamic rating models for advanced transmission networks congestion controls are derived. Focus here is on optimal congestion management techniques to be included in Extended Energy Management Systems and the implementation of these management procedures into a specific computation environment able to meet the stringent computational burdens required by real-time applications.

**Status of project and main scientific results of workgroups**

The project comprises several aspects that are clustered in four work packages (WP). The first two have started early 2012 and are finished, the other two started in summer 2013 and are ongoing.

**Electro-thermal properties of Aldrey conductors at the operating limit**

WP A investigated and developed reliable thermal models of the transmission line, as Ampacity levels are based on accurate estimations of the line temperature. All the goals of WP A have been reached and delivered. Furthermore, WP A delivered additional results and a continuing research line has been planned.

One of the goals delivered by WP A was to investigate how the higher internal conductor temperature influences the maximum current capacity of AAAC (the current practice is that only the surface temperature is considered). In ETHZ a laboratory test facility was built and measurements of the internal line temperature were performed as a function of electrical current and tension. Using this data, the effective radial conductivity of an AAAC line was found as a function of the tension in the line. This finding can be used to accurately determine in a simple way the maximum current capacity of an AAAC line for a given maximum operational temperature (which is obtained by the methods developed in WP B and C).

Another objective delivered by WP A was the development and benchmark of a reliable thermal model for the surface temperature of AAAC. Starting with the standard rating models, improvements were done to the wind cooling terms as well as to the thermal-radiation term. In addition, a procedure to calculate the effective solar radiation on the line was presented. The results obtained were benchmarked against data taken in a real transmission line. The accuracy of the model was found to be 1°C with a precision of 3°C.

Since the line temperature of normal transmission lines is considerably lower than the maximum one allowed, the line temperature model was also tested at high conductor temperatures in the new outdoor test facility built in ETHZ (figure 1). The results showed that the line temperature model is also reliable at high conductor temperatures, with an accuracy of 1.5°C and a precision of 3.5°C. Aside from benchmarking line temperature models, it is planned to use the new outdoor test facility to test the reliability of different dynamic line rating (DLR) schemes in future projects.

WP A further delivered contributions towards the development of a dynamic line rating scheme suitable for the Swiss transmission network. Most important, a study of the performance of a zero-wind-based dynamic rating scheme was delivered. In this study it was found that during the summer this dynamic scheme produced maximum current capacities which are larger than the standard ones, but in winter they were smaller. This study set the base line for other dynamic schemes since a zero wind as-
TeKaF
Temperature Dependent Ampacity Limit Modelling of Overhead Power Lines

Consumption is the most conservative scenario.

**Mechanical and physical properties of Aldrey at elevated temperatures**

WP B investigated the mechanical and physical properties of the material, the wires and the whole conductor. The experimental campaign for the assessment of the effect of aging at elevated temperature on material properties was completed. A representation using a time-temperature parameter was applied to rationalize the observations with respect to data in the literature. The results allow predicting, e.g., the time at given temperature for a specific strength reduction of Aldrey. This information could be used for a lifetime assessment of existing overhead lines (OHL). The data indicate that resistivity is proportional to strength so that aging leads to a reduction of Ohmic losses. The next criterion for a safe operation of the conductors is the progression of sag with time. The analysis of the creep response of wires and whole conductors was improved and used to determine refined model equations for sag prediction.

Finite element calculations were performed to determine the short and long term tensile response of a conductor for a given temperature distribution (see WP A). Non-linear constitutive equations (elastic visco-plastic), internal stress states from the stranding process and wire contact interactions were defined to represent the complex behaviour of the helical structure. Validation of the 3D model was based on short term tensile data reported in the literature as well as own measurements using a dedicated whole conductor test setup. Long term (up to 1000 hours) high temperature tensile tests were performed on conductors test pieces of 9 m length (figure 2). The measurements confirmed the accelerated creep elongation predicted using the model, associated with relaxation of internal stresses in the conductor (figure 3). The overall good performance of the numerical model was confirmed for a temperature and force range that is relevant for conductor operation. Based on the 3D finite element model a 1D sag calculation was performed, demonstrating the potential use of the present results for the calculation of retightening force and corresponding history of sag of overhead line conductors.

**Coupled electrical-thermal-mechanical simulations of Aldrey conductors**

WP C aims to develop a simulation tool to predict the lifetime of AAACs dependent on the electrical-thermal-mechanical coupled phenomena.

As the goal of the TeKaF project is to increase the efficiency, reliability, and safety of the Swiss transmission grid, OHLs would occasionally be operated closer to the limit. Thus, this limit and the impact of different load scenarios and weather conditions on the conductor lifetime are investigated in this WP. The findings of WP A and B as well as further experimental measurements are required to perform entirely coupled electrical-thermal-mechanical simulations of the AAAC.

First, the focus is on modelling and understanding the region of the tension clamp, where the conductor is compressed and all the tensile force is introduced. On the other hand, this zone is investigated for classifying the risk of failure due to the locally elevated mechanical stresses and strains, which can cause increased material weakening and creeping. The ongoing investigations are on quantifying the effects of fewer heating and increased cooling, which are both resulting in lower temperatures of the conductor near the clamp. The magnetic field is influenced by the manner of how the current flows through the clamp. By measuring and simulating the magnetic field (figure 4) near the clamp, the electric losses and thus the heating power at this location can be quantified. As creep is enhanced by higher temperatures and by elevated
stresses, it is currently studied if the lower temperature in this zone can compensate the higher stresses. On the other hand, the transition from a clamped to a homogeneously loaded conductor is of interest because suitable boundary conditions are required for the 3D finite element simulations of homogeneously loaded conductor models. This mechanical transition from the clamp to the free span is analysed by the newly developed adaptive computer tomography method (see figure 5). This X-ray imaging method enables measurements of wire displacements of the inner conductor layers.

Second, the findings of the complex conductor behaviour in the clamping zone can be implemented in the model of the homogeneously loaded conductor for the free span. Comparing and combining the models as well as the experimental data of these two zones of the OHL allow appropriate evaluation of case specific transmission limits and conductor lifetimes. Thus, the permitted operating time for a given overcurrent or the maximum possible steady-state current can be assessed.

**Extended-energy management system**

WP D aims to integrate the DLR of the transmission lines into the optimal operation of power systems. In particular, it integrates the DLR into the optimization of Extended-energy Management Systems (EeMS) including: day-ahead market, balancing market and real-time operation.

Figure 6 shows the links between this work package and the other ones. On the basis of the proposed DLR model in different time scales in power systems operation, several aspects of the OPFs have to be investigated in the EeMS. To complete the previous studies («Day ahead scheduling: Security Constrained Unit Commitment (SCUC)»), the following two studies have been addressed:

- Real-time operation: AC Optimal Power Flow (AC-OPF)
- Contingency analysis.

In the first study, we propose a suitable integration of the Heat Balance Equation (HBE) equations applied to OHL conductors into an AC-OPF that deals with the case of real-time dispatching. The different terms of the HBE have been properly integrated into the OPF. A linearized AC-OPF formulation is used to consider the non-negligible effects of reactive power flows as well as the voltage constraints. The short term overloading of the conductors following a contingency is modeled and added to the optimization problem. Making reference to a simplified 5 bus system and to standard IEEE benchmark systems, we have compared the performances of the proposed DLR model with the case of Static Line Rating (SLR). Numerical results (e.g., figure 7) show that even if the SLR contingency ratings are used for a short time after the contingency, it cannot exploit the thermal inertia of the conductors as well as the dynamic of the HBE. The proposed method exhibits several advantages in terms of both optimality of the solution and security of the system and might be considered in realistic operation practices of interconnected power transmission grids.

The aim of the second study is to integrate the concept of DLR in power system contingency analysis. Here, it is assumed that the schedule of generators under normal operation of the system is known in advance. Then, we investigate the effect of the outage (contingency) of each component of the system including the generators and transmission lines on the security of supply considering the dynamic thermal rating of the remaining transmission lines. The validation of the proposed method relies on simulations using a realistic transmission system such as the Swiss one. Moreover, the thermal parameters of the transmission lines are derived from the results of the other WPs.
HydroNet 2
Modern Methodologies for the Design, Manufacturing and Operation of Pumped Storage Power Plants

Scope of project

The HydroNet II project aims at improving the design, manufacturing and operation of hydropower plants. Thanks to its multidisciplinary consortium, the project involves hydrodynamic, electricity, civil engineering and environmental aspects with a focus on the development of a joint and non-intrusive methodology for the monitoring of the entire hydropower plant.

Status of project and main scientific results of workgroups

The main scientific results obtained during the overall project are summarized hereafter. In addition, all the results are to be presented in a wide and open workshop, which will be held in Lausanne in February 2016, under the theme «Current downturn of hydropower generation: Technological and political responses» (more information is available on http://hydronet.epfl.ch/Workshop).

Sand erosion of Pelton turbines

Numerical simulation

In this subtask, a new model for silt erosion in which the motion of the fluid and silt, the solid deformation and material removal are simulated. The flow is assumed viscous and weakly compressible. The solid deformation is derived from an elasto-plastic constitutive model with isotropic linear hardening. Silt particles are assumed rigid and spherical and their motion is driven by Newton’s second law. Fluid and solid equations are discretized using finite volume particle method (FVPM), which combines attractive features of smoothed particle hydrodynamics (SPH) and conventional mesh-based finite volume method (FVM). The solver (SPHEROS) was developed at EPFL using parallel computing. The method was successfully validated against several academic case studies. The related PhD thesis was examined and accepted in 2014.

Sand erosion of hydraulic turbines

Experiments

We have initiated an experimental study of sand erosion in hydraulic turbines in 2014 with additional funding provided by EOS-Holding. The main purpose of this task is the development of a non-intrusive method to monitor the erosion rate in hydropower plants. To this end, we propose to measure the erosion rate in-situ on metallic samples using a high speed jet derived from the penstock upstream to the turbine inlet. The typical jet diameter is 1 mm and the deviated flowrate has almost no effect on the output power. Our method has several advantages:

- it is non-intrusive,
- it uses water with the same particles distribution as the one crossing the turbine,
- it is portable,
- it may be used to evaluate the resistance to silt erosion of new materials in a realistic environment.

The Electra Massa power plant has been selected for the deployment of the 1st version of our monitoring device. Besides the validation of the operation safety, substantial erosion on stainless steel samples have been obtained in a relatively short time (few hours). It was also found that the particles concentration may vary significantly within a day, which requires an online monitoring of water quality. Following these preliminary tests, we have designed a portable and automated device for sand erosion monitoring, which is being tested in Electra Massa power plant. Talks are underway with Alpiq to deploy the monitoring device in other power plants.

Tip vortex cavitation in axial turbines

Experiments

The tip leakage vortex (TLV), which develops in the clearance between the rotor and the stator of axial hydro turbines, has been studied for decades. Yet, many associated phenomena are still not understood. For instance, it remains unclear how the clearance size is related to the occurrence of cavitation in the vortex, which can lead to severe erosion.

Experiments are carried out on the EPFL cavitation tunnel on a NACA0009 hydrofoil with adjustable gap. The 3D velocity fields are measured using stereo particle image velocimetry.
HydroNet 2
Modern Methodologies for the Design, Manufacturing and Operation of Pumped Storage Power Plants

Figure 1: Left: visualization of the mean trajectory of the cavitating TLV for two values of the normalized clearance. The yellow crosses represent the location of the SPIV measurements. Right: Corresponding vorticity maps and isocontours of the tangential velocity around the vortex, derived from the SPIV measurements. The hydrofoil chord length = 100 mm.

(SPIV) in three planes located downstream of the hydrofoil for different flow conditions. Moreover, high-speed visualizations are used to highlight the vortex core trajectory and gap flow (figure 1).

The measurements clearly reveal the existence of a specific tip clearance for which the vortex strength is maximum and most prone to generating cavitation. The results have been published in Experiments in Fluids in 2014 and the related thesis was successfully presented in 2015.

CFD modelling

3D numerical simulations of tip vortex cavitation have been performed. The case study is similar to the one tested experimentally. The influence of the gap width is investigated with and without cavitation using RANS and LES simulations (figure 2). The results were used to describe the flow topology in the gap region for two different values of the gap width. A semi-empirical law for the vortex trajectory above the blade has been derived. The experimental data were used to validate the simulation procedure and the outcome was published in Journal of Turbulence in 2014. We are currently investigating new avenues for active control of the cavitating tip vortex. The results were published in CAV2015: International Symposium on Cavitation, hosted by EPFL in December 2015.

Flow instabilities in pump turbines

The work in this area is continued on several levels.

First, the results of the unsteady computational fluid dynamics (CFD) simulations of a medium specific speed pump-turbine were compared with the detailed experimental data (particle image velocimetry, PIV) obtained from the Techni- cal University Graz (figure 3). Here, the secondary flow distribution in the vaneless space between the runner and guide vanes is depicted. The pump-turbine is operating in turbine mode at «speed no load» conditions for a guide vane angle of 6 degrees near the unstable characteristics. A good agreement was obtained between the CFD and PIV data.

Further unsteady CFD simulations are carried out on the medium specific speed pump-turbine focusing on the flow in the vaneless space in order to better understand the flow blockage effects. It is observed that a primary vortex core is blocking the flow passage at the runner inlet that is triggering later the instability. A secondary vortex core, which is interacting with the primary vortex within the flow passage, is also determined. Finally, on the experimental side, a low specific speed (nq = 25) pump-turbine model is installed and instrumented in the laboratory. Currently measurements are ongoing on this pump-turbine model for determining the characteristics in four quadrants of the pump-turbine operation.

Hydropower design under uncertainties

The design of hydropower plants is determined by long-term forecasts, which are highly uncertain. In fact, the engineering and economic approaches that underlie virtually all water planning assume that the hydrological and market processes are stationary, even if it is well known that they change. Additional uncertainties may also stem from interpretation of incomplete data. An aberration of the effective values from the forecasts can highly affect the success of a project. Despite the high risks taking over hydropower projects, surprisingly little systematic knowledge exists about the incorporation of risk management into the design of hydropower plants. Furthermore, the increasing proportion of private investors for hydropower projects reinforces the trend towards control or limitation of risks when making investment choices. The largest dataset of realized small hydropower projects has been elaborated and analyzed. The results of the two main sources of uncertainty, namely cost overrun and production overestimation, suggest that...
small hydropower projects face significant risks. The average cost overrun is about 40%, and more than half of the projects suffer a cost overrun. In addition, the study indicates a significant production overestimation (average of 35% lower). Based on the analysis of the uncertain parameters, evaluation methods are applied which capture a more comprehensive picture about the pros and cons of projects or design alternatives. The performances of different alternatives are compared under the criteria of expected net present value (ENPV), value at gain (VaG) and value at risk (VaR). In a next step, the approach will be extended to large hydropower projects in Switzerland. This will allow a comparison of the risk profile of small and large hydropower projects. Finally, design methods to manage uncertainties by design adjustments will be elaborated and applied for hydropower projects.

**Pressurized Shafts and Tunnels**

Due to increasing demand for energy along with the fast growing contribution of new renewable highly volatile energies, pumped-storage hydropower plants are subjected to more and more severe operation conditions because of highly dynamic pressures in steel-lined pressure tunnels and shafts. The development of high-strength steels addresses these harsh mechanical requirements. However, these steel grades are difficult to weld and subjected to fatigue. Design guidelines for steel-lined pressure tunnels and shafts exist for ductile steels, but they are no longer sufficient for high-strength steels. In this task, the finite element method is used to address the influence of the surrounding materials (namely the backfill concrete and the rock mass) on stresses and deformations in the steel liner, considering rock anisotropic behavior, as well as the presence of geometrical imperfections and cracks in the welding zone (figure 4). In 2014, the influence of anisotropic rock behavior on stresses and displacements in the steel liner was studied. A systemic parametric study was performed and empirical formulas were derived. In parallel, the influence of geometrical imperfections and the initial gap between the steel liner and the backfill concrete was studied by means of the contact technology. We intend to assess the dynamic response of the multilayer system, as well as the influence of cracks in the weld using innovative approaches such as probabilistic fracture mechanics.

**Non-intrusive monitoring of pumped storage power plants**

The scope of the work is to investigate the effectiveness of energy saving mechanisms for wireless sensor networks such as low power sensing hardware, embedded data processing, event driven monitoring and network layout optimization. The hard- and software tools that have been developed in the previous years (generic analog front end, event recognition sensor nodes with alerts, embedded cycle counting identification and fast Fourier transform algorithms) were implemented and assembled into a wireless sensor network. The system performance was evaluated with laboratory and outdoor tests. This has led to some fine-tuning enhancements, mainly to reduce the average latency time of the alerting mechanism when the communication was operated over several hops. Finally, a demonstration wireless sensor network consisting of nodes monitoring vibrations, noise and temperature has been deployed in the Laboratory of Hydraulic Machines (LMH) of EPFL. The deployed monitoring system works reliably with a data loss rate of less than 1%.

**Real time monitoring**

The objective of this task is to develop and test an advanced and intelligent monitoring system based on real-time monitoring simulation (RTMS), and to implement it within an operating hydropower plant. The system operates a well validated simulation model of a hydroelectric power plant in real-time, and takes into account both the system boundary conditions (such as reservoir water level...
Electricity

HydroNet 2

Modern Methodologies for the Design, Manufacturing and Operation of Pumped Storage Power Plants

and power network voltage) and the control system set points (such as turbine guide vane opening, valve opening, generator excitation system voltage, circuit breaker state) directly measured on site to simulate the dynamic behavior of the power plant. Thanks to the comparison between simulated and measured quantities, this advanced system enables the identification of possible power plant dysfunctions if deviations are detected. Moreover, a test bench has been developed in order to validate the monitoring concept and the simulation model implemented in SIMSEN (which is a simulation software for power networks, developed by EPFL and PowerVision Engineering Sàrl). Finally, to corroborate the good measurements achieved in the laboratory, a measurement series has been realized in the Mottec power plant. The tests included variation of active and reactive powers in order to cover a wide operation range and have validated the simulation model of Mottec, including hydraulic and electrical systems (figure 5). A satisfying agreement was obtained between the model and the measurements.

Study of the drivers and asset management of PSPP

Pumped-storage power plants (PSPP) represent the only mature option for large-scale electricity storage, and offer a wide range of grid management services, ranging from peak power production to ancillary services. This technology has undergone drastic progress in reliability, efficiency and generation capacity, with modern PSPP being able to switch from pumping to generating mode in a few minutes and working at different levels of part load. This task has led to the submission of a review article to Energy in 2015, presenting a historical perspective and the current trends in PSPP deployment at a global level. It covers initial investment rationale, the evolution of the operational management and trends in installed capacities, and a systematic overview on the contribution of PSPP to electricity system flexibility and reliability to different electricity markets and different power grid configurations. Particular attention is devoted to the electricity production mix evolution in the selected countries. The role and operation of PSPP have evolved significantly over time to adapt to new electricity mix and market conditions. Insights regarding the prospects and barriers of PSPP in the coming decades are discussed, and estimates of remaining potential are compared with future storage needs, highlighting that alternative energy storage technologies will need to emerge alongside PSPP to meet the future needs.

Remote sensing of particle mass concentration in Alpine reservoirs

The Grimsel reservoirs in the Bern Canton are well known for their high load of suspended mineral particles which originate from glacial erosion, notably from the Unteraargletscher. Particles are deposited into the reservoirs by glacial melt, snowmelt and heavy rain events. Seasonal trends on Grimselsee, Oberaarsee, and Raeterichsbodensee have been followed thanks to various methods, especially by conductivity, temperature and depth profiling (CTD) and estimation of particle mass concentration (PMC). Particle size analysis revealed that suspended particles cover the size range from submicron to a few microns. These particles hardly settle out and influence the turbidity also of the downstream river and lake. Measurements of inherent optical properties were carried out in situ and in the lab, as well as reflectance above and below surface, to compare in-situ and remote sensing measurements. Simultaneous airborne spectroscopy data were acquired in 2013, and satellite data (Landsat-7, Landsat-8, Rapid Eye) have been used to investigate the feasibility of atmospheric correction in high-alpine conditions.
Geotherm 2

Geothermal Reservoir Processes: Towards the Implementation of Research into the Creation and Sustainable Use of Enhanced Geothermal Systems

Scope of project

Geotherm-2 (May 2013 – April 2016) is the continuation of Geotherm-1 (2009–2011). It was conceived as a bridge to a major nationwide project in geothermal energy, the Swiss Competence Center Energy Research – Supply of Energy (SCCER-SoE), which was in its planning phase when Geotherm-2 was proposed, and became operational in December 2013. Geotherm-2 conducts cross-disciplinary research targeted to the development of enhanced geothermal systems (EGS). The research addresses aspects concerning the geomechanical characterization of reservoirs, the numerical simulation of a reservoir creation, the long term effects of geochemical reactions on permeability and heat extraction, the assessment and management of the induced seismicity risk, the social acceptance and comparative assessment of the risks inherent to an EGS project, and the analysis of geothermal energy usage in cities, with the case study of Lausanne.

Status of project

Geotherm-2 is organized in 6 work packages (WP) and has now entered in its final phase, with no major variations from the original schedule. A few adjustments of the original research plan were necessary, due to the large time lapse from the first proposal application to the effective start of the project. The work accomplished under the umbrella of Geotherm-2 has been presented in various international meetings for a total of 40 presentations to date; 26 publications in peer reviewed scientific journals have been published so far, numerous more are on the way.

Main scientific results of workgroups

WP 1: EGS reservoir characterization and geomechanics

In order to predict reservoir injection and production behavior, the knowledge of permeable fractures in reservoirs is essential. Faults inferred from the microseismic cluster dataset of Kraft & Deichmann (2014) were compared in orientations with borehole fracture data and with the most-likely fault planes inferred from fault plane solutions by Deichmann et al. (2014).

Considerable agreement was found between the strike directions of microseismically inferred faults (figure 1a), and the mean strike directions of fractures previously identified from image logs run in the Basel-1 well (figure 1b). However the fault planes from seismic event clusters cover a narrow range of vertical orientations, while the fracture zones imaged in the well show a much larger dispersion in orientation. Planes that slip aseismically also remain undetected. Microseismic clusters of larger sizes identified by Dyer et al. (2010) are now investigated, with a view towards more complete integration of the microseismic and borehole datasets.

Main Investigator
Stefan Wiemer, ETHZ

Project Partners
ETHZ
EPFL
PSI

Time frame of Project
2013–2016

Project Website
www.cces.ethz.ch/projects/nature/geotherm-2

Part of SCCERs
SoE (Supply of Electricity)
Electricity

Geotherm 2

Geothermal Reservoir Processes: Towards the Implementation of Research into the Creation and Sustainable Use of Enhanced Geothermal Systems

WP 2: Induced seismicity – monitoring, risk assessment and management

The work of this WP tackles various aspects of induced seismicity. A database of induced seismicity, has been implemented and is now setup at the Swiss Seismological Service. A new hydro-mechanical model coupled with a rate- and-state frictional behavior has been performed to study rupture propagation of induced earthquake and derive implications on the maximum possible magnitude. A new hybrid model combines numerical modeling of flow with the so-called “seed model”, that stochastically generates seismicity according to the flow solutions provided to it. This hybrid model is currently exploited in Monte Carlo-like simulations.

An Induced Seismicity Test Bench has been used to test and rank models designed for earthquake forecast systems operational during stimulation projects. The Test Bench has been applied to the data from Basel 2006 and Soultz-sous-Forêts 2004 geothermal projects, to assess forecasts of two models – the Shapiro in Space (SiS) and the Hydraulics and Seismics (HySei) model. The time-dependent properties of the ambient seismic wavefield have been used to detect, resolve, monitor, and image the deformation induced by the water injection associated with the stimulation of the 2006 Basel and St. Gallen projects.

A multi-trace cross-correlation detector allows to exploit waveform similarity to derive accurate earthquake magnitudes and a similarity-distance relationship is used to locate micro earthquakes.

WP 3: Comparative assessment of accidental risks and social acceptance

This module provides risk indicators (e.g., fatality rate), to comprehensively describe the accident risk associated with deep geothermal energy systems. The assessment is in continuous evolution: recently the risk indicators have been updated according to the new assumptions and plant capacity cases defined within the joint activities of SCCER-SoE.

A teaching course called Trans-disciplinary Case Study (tdCS) was organized at the ETH Zurich (Masters Program in Environmental Sciences). Master students retrospectively analyzed the project of St. Gallen especially focusing on public and stakeholder involvement. A media analysis on newspapers from the Romandie is ongoing in order to assess the public perception of Deep Geothermal Energy in French speaking Switzerland.

In parallel a fieldwork based case-study on the involvement of the public in the development of the Haute-Sorne deep geothermal energy in Jura has started.

WP 4: 3-dimensional simulator for EGS reservoir creation and production

The work in this WP seeks to provide a simulator that can improve our understanding of how a reservoir responds to pressure and temperature stimulation and high flow rates. A new finite volume based method is developed to model shear failure which includes special basis functions for discontinuity. The mechanical solver is coupled with a flow solver which relies on a hierarchical fracture network modeling approach, and it allows to compute flow induced shear failure along pre-existing frac-
Geotherm 2
Geothermal Reservoir Processes: Towards the Implementation of Research into the Creation and Sustainable Use of Enhanced Geothermal Systems

Investigation on thermo-elastic effects is under progress.

WP 5: Geochemical effects on long-term permeability evolution & heat extraction

The WP has developed the prototype of a simulation tool capable of simulating reactive transport in 3D complex geometries. The improved computational efficiency of the simulator and the accuracy of the solutions allow now to include realistic geometries. Some first reconnaissance simulations have been performed to test the effects of fracture aperture variations on reactive flow. Figure 3 shows how the reaction front progresses irregularly inside the fracture, in response to differential supply of reactive components imposed by aperture variations (smaller aperture limits the amount of fluid that can pass).

The authors of the simulator will contribute to a chapter on «Reactive Transport Modeling: Applications in Subsurface Energy and Environmental Problems» to a new book on reactive transport, which is supposed to be edited and published towards the end of 2016.

WP 6: Geothermal energy usage in cities

The module studies the usage in cities of geothermal energy from sources at different depth and aims to develop a decision support tool, which includes geographic information (GIS) to geo-localize and characterize the demands and the geothermal resources. A methodology to cluster urban systems has been developed, integrating both GIS existing information about the building stock (location, construction date, demand in energy services, etc.) and the distribution of geothermal resources.

Figure 4 shows the application of the methodology to the case study of Lausanne. The goal was to identify suitable zones of the urban system for a medium depth geothermal application (Malm Aquifer, depth: ~2 km). The methodology is general and can be extended to various cities in Switzerland.

A subtask in this module has developed a full life cycle impact assessment procedure for EGS power plants, revealing that the major part of the environmental impact is caused by the drilling of the geothermal wells during the construction phase. Further plans are to include also induced seismicity in the impact assessment and find ways how to compare the environmental effects in different impact categories.
Electricity

FAMSADI
Swiss High Energy Density Batteries – From Advanced Materials to a Safe Device

Scope of project
The goal of the CCEM project «Swiss High Energy Density Batteries – From Advanced Materials to a Save Device» (FAMSADI) was to develop a cost-effective prototype for a high energy density rechargeable lithium ion battery on the cell level based on abundant and environmentally friendly materials. The focus of the project was on developing innovative synthesis processes enabling production of novel nanostructured electroactive materials with improved electrochemical performance at industrial scale and on demonstrating industrially relevant prototype cells to push these materials to market. The project also offers a criticality and life cycle analysis to assess the competitive advantages with respect to established lithium ion battery technologies.

Status of project
The project was completed on schedule end of March 2015. The project resulted in several patents and publications in peer-reviewed journals and also fulfilled its mission in training young scientists to support Swiss industry as two postdocs trained at ETH Zurich and Empa within the FAMSADI project were hired by the industrial partner to accelerate developments towards a commercial product and a PhD student successfully defended his PhD.

A pilot production line is currently under development at the industrial partner.

Main scientific results of workgroups
The main outcome of the FAMSADI project is the development of a cathode based on H₂V₃O₈ (see figure 1) exhibiting a very high capacity to accommodate lithium ions resulting in a theoretical charge capacity of up to 400 Ah/kg.

Reliable hydrothermal synthesis processes were developed and refined to enable the industrial partner to scale production to pilot line level. The oxidative synthesis route described in the literature making use of sulfuric acid was abandoned in favor of a newly developed synthesis route involving an organic reducing agent facilitating scale up. Various other electroactive materials were investigated as candidates for the cathode during the course of the project including magnesium and vanadium oxides, oxynitrides, and borates. While some of these materials demonstrated good performance, the possibility to synthesize and process H₂V₃O₈ in aqueous media provides a significant advantage from a manufacturing and cost perspective.

For the anode side, a silicon-carbon composite was developed, successfully tested in half-cell configuration, and patented by Belenos. However, the absence of lithium in the as-synthesized cathode material causes silicon based anodes to be unsuitable for a commercial device, as a supplementary pre-lithiation step becomes necessary. More recent efforts have focused on developing a lithium metal based anode for the FAMSADI battery.

Initial challenges concerning the cycle life of H₂V₃O₈ were addressed applying a protective surface coating jointly developed and patented by Empa and Belenos. Stable cycling over more than 500 cycles was finally demonstrated operating H₂V₃O₈ against metallic lithium in a coin cell in combination with a newly developed electrolyte improving Coulombic efficiency from 99.06 % to 99.95 % and more than 75 % capacity retention after 500 cycles (figure 2).

To enhance the conductivity of H₂V₃O₈ at high lithium content, a doping process was developed jointly by Empa and Belenos. Substitution of vanadium with several other transition elements was found to improve the electrochemical performance of H₂V₃O₈. This work led to the development of a new material class of anode materials with improved performance at high lithium contents.

Figure 1:
Stick and ball model of the atomic structure of H₂V₃O₈.
metal elements was demonstrated enabling fine tuning of the electrochemical performance.

Initial tests with reduced graphene oxide as a conductive agent for the cathode yielded promising performance. In particular the carbon content in the electrodes could be minimized to as low as 1% by weight while maintaining good performance. Nevertheless, as the supply of graphite oxide is limited and unreliable, and the exfoliation at large quantities challenging due to the large surface area, electrodes making use of standard carbon additives were developed with comparable performance.

Progress in materials chemistry and electrochemistry during the project enabled the demonstration of a prototype cell with a very high energy density of 400 Wh/kg. In comparison, a commercial high energy lithium ion battery currently reaches an energy density of about 220 Wh/kg.

A prototype FAMSADI pouch cell shown in figure 3 integrating two larger cathodes and two matched anodes with dimensions 5x10 cm² was fabricated by Belenos and tested by Empa. While the large weight contribution of the pouch foil in this double cell stack configuration resulted in a measured energy density of 100 Wh/kg, an extension of this cell architecture to multiple cell stacks results in a significant increase in energy density. In fact a prototype cell with 10 cell stacks would already reach energy densities in excess of 400 Wh/kg.

**Assessment of operational safety**

First steps towards the assessment of operational safety at the material level were taken. The thermal decomposition of H₂V₃O₈ based cathodes at different states of charge was investigated by Empa using differential scanning calorimetry and compared to several commercial cathode materials. As for most cathode materials, thermal decomposition is also exothermic for vanadates. With respect to the amount of heat released and the heat release rate, as well as the onset temperature for heat release, H₂V₃O₈ based cathodes rank among the safer commercial lithium nickel-manganese-cobalt (NMC) oxide based cathode materials and is more stable than lithium nickel-cobalt-aluminum (NCA) oxide based cathodes with respect to thermal events.

**Criticality and life cycle analysis**

Within the FAMSADI project, Empa performed both a criticality and a life cycle analysis for the FAMSADI battery. The criticality assessment is directly influenced by geopolitical factors and market demands and may therefore change over time. While cobalt has been classified as a critical raw material by the European Commission, vanadium remains a non-critical element with relatively low supply risk despite its higher economic importance. In addition, due to the relatively low synthesis temperature of H₂V₃O₈ of typically only 200 °C as compared to 800–900 °C for NMC materials, the global warming potential for the FAMSADI battery is projected to be lower than for state-of-the-art lithium ion batteries, despite a significant contribution of the lithium metal anode, as shown in figure 4.

Belenos is currently scaling production of H₂V₃O₈ to kg scale and building a pilot production line for the FAMSADI battery. A collaboration between Belenos and Empa is ongoing to further improve the understanding of this new materials which thanks to the FAMSADI projects promises to grow from an academic curiosity to a commodity.
MeAWaT
Methods of Advanced Waste Treatment

Scope of project

MeAWaT (methods of advanced waste treatment) is a follow up project of PINE, where an advanced nuclear fuel designed for waste transmutation was studied; the so called sphere-pac fuel. MeAWaT extends the previous efforts by implementing the production unit in an active environment, allowing working with plutonium and minoring actinides. Furthermore thermal-hydraulics plus neutronics aspects are investigated for subcritical reactor systems (ADS), which are especially designed for efficient transmutation of actinides. In order to improve the heat transfer a new pin design is suggested. The project is divided in 4 tasks, where task 1 regards a new pin design. Task 2 treats the thermal hydraulics and task 3 the neutronics aspects. Task 4 is concerned with the production of actinide containing fuel, which also requests the enclosure in a glove box.

Status of project and main scientific results of workgroups

Task 1: New pin design

In task 1 the thermal conductivity and heat transfer of an annular pin design is being studied as a function of the sphere-pac composition of small and coarse sized spheres. This task was reported.

Task 2: Thermal hydraulics

During last year, we focused on the preparation of an article with the findings from computational fluid dynamics (CFD) simulations of a wire-wrapped fuel pin bundle. In the numerical simulations, we put special emphasis on the calculation of the pressure drop and on the formation of recirculation areas, which could potentially lead to the development of hot spots. Several simulations were carried out and, based on the results, a modification to the Darcy-Weisbach correlation was proposed.

Figure 1 shows the geometrical configuration of the studied bundle. The main parameters for a single subchannel are the wire pitch \( H_w \), wire diameter \( D_w \), the outer pindiameter \( D_p \) and the pin length \( L_p \). Considering these geometrical parameters, the newly modified Darcy-Weisbach correlation reads,

\[ \Delta P = \beta \times \frac{L_p \rho V^2}{D_p} \]

where the geometrical factor \( \beta \) is given by

\[ \beta = 1 - 7.46 \left( 1 - \frac{1}{1 + \pi \left( \frac{D_p + D_w}{H_w} \right)^2} \right) \]

When comparing the pressure drop predicted with equation (1) with that from the well-known Cheng-Todreas correlation, the results are in good agreement (see figure 2). However, when using equation (1) to predict experiments with water as coolant, the results are not very satisfactory.

We believe that the main reason for the disagreement lies in the geometric factor given in equation (2). We are still investigating several improvements for this factor, and the results are expected to be published soon in a new article.

Task 3: Neutronics aspects

In task 3 the core design and optimization procedure was developed and applied to the analysis of the MeAWaT core, i.e. sub-critical Gas-cooled Fast Reactor for waste transmutation. The task was mainly concluded in the last reporting period.

The finally chosen core design features thermal power of 400 MW at the subcriticality level of 0.97, the SiC cladding with the W-Re inner layer and Yttrium-Stabilized Zirconia as inert matrix for a fuel exclusively composed by transuranic elements from Light Water Reactor, with an initial fuel inventory of about 6 t and 4 year irradiation time, resulting in fuel burnup of about 10% (maximum achievable).

The americium fraction in the discharged fuel is significantly

List of abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADS</td>
<td>Accelerator-Driven System (subcritical reactor system)</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
</tbody>
</table>

Main Investigator
M.A. Pouchon, PSI

Project Partners
PSI
Empa
EPFL
ETHZ
Institute of Modern Physics, Chinese Academy of Sciences

Time frame of Project
2012–2015

Figure 1:
Fuel bundle geometry. The spacer wires are displayed in green and the inner cooling channels in yellow.
MeAWat
Methods of Advanced Waste Treatment

Electricity

reduced mainly due to the increase of the Pu-238 fraction. The use of the annular pins allows 20% higher power density compared to standard pins while reducing pressure losses across the core. The negligible Doppler and positive void effects are counterbalanced by negative reactivity effects of core thermal expansion in radial and axial directions.

The two main problems of the proposed core design were found to be
1) the limitation of the core power density at the level of 50 MW/m³ because of the low fuel conductivity and
2) the high reactivity swing (~3000 pcm), which suggests the use of control rods to avoid a significantly oversized proton accelerator.

Task 4: Production of actinide containing fuel

Task 4 is divided into three subtasks. The first one is concerned with an advanced feed-solution preparation by short-term mixing, which allows the preparation of actinide containing solutions, not being affected by decay heat and changes in chemistry. Here the device already mentioned in last year’s report was further developed and many tests were conducted with inactive materials, proving the quality of the produced spheres.

The second task deals with the production integration into...
the glove-box. Here major achievements were reached, as the glove box is fully functional and only waits for the license from the Swiss Nuclear Safety Inspectorate to produce Pu containing samples.

Figure 3 shows the new glove-box on the left side, and all the external microwave equipment plus the solution preparation on the right side. The figure also shows an inside view of the glovebox, with the mixing device, the nozzle and the microwave cavity.

One of the key components developed for this project is the microwave window, which is also shown on the picture. It is important to minimize losses in intensity and quality of the microwave signal, in order to still efficiently heat in the microwave cavity. At the same time the safety aspects are assured, as the window has two hermetic barriers, in case one fails.

The spheres shown in figure 4 are produced using the new in-situ mixing technique, and the microwaves being transmitted thought the newly developed microwave window. The numerous gelation tests with the optimization of the chemistry were performed together with a guest from the Institute of Modern Physics (IMP) from China. Technically the task has been accomplished, and only the license for the production of active material is pending.

In the third subtask «Microwave Sintering», the PhD candidate Hussein Hammoud under the supervision of Dr Sébastien Vaucher (Empa) and Prof François Valdivieso (Ecole Nationale des Mines de Saint-Etienne) is now finalizing his thesis. The final examination will take place in March 2016.

In 2015, the final year of the PhD, the effort has been concentrated on investigating the effect of particle size and necks on the microwave sintering behavior. Based on experimental data acquired in the previous reporting periods, a multi-physics model has been developed and tested.

The results have been reported in three conferences (oral presentations) and a paper (submitted).
SLIB
All Solid State Li-Ion Batteries based on New Ceramic Li-Ion Electrolytes

Scope of project

Renewable energy production and storage are critical in terms of enabling new technologies (e.g. electric cars) and reducing CO₂ emissions & environmental pollution. However, current Li-ion battery technologies based on liquid electrolytes are not sufficient to provide high practical energy densities. Novel battery technologies based on solid inorganic electrolytes could enable the use of high capacity electrode materials in a safe way. The SLIB project focuses on new and safe solid state materials and device design concepts for next generation, all solid Li-ion batteries, offering an alternative to current liquid/polymer based Li-ion batteries. In this sense, new doped garnet electrolytes are investigated in depth.

Status of project

In the second meeting of the project (17.4.2015) at Paul Scherrer Institute (PSI), the current status of the project was evaluated. Then, bilateral meetings between the subgroups and active sample and know-how exchange were intensified. The industrial partners were also informed to get feedback and make improvements on a more applied level. The third meeting of the project (29.10.2015) was held at ETH Zurich with the participation of the project evaluator. The current results from the individual groups were delivered and active synergies between groups evaluated. The second year plans in terms of actual collaboration and scientific outcome were also discussed.

Up to this point in the project, the work packages (WP) 1, 3 and 6 were focused and milestones in these packages have been fulfilled. The novel garnet type electrolytes for all solid batteries were synthesized and characterized. Li-ion conductivities for these electrolytes are determined and electrochemical cells were suggested for Li-based solid state electrolyte/electrode configurations based on garnet-type solid ceramic electrolytes.

Main scientific results of workgroups

**WP 1: Garnet-type Fast Li-Ion Conductors (Li₆.7₅La₃ₓMₓZr₁.₇₅Ta₀.₂₅O₁₂)**

The cubic phase of Li₆.7₅La₃ₓZr₁.₇₅Ta₀.₂₅O₁₂ garnets and doped variants are interesting solid electrolyte candidates with high Li-ion conductivities in the range of ~10⁻⁸ S/cm at room temperature (RT). New doping strategies to obtain the highly conductive cubic phase have been reported.

A series of new compounds with the general formula of Li₆.₇₅La₃ₓMₓZr₁.₇₅-Ta₀.₂₅O₁₂ have been prepared and characterized in terms of structural and electrical properties for M = Er³⁺, Y³⁺, Nd³⁺ and also in the plain form. All prepared materials exhibit cubic garnet phase confirmed with Raman Spectroscopy (figure 1a). The activation energy of Li⁺ conductivity in a range of 0.38 eV has been determined, and both activation energy and ionic conductivity values (figure 1b) are comparable to the results in literature for the cubic phase of Li₆.7₅La₃ₓZr₁.₇₅Ta₀.₂₅O₁₂ garnets. This forms an important base to make larger and micro-batteries for testing and is a prerequisite for the following success of the project; which was matched in the 1st year.

**WP 2: Silicon thin film anodes for Li-ion Batteries**

Si thin film anodes in liquid electrolyte systems are investigated prior to their measurement in all-solid-state Li-ion batteries. Si thin films
Electricity

SLIB
All Solid State Li-Ion Batteries based on New Ceramic Li-Ion Electrolytes

WP 3: Thin film \( \text{Li}_4\text{Ti}_5\text{O}_{12} \) anodes for \( \text{Li}_{6.25}\text{Al}_{0.25}\text{La}_3\text{Zr}_2\text{O}_{12} \) based batteries

Stoichiometric, 91\% dense pellets of \( \text{Li}_4\text{Ti}_5\text{O}_{12} \) have been fabricated, characterized by x-ray diffraction (XRD) and used as target materials for thin film deposition by means of pulsed laser deposition (PLD). Thin films (thickness around 630 nm) of \( \text{Li}_4\text{Ti}_5\text{O}_{12} / \text{TiO}_2 \) mixed phase have been deposited on a dense \( \text{Li}_{6.25}\text{Al}_{0.25}\text{La}_3\text{Zr}_2\text{O}_{12} \) pellet of 250 \( \mu \)m thickness. The electrochemical cells constructed with gold top electrodes and Li metal anodes (figure 3a) showed initial open circuit voltages (OCV) of \( \sim 1.6 - 1.8 \) V and reversible cycling (figure 3b). The optimizations to obtain practical capacities from such cells close to the theoretical values (ca. 175 mAhg\(^{-1} \)) at 1.55 V for \( \text{Li}_4\text{Ti}_5\text{O}_{12} \) are ongoing.

WP 3: Colloidal BiF\(_3\) nanocrystals – an approach to conversion-type Li-ion cathodes

New electrode materials that could be implemented to half-cell all solid state batteries within the scope of the project were synthesized and characterized. BiF\(_3\) is a highly promising cathode material due to its conversion to BF\(_3\) + 3LiF (during discharge), occurring at an average voltage of \( \sim 3 \) V. The theoretical specific capacity of BiF\(_3\) is very high (302 mAhg\(^{-1} \)), corresponding to an energy density of \( \sim 900 \) Whkg\(^{-1} \). However, BiF\(_3\) is an electrical insulator and cannot be used as an electrode material in the bulk form. The size reduction is necessary for electrochemical activity as an electrode material for Li-ion batteries.

We report the synthesis of BiF\(_3\) nanocrystals (NC) employed Bi(III) trifluoroacetate, Bi(TFA)\(_3\), as a single-source precursor, using inexpensive starting reagents (figure 4). Namely, thermal decomposition was triggered by the injection of Bi(TFA)\(_3\) precursor solution into hot (230°C) oleylamine, yielding BiF\(_3\) NCS in several minutes. Oleylamine served as both a high-boiling solvent and the surfactant.

After removal of the capping surfactant molecules, BiF\(_3\) NCS were tested as a cathode material for Li-ion batteries using liquid Li electrolyte (1M LiPF\(_6\) in dimethyl carbonate). Close to theoretical Li-ion storage capacities of up to 300 mAhg\(^{-1} \) at an average voltage of 3 V were obtained at a current density of 50 mAg\(^{-1} \).
WP 3 & 6: Li$_7$La$_3$Zr$_2$O$_{12}$ thin film growth and optimization through PLD

The optimization of both electrolyte and cathode thin film deposition using PLD and radio frequency (RF) sputtering is investigated. The primary obstacle has been a general Li deficiency in the deposited films leading to the formation of some Li deficient phases (e.g. La$_2$Zr$_2$O$_7$). By studying the effect of a post Li treatment on Li$_7$La$_3$Zr$_2$O$_{12}$ thin films, several previously unknown mechanisms occurring in the thin film regime can be identified – a substantial contribution to the discussion of optimal Li-content to the electrolyte stability where currently almost no investigations are available.

Graphite anodes, which, despite being the most common anode material, are rarely studied because carbon’s low core charge number results in weak X-ray attenuation contrast between graphite and the other pore space filling components in an electrode microstructure. It has been demonstrated that a combination absorption and phase contrast X-ray tomography (figure 6a) can be used to distinguish between the graphite particles and the electrolyte-filled pores, allowing the microstructural dynamics during electrochemical cycling to be tracked non-invasively. Furthermore, it has been shown that applying digital volume correlation can be used to capture the dynamic evolution of the microstructure of the electrodes during operation and to quantify local electrochemical activity as a function of 3D space and time (figure 6b).

Conclusion

New type of doped Garnet-type Fast Li-Ion Conductors Li$_{6.75}$La$_3$M$_x$Zr$_1.75$Ta$_0.25$O$_{12}$ (M = Er$^{3+}$, Y$^{3+}$, Nd$^{3+}$) are synthesized, processed and Li-ionic conductivities are determined based on solid state processed sintered ceramics. Thin films of Li$_4$Ti$_5$O$_{12}$ and silico anode materials for Li-ion batteries are fabricated and electrochemical tests are performed in solid electrolyte and liquid electrolyte systems, respectively.

The imaging techniques to analyze microstructure and degradation in lithium ion batteries in the future steps of the project are investigated and improved based on available battery materials and electrodes (e.g. graphite anodes) before switching to all solid state batteries. The results of the work packages have been communicated in respectable conferences and journals.

WP 5: Computer simulation and imaging of Li-ion batteries

The imaging techniques to analyze microstructure and degradation in lithium ion batteries were improved in the first year of the project. The focus was on improving the capabilities for visualization of Li-ion batteries using commercially available battery materials and electrodes before switching to all solid state batteries.

The segregation of Li to the film surface observed by Raman spectroscopy is coupled to the formation of amorphous lithium carbonate upon exposure to air. A first model between film thickness and phase formation/morphology has also been established. Through a novel post-annealing treatment a 650 nm film was formed with a high density and a large proportion of cubic Li$_7$La$_3$Zr$_2$O$_{12}$ phase (figure 5).

Figure 5: XRD powder pattern of a thin film of c-Li$_7$La$_3$Zr$_2$O$_{12}$ mixed with La$_2$Zr$_2$O$_7$ phase. Inset shows a scanning electron microscope image of the high density film.

Figure 6: a) 3D reconstructions of a sub-volume of graphite anode using pure absorption contrast tomography (top) and a mix of absorption and phase contrast tomography (bottom). The combination of absorption and phase contrast tomography preserves the high-resolution of the absorption contrast while offering more contrast between particle and pore space to facilitate microstructural analysis.

b) Divergence maps from digital volume correlation plotted overlaid on the corresponding slices of electrode. Brighter colors indicates volume expansion due to lithiation, while darker shading indicates contraction due to delithiation. Vertical cuts through the cell (bottom) reveal uniform lithiation in the bottom electrode until about 50 % state of charge (SOC), after which a lithiation front moves through the electrode: yellow color propagating from the middle of the image (separator-graphite electrode interface) to the bottom (current collector interface).
ISCHESS
Integration of Stochastic Renewables in the Swiss Electricity Supply System

Scope of project

The project goal is to study the integration measures required to increase the penetration of distributed stochastic generation in the Swiss electricity supply system. The first project phase evaluates the impact of intermittent renewable energy sources (RES) at the distribution voltage level, whereas the second project phase will extend the study to the national scale of the transmission grid. More specifically, the following alternatives for the stochastic RES integration will be analyzed and compared within the scope of the project:

• One alternative is to reinforce and expand the network as required by the increasing energy flows in the grid. Conceptually, this is the traditional way to accommodate for varying power levels in the network and can therefore be denoted as business as usual (BAU).

• Another option is to use local storage elements like batteries: in a system with bidirectional and less predictable power flows, electrical storage devices in the distribution grid could balance supply and demand, since they offer the potential to store generated (excess) electrical energy and release it at a later point in time when there is a shortage of energy supply.

• Dispatchable loads (such as electrolyzers for hydrogen production or water heaters) represent another alternative to shift the electricity demand in time to maintain the generation/load balance.

• A final option is to directly curtail RES generation when too much generated energy is available, in order to preserve the energy equilibrium in the grid.

Status of project and main scientific results of workgroups

Table 1: Capital costs for PEM hydrogen electrolyzers by size classes (DOE 2014).

<table>
<thead>
<tr>
<th>Size</th>
<th>Total Cost</th>
<th>Average Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>kg/day</td>
<td>$/kg/hr</td>
<td>$/kW</td>
</tr>
<tr>
<td>10</td>
<td>0.42</td>
<td>13.9</td>
</tr>
<tr>
<td>100</td>
<td>4.17</td>
<td>138.9</td>
</tr>
<tr>
<td>1’000</td>
<td>41.67</td>
<td>1388.9</td>
</tr>
<tr>
<td>1’500</td>
<td>62.50</td>
<td>2083.3</td>
</tr>
<tr>
<td>50’000</td>
<td>2’083.33</td>
<td>69444.4</td>
</tr>
</tbody>
</table>

Technology and life cycle assessment

In 2015, the major focus has been on the technology characterization, and especially costs, for two of the four major alternatives considered, in particular electricity storage and dispatchable loads.

Battery storage

For the distribution voltage level, the choice of batteries was restricted to lead acid and lithium ion batteries, based on size, costs and battery life. Battery degradation as a function of use was a particular focus. A simple hybrid model using lifetime energy storage capacity and state of charge was developed for both battery technologies, based on the literature and consultation with PSI battery specialists. The cost model developed degradation was then used in the network analysis.

Dispatchable loads

The focus for dispatchable loads was on hydrogen electrolysis. The polymer electrolyte membrane (PEM) electrolyzer technology was selected, based on size, life, and particularly its fast response time characteristics. The PEM technology was surveyed for costs, cost scaling by size, life and average generation costs. In particular, 2008 NREL results for size classes and scaling were calibrated to later 2014 DOE costs to give capital costs shown in table 1. In addition, Swiss industry assumptions for hydrogen distribution costs were gathered to help determine location-specific hydrogen value at the distribution substation level.

The life cycle assessment (LCA) results for the selected environmental indicators – climate change impacts, human health impacts and ecosystem quality – have been provided in order to allow for the assessment of the environmental performance of different RES integration scenarios (table 2). Inventory data for conventional lead acid and Li-Ion batteries have been further improved using latest literature data and information from manufacturers. Furthermore, new inventories for redox flow batteries have been compiled in collaboration with EPFL and Gildemeister Energy Solutions. Redox flow batteries can be designed for storage of comparatively large amounts of electricity and will therefore be
of importance in the 2nd phase of the project.

In addition and in collaboration with Leclanché SA and EPFL, new inventories for a certain Li-Ion battery technology (cathode: Lithium-Nickel-Cobalt-Oxide; anode: Lithium-Titanium-Oxide), specifically designed for stationary applications, are in development. This new battery is supposed to perform much better than current conventional models for large-scale, stationary electricity storage due to its robustness to deep discharge, long cycle life and inherent safety.

The comparatively lower gravimetric energy density does not pose a substantial obstacle for stationary applications.

**Grid modelling and assessment of RES integration strategies**

A number of components have been selected and implemented for the case study in collaboration with PSI-TAG. Electrochemical storage components include lithium-ion and lead-acid batteries. To incorporate various types of battery models and parameterizations, a generic piecewise cost function depending both on the state-of-charge (SOC) and the battery power has been implemented. Hydrogen generation is implemented at the feeder bus to investigate the interaction between potential electrolyzers and the electrical grid. Household load components are modeled in accordance with an assumed coincidence factor of the loads in the distribution grid. Demand side management components are assumed to be available in a certain range of the households to shift the households’ consumption throughout the day. They are implemented in the same framework as the storage components. Electrical line upgrades are modeled in accordance to the distribution grid data and generic system properties of the grid under investigation. PV curtailment is used when the available PV power can not be integrated in the network example without the violation of security constraints.

All models and cost functions have been implemented within the MATLAB-based simulation framework. The key step is the formulation of the operation and planning problem as large nonlinear optimization problem that is solved using tailored external solver packages.

Since the planning outcome is very sensitive to the parameter variations of the system components, scenarios and cost functions, the planning problem is solved for the full ranges of key parameters rather than specific uncertain values.

This provides the sensitivity of the outcome to key system parameters and also leaves room for strategic planning adjustments of the individual system planner.

The component models and grid scenarios have been applied to a selected distribution grid. They illustrate the optimal planning decisions under different modelling assumptions and price predictions. The main challenge to the system stability comes from a large infeed of distributed PV sources. The planning objective captures the overall social costs for electricity import, component degradation and grid upgrades.

The results show a large sensitivity of the planning outcome to the assumed storage costs. A prominent and cheap solution under various scenarios

---

### Table 2: Life Cycle Assessment results for different components of a regional energy grid.

<table>
<thead>
<tr>
<th>Component</th>
<th>Climate change impacts kg CO2 eq</th>
<th>Human health impacts w/o climate change</th>
<th>Ecosystem quality w/o climate change</th>
<th>DAILY species yr</th>
</tr>
</thead>
</table>
ISCHESS
Integration of Stochastic Renewables in the Swiss Electricity Supply System

The parametric result for a whole range of battery storage cost parameters is shown in figure 2. Here, the vertical axis indicates the total cost of the optimal system operation and extension (indicated by a star in figure 1) as a function of different storage cost parameters, shown on the two horizontal axes.

With regard to the second project phase, investigating the transmission level aspects of the large scale RES integration in Switzerland, a network model is being developed in collaboration with PSI-EEG to meet their demands for the studies with the STEM-E model. A key step is the reduction of a detailed power system model to a reduced model that still incorporates all security constraints of the underlying network. A reduction algorithm has been developed and tested on a benchmark European network model, allowing a flexible generation of reduced models according to the specifications of the system planners and research partners.

The scope of the Swiss TIMES Electricity Model (STEM-E) has been extended to include storage technologies, ad-hoc representation of the electricity grid, grid balancing markets and heat demands. In addition to pumped-hydro storage in STEM-E, a number of electricity storage technologies, such as batteries, compressed air storage and power to gas, have been introduced. The model is also extended to include heat demands from all end use sectors. Figure 3 shows the schematic of the Swiss TIMES Heat and Electricity Model (STEM-HE). The new model also includes thermal storage options (hot-water tanks / thermochemical storage) for water and space heating applications.

For the newly introduced electricity storage technologies, provisional technical-economic characterization data are pooled. The data will be finalized during scenario analysis. Two new features developed within this project include an ad-hoc representation of the electricity grid and endogenous modelling of grid ancillary services. The area shaded in orange in figure 3 shows the model developments within the ISCHESS project. To this end, electricity grid levels 1 to 7 have been modelled in aggregated form, i.e. without any spatial aspect, to characterize energy losses and simplified grid infrastructure costs. The modelling of various grid levels makes it possible to distinguish the role of centralized and decentralized sources of

Figure 1: Two day operational example of a CKW 20 kV/400 V distribution grid (390 nodes, 16 transformers, 1 feeder) with high PV share, high demand and controlled battery storage. Top plot: Hourly power demand and power import. Bottom plot: Cumulative trajectories for total system operating costs, energy import costs and battery degradation costs (with state-of-charge, charging power, and constant degradation components); using fixed battery degradation cost parameters.

Figure 2: Planning example of a CKW 20 kV/400 V distribution grid (390 nodes, 16 transformers, 1 feeder) with high PV share, high demand and controlled battery storage. Total system operating costs for variable battery degradation cost parameters (for state-of-charge and charging power).

Integration of energy system and grid modelling

is using simple curtailment of the PV sources during peak hours. Additional flexibility in the network is more profitable compared to traditional grid extension with typical upgrade cost ranges. A typical operational example is shown in figure 1. For a fixed set of battery storage cost parameters, the optimizer selects the optimal storage allocation in the network, as well as the optimal system operation, yielding the minimum total cost for this scenario, indicated by a star in the figure.
Electricity

**ISCHESS**
Integration of Stochastic Renewables in the Swiss Electricity Supply System

Electricity supply. The second enhancement is the representation of demand for ancillary services for electricity grid balancing. The provision of primary and secondary control power (both negative and positive) is endogenously determined based on the levels of intermittent sources, electricity supply and electricity demand. The power plants bid their true capacity in order to participate in the grid balancing markets. However, activation of the reserve capacity is not modelled because this requires a stochastic modelling framework. In the power-to-gas option, hydrogen is produced through electrolysis. The hydrogen can be used in fuel cells or stored or injected into the natural gas grid either as pure hydrogen or after conversion to methane.

A conceptional method to integrate the STEM-HE model and the FEN-planner model has been established and illustrated in figure 4. It will be a soft coupling to exchange insights from the both modelling frameworks.

For example, the STEM-HE offers long term electricity demand and supply (mapped to the 288 typical hours represented in the model), the international electricity exchanges and the required net transfer capacity (NTC) to the neighboring countries.

In order to define the international boundary conditions on electricity trade, the European Swiss TIMES Electricity Model (EUSTEM) will be used. Using this information, the FEN-planner framework offers insights to STEM-HE via a 3-5-nodes of aggregated electricity grid network with NTC among the nodes.

The FEN-planner also provides 1) possible allocation of the Swiss electricity generation portfolio to the selected nodes; 2) admissible additional power generation at each node, and 3) import/export boundaries between them.

The soft-coupling is envisaged in three steps, viz.

1. definition of international boundary conditions using EUSTEM;
2. running the STEM-HE model; and
3. iteration with FEN-HE to incorporate potential transmission network upgrades.

Using the coupled framework above, a set of long term electricity scenarios will be analyzed next year.
IDEAS4cities
Integration of Decentralized Energy Adaptive Systems for cities

Scope of project

Decentralized renewable energy generation by solar photovoltaic, solar thermal and biomass, waste heat use, and respective storage technologies, will become increasingly significant for the future Swiss energy system. In this project urban energy system concepts are developed and analysed that, within a city quarter or community, dynamically manage energy supply inputs with the respective demands for heating, cooling and electricity, with storages interacting with the devices to achieve optimal functionalities. Application potentials for real cases are evaluated, and respective technologies are installed and tested in two demonstration facilities.

Status of project and main scientific results of workgroups

WP A: Design procedures

Recent work focused on methods to generate and map time-resolved energy demands and potentials of decentralized energy systems. Building data are collected and energy demand profiles for different building types in neighbourhoods determined. Potentials for renewables in urban environments are also determined and integrated into GIS database.

Energy related infrastructure including different energy conversion technologies as well as district heating/cooling networks and thermal energy or power-to-gas storages can be optimised using a bi-level multi-objective optimization framework, solving the scheduling problem through MILP models with model predictive control at the lower layer, and at the upper layer objectives such as total capital expense and the dwelling self-sufficiency. Lifetime energy system costs were minimized using robust optimization techniques by integrating solar renewables and buffer as well as seasonal heat storages. A trade-off between an optimal system versus a robust system that can deliver the required services under worst case conditions can be made for cost or different components size as e.g. solar panels (figure 1).

WP B: Global urban energy model

Existing Energy Hub and Power Nodes modelling frameworks figure 1: For the objective value costs and the key indicator solar thermal panel size, the respective result is given as a function of the number of input parameters at worst case value (J. Rager, EPFL thesis n° 6731, 2015).

Figure 2: Impact of climate change on an office building’s energy requirements using multi-year predictions for the period of 2021–2040 from multiple climate models. Today’s period corresponds to the average conditions in 1981–1990. Data from the CORDEX project (Giorgi et al., 2006) downscaled further using the «morphing» technique (Belcher et al., 2005).
IDEAS4cities
Integration of Decentralized Energy Adaptive Systems for cities

are further developed and extended for realistic building blocks and city quarters modelling. This includes the different energy carriers, fluctuating distributed generation and load demand, energy storage efficiencies and limitations and other storage-like functionalitv, and optimization & control techniques for multi-energy grids. Time aggregation significantly reduces the computational effort for predictive power dispatch problems for large-scale power & energy systems. Asset aggregation can reduce the computational effort for simulation by a factor up to 20 000 (in case minimum power output constraint is active) (Deml et al. 2015). The approximation quality, however, strongly depends on the procured energy from the units and their power ratings and constraints.

For better integration of stochastic resources into the urban microgrid model, the COMMELEC (see link to website) method has been developed. It is based on a common abstract model characterized by the main properties of composable subsystems which can be aggregated into virtual devices. For this purpose, several elements have been modelled to cope with the control method, taking into account real scale devices such as installed in the EPFL microgrid facility (see WP C2).

**WP C1: Case studies**

For different climatic models, a range of possible futures climate data and related uncertainties was derived, and used to quantify the impact of different climate data on building heating and cooling demands (figure 2). Considering such effects allows for more robust buildings and energy systems design. The method used is now extrapolated to the district scale applications, considering the possible future building energy demand ranges, and used for more informed design decisions for future energy systems.

With data already gained on the village of Zernez, a cost optimization study, considering different carbon mitigation policies, indicates that decentralized generation and storage technologies can significantly reduce the community’s electricity grid usage through the deployment of local small hydro and photovoltaic panels (figure 3). Further work focuses on a study for the city of Basel where, compared to the rural case, the set of energy consumers is larger and more diverse; gas and district heating networks are available; and several local power stations help meet demand.

Hourly heating demand and building integrated PV generated electricity were determined for the EPFL campus for actual and future different climatic scenarios, using the city energy simulation tool CitySim. Thermal energy storage in the building structure, and heat and electric storage devices were considered. The heat distribution system was optimized by a MILP approach. Such, future challenges for the electric distribution grid were identified.

**WP C2: Microgrid test facility**

The EPFL-DESL microgrid facility contains realistic-scale devices such as large PV power plant, lithium-titanate batteries (figure 4), supercapacitors, electrolyser, PEM fuel cell, and building load emulator for HVAC and appliances. Performances using COMMELEC are
studied, and a first validation was successfully performed. This control method simplifies grid controller decisions methods, keeping safe network conditions and considering several devices/energy resources. Full renewable operation is sought, both in islanded and grid-connected mode, providing also ancillary services to larger grids. Figure 5 shows a screenshot of the microgrid operation, showing how COMMELEC can track the request with the stochastically fluctuating PV production and exploiting the flexible resources without knowing their nature.

**WP C3: Energy hub in NEST**

The control system is specific for NEST and allows for a very flexible integration of new control strategies.

**Main achievements / outreach**

Urban energy system models and techniques are available and are further developed and applied to real cases. GIS-based demand and potential models are developed. In energy hub modelling, the focus is on holistic optimization for design and operation, on uncertainty handling, and on flexibility / resilience / robustness assessments. Many activities are in close relation to SCCER FEEB&D and SCCER FURIES. The EPFL microgrid test facility is operational and ready for testing of new grid control techniques. More components are envisaged to be installed in the facility in the next months and further validations in presence of more complex scenarios are planned. The inauguration of NEST building is planned for May 2016. The EH will be made operational in parallel. Development of EH models and control is ongoing. The extension of the EH with smart grid components (system of EPFL-DESL) is planned in Q3/2016.

**Websites**

Zernez Energia 2020: zernezenergia2020.ch
Empa NEST Energy Hub: empa.ch/web/energy-hub
EPFL low voltage microgrid: dest-pwrs.epfl.ch/microgrid
Smart Heat Design: crem.ch/SmartHeat
COMMELEC real-time control framework: arxiv.org/abs/1403.2407
SCCER FEEB&D: sccer-feebd.ch
SCCER FURIES: sccer-furies.epfl.ch

Figure 5: Active power of energy resources in the microgrid under the COMMELEC control framework:
- Uncontrollable and stochastic: photovoltaic power (red).
- Controllable: consumption of 8 electric-space-heaters (green); power of a battery (white). Given power request at the point of connection of the microgrid with the main grid (yellow). Actual implementation (cyan).

Figure 6: The NEST Energy hub components. Different energy hub configurations can be demonstrated and tested, in relation to applications such as hybrid storage, smart grid, or combinations with mobility.
SECURE
Synergistic Energy and Comfort through Urban Resource Effectiveness

Scope of project

The two principal natural driving forces for urban environmental systems are atmospheric (wind, temperature and humidity) and solar (daylight, heat gains and power generation). This system should be considered at two scales: district-level (relationships and interactions between buildings) and building-level (abstracted in a simplified manner where appropriate). This project aims to enable effective use of resources (land area, solar gains, air flows) to achieve synergies that benefit both energy use and comfort in urban areas.

Metrics and indicators will be explored that can provide a means of using climate and solar data as energy stimuli for buildings. A modular simulation platform is being developed to combine many existing software packages to achieve the holistic analysis required. Statistical emulation of results to more abstract levels will also be incorporated to bridge the different scales and levels of detail. Advanced optimization processes will use the co-simulation environment to explore the design space at a detailed level. This will inform decision support systems that are applied early in the design process. Verification and validation will accompany usability and effectiveness appraisal during the application of the developed tools on case study projects in conjunction with industry partners.

Status of project and main scientific results of workgroups

The CCEM project officially started on January 1, 2015. An overview of the project topics and their interactions is given in figure 1. It is organized into two closely linked work packages (WP) as follows, each divided into two strands.

WP 1A: Metrics and indicators

Solar indicators are used to help predict cooling and heating needs as well as daylight autonomy and PV potential. A meta-model is fitted to the results of many simulation runs, as shown in figure 2. This uses multiple linear regression, though a Bayesian technique based on Gaussian processes is also being investigated. Key input parameters identified include plot ratio, form factor, south facade ratio, window-to-wall ratio, window-to-floor ratio, facade irradiation per floor area and roof irradiation per floor area. The results were presented at the PLEA conference.

WP 1B: Co-simulation platform

The simulation platform development is continuing. An extension to the SECURE project will facilitate better integration of this with ongoing work on other projects, and broadening the scope of the platform to include energy systems modelling.

The detailed underpinnings of micro-climate indicators are being investigated across the following areas:

- Bridging the meteo and micro-climate scales.
- Development of both city (roughness & energy balance) and neighborhood (porous media, sources & sinks) models.
- Understanding the importance of buoyancy effects.

Figure 1:
The SECURE concept bridges the building and micro-climate domains, and addresses issues of comfort as well as energy use.
in low wind conditions, including the use of unsteady RANS models instead of full LES models.

- Inclusion of vegetation modelling (drag, evaporation, radiation impact).

This will interact with the wider SECURE project via boundary conditions for surface temperatures/solar radiation, use of spatially-resolved city temperature profiles for climate indicator work, and the use of common typologies between solar metamodelling and urban microclimate modelling.

**WP 2A: Optimization**

Progress with the optimization work package includes:

- A sequential assessment methodology in which an approximate but fast simulator is used in the early stages of the optimization process, then substituted for a detailed but slower simulator for the later stages. To be published at Building Simulation 2015.

- Inclusion of a mixed-integer linear programming (MILP) solver within the Grasshopper environment, to allow urban energy systems design and scheduling problems to be included using the “energy hub” approach. To be published at the Sustainable Built Environment conference in Zurich next year.

- Application to the Empa campus energy hub design, presented at the CISBAT conference.

- Extension of the meta-heuristic optimization methods to a hyper-heuristic approach in which a high-level search (in heuristic space) is performed for the best low-level operators to perform an optimization (in design space). This can be seen as “optimizing the optimizer”, and has great potential for improving optimization performance, especially on repeat runs of similar problems. The process is outlined in figure 3.

There is ongoing collaboration work between this WP and WP 2B on the inclusion of optimization in the design exploration process, which will hopefully lead to a joint paper covering the use of optimization algorithms with metamodelling.

**WP 2B: Decision-support tools**

The main achievement in this work package was the organization of a workshop to evaluate a prototype decision-support tool.

Three workshop sessions were organized to test a design decision-support prototype developed for assessing the solar/energy performance of early-design phase neighborhood variants automatically generated from a set of user-inputs. The workshop included...
ed 2 questionnaires, 2 design phases, and 2 ranking phases. The first session, considered a test-run, was conducted with 4 colleagues (all architects), while each of the following «official» sessions involved 4 professionals (architects/urbanists and one engineer) coming from different architectural offices in Lausanne.

The core of the prototype that was tested is coded and packaged as a Grasshopper plug-in for Rhino¹, with a customized interface for gathering the user-inputs. The tools and languages used are shown in figure 4. The prototype automatically generates 20 design variants, based on the inputs given by the user, and assesses their performance for three criteria.

Participants were first asked to design a neighborhood project using their usual methods and tools. They were then introduced to the prototype tool and asked to explore the solutions it generated based on their inputs, which were meant to recreate something similar to their initial design, and to later submit a revised design. In between the design phases, based on various levels of information and before/after using the tool, participants were asked to rank their own variants as well as 3 given example variants with respect to each performance criterion. Feedback from the participants were gathered through a final questionnaire.

The objectives of the workshop, and the degree to which they were met:

(i) Assess the potential of the proposed workflow as a solar/energy performance-based design decision-support method for the early-design phase of neighborhood projects. Significant information was gathered on this subject; the feedback received during the workshops and the final questionnaire allows to draw positive conclusions on the relevance and potential of the prototype if further developed and improved to overcome the current, mainly technical, obstacles.

(ii) Verify if the workflow can bring new knowledge and help to improve the performance of a design. Due to the technical difficulties encountered, e.g. when trying to recreate Variant A, it is difficult to draw conclusions on the informative and guidance features of the prototype. Results from the ranking phases do not provide convincing evidence. A closer look on the most successful sessions (i.e. from participants that could reproduce their Variant A and learn something from the tool) is necessary to deepen the analysis.

(iii) Identify bugs and improvements in the interface and workflow. This objective was achieved; various bugs were identified and multiple improvements were gathered through feedback from the users.

(iv) Assess the predictive accuracy of the underlying mathematical functions which were developed to obtain a quick estimate of the passive solar and daylight potential (respectively quantified by the energy consumption for heating and cooling and spatial daylight autonomy).

Main achievements / outreach

Work from the project was presented at the International Conference On Computational Science in Porto in June, the PLEA conference in Turin and the CISBAT conference at EPFL in September (2 papers) and the Building Simulation conference in India in December (3 papers).

¹ Grasshopper is an extensible parametric modelling environment for the Rhino 3D modelling program, see www.grasshopper3d.com.
UMEM
Urban Multiscale Energy Modelling
Sustainable Cities and Urban Energy Systems of the Future

Scope of project

There is a worldwide trend towards urbanization. Cities have to improve their sustainability by saving natural resources and energy, in order to mitigate the impact of climate change. Therefore growing cities need to optimize the energy demand of their new and existing buildings. On city quarter scale new energy concepts are needed based on decentralized and renewable energy supply and related sustainable energy conversion, storage, distribution and management.

In this project, building and city energy design and analysis models are developed and linked in a multiscale approach with urban microclimate as well as occupancy and mobility models. Possible designs of existing neighborhoods are analysed leading towards energy self-regulating communities by a decentralized energy adaptation concept, considering also urban heat islands and climatic change scenarios.

Status of project and main scientific results of workgroups

The CCEM project started on October 1, 2012 and was finalized in 2015. It was organized in four closely linked work packages (WP). In the last year of this project additional models for renewable energy systems were developed and integrated into the building energy simulation (BES) model CitySim. Also the occupant activity model was improved in CitySim.

Two case studies were conducted. In the first case study the urban microclimate at the ETH Hönggerberg campus was studied with nested LES (Large Eddy Simulation) simulations. In the second case study building energy demands for two different zones in the city of Geneva were analyzed for two climate scenarios.

WP 1: Microclimate modelling

The work of this WP focused on the development and demonstration of a nested multi-scale method for time-resolved LES simulations. To resolve the detailed flow between urban obstacles (e.g. buildings) and to avoid large computational costs, a multiscale approach is needed. Two computational domains using different spatial and temporal scales are nested together. A large scale model, which resolves only the small flow features. Depending on the range of order of magnitude, several nested models can be used (nesting cascade), each of them dedicated to a specific scale.

A one-way downscale nesting procedure is implemented into OpenFOAM. It allows coupling a small-scale model into a large scale one. The nesting, is achieved by interpolating the three dimensional fields of the large scale CFD (Computational Fluid Dynamics) on the boundaries of the small scale CFD. To achieve a smooth coupling between both CFD models a blending region around the small scale CFD boundary conditions is used. The small
scale CFD has a finer spatial and temporal discretization than the large scale CFD.

The Hönggerberg campus is used to demonstrate the applicability of the nesting procedure to a real test case. The Hönggerberg campus is one of the two sites of ETH Zurich. The campus sits on a shallow pass of the Hönggerberg hill (figure 1, left). The campus itself is a cluster of about 20 heterogeneous buildings as can be seen in figure 1 (right). The flow through the campus is strongly influenced by the hill and the surrounding inhomogeneous roughness elements (forest, crops, city blocks). Therefore a nesting procedure is used. The outer domain is dedicated to computing the atmospheric boundary layer only, the roughness elements being parametrized by a wall-model. The inner domain computes only the flow through the campus, which is discretized by a well-resolved grid. Figure 1 (middle) shows the potential temperature difference on a terrain-following cut-plane at 20 m above the ground. In the central part of the campus, the air is 1.25 K to 1.75 K warmer than the air outside the campus. It denotes a small heat island effect as is usually the case in urbanized areas. The case study showed that the nesting procedure is able to produce high quality results for a fraction of the computational time required by a single domain LES with similar land cover and grid refinement.

WP 2: Urban buildings and energy systems

The first subtask in WP 2 aims at building information modelling (BIM) based building descriptions and the linking of the building energy simulation model design performance viewer (DPV) with the city energy simulation (CES) model CitySim and, based on WP 1, with the urban microclimate model. An automated workflow, illustrated by figure 2, was established that extracts both a BES model and a CES model from the BIM model and co-simulates these with a two-way-coupling of specific variables. Data about local climate conditions is passed from the CES to the BES. The BES then reports back fine-grained energy consumption for specific thermal zones as well as surface temperatures. The BES engine, EnergyPlus, was modified to overcome its long wave radiation calculation with a more detailed calculation performed by the CES engine as part of the co-simulation exchange. An automated workflow was established that extracts a BES model from a CES model using the same co-simulation techniques to provide an enhanced “drill-down” version of the city energy simulation for case studies that cannot easily be modelled in the BIM.

In the second subtask, modelling capabilities of CitySim are further enhanced by integrating simulation models of local renewable energy sources in the software, allowing decentralized energy conversion to be considered within buildings. Models for the following components have been set up, verified and implemented in CitySim:

- Building integrated solar photovoltaic (BIPV) power plant, which was compared to PVSYST simulations, a PV system design software, as well as field data;
- Solar thermal collector, which was compared with field data obtained from SPF (Institut für Solartechnik, Rapperswil), and sophisticated control strategy for coupling with domestic hot water and space heating;
- A ground-connected heat pump model, which was verified using field data obtained from University of Applied Sciences Buchs, as well as a ground model, which was developed to determine the source temperature of the heat pump;
- A wind turbine model, which was compared with field data;
- A solar combsystem (space heating tank and domestic hot water tank) model was developed. Further, the domestic hot water storage tank model was verified using monitored data. The model supports also phase change materials (PCM) for more efficient heat storage.

WP 3: Urban energy and resource flow modelling

The aim of this work package was to develop an occupant activity model for residential buildings and further extend it to non-residential buildings. The following methodology has been developed to implement a simplified occupant model in CitySim:
UMEM
Urban Multiscale Energy Modelling
Sustainable Cities and Urban Energy Systems of the Future

- Occupant presence profiles issued from the SIA 2024 guideline are used where the occupancy rate is based on presence probability;
- A random number is generated to make a binary choice (presence or absence) for each person in the house;
- The activity profile from a French dataset is used;
- A random number is generated to select the activity for the occupant;
- And the activity is associated to a household electrical equipment.

The model was verified using the occupant presence data obtained from monitoring campaigns carried out in the LESO building on the EPFL campus (EIB database). The following four scenarios were considered for the testing (figure 3):
1. Case A: CitySim with occupants and blinds.
2. Case B: CitySim with blind but no occupant.
3. Case C: CitySim with occupants but no blind.
4. Case D: CitySim with no occupants and no blind.

Main achievements / outreach

Multiscale CFD simulations using a one-way downscale LES to LES nesting procedure has successfully been demonstrated for the ETHZ Hönggerberg case study. An automated workflow for two-way-coupled BES/CES was established that extracts both a BES model and a CES model from the BIM model and co-simulates these. All renewable energy system models were successfully validated and implemented in CitySim. A methodology for the occupant model has been developed and implemented.

A case study for the city of Geneva has been conducted, where two city zones have been identified and energy demands have been determined for different climate change scenarios.
Fuels

HYDROGEN
BIO NATURAL GAS
SOLAR POWER

SAUBER FAHREN - ROULER PROPRE - C

shop

3.7m
Syngas Diagnosis
Online Diagnostics for Performance Assessment of Biomass Gasification Processes

Scope of project

The technological objective of this investment project is the development and improvement of a diagnostic toolbox which allows characterisation and monitoring of different process units within biomass gasification related plants, i.e. plants which produce and/or use producer gas from biomass gasification for synthesis of fuels or for electricity production. A specific combination of a sampling system and an analytical instrument is a diagnostic system. A combination of a multitude of sampling systems and analytical instruments measuring several components in a single sample is a diagnostic toolbox. Such flexible online process diagnostics tools applicable for field measurements in industry as well as for research performed by academia are not off-the-shelf technologies.

By measuring the composition of gas streams, liquid effluents and solid streams further optimization of process units and development of technologies are possible. In addition, it allows the validation of physico-chemical models of individual unit operations as well as of whole process chains.

The developed and validated diagnostic systems within this CCEM project can be applied for other thermochemical conversion processes such as pyrolysis, torrefaction or combustion as well as biochemical conversion processes, i.e. anaerobic digestion. The basic knowledge on selecting the appropriate analytical instruments and the corresponding sampling systems is the same.

Status of project and main scientific results

In the framework of this CCEM project method development of sampling systems and analytical instruments is performed. Purchase of complementary analytical instruments and equipment was needed to realize and optimize diagnostic systems according to the requirements of biomass gasification processes.

Sophisticated sampling systems are one of the keys for a robust and sensitive analysis of gas streams.

Considerable progress has been made for the continuous alcohol liquid quench (LQ), which is the back bone of sampling systems at PSI. It is a reliable system that allows simultaneous real-time measurements of condensable in the solvent (water, tars, etc.) and non-condensable compounds in sampled gases (H₂, CO, CO₂, CH₄, C₂H₆, etc.). By adjusting the ratio between sampled gas and quenching liquid flow, condensable components at low concentrations are accumulated in the liquid phase, improving the limit of quantification (LoQ) of the diagnostic tool.

For the characterization of condensable components in the liquid stream, a variety of analytical instruments such as gas chromatography / mass spectrometry (GC/MS), gas chromatography / flame ionization detector (GC/FID) or gas chromatography / sulphur chemiluminescence detector (GC/SCD), inductively coupled plasma optical emission spectrometry (ICP-OES) and inductively coupled plasma mass spectrometry (ICP-MS) are available.

Online density measurements can be used to determine water content in liquid samples. Content of tars in liquid samples can be measured online with ultraviolet-visible spectroscopy (UV-VIS). For simple gas cases UV-VIS is also applicable for online gas phase measurements.

The continuous solvent flow allows taking continuously samples of the liquid stream for offline analysis with a fraction collector system. Measurements of liquid samples can therefore provide time resolved quantitative information about tars, sulphur containing tars and other contaminants in sampled gas. Optional sample post treatments of the liquid samples allow a further increase of the concentration level in the liquid, which improves further the LoQ.

Progress with liquid phase sampling systems

A prototype control/data logging system for temporarily unmanned operation of the LQ sampling system was implemented. The prototype was tested successfully in the framework of a joint cam-

Co-financed by CCEM and swisselectric research

List of abbreviations
CI Condensation Interface
FTIR Fourier Transform Infrared Spectroscopy
GC/FID Gas Chromatography – Flame Ionization Detector
GC/MS Gas Chromatography / Mass Spectrometry
GC/SCD Gas Chromatography / Sulfur Chemiluminescence Detection
ICP-MS Inductively Coupled Plasma Mass Spectrometry
ICP-OES Inductively Coupled Plasma Optical Emission Spectrometry
LQ Liquid quench
LoQ Limit of Quantification
LoD Limit of Detection
RDD Rotating Disk Diluter
SCD Sulfur Chemiluminescence Detection
SMPS Scanning Mobility Particle Sizer
TGA Thermogravimetric Analyzer
UV-VIS Ultraviolet-Visible Spectroscopy

Main Investigator
Serge Biollaz, PSI

Project Partners
PSI

Time frame of Project
2010–2015

Part of SCCER
BIOSWEET (Biomass)
Syngas Diagnosis
Online Diagnostics for Performance Assessment of Biomass Gasification Processes

Figure 1: Semi-automated continuous liquid quench (LQ) sampling system.

The implementation of a gas phase sampling system is motivated by different analytical instruments such as FTIR, gas online measurements with GC/FID, GC/SCD, GC/ICP-MS, ICP-MS, ICP-OES or SID. Therefore there is not one single design for all analytical instruments due to the different sensitivity of analytical instruments and the gas flows needed. Nevertheless experience gained from one application is transferred to the other applications.

For online ICP-MS measurement of gases/aerosols in hot gases two sampling interfaces are successfully coupled to the ICP-MS instrument. The first method is achieved by setting an appropriate arrangement of gas dilution, while in the second one a combination of a condensation interface (CI) and rotating disk diluter (RDD) is used to preserve and dilute the gas and the aerosol generated in the process to be investigated.

The ICP-MS instrument was in operation for online measurement of gaseous metalloid contaminants in the lab at PSI for the first time. Sorption of H₂Se on a ZnO/Al₂O₃ bed was selected as a test case. In this setup, a gas mixture of H₂, H₂O and Ar was used as matrix for H₂Se. Online calibration was performed for different Selenium concentrations and H₂/ H₂O contents which resulted in a LoQ of 1.35 ppbv.

Breakthrough curves of Se sorption were measured for two different Zn concentrations. The Zn loading was of 0.89 wt% and 8.21 wt% respectively. Feed gas concentration of H₂Se was 4.77 ppmv. As can be seen in figure 2, ICP-MS is very sensitive and detects easily very low concentration changes. This allows,
Syngas Diagnosis
Online Diagnostics for Performance Assessment of Biomass Gasification Processes

amongst others, fast screening of sorbent materials.

With the same sampling and analytical approach as for H$_2$Se other critical very volatile compounds such as AsH$_3$ or PH$_3$ should be measurable.

**Progress with ICP-MS and ICP-OES**

Meanwhile the ICP-MS system is routinely used for the elemental analysis of liquid samples which are sampled from gasification processes or obtained by microwave digestion of solid samples such as biomass (e.g. wood) and synthesized materials used in catalytic processes.

Using CI-RDD as a gas sampling system, the ICP-MS is coupled to a thermogravimetric analyzer (TGA) and a scanning mobility particle sizer (SMPS) for the online analysis of gases produced from impregnated wood samples. This setup allows simultaneous particle size and elemental composition measurement. In this study saw dust was impregnated with CuSO$_4$, KCl and/or CuCl$_2$ (as contaminants). The volatile carbonaceous particulate matter, which was generated during wood combustion, was removed by using an evaporating tube. Varying the TGA temperature, elemental intensity of different elements (Cu, K, S, Cl, C) and size distribution were recorded. These three dimension data were then presented in 2D color plots, allowing to correlate the size-resolved SMPS signal to the ICP intensities and to distinguish between gas and particulate species.

A new ICP-OES was purchased in 2015 and will be coupled with the developed CI-RDD online sampling system. For gas diagnostics the two ICP systems, MS and OES, can be seen as complementary analytical instruments regarding different factors (including sample matrix, used gas/aerosol source, and concentration of contaminant) to be measured.

**Progress with FTIR**

In 2015 evaluation of potential suppliers of Fourier transform infrared spectroscopy (FTIR) equipment was consolidated. A FTIR has to be applicable for all relevant syngas such as raw gases from fluidized bed gasification and entrained flow gasification as well as for cleaned gases. The analytical instrument FTIR combined with an appropriate sampling system (i.e. heated dilution system) is a very powerful tool, especially for monitoring biomass gasification processes with a high time resolution (few minutes) and low labour effort.

Compounds of interest are NH$_3$, HCN, HCl, H$_2$O, CO, CO$_2$ and hydrocarbons (C1 through C5 compounds). These compounds are well known for FTIR applications for flue gas analysis/monitoring. In principal compounds such as benzene, thiophene and naphthalene can be measured with FTIR as well. Tests will have to show what the actual detection limits (LoD, LoQ) for these individual compounds are.

A FTIR from the supplier AVL has been in operation at PSI for 6 years for flue gas measurements (SESAM version 4). This device has been cofounded by CCEM. There is an excellent technical/scientific exchange with the FTIR experts from AVL. With the support of AVL this system is adapted for syngas analysis, i.e. to include specific spectres in the data base. There is no mechanical or software modification on the SESAM system required, so it can be used for flue gas measurement and syngas measurement as well. This system is transportable and can be used for measurement campaigns at PSI, but not outside.

For field measurements outside PSI a portable and compact FTIR instrument is needed. Potential suppliers for such a system have been reviewed. The FTIR technology made considerable progress over the last few years. Offers from three suppliers have been requested. The selected supplier for such a compact FTIR is the company GASMET. The compact FTIR of the company GASMET is shown in figure 3.

The sampling system will include eight individual inlet ports, which is not an off-the-shelf system. This allows...
having six sampling ports available at any time which is of particular interest in industrial plants. Two sampling ports are for reference gases in order to monitor drifts of the FTIR equipment.

**International and national exchange of knowledge**

International exchange of knowledge was further intensified by Webinars and a workshop. The fifth analytical workshop took place on June 5th in Vienna just after the 23rd European Biomass Conference & Exhibition (EUBCE). The European network of biomass gasification specialists with a common interest in diagnostic toolboxes includes meanwhile nearly 20 research organizations (universities and national labs).

In order to further strengthen the international exchange of experiences on diagnostic purposes, contacts to biogas experts were intensified. For instance personal contacts have been established to the EMRP project «Metrology for Biogas». This European project aims to develop and validate traceable methods for determining key impurities, moisture, particulates, calorific value, and density in biogas in order to meet the requirements of this quality specification.

In the Metrology for Biogas project considered organic impurities in biogas are siloxanes, sulphur-containing compounds, monocyclic aromatic hydrocarbons, polycyclic aromatic hydrocarbons and halogenated hydrocarbons. The considered inorganic impurities in biogas are ammonia, hydrogen cyanide, hydrogen chloride and carbon monoxide. Except of siloxanes all the considered impurities in biogas are relevant impurities for biomass gasification processes as well. Therefore a fruitful collaboration is expected in the near future.

On the national level the exchange of experience on diagnostic purposes was stimulated via the SCCER BIOSWEET. Experts from gasification, combustion and anaerobic digestion work together in that competence centre and network and develop a common understanding or joint interest in diagnostic skills and needs.

This CCEM project is finally coming to an end. Sampling systems were successfully developed and high end analytical instruments purchased. This equipment, as shown in figure 4, will be used for many different applications. These flexible online process diagnostics tools will be used for field measurements in industry as well as for research facilities.

---

**Figure 4:** Example of a diagnostic toolbox.
ARRMAT – ARRMATplus
Attrition Resistant Fluidized-Bed Materials and Methanation Catalysts

Scope of project

Project «ARRMATplus» deals with manufacturing of attrition resistant catalysts with desired properties for the application in fluidized-bed methanation and with the experimental testing of these materials to identify optimal operation conditions. Very promising support materials with excellent attrition resistance and temperature stability have been developed in the completed CCEM project «ARRMAT» for high temperature applications (700 °C and 900 °C).

A first aim of CCEM project «ARRMATplus» is to further investigate these diatomite and boehmite based porous granulate materials as support for methanation catalysts to be applied within the production of synthetic natural gas (SNG) at temperatures around 300 °C to 400 °C.

A second aim of the project is to consolidate testing procedures for testing mechanical and chemical performance of attrition resistant reactive bed materials and identify suitable performance indicators. These tests are very important to support material development and keep the effort in testing new materials at a reasonable level. For this research activity, natural reference materials such as Al₂O₃, dolomite, pumice, sepiolite or olivine are considered, which cover a wide range of possible applications of attrition resistant reactive bed materials.

Finally the methodical knowledge can be applied to a number of cases, where attrition resistant reactive bed materials are relevant. This is true for natural and synthetic materials, where either catalysis or sorption reactions are of importance. The case of nickel impregnated methanation catalyst is one of the most challenging cases due to the fact that high activity is needed at low temperatures.

Status of project

The process from wood to biomethane includes four major process steps. Wood has to be gasified; the producer gas from the gasifier then needs to be cleaned to remove particles, impurities and potential poisons to the catalyst that is applied in the third step, the methane synthesis (methanation). The raw-SNG from the methanation needs to be up-graded, i.e. water, carbon dioxide and unreacted hydrogen have to be removed to meet the gas quality required for feeding into the natural gas grid.

Catalysts applied in fluidized bed methanation have to fulfil certain requirements to avoid failure of the process step.

- Catalysts must be mechanically stable, i.e. attrition resistant.
- Internal surface area should be sufficiently large to facilitate sufficient nickel loading without danger of sintering or yielding too low dispersion.
- Active nickel must not be separated from the support to avoid selective transport out of the reactor into the filter.
- Depending on the reaction rates and the particle diameters, intra-particle diffusion limitations can have an influence on the activity, but even more on the selectivity.

All these requirements at temperatures around 300 °C to 400 °C are challenging. Targeted materials development therefore also requires appropriate testing procedures, which have been developed to some extent as well. Studying the attrition resistance of nickel catalyst for reactive conditions requires special online or inline particle measurement methods due to the operation conditions and safety issues related with active catalysts.

Main scientific results of workgroups

Assessment of attrition and elutriation

Catalyst attrition has often been a major obstacle in the development of new fluidized-bed processes and is still of concern for existing processes whenever the catalyst is changed. A quantitative prediction of attrition and elutriation effects in a given process requires a detailed understanding of basic attrition and elutriation mechanisms.

In general, the mode of attrition may vary from pure abrasion to total fragmentation of particles.

There is a need to consolidate testing methods for the assessment of attrition performance of bed materials especially for different phase in material development. In figure 1 different methods for

List of abbreviations

BFB Bubbling Fluidized Bed
μBFB Micro Bubbling Fluidized Bed
DFB Dual Fluidized Bed
FICFB Fast Internally Circulating Fluidised Bed
PSD Particle Size Distribution
SNG Synthetic Natural Gas
TRL Technology Readiness Level
WP Work Package

Major partners in the ETH domain

- Empa – Laboratory for High Performance Ceramics (LHPC)
- PSI – Catalysis for Energy Group (CEG)

Main Investigator
Serge Biollaz, PSI

Project Partners
Empa
PSI

Time frame of Project
2009–2015

Thematic Relationship to SCCER
BIOSWEET (Biomass)
ARRMAT – ARRMATplus
Attrition Resistant Fluidised-Bed Materials and Methanation Catalysts

Fuels

Mechanical characterization of bed materials are shown, i.e. ARI tests and tests on a bubbling fluidized bed (BFB) plant. Further methods for analyzing the tested material are applied such as laser diffraction measurement and scanning electron microscopy analysis of the coarse particles. This allows comparing ARI results with the results of the BFB tests focusing on the particle size distribution (PSD).

Further long duration elutriation experiments up to 100 hours were conducted at PSI for different gas flows, using further natural materials like pumice and sepiolite. Pumice has been chosen for being a very lightweight material, due to its low density and high porosity. Results showed unexpectedly high attrition resistance for long hours of fluidization, proving that material hardness is not completely defining the attrition resistance behavior of a material.

All results were successfully implemented in a simple two parameter model already developed for previously tested materials. Good predictions in every case were obtained. The model was also able to predict the behavior of long duration tests by only introducing data corresponding to the first 6 hours of fluidization (see figure 2).

The need of measuring elutriation and nickel emissions downstream a reactive bubbling fluidized bed requires special online or inline measurement methods. An evaluation of different particle measurement technologies has been made in collaboration with experts from the Department of Pretreatment and Gas Cleaning at KIT. Finally, an inline electrostatic particle counter system (PCME) was selected as best measurement system.

Different experiments have been performed, measuring elutriation and particle emissions under atmospheric conditions testing natural bed material. The sensor has been proved to measure particle concentration in raw and clean gas properly. This inline technique performs a constant monitoring of elutriation and emissions, providing high time resolution data and improving our study of attrition behavior as well as the model predictions. Testing this particle measurement system with nickel catalyst is foreseen in follow up experiments in order to ensure proper detection of the particles present under reactive conditions.

Assessment of catalyst activity

In the framework of the European project BRISK, considerable effort was invested to build a new and improved micro fluidized bed (μBFB) methanation system. In figure 3, the lab μBFB-reactor for methanation is shown.

One of the specialities of this test rig is a movable sampling tube, which can be submerged into the BFB. Temperatures and gas compositions can be measured with a very high local resolution. The dried gas composition is measured by micro gas chromatography. This allows to observe changes during the experiment and to determine deactivation phenomena much easier and earlier as this would be the case, if the gas composition is measured only at the exit of the μBFB reactor. The μBFB system is designed in such a way that typical temperatures in fluidized methanation can be investigated, i.e. 250 °C up to 400 °C. The operation pressure is between 1 and 3 bara.

One of the applications of the μBFB is to test activity and selectivity of a specific methanation catalyst for a specific syngas quality (bulk gas composition, impurities). Any attrition resistant catalyst can be tested for a wide range of syngas compositions, in order to find optimal operation conditions, i.e. temperature and steam content. The μBFB unit corresponds in such an operation mode to a technology readiness level 3 (TRL 3)
ARRMAT – ARRMATplus
Attrition Resistant Fluidised-Bed Materials and Methanation Catalysts

Fuels

Table 1: Tested gas mixtures for methanation experiments for ECN gas.

<table>
<thead>
<tr>
<th>Gas mixture</th>
<th>Feed gas composition in mol-%</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>H2</td>
</tr>
<tr>
<td>ECN-Gas, 23.3g/h H2O, 320°C</td>
<td>23.8</td>
</tr>
<tr>
<td>ECN-Gas, 29.5g/h H2O, 320°C</td>
<td>22.6</td>
</tr>
<tr>
<td>ECN-Gas, 29.5g/h H2O, 320°C, 0.3% Benzol</td>
<td>22.0</td>
</tr>
<tr>
<td>ECN-Gas, 29.5g/h H2O, 320°C, 1% Benzol</td>
<td>22.0</td>
</tr>
<tr>
<td>ECN-Gas, 29.5g/h H2O, 340°C, 1% Benzol</td>
<td>21.9</td>
</tr>
<tr>
<td>ECN-Gas, 29.5g/h H2O, 360°C, 1% Benzol</td>
<td>21.9</td>
</tr>
</tbody>
</table>

From historic experiments performed by PSI staff, it was known that benzene should be no problem for the BFB methanation technology. Depending on the operation conditions, C6H6 is either converted to CH4 or C3H8. A conversion to C3H8 is favored as this compound increases the volumetric heating value of the gas and lowers the requirement on the downstream processes, i.e. CO2 and H2 separation.

In order to investigate the influence of benzene on the BFB methanation, benzene concentration was varied between a benzene-free gas and 1 vol% of benzene. First tests were performed at a constant bed inlet temperature of 320 °C. The results indicate that a certain amount of benzene can be easily tolerated for a short time at this temperature.

For higher concentrations such as 1 vol% benzene, the amount of C3H8 measured at the exit of the BFB gasification is increasing very fast. C3H8 is well known as an excellent indicator for the stability of the process. Therefore it is clear that these operation conditions (i.e. 320 °C bed inlet temperature) are not sustainable for the methanation catalyst. By increasing the methanation temperature by 20 °C a stable methanation process was achieved again. These results confirm the robustness of the BFB methanation process.

The amount of CH4 is already high in the syngas produced by dual fluidized bed (DFB) gasification systems. This CH4 is a pyrolysis product of the gasified biomass due to the low gasification temperature. Other compounds such as C2H4, C2H2 and C2H6 are produced as well in the gasification process and correlate with the concentration of CH4. It is well known that olefines typically lead to a deactivation of methanation catalysts operated in fixed bed. This has been reconfirmed in the framework of the ARRATplus project.

In order to get maximum efficiency from feedstock to biomethane, all key processes i.e. gasification, gas cleaning and methanation should be optimized in an intergraded way. An olefine tolerant methanation process allows such an optimization. The new μBFB setup allows to conduct investigations in order to assess the performance of the methanation catalyst or to see if the gas cleaning strategy is promising for a thermo-economic optimized process chain from feedstock to biomethane.

ECN’s MILENA gasifier followed by the OLGA gas cleaning is known as one of the processes with the highest concentration of olefines, benzene, toluene and xylene (BTX) in the syngas. Therefore this system is considered as one of the most challenging systems for the BFB methanation technology developed by PSI. The MILENA system is also one of the most interesting DFB systems due to the potential of pressurization of this DFB gasification system up to 6 bar.

Interestingly, the concentration of CH4 and C2H4 measured at the exit of MILENA/OLGA system meanwhile is similar to the fast internally circulating fluidised bed (FICFB) gasification process, an other well known DFB gasification system. Therefore, most of the experimental knowledge acquired over the last decade at PSI based on the FICFB gasification system can be transferred to the actual MILENA/OLGA system. In table 1 the concentrations investigated for the experiments for the ECN gas are listed.
OPTIWARES

OPTImization of the Use of Wood as a Renewable Energy Source

Scope of project

OPTIWARES is a joint CCES-CCEM project focusing on wood combustion. Wood combustion and other biomass combustion represent renewable energy sources, and means to reduce global CO₂ emissions if the biomass stems from sustainable agriculture and forestry. On the other hand, biomass combustion inherently produces high emissions of particulate matter. These aerosol particles exert a climate forcing and have adverse health effects, affecting population morbidity and mortality. Therefore, the four key objectives of OPTIWARES are:

• to assess the influence of wood burners on air quality;
• to improve the application of energy conversion systems using wood;
• to assess the regional climate effect of wood combustion;
• to calculate the external costs of the various types of wood usages.

The results will be made available to the involved industrial partners, enhancing their competitiveness in the market in Switzerland and worldwide.

Status of project and main scientific results of workgroups

OPTIWARES started on May 1, 2012. Since then, many activities have successfully been started, with a wide variety of results as exemplified in the following.

Results

A major goal of OPTIWARES is to assess the total aerosol concentration emerging from wood combustion, i.e., including both the primary emission (direct emission of particulate matter) as well as the secondary aerosol which is formed through oxidation of volatile (gaseous) organic compounds in the atmosphere followed by condensation of the products to the aerosol phase. It has been shown that the latter often presents the dominant fraction. From this perspective, it is important to know which gas phase compounds have the highest secondary organic aerosol (SOA) formation potential. Although hundreds of organic gases are emitted during wood combustion, SOA is dominated by the aging products of only 22 compounds. In some cases, oxidation products of phenol, naphthalene and benzene alone comprise up to ~80% of the observed SOA.

Since SOA is formed from the oxidation products of volatile organic compounds (VOCs), removal of VOCs from the exhaust can reduce the SOA formation potential from emissions. While primary particulate emissions may be reduced by applying mechanical measures (e.g., electrostatic precipitators, see below), catalytic conversion is required to reduce VOCs and subsequently reduce the SOA formation potential. Therefore, we studied the influence of catalysts coated on cordierite monoliths on primary and secondary wood burning products. We sampled exhaust gas from a log wood stove fueled with dry beech wood into a 3 m³ teflon batch chamber. The well-mixed sample allowed the investigation of the effect of catalyst temperature on the conversion of carbon monoxide (CO) and VOCs in the exhaust, and the associated effect on the SOA, simulated with a potential aerosol mass simulation chamber (PAM).

A speciation of the different VOCs (measured by PTR-ToF-MS) showed temperature dependent conversion and breakthrough of different aromatic hydrocarbons, such as benzene, toluene, styrene and naphthalene. These compounds have adverse health impacts and are important precursors for SOA. They are efficiently removed using a catalytic converter, at realistic exhaust gas temperatures of 200–300 °C. Their reduction also leads to a significant decrease in the SOA potential of the emissions (figure 1 and 2).

We also performed measurements using an emissions conditioning system called NOSMOG (prototype developed by Hexmodul AG, Oekosolve AG and Salermo Engeler GmbH). NOSMOG is a multifunctional flue-gas conditioning system with particle-precipitation properties for biomass combustion in small combustion installations (SCI). The electrostatic precipitator of NOSMOG efficiently reduces the primary emissions to less than 1 mg/m³ at 13 % O₂ independently of the tested appli-
OPTIWARES
OPTImization of the Use of Wood as a Renewable Energy Source

ance, the combustion phase or the quality of the combustion. However, the system also reduces the temperature of the flue-gas down to ~50 °C, affecting partitioning and therefore the emission of SOA precursors. Measurements performed on a logwood stove are shown in figure 2. When the electrostatic precipitator (ESP) was operated at low temperatures, the SOA production potential was decreased significantly, especially during the start-phase of the cycle. At low temperatures (in this case below 70 °C), the raw gas partition is shifted towards the particle phase and, thus, the ESP is capable of removing the substances that would otherwise produce secondary organic aerosol. There was, however, no evident reduction of non-methane hydrocarbons due to the use of NOSMOG (figure 2c). This suggests that NOSMOG removes only a small fraction of low-volatility non-methane hydrocarbons which are however responsible for most of the SOA production. As the system is heated up again (experiment 4 in figure 2a and 2b), the captured low-volatility species will be revolatilized and cause the production of SOA, and a higher concentration of non-methane hydrocarbons is measured after the ESP.

In addition to the removal of SOA precursors, the filter efficiency of the filter in the NOS-
OPTIWARES
OPTImization of the Use of Wood as a Renewable Energy Source

MOG system in terms of mass is also increased. Whereas the mechanism for SOA reduction is quite obvious, the reason for the increase in efficiency is still unclear; this is topic of an ongoing project.

Figure 3 shows a comparison of the useful heat that can be derived from the same input of wood energy (100% in the figure) with different heating systems. The net output (relative to the wood energy input) is the sum of useful heat outputs corrected by the life cycle energy penalty. Outputs above 100% relative to the wood energy input are possible because environmental heat from the ground is added.

- System (a) in figure 3 is a log wood heating with an assumed efficiency of 90%.
- System (b) is a combination of a wood SNG (synthetic natural gas, i.e. essentially methane) plant, a highly efficient (i.e. large, order of 400 MWel) combined cycle (CC) gas plant and heat pumps.

For the ground-based brine-water heat pumps an average SPF (seasonal performance factor) of 3.9 for existing buildings in Switzerland was assumed. Current conversion efficiency of wood to SNG/methane in ecoinvent is assumed at 56%. Data is based on the Güssing SNG plant. For near future systems, a conversion efficiency wood to SNG of 65% with a total efficiency of 90% including use of heat is expected. Conversion efficiencies in the order of about 70% for wood to SNG have been estimated for advanced future systems.

Figure 3: Different options for the use of wood as energy source for heat production. SPF: Seasonal performance factor; LCEP: Life cycle energy penalty. (Source: Heck, 2015).
Scope of project

The RENERG² project is based on the new Swiss energy strategy with a strong development in renewable electricity production resulting in large quantities of excess electricity in summer, depending from the degree of photovoltaics and wind power installations.

The project will show how the excess electricity could be used to substitute fossil energy. The utilization of excess electricity includes the transformation to a chemical energy carrier as hydrogen and methane for example. In this form, the excess energy could be used in the mobility sector.

Status of project and main scientific results of workgroups

**WP 1: Electrolysis**

The goal of WP 1 is to generate new anode catalysts for both PEM water electrolysis and co-electrolysis. In one path, we are focusing on the development of new electrocatalytic systems for the oxygen evolution reaction (OER) with a reduced amount of noble metals (e.g. Ir), a reaction taking place in both water electrolyzers and co-electrolyzers. In addition, in the second path, we are focusing on the development and understanding of efficient catalysts for the electrochemical reduction of CO₂. Both pathways are supported by theoretical modelling using density functional theory (DFT) of the stability and activity of the respective systems.

In the current reporting period, we could achieve the successful synthesis of high surface area IrO₂ following a modified Adams route without the use of chloride containing precursors, as we found out that formation of trace amounts of oxy-chlorides hamper the final OER activity. The resulting catalyst of 150 m²/g specific surface area shows a ca. 100 mV improvement for the OER as compared to commercially available IrO₂ catalysts. Furthermore, we followed a strategy to replace Ir with less noble metals by producing pychlore-type catalysts. In this effort, we could identify Y₂Ir₂O₇ as a compound with similar mass activity than the aforementioned high surface area IrO₂.

**WP 2: Methanation**

In WP 2 the goal of the activities is to increase know-how on CO₂ methanation which converts biogas and pure CO₂, e.g. from industrial sources, as well as on (dynamic) hydrogen addition to methanation of gasification derived producer gas or to a hydrothermal gasification process. The activities cover modelling and (dynamic) pilot scale experiments that can be used for model validation.
The pilot scale setup «Gany-Meth» that shall be used for the experimental part is still under construction; the erection of the setup however is funded by another project. Delivery of the complete setup is still delayed and the reactive runs will start after summer break 2016.

Meanwhile, modelling of the complete process chain for direct methanation of biogas was conducted showing that full conversion can be achieved when either a hydrogen recycle or a small second methanation unit are included in the process. A maximum methane concentration of 88 vol% was found for the typical operating conditions of 420 °C and 28 MPa if pressurized H\textsubscript{2} was added stoichiometrically to the feed containing a water-glycerol mixture.

**WP 3: Combustion fundamentals**

WP 3 is focused on experimental and numerical investigations of the early flame phase of methane and hydrogen enriched methane combustion. Spark induced breakdown spectroscopy within the constant volume combustion chamber at Empa leads to design specifications of an optical spark plug. This spark plug will provide additional information about the early flame propagation for reactive measurements.

A numerical study has identified a suitable way to achieve engine relevant turbulence levels at spark timing in the Rapid Compression Expansion Machine (RCEM) at ETHZ/LAV, enabling the investigation of the turbulence influence on flame propagation. A high-speed particle image velocimetry system has been commissioned and is used for flow field characterizations of the RCEM. A novel flame speed closure has been implemented and investigated towards its predictive capabilities and compared to a commonly used flame speed closure by means of experimental data from the 250 cm\textsuperscript{3} single-cylinder engine for which measurements are planned in WP 4.

A Large Eddy Simulation (LES) study on a canonical engine like setup and comparison with Direct Numerical Simulation data identified the capability of different LES models to capture the cyclic variability of the flow field.

**WP 4: HCNG field testing**

In WP 4 laboratory and field testing of 3 vehicles running on hydrogen-enriched compressed natural gas (HCNG, fuel mixture with 2 vol-% H\textsubscript{2}) were concluded in 2015. Results show that, despite the little hydrogen addition, measurable improvements regarding engine start behavior are observable. The recorded data also show positive trends with respect to engine efficiency and CO\textsubscript{2} emissions.
The ad-interims HCNG dispenser specifically built to refuel these test vehicles was decommissioned in the 3rd quarter of 2015 and was replaced by the permanent HCNG dispenser enabling hydrogen contents from 2 to 30 vol%. The hardware of this dispenser was assembled in 2015 whereas its control will be implemented in 2016. This will allow laboratory and field tests on the newly acquired test vehicle (Iveco Daily) used for measurements with higher hydrogen content up to 25 vol%.

Regarding the investigations on HCNG decentralized power (co)generation, the engine and test bench as well as the measurement concept were prepared in 2015. Various calculations and simulations were conducted to identify resulting deviation caused by using synthetic instead of real exhaust gas recirculation.

**WP 5: Markets and Grids**

In WP 5 the modelling of the financial side is one issue. A collaboration with Ariadne Software AG allows to use their platform, offering the corporate modelling capacities including the integration of the energy part. Financial issues around property plant investments plans, depreciation effects, effects of financing instruments, stochastic sales volumes and prices as well as risk-based cost modeling are included. The possibility to define business scenarios is essential.

Furthermore, a simulation tool was built that allows computing the profitability of the power-to-gas technology. The most important input parameters can be chosen and the simulation will compute the present value of an investment in this technology, based on a given interest rate. These simulations allow quantifying the improvements that are required for this technology to become profitable. Furthermore, it is possible to quantify the monetary subsidies from the government, which are required for a successful power-to-gas project.

In the field of optimal grid integration, the feasibility and applicability of power-to-gas technology in the Swiss electric grid in light of its Energy Strategy 2050 was evaluated. This period was focused on implementing scenarios for integrating renewable energy generation through power-to-gas technology at the Swiss grid level while treating Switzerland as a single node. To this end, three scenarios were established through Matlab models and run on Model Predictive Controller (MPC) with realistic load and generation data.

Future project activities will continue simulations of the power-to-gas integration at the Swiss grid level as multi-node. It is planned to conduct a power-to-gas feasibility study based on previous study results related to the excess energy due to an increased photovoltaics production at a low voltage level.

![Figure 4:](image)

Left: Emissions- and fuel consumption investigations of a delivery vehicle with 2 vol% hydrogen blending on a chassis dynamometer. Right: Engine cranking data with CNG (green line) and HCNG (blue line), showing a bisected duration for HCNG with 2 vol% H₂ blending.
SCHE-dual
Stable and Clean, High-Efficiency Diesel and Dual-Fuel Combustion

Scope of project

The project is aiming at the further development of both diesel and dual-Fuel engines towards higher efficiency and lower emissions. This requires a better understanding of the fundamental in-cylinder phenomena at the more challenging future conditions during fuel injection and combustion. In order to achieve this goal, this project builds upon, extends and further strengthens the well-established framework among the Combustion Research Laboratory at the Paul Scherrer Institute (PSI-CRL) and the Laboratory of Aerothermochemistry and Combustion Systems at ETH Zurich (ETH/LAV), combining their expertise on spray, ignition and combustion behavior both for smaller (passenger car) and larger (heavy-duty, marine) engine configurations. The activities within SCHE-Dual are targeted at filling the gap between these extremes and to further extend the range of application and consequently enhance the competences of both participating institutions.

Status of project and main scientific results of workgroups

WP 1: Task 1

In the context of WP 1 task 1 a complete methodology for quantitative two dimensional detection of fuel vapor concentration in a diesel spray has been developed. The methodology is based on the two-color PLIF of the TMPD tracer substance, with liquid phase detection via the Mie scattering. A red-shift of the TMPD fluorescence spectrum with rising temperature has been used to extend the tracer PLIF method to the two color approach, where a two dimensional temperature field of the fuel vapor is measured based on the ratio of fluorescence signal in two wavelength bands. Based on the known fluorescent yield at each temperature, a two dimensional fuel concentration is calculated.

We have achieved a proof-of-concept of the methodology by application of the method to measure fuel concentration and temperature in a surrogate diesel spray in the HTDZ (figure 1) under diesel engine relevant conditions. The precision of thermometry is in the range of 20–40 K. Good fluorescent yield of the employed tracer will enable time resolved measurements of fuel concentration in a diesel and micro-pilot fuel spray using a high speed laser system.

Furthermore, LII in combination with the two dimensional DBI technique was applied for quantitative measurements of soot concentration in the HTDZ. This methodology proved to yield quantitative results for moderate soot concentration. The methodology is sufficient to study soot formation in the dual-fuel operation as well as under moderately sooting diesel operating conditions.

WP 1: Task 2

Proof of feasibility of OH PLIF and CH\textsubscript{2}O PLIF for detection of high temperature ignition and low temperature flames, respectively, has been accomplished. The aim of the investigations was to study the limits of applicability of both methods regarding the required laser energy and permissible pressure level. Positive results can be reported regarding the applicability limit of the OH and CH\textsubscript{2}O PLIF under engine relevant conditions. Environmental conditions up to 60 bar and 900 K have been probed.
WP 2: Task 1

In the context of WP 2 task 1, a priori studies with LES at non-reactive conditions have been conducted in 2013, whereas a detailed analysis on averaging methodologies for LES has been carried out in 2014. Here, the developed methodology has been partially adopted to strongly reduce computational effort allowing for detailed investigation of combustion and soot dynamics in diesel sprays.

Formation of soot in an auto-igniting n-dodecane spray under diesel engine relevant conditions has been investigated by means of LES and RANS turbulence treatment, using the WM approach for combustion. Since the WM model is readily suitable for combustion involving two fuels this model is studied here while developments are ongoing in parallel to further develop an in-house CMC combustion model for dual-fuel capabilities.

Analysis of the intermittent soot dynamics revealed that the enhanced flow structures captured by the LES model affect the distribution and magnitude of soot mass fraction by shaping the chemical and advective terms, which were found to be the most prominent ones. The chemical term was linked to the flow field both on the side of soot formation and soot oxidation. It was shown that the LES model predicts an inherently unsteady evolution of soot distribution, because the advective term and the chemical term do not balance each other, as is the case in RANS.

Overall the simulation results are in good agreement with experiment and the WM model appears to adequately reproduce the combustion process during the quasi-steady combustion phase. This reference modelling approach will serve as an interesting benchmark for the CMC combustion model for which developments are currently underway.

WP 2: Task 2

The modification and preparation of the HTDZ test rig and all involved parts is the first priority of this task in order to be able to produce then a detailed experimental database for purposes of model validation and for deeper understanding of combustion processes occurring at different fuels.

In that view, single axial-hole injector nozzles have been initially employed. After the characterization of the injector behavior by a Bosch tube injector rate analyzer, it was found that there is a strong influence of caviation effects on the injectors.

Since the already employed injectors are not suitable for comparison with the current state of the art injectors used in automotive applications, new conical single-hole injectors were fabricated. The new improved injectors bare conical nozzle holes including hydro-erosive grinding of the hole inlets and were manufactured in four different hole diameters: 0.090, 0.120, 0.180 and 0.240 mm. Multiple copies of each diameter were prepared in view of performing parallel tests in the two nominally identical facilities at the ETH/ LAV and PSI. The characterization of the injectors showed that the new injectors are operating properly and are free from cavitation effects (figure 3), while the injected mass can be tuned easily by adjusting either the energizing time or the injection pressure.

In the next steps, optical measurements will be performed in both facilities in order to gather information about the spray penetration and liquid length (Mie scattering imaging) and about vapor phase penetration and ignition delay (double-pass Schlieren imaging, OH* chemiluminescence imaging).
PAWaSto

Photovoltaic Assisted Algae Production and Waste Water Treatment for Combined Heat and Power Generation and Storage

Scope of project

This project aims to the study of photovoltaic (PV) assisted microalga generation and their non-catalytic hydrothermal gasification for heat and power generation and storage. However, the option to produce methane using a catalytic hydrothermal process, like in the SunChem process, remains an interesting option (see CCEM project SunChem). The PAWaSto project focuses on a new concept of efficient hybrid electricity-biomass production system for the production of microalga, and at the same time converting the non-used part of photons to produce additional electricity via the semi-transparent PV cell. The produced electricity will reduce the energy need for maintaining the microalga culture. High value compounds can be extracted from the produced biomass. In the frame of this project we will evaluate the potential of treating the remaining algal residues together with wastewaster effluents for energy and nutrients recovery purposes. Additionally, detailed mathematical models of the hybrid PV-microalga reactor, and non-catalytic hydrothermal gasification of microalgae will be investigated.

Status of project

The activities in the frame of the PAWaSto project started in 2015. The mathematical models for microalga growth in open pond and horizontal flat panel were validated and detailed studies were made on mass and energy balances. In addition, synthetic natural gas production from microalgae through hydrothermal gasification was optimized. In the middle of 2015, EPFL-GMF group joined the team and mainly worked on the PV part. Together with PSI-CPM a PV-microalga bioreactor system was designed and built. Several alga species were selected and tested and a significant improvement of algae growth was observed.

«Scientastic», EPFL's new science festival, focused on the theme of energy. PSI-CPM was invited to present the algae related activities (figure 1). The event was held on November 21 and attracted more than 6000 visitors. Major activities performed and results obtained in the work packages (WP 1, WP 3, and WP 3) of the project PAWaSto are described in the following sections.

Main scientific results of workgroups

Photovoltaic-algae engineering and optimization

WP 1 deals with building the mathematical models for a hybrid PV-microalga bioreactor, and the non-catalytic hydrothermal gasification of microalgae for the production of heat and power. Partner is mainly EPFL-IPESE.

Based on the earlier theoretical study on algal biomass production, using vertical photo bioreactors, the IPESE group has assembled and validated dynamic models for microalga growth in open ponds and horizontal flat panels in 2015. In these models the effect of light, temperature, mixing, pH value, nutrients, and CO₂ on the growth of microalgae has been considered (figure 2). Further, detailed studies on mass and energy balances have been completed for microalga growth models in open ponds and horizontal flat panels.

Recently, synthetic natural gas (SNG) production from microalgae through hydrothermal gasification was also studied for multiple objectives. SNG from hydrothermal gasification can be exported to the grid after the separation of water (using absorption tower) and CO₂ (using membranes). Alternatively, partially purified SNG (i.e., only water separation) can be used in solid oxide fuel cells with a gas turbine (SOFC- GT) for electricity production. Currently, the performance of the SOFC-GT is optimized, assuming typical SNG composition, for the electrical efficiency and total annualized cost of the system, simultaneously.

In 2016, the existing model for microalga growth in a flat horizontal panel will be adapted for microalga growth in a flat vertical panel with photovoltaic surface (PV-algae), using experimental data. Then, this PV-algae model will be validated using experimental data from WP 2 and WP 3. In addition, a renewable energy production process, using PV-algae, hydrothermal gasification and SOFC-GT, will be designed, analyzed and optimized. Finally, the effect of uncertain market parameters on
the performance of a complete energy conversion system will also be explored.

**Photovoltaic-algae lab-scale tests**

WP 2 deals with the experimental setup of the lab-scale tested PV-algae bioreactor system. Partners in the ETH domain are PSI-CPM, EPFL-GMF, and EPFL-IPESE. The main aim is to design a semi-translucent PV-algae bioreactor setup, which will be used to test algae growth using waste water. The PV will be used for additional electricity generation as well as a light filter for assisting algae growth. These two methods of energy production use different absorption wavelengths from the same energy resource (sunlight) allowing the production of an additional energy output.

The photovoltaic-algae bioreactor system was designed as shown in figure 3. The dye-sensitized solar cell (DSC) was...
Fuels

PAWaSto
Photovoltaic Assisted Algae Production and Waste Water Treatment for Combined Heat and Power Generation and Storage

The effect of DSCs in the growth of C. Vulgaris

Figure 4: Cell concentration of Ch. vulgaris (green micro-algae) growth under different DSCs panels.

Figure 5: Microalgae bioreactor equipped with a 770 cm² DSC panel. Experiments performed in collaboration with the group of F. Fischer at HES-SO Valais-Wallis (Sion, Switzerland).

chosen as the photovoltaic filter considering about the inexpensive fabrication costs, good performance, stability, and transparency. By choosing different sensitizers, the absorption region and the color of the DSC panels can be easily adjusted. According to the photons needed by different kinds of algae, the DSC panels with corresponding color and transparency can be prepared.

In 2015, DSC panels with the color of orange, red, and green (with the size of 144 cm² and 770 cm²) have already been prepared and used together with the algae bioreactor.

Three different algae species were tested in our PV-bioreactor system together with the red, orange and green DSC panels (144 cm²) under a solar simulator as light source. It was quite promising that in the presence of the red DSC panel, which exhibited a power conversion efficiency of 3.1 %, a significant improvement of the growth rate for the green microalgae Ch. vulgaris was observed (figure 4). The results show that by carefully matching the properties of the PV and the algae, the DSC panel can be used as a PV filter to enhance the growth of algae, indicating that our idea to combine the electricity and biomass production works.

Additional experiments with non-synthetic human urine are planned for a comparative study.

In a hydrothermal treatment the inorganic fraction can potentially be separated and concentrated in the salt brine after the conversion process. Therefore, nutrients can be reused in the algae culture or alternatively a fertilizer suitable for the application in agriculture applications could be produced.

Algae choice and waste water treatment using PV-algae systems

WP 3 focusses on options to create added values related to energy use of microalgae. One way is to use wastewater as nutrient supply with the designed PV-algae system developed in WP 2. It is planned to further evaluate the potential of using waste waters such as urine from a housing district. Using a hydrothermal gasification process, even black waters could be used for energy recovery from wastes as well as nutrient source for algae production. Partner is mainly PSI-CPM.

In 2015 a preliminary microalgae cultivation study was performed with four microalgae strains, i.e. Ch. vulgaris, Ch. sorokiniana, Ph. tricornutum, H. pluvialis using 10 times diluted synthetic urine. Except for Ph. tricornutum, all the others species were able to acclimate with their medium. Additional experiments with non-synthetic human urine are planned for a comparative study.

At the end of 2015, a bigger setup was tested at HES-SO in Sion using the DSC panels with the area of 770 cm² together with a «Labfors 5 Lux» reactor equipped with cool white LED as lighting source (figure 5). The experiments are still in progress.
Solar Fuels

Solar Thermochemical Production of Fuels from CO₂ and H₂O Using Ceria Redox Reactions

Scope of project

This project is aimed at developing the science and technology required to efficiently produce liquid hydrocarbon fuels from H₂O, CO₂, and solar energy. A 2-step H₂O/CO₂-splitting thermochemical cycle is investigated based on non-stoichiometric ceria redox reactions. The first step involves the high-temperature reduction of ceria (T > 1673 K) driven by concentrated solar energy. In a second lower temperature step the reduced ceria is oxidized with H₂O and CO₂ to produce H₂ and CO, a mixture known as syngas, which is a precursor to diesel, kerosene, and other liquid hydrocarbon fuels. The optimization of the ceria-based materials and structures for improved radiation heat absorption, chemical kinetics and thermodynamic potential (i.e. doping) is an essential endeavour for reaching high solar-to-fuel energy conversion efficiencies.

Status of project and main scientific results of workgroups

The project encompasses 3 work packages:
- ceria synthesis and structural development;
- ceria doping and mixed oxides;
- transport phenomena, pore level engineering, kinetics.

Porous ceramics

Reticulated porous ceramic (RPC) foam-type structures have been developed featuring dual-scale porosity: mm-size pores for volumetric radiation absorption during reduction and μm-size pores within its struts for enhanced mass transfer and kinetic rates during oxidation. We investigated the quantity of interconnected pores produced with 50 vol-% carbon pore forming agent, remaining in undoped and doped ceria ceramics after sintering for 5 h at 1600 °C. In undoped ceria 40.5 vol-% porosity (interconnected pores) remains after sintering, as presented in figure 1. With increasing doping concentrations of ZrO₂, HfO₂ or Pr₂O₃ into the CeO₂ structure, pore sizes are decreasing, pores are eventually isolated, and the interconnected porosity of the infiltrated ceramic was reduced. Doping with TiO₂ leads to complete pore isolation. The only ceramic effectively retaining interconnected porosity is Li-Hf co-doped ceria. While undoped Hf₀.₃Ce₀.₇O₂ has a porosity of 34 vol-%, Li-doped Hf₀.₇Ce₀.₃O₂ exhibits a porosity of 41, 39, and 43 vol-% for 2-, 6- and 10 mol-% Li co-doping respectively. The isolation of pores is a consequence of grain coarsening at high temperatures which, in the case of porous ceria ceramics, is driven by grain boundary diffusion mainly. Dopants such as Zr⁴⁺, Hf⁴⁺, Ti⁴⁺ and Pr³⁺/⁴⁺ increase diffusion rates across the grain boundary, while Li⁺ inhibits diffusion processes. Concerning the latter we propose that a glassy Li-Ce-O layer is formed along the grain boundaries in which the bulk (ceria) has a low solubility, thus preventing mass transfer, which also has been suggested in other studies.

Structural analysis

Using a specially designed high temperature cell, in situ X-ray absorption experiments were carried out at the Swiss-Norwegian Beamline BM01B at the ESRF in Grenoble, France. In situ X-ray absorption spectroscopy (XAS) measurements at the Ce, Zr and Hf K edges were carried out in transmission mode under relevant conditions present in a solar reactor. Samples were exposed to temperatures up to 1773 K in a flow of argon for reduction and a flow of carbon dioxide for oxidation. The shift of the Ce K edge position allows the determination of the non-stoichiometry of ceria. Spectral changes that indicated structural differences pointing to reduction and oxidation could be observed at both Ce and Zr absorption edges under different conditions.

Figure 2 shows results of a typical in situ XAS experiment under thermochemical looping conditions. A Ce₀.₃Zr₀.₇O₂.₈ sample was heated from 1073 K to 1773 K in a flow of argon and subsequently, isothermal switches between a flow of argon and carbon dioxide were performed. The background colors indicate the feed gas composition: white indicates argon and blue carbon dioxide, respectively. The top panel in the figure shows...
the temperature in the reactor and the mass spectrometer signal of oxygen in the product gas. The bottom panel shows the non-stoichiometry \( \delta \), which was determined from time-resolved absorption measurements at the Ce K edge. The non-stoichiometry \( \delta \) is proportional to the shift in the energy of the Ce K absorption edge. Upon heating in argon, the mass spectrometer (MS) signal indicated the release of oxygen from the sample. Concomitantly, the position of the Ce K edge shifted to lower photon energies, providing quantitative information on the changes in the electronic structure of cerium.

**Thermodynamics & kinetics**

The thermodynamic characterization and critical evaluation was carried out for \( \text{Zr}^{4+} \) doped ceria. As a case study, we experimentally examined 5 mole-% \( \text{Zr}^{4+} \) doped ceria and presented oxygen nonstoichiometry measurements at elevated temperatures ranging from 1573 K to 1773 K and oxygen partial pressures ranging from \( 4.50 \times 10^{-4} \) atm to \( 2.3 \times 10^{-4} \) atm, yielding higher reduction extents compared to those of pure ceria under all conditions investigated, especially at the lower temperature range and at higher \( p_{O_2} \). Thermodynamic properties were determined, namely: partial molar enthalpy, entropy, and Gibbs free energy, shown in figure 3. Although reduction extents increase greatly with dopant concentration, the oxidation of \( \text{Zr}^{4+} \) doped ceria is thermodynamically less favorable compared to pure ceria. This leads to substantially larger temperature swings between reduction and oxidation steps, ultimately resulting in lower theoretical solar energy conversion efficiencies compared to ceria under most conditions. In effect, these results point to the importance of considering oxidation thermodynamics in addition to reduction when screening potential redox materials.

The thermochemical redox performance and analytical characterization was carried out for \( \text{Hf}, \text{Zr} \) and Sc doped ceria solutions, all of which are promising redox materials for the two-step solar thermochemical splitting of \( \text{H}_2\text{O} \) and \( \text{CO}_2 \) to \( \text{H}_2 \) and \( \text{CO} \). Dopant concentrations ranging from 5–15 mol-% have been investigated and thermally cycled at reduction temperatures of 1773 K and oxidation temperatures ranging from 873 K to 1073 K by thermogravimetry. Results are shown in figure 4. The degree of reduction of \( \text{Hf} \) and \( \text{Zr} \) doped materials was substantially higher than those of pure ceria and Sc doped ceria, and increases with dopant concentration. However, it may still result in lower overall solar-to-fuel efficiencies because of the high concentrations of the oxidizing gas needed to drive the oxidation reaction and because of the energy penalty associated with the temperature swing between reduction and oxidation steps.

**Figure 2:** Top: Experimental conditions of isothermal thermochemical looping – temperature, mass spectrometer signal of oxygen (m/z = 32) and reduced gas (white = argon, blue = carbon dioxide). Bottom: Shift in the Ce K edge energy and corresponding non-stoichiometry of a \( \text{Ce}_0.5\text{Zr}_{0.5}\text{O}_2 \) compound. Filled circles: sample, hollow circles: aligned reference (\( \text{CeO}_2 \)).

**Figure 3:** Left: Gibbs free energy change versus temperature for the reduction of \( \text{CeO}_2 \) (black), \( \text{CZO}_2 \) (blue) and \( \text{CZO}_2 \) (red) from \( \delta_{\text{ox}} = 0 \) to \( \delta_{\text{ox}} = 0.1 \) (solid lines) and \( \delta_{\text{ox}} = 0 \) to \( \delta_{\text{ox}} = 0.05 \) (dashed lines). Right: Gibbs free energy change versus temperature for the oxidation of \( \text{CeO}_2 \) (black), \( \text{CZO}_2 \) (blue), and \( \text{CZO}_2 \) (red) with \( \text{H}_2\text{O} \) from \( \delta_{\text{red}} = 0.1 \) to \( \delta_{\text{red}} = 0 \) (solid lines) and \( \delta_{\text{red}} = 0.05 \) to \( \delta_{\text{red}} = 0 \) (dashed lines).

**Figure 4:** (a) The initial redox cycle for 10 mol-% dopant (Sc, \( \text{Hf}, \text{Zr} \) compositions and pure ceria reduced at 1773 K (\( p_{O_2} = 10^{-4} \) atm) and oxidized at 1073 K (\( p_{O_2} = 0.4 \) atm). b) Subsequent cycles oxidized at 973 K and 873 K (\( p_{O_2} = 0.4 \) atm) and reduced at 1773 K (\( p_{O_2} = 10^{-4} \) atm).
SOLAR-HTG
Solar Assisted Hydrothermal Gasification Process

Scope of project

The goal of the project is to develop a solar assisted hydrothermal gasification (HTG) process that converts wet biomass into methane with the help of solar heat. Wet biomass represents a very important part of the biomass resources sustainably available in the world (e.g. sewage sludge, wastewater of biofuel production, manure etc.). Hydrothermal gasification is a relatively new technology that is able to convert wet biomass in supercritical water into gas, clean water and salts. This technology is suited for the energetic valorization of wet biomass and also for recovering the salts contained in the biomass which can then be used again as fertilizer.

Status of project

In the previous project phases modelling and optimization of a solar-hydrothermal gasification process system were performed, analysis on size of the solar thermal utility with respect to heat transfer fluid and operating temperatures was investigated at EPFL. In this last year the scope has been moved to the development of a methodology that not only allows for process targeting or conceptual design, but allows to determine a plant configuration by means of heat exchanger networks.

The ETH-PSI group aims at the development of a solar assisted high-temperature salt separator. A combined numerical and experimental approach is adopted to identify operating conditions and salt separator configurations that lead to an efficient salt separation. Based on these findings, an improved solar-heated salt separator will be designed.

Main scientific results of workgroups

LENI-EPFL: Status

The EPFL group focused on research in the field of catalytic hydrothermal gasification at process superstructure level. It developed mathematical methods for the synthesis of heat exchanger networks (HEN) including thermal storage utilities.

Concerning design methods, two publications have been developed. The first one concerns the simultaneous plant design framework which includes the HEN design. The second one covers the extension of the framework in order to account for thermal storage utilities. Additionally, a publication regarding the application of the developed framework to the solar assisted gasification plant will be included in the final project report.

LENI/EPFL: Results

The design and optimization of heat exchanger networks including thermal storage options has been addressed. The Framework description is graphically reported in figure 1.

First, the set of utilities (solar thermal plants, storage options, heat transfer fluid options) needs to be specified as inputs. Successively the problem is decoupled in a bi-level framework, where the «Particle Generating Set – Complex» method proposed in Martelli and Amaldi (2014) is coupled.
with the three-steps sequential framework for utility integration and HEN design (Mian et al. 2015a). The validity of the method has been tested considering a literature example and showing that the energy efficiency can be highly improved, as well as the related operational expenditure (OPEX) and capital expenditure (CAPEX) (Mian et al. 2015b).

The application of the framework to the solar assisted HTG would require to take into account multiple objectives and generate multiple solutions. For this reasons the framework has been modified by coupling the upper level Multi Objective Optimization tool developed at the IPESE laboratory of EPFL with the lower level three-steps sequential framework. A representation of the framework proposed as alternative to the one reported in figure 1 is depicted in figure 2.

**ETH-PSI: Status**

The research at PSI focussed on the development of design tools to understand the effect of different salt separator configurations on salt separation, and to ultimately predict the performance of a particular separator design. Computational fluid dynamics (CFD) simulations and experiments have been combined in order to achieve this goal.

On the experimental side, a lab-scale setup has been built using a dip-tube salt separator. This separator is a vertically aligned pressure vessel; salt solution is fed from the top through a dip-tube. Separated salts are ideally removed at the bottom as concentrated salt brine while the salt-free stream exits at the top of the vessel. The vessel is heated through the outer wall via several electrical cylinder heating bands. The electrical power input to each of these heating elements can be adjusted individually, and it is thus possible to investigate the influence of different axial temperature profiles in the salt separator.

Deposition of salts can be detected by measuring the temperature at the outer wall of the salt separator: Deposited salts introduce an additional heat transfer resistance at the inner wall of the separator vessel, locally inducing a rise in temperature of the outer wall. Therefore, the temporal change of the outer wall temperatures serves as an indicator for the salt deposition. The experimentally observed salt depositions were compared to the temperature and flow field of pure water in the salt separator computed using CFD. From this comparison, we attempt to identify temperature and flow patterns that correlate to the location of the experimentally observed salt deposition.

**ETH-PSI: Results**

To validate the salt deposition detection method, salt depositions in the separator have been visualized using an endoscopic camera. Comparing the location of major salt depositions based on deposition detection and visual inspection, it can be concluded that the presented method is a cost-effective and simple way for detecting salt deposition in the separator. Comparing experimentally observed salt deposition to the simulated temperature and flow field of pure water in the salt separator, results as shown in figure 3 suggest that both temperature and flow field determine the location of the salt plug. The salt deposition is located within the zone where the temperature of the fluid exceeds the saturation temperature of the fed salt solution. However, the salt plug is situated at the bottom end of this zone; it coincides with the location of the recirculation zone of the flow field. This agreement suggests that the formed salt particles separate from the flow as the flow decelerates and reverses its direction. The particles do not follow the upwards curvature of the flow field but keep moving in radial direction until they impact on the inner wall of the salt separator pressure vessel.

**SOLAR-HTG**

**Solar Assisted Hydrothermal Gasification Process**
Hy-Form

Formic Acid – Chemical Storage of Electrical Energy and On-Site Hydrogen Production for Use in PEM Fuel Cells

Scope of project

The purpose of this research project is to develop a medium scale reactor for on-demand hydrogen generation from formic acid (FA) for use in a downstream fuel cell. In order to realize an efficiently functioning reactor and fuel cell couple, three independent but interrelated research areas are involved. The first concerns the design, prototyping and testing of a suitable reactor, which is carried out at EPFL. A second, concurrent task at ZHAW involves computer modelling of precise flow dynamics, heat transfer mechanisms and effects of particle size. The third arm of the project, based at PSI, studies the compatibility of the reactor gas outflow with single- and multi-cell PEM (proton exchange membrane) fuel cells.

Status of project

WP1 – Reactor design and prototyping:
Still ongoing but progress has been made in 2015.

WP2 – Computer modelling:
The experimental validation of the mathematical model of the reactor is delayed due to lack of stable reactor measurements. Unexpected reactor behavior was described with model extensions (azeotrope and catalyst floating). Reactor designs were suggested based on unvalidated model.

WP3 – Compatibility studies:
Basic hookup tests were performed using an alternative reactor supplied by EPFL. There were some fuel cell performance issues with CO, but they can be alleviated by changing the fuel cell type or adding additional components which preferentially remove this impurity.

Main scientific results of workgroups

WP 1: Reactor design and prototyping

As discussed in the previous report, at the end of 2014 the team at EPFL realized that the reactor wall was being compromised by hot formic acid. It was sought to rectify this issue by electropolishing and gold-plating the internal surfaces of the concentric-tube reactor. Reactor installation was completed with external heating by an oil circulator in the outer chamber, and gas workup was carried out with a heat exchanger and magnesium oxide trap for formic acid vapors. Maximum production of ca. 640 mL per minute was attained using 5 mL catalyst at a reactor temperature of 126.7 °C.

Some abbreviated points of learning:
- It has been discovered that using 99% pure formic acid as feed will always tend towards an azeotropic mixture containing approximately 40 mol% water.
- Small imperfections in the gold plating are sufficient for acid to penetrate through to the main wall.
- Formate is necessary to stabilise the polymer-bound ruthenium catalyst.

The next generation of reactor was designed and built (figure 1). It consists of a 400 mm pressure resistant glass tube with internal surfaces made from acid resistant Inconel. Heating is performed by circulating oil through a set of tubes placed inside. When the reactor was charged with catalyst and formic acid, a strange flotation effect has been encountered. At low temperatures the solid material settled to the bottom of the reactor as its density is greater than that of the liquid phase. However during gas production at elevated temperatures the solid began to float to the top of the reactor. After some time, gas production essentially ceased due to this phase separation. The phenomenon seems to originate from a combination of the heating regime and the reluctance of gas to desorb from...
the polystyrene surface. Interestingly this effect was not observed in our previous reactor nor in standard equipment such as glass tubes heated from the outside.

The strategies to overcome the maldistribution are:
- to increase the non-heated interior volume in an effort to promote better convection (by using a larger glass tube);
- to add a surfactant that is stable towards hot acidic media and hydrogen that still allows formic acid to interact with the catalyst;
- to prepare different structuring/size of catalyst particles to increase their density.
- to find a suitable recirculation pump to enforce proper distribution of the catalyst in the liquid phase.

**WP 2: Computer modelling**

The model theory from the previous reporting year (before the experimental results were available) was published in January. During 2015 ZHAW-ICP continued systematic extension of this multi-phase model of the reactor based on the experimental testing of the reactor by Granit SA and EPFL. The effect of the water content within the formic acid solution entering the reactor has been implemented. The mixture of water and formic acid forms an azeotrope (constant boiling) mixture, which does not change its proportion by distillation (evaporation). After some time the liquid mixture within the reactor adopts the proportion of the azeotrope, but on the input/output the proportions remain unchanged. The effect of azeotropic liquid mixtures has been implemented in both theory and simulations.

After the experimental tests on the 30 cm high reactor with inner heating experiencing flotation of the catalyst particles on its top (described in detail in WP 1), ZHAW-ICP implemented this phenomena by additional equations for the solid catalyst distribution. In order to obtain similar floating behavior of the simulated and experimental catalyst distribution, the effective density of the catalyst particle has been extracted as 1000 ± 50 kg/m³. It was jointly agreed with EPFL and Granit SA that currently the flotation effect is a consequence of an artificial lift-up by gas bubbles sticking to the surface of catalytic particles. Simulation of the floating of the catalyst and temperature map is shown in figure 2 (in 40 mm high reactor with outer heating). The floating of the catalyst is less pronounced for this low profile (height) reactor, reaching a maximum catalyst concentration of 28 %, as compared to a 300 mm profile reactor where 45% catalyst concentration was reached on the top of the reactor (not shown).

Having the full model containing the effect of azeotrope and catalyst floating, different reactor designs are investigated in order to obtain the best possible performance. Two low profile reactor designs with different heating positions are proposed and their performance as well as their advantages and disadvantages examined. Simulation predictions currently need to be taken with precaution, the model is undergoing experimental validation.

**WP 3: Compatibility studies**

The task of the PSI in the framework of the HyForm project is to demonstrate the operation of a fuel cell with the reformate obtained from the fuel processor located upstream. Considering that the current reactor so far cannot supply the required flow rates, an existing installation is used based on a similar homogeneous ruthenium catalyst. Operating temperatures are 80–100 °C and flow rates of up to 30 L/min at 8 bar pressure are possible.

The formic acid reformer was moved to PSI and operated next to the fuel cell test bench. The fuel gas stream (with nominal composition of 50 % H₂ and 50 % CO₂) fed to the fuel cell was adjusted in the range up to 5 L/min, according to the required amount given by the current and number of cells.

Two types of polymer electrolyte fuel cells (PEFC) were linked to the reformer. The low-temperature (LT) PEFC is based on a sulfonic acid iono-
Hy-Form
Formic Acid – Chemical Storage of Electrical Energy and On-Site Hydrogen Production for Use in PEM Fuel Cells

A polymer membrane that operates at around 80 °C. Here, a 6 cell stack with active area of 58 cm² was used, which has a nominal power output of 250 W using pure H₂ as fuel. The anode flow field had previously been adapted to the use of the (50/50) H₂/CO₂ fuel by adjusting the flow channel geometry.

The polarization curves shown in figure 3a indicate that with the reformate from the formic acid fuel processor a substantial loss in performance is observed at low current density. The behavior of the cell strongly indicates the presence of CO in the fuel gas, which could be proved to be around 50 ppm. The polarization curve with synthetic reformate containing 50% CO₂ shows that in the absence of CO performance should be close to that obtained with pure H₂, with somewhat more pronounced losses at high current density, owing to increased mass transport resistance. At the typical operating temperature of a LT-PEFC of around 80 °C, the CO tolerance of the pure Pt catalyst used on the anode side is only around 10 ppm. Even though this reactor is not the actual one designed for this project, one should be aware that CO production is possible, and that steps to mitigate its effect must be considered.

To alleviate the effect of CO-poisoning, additional experiments were carried out in the HT-PEFC, which operates at a temperature of around 160 °C (figure 3b). Under these conditions, the performance of the cell operated on the reformate was equivalent to the performance of the cell operated on diluted H₂. This demonstrates the superior CO tolerance of the HT-PEFC. There are, however, a few shortcomings of the HT-PEFC. Firstly, it takes more time for start-up and shutdown from/to ambient conditions due to the higher operating temperature. Secondly, since the electrolyte is based on a polymer doped with phosphoric acid, condensation of liquid water in the cell is to be avoided to prevent leaching out of the phosphoric acid. Furthermore, the overall noble metal loading is higher in the HT-PEFC, and also the power density obtained is lower, which is a consequence of the blocking of active catalyst sites by phosphate anions.

Figure 3: Fuel cell performance with the formic acid reformate and defined fuel gas mixtures, using air as oxidant. (a) Results obtained in the LT-PEFC at a temperature of 80 °C and a gas pressure of 2.5 bar absolute. (b) Polarization curves obtained in the HT-PEFC at 160 °C and 1 bar absolute pressure.
**HyTech**

**Sustainable Hydrogen Utilization**

**Scope of project**

The intermittency of renewable power sources such as hydroelectricity, wind turbines and photovoltaics necessitates energy storage systems. Of the various systems available hydrogen and other chemical energy carriers are expected to become of increasing importance in Switzerland and elsewhere. Abundant renewable hydrogen would facilitate a wide range of future renewable energy technologies, including hydrogen powered vehicles, the development of synthetic fuels from carbon dioxide, the transformation of biomass into fuels and, more broadly, employment in many industrial applications where current hydrogen demand is largely met by steam-reforming of methane. In the Hytech project both sustainable hydrogen production and storage were studied.

**Status of project and main scientific results of workgroups**

Since the start of the HyTech project key advances have been made related to the development of new catalysts for hydrogen generation and storage, spanning new catalysts, materials and modelling studies. Many new fundamental insights have been gained providing molecular level mechanistic insights that will facilitate future rational material and catalyst design. Much of the research undertaken within the HyTech project involves collaborations between the workgroups and other CCEM projects although in the text below each project is listed under the main investigator.

**Hydrogen production**

ETHZ-LSK has been designing and testing homogeneous and immobilized heterogeneous catalysts for hydrogen evolution (water oxidation and reduction catalysts). The catalysts were inspired by anthropogenic and natural catalysts. A limitation of homogeneous hydrogen evolution catalysts is their instability. To overcome this problem multidentate N-heterocyclic carbenes were employed, as these ligands stabilize metal centers. Although some of the complexes were active catalysts, e.g. KM86 (see figure 1), it was found that they convert to ruthenium nanoparticles that are catalytically inactive.

Photo-receptive heterogeneous catalysts based on a functional metal organic framework (MOF), MIL-125-NH$_2$(Ti), were developed in collaboration with SABIC (Saudi...
The photo-catalytic activity of a new MOF composite comprising a hydrogen evolving nickel catalysts and MIL-125-NH2(Ti), prepared using a ship-in-the-bottle technique and termed Ni@MOF, was studied (figure 1). The activity of the Ni@MOF catalyst is superior to that of the constituent parts. Other classes of photocatalytic water splitting catalysts were studied including titania doped with platinum nanoparticles and biomimetic metal organic framework systems inspired by hydrogenases.

EPFL- LSCI has focused on solar hydrogen production. Numerous significant results were obtained including the development of a simple and scalable solid-state reaction to produce polydisperse dinickel phosphide nanoparticles that are excellent catalysts for the electrochemical hydrogen evolution reaction. Related materials were also found to be efficient co-catalysts for the oxidation of formic acid in direct formic acid fuel cells and were found to catalyze the oxidation of methanol in direct methanol fuel cells.

A series of non-precious metal hydrogen evolution catalysts were discovered and developed. These catalysts are based on amorphous molybdenum sulfides, molybdenum carbides, molybdenum borides and nickel phosphides (figure 2). The active sites of the hydrogen evolution catalysts were established using a combined experimental and computational approach.

PSI-STL in close collaboration with ETHZ-PREC has been advancing two-step H$_2$O/CO$_2$-splitting cycles based on metal oxide redox reactions using concentrated solar energy for solar H$_2$ production. Effective heat/mass transfer properties of complex porous media and dynamic reactor modelling are used to facilitate engineering design, optimization, and scale-up of thermochemical reactors and processes.

As part of this research a non-linear dynamic model was developed and applied to a solar reactor for ZnO reduction under ambient pressure conditions. The model includes 3D governing unsteady mass and energy conservation equations, combined radiation-conduction-convection heat transfer coupled to reaction kinetics, and radiative exchange within absorbing-emitting-scattering particle bed undergoing thermochemical transformations. The model was validated by comparisons with experimental data obtained from a 10 kWth solar reactor prototype and a 100 kWth solar pilot reactor.

A drawback of thermochemical H$_2$O/CO$_2$-splitting cycles is the inert gas consumption during the reduction step to decrease the oxygen pressure for shifting the thermodynamic equilibrium towards lower operating temperatures. In one approach, a combined computational/experimental study of perovskite redox materials was conducted to design compositions that allow for low-temperature and high-efficiency thermochemical separation of O$_2$ and thermochemical splitting of H$_2$O and CO$_2$ (figure 3).

Another approach aims at operating the solar thermochemical reactor at reduced pressure, which was experimentally demonstrated for the solar assisted carbothermal reduction of ZnO.

The results obtained in this study will facilitate the further development and design of continuous solid particle vacuum solar-thermochemical reactors for fuel production.
Hydrogen storage

EPFL-LMER (formerly EPPM-H2E) has explored complex hydrides – potential, reversible hydrogen storage materials. Some complex hydrides are liquid at room temperature, e.g. Al(BH₃)₃ and Ti(BH₄)₃, which potentially offers advantages over solid metal hydrides. Empirical correlations based on vibrational spectroscopy were developed to estimate the stability and melting point of these borohydrides. Their decomposition mechanisms were also determined and a new approach was successfully evaluated in which unstable and volatile metal hydrides may be incorporated into high surface area materials thereby extending the decay time from minutes to months. Specifically, Ti(BH₄)₃ was trapped in MOF UiO-66 (see figure 4). This work provides a general route for stabilizing thermodynamically unstable energy dense species while allowing their safe storage and easy handling.

Additional studies on the separation and concentration of CO₂ using ammine modified silica foams and the synthesis of hydrocarbons from hydrogen and CO₂ with a full life cycle analysis were undertaken. New catalysts for the hydrogenation of CO₂ are also under development. An important part of the work comprised the construction of a new experimental station to measure and identify in situ the products resulting from the reduction of CO₂. Using this equipment it was possible to demonstrate that water absorption enhanced catalysis greatly increases the conversion of CO₂ using a methanation catalyst leading to the development of a new catalysis/absorption reactor.

EPFL-LCOM has focused on direct hydrogen capture and storage materials based on ionic liquids. The team has also developed the first ionic liquid that can activate hydrogen, absorb and reduce CO₂. Such ionic liquids could be used to trap hydrogen generated from hydrogen evolution catalysts while allowing the oxygen produced to pass through. Following experimental validation of the first system of this type, i.e. the [PrN(CH₂)₂mim][Tf₂N]-B(C₆F₅)₃, quantum-chemical computations were employed to rationalize the formation of the hydrogen-complex, [PrN(CH₂)₂mimH][Tf₂N]-B(C₆F₅)₃H. Dihydrogen can be released from the system or, alternatively, CO₂ can be absorbed in the hydrogen-rich liquid which leads to the direct reduction of CO₂ and the formation of formic acid (in the absence of a catalyst). Further optimization is required to improve the efficiency of this latter process. Numerous applications can be envisaged since the ionic liquid can selectively trap hydrogen, activate it for further reaction if necessary, and forms a separate phase to water and organic solvents.

Work on other catalysts that transform CO₂ into fuels has also been undertaken and a new, inexpensive organocatalyst derived from vitamin B1 has been discovered.
**CO₂ to Methanol**

**Highly Efficient and Selective Catalysts and CO₂ Sorbents for the Electrochemical Production of Methanol from CO₂**

**Scope of project**

Conversion of CO₂ into useful carbon neutral fuels using renewable energy sources is an attractive way to sustainably reduce CO₂ accumulation in the atmosphere and recycle this greenhouse gas. However, CO₂ reduction into a desirable fuel is challenging due to the kinetic limitations (multiple proton-coupled electron transfer steps), which results in the need of high over-potentials to drive this reaction. Other challenges include finding an efficient and selective catalyst which enables to form controllable yield of valuable products such as methanol, essential to achieve a cost-effective process, and having a concentrated source of CO₂. This work is thus divided into three main sub-projects: identifying the best Cu-based catalysts for the selective conversion of CO₂ to hydrocarbon products (WP 1), and developing powdered catalysts on carbon supports (WP 2) and methodology to capture CO₂ (WP 3) with the goal to develop an effective CO₂ conversion (demonstration) process into fuels (WP 4). These workpackages are carried out by ECL@PSI, SIC@ETHZ, and LESE@ETHZ with their respective complementary expertise.

**Status of project and main scientific results of workgroups**

With the goal to understand what is the best suited catalyst composition (WP 1), the group of Prof. Schmidt (PSI) has prepared Cu-based catalysts by sputtering techniques and developed methodologies to monitor the reaction by combining electrochemical measurement with liquid and gas analysis of reaction products. Preliminary results show a promising route for the selective electroconversion of CO₂ to isopropanol. Understanding the origin of the selectivity, and further tuning the activity and the selectivity of the catalysts is currently under way; the primary focus is directed at developing metal-doped catalysts.

In parallel, the group of Prof. Copéret (ETHZ – D-CHAB) has developed robust methods to prepare Cu nanoparticles using colloidal approaches (WP2); this approach allows controlling the particle sizes between 3 and 5 nm using various stabilizing ligands and Cu molecular precursors. Alternative approaches via precipitation – deposition method have also provided promising results, but still yield very large nanoparticles. The research effort is now directed at finding improved deposition methods to prepare the corresponding supported nanoparticles. In addition, evaluation of the catalytic performances is currently underway in order to compare them with what has been obtained for model systems prepared using sputtering techniques.

Finally, the group of Prof. Mueller (ETHZ – D-MATV) has obtained promising CO₂ sorbent materials using carbonaceous templates and atom layer deposition approaches (WP 3). A further improvement of the structure of these materials is expected to increase further their CO₂ uptake.

With these promising results in hands, each team will continue improving the respective component of the process (WP 1–3) before starting to integrate them into a demonstrator with the goal to achieve an efficient process for the electroconversion of CO₂ to fuels (WP 4). In addition, a major effort in computational modelling will be carried out to help understanding the catalyst performance and proposing more rational development approach (WP 1–2).

**Main achievement and outreach**

This research program has been integrated in the SCCER Heat and Energy storage. With promising results in hands, it is expected that publications through posters at conferences and in scientific journals will be done in the coming year.

---

**List of abbreviations**

SCCER Swiss Competence Centers for Energy Research
WP Work Package

**Major partners in the ETH domain**

- ETHZ – Surface and Interfacial Chemistry (SIC)
- ETHZ – Laboratory of Energy Science and Engineering (LESE)
- PSI – Electrochemistry Laboratory (ECL)

**Main Investigator**

Christophe Copéret, ETHZ

**Project Partners**

ETHZ
PSI

**Time frame of Project**

2014–2017

**Part of SCCER**

HaE (Energy Storage)

**Thematic Relationship to SCCERs**

CREST (Transition)
GasOMeP
Gasoline Vehicle Emission Control for Organic, Metallic and Particulate Non-Legislative Pollutants

Scope of project

Gasoline direct injection (GDI) vehicles will quickly replace port-fuel injection vehicles in the next years. It is estimated that about 50 million GDI vehicles will be operated on Europe’s roads by 2020. In the GASOMeP project, we comprehensively study exhaust composition of various GDI vehicles including particle-bound, condensable and gaseous pollutants. Effects of fuel quality and converter technology, especially the potential of gasoline particle filters (GPFs), which are currently developed by our industrial partners, will be studied. Particle characterization including size distribution, number and metal content as well as the emissions of genotoxic compounds like polycyclic aromatic hydrocarbons (PAHs), their alkylated and nitrated forms are studied. These semi-volatile compounds are expected to penetrate filters to some degree and are important precursors of secondary organic aerosols (SOA) formed upon atmospheric oxidation. Respective SOA forming potentials are investigated in smog chamber experiments and two different flow reactor approaches in the project.

Status of project

After two years we can now look back to four intense sampling campaigns of 3 to 4 weeks each at the chassis dynamometer at the University of Applied Sciences Biel (UASB). One from the PSI, one from the University of Applied Sciences Northwestern Switzerland (UASWN) and one from Empa met the one at the UASB to investigate, according to the different work packages, emissions of regulated pollutants and nanoparticles (UASB, UASWN), non-regulated pollutants and metals (Empa) and secondary organic aerosols (PSI, UASWN).

So far, five different GDI vehicles from Euro-3 and Euro-5 legislation were tested and compared with a Euro-5 diesel vehicle with particle filter as the bench mark vehicle. A flex-fuel vehicle (Volvo V60 T4I, 1.6I, Euro-5) which was operated with (bio)ethanol/gasoline blends is the reference GDI vehicle available in the 3-year campaign. In addition, two of our industrial partners contributed two coated and two non-coated gasoline particle filters (GPFs). These filters were tested with the conditions and in a steady state cycle (SSC) with constant vehicle operation at 94, 61, 45, 26 km/h and idle.

Main scientific results of workgroups

GDI vehicles release up to 2000 \( \times \) more particles than current diesel vehicles equipped with filters: The five GDI vehicles studied so far released substantial numbers of nanoparticles (PN) in the range of \( 7 \times 10^{11} \) to \( 2 \times 10^{12} \) particles/km. Emissions were about 2–10 times higher under cold start conditions. In other words, PN emissions of these GDI vehicles are clearly above the threshold limit for diesel passenger cars of \( 6 \times 10^{11} \) particles/km.

Figure 1: Emissions of genotoxic PAHs and precursors for genotoxic nitro-PAHs in GDI vehicle exhausts (ng/m\(^3\)).
Comparing these values with those of the benchmark diesel vehicle (Peugeot 4008, 1.6 l, Euro-5), which is equipped with a particle filter, revealed 30–2000-fold higher particle emissions of the GDI technology. This clearly indicates that filters must have a large potential to detoxify GDI vehicles with respect to their high particle emissions.

**Comparable emissions of genotoxic PAHs from GDI- and diesel vehicles**

Figure 1 displays emission factors (ng/m³) of various 4-, 5-, 6- and 7-ring PAHs, including those PAHs relevant for the genotoxic potential, of five GDI vehicles and the benchmark diesel vehicle equipped with a filter (Peugeot 4008, 1.6 l). PAH emissions varied considerably among the different GDI vehicles. They were highest for the oldest vehicle (Mitsubishi Carisma, 1.8 l, Euro-3) but comparable for the Euro-4 and Euro-5 vehicles. In comparison with the diesel vehicle, one can state that PAH emissions of the GDI vehicles are at or slightly above those of the diesel vehicle. In other words, GDI vehicle exhausts will also contribute to the overall burden for these genotoxic compounds in areas which are affected by traffic.

**Impact of (bio)ethanol on PAH and particle emissions**

Figure 2 displays emission factors (µg/km) of various 2-, 3-, 4- and 5-ring PAHs of the reference vehicle (VOLVO V60 T4F, 1.6 l) operated with gasoline (E0) and ethanol/gasoline blends (E10, E85) in the cold and hot started WLTC and the SSC. Transient driving (WLTC) has a substantial impact on PAH emissions which were 1–3 orders of magnitude higher than those under steady state driving. The cold start effect is moderate (<10x) whereas blending with ethanol lowered PAH emissions by more than one order of magnitude. Effects tend to be larger with increasing PAH ring number.

For comparison, figure 2 also includes particle number emissions in the WLTC which were 10¹³ particles/km with E0 but only about 10¹¹ particles/km with E10 and E85. This indicates that blending of gasoline with ethanol has beneficial effects on particle and PAH emissions including the genotoxic PAHs. However, these promising effects will be verified again in next year’s campaign on additional GDI vehicles.

**Particle filters for GDI vehicles successfully applied**

So far, four different filters, two with catalytic coatings, two non-coated ones, have been tested on the reference vehicle under comparable conditions. Data evaluation is ongoing and will be reported later in the project.

**Time-resolved secondary aerosol analysis of GDI vehicles**

Time-resolved secondary aerosol analysis of GDI vehicles was conducted using the micro smog chamber. A continuous-flow reactor-tube was applied to study the formation of secondary aerosols (SA) by taking the gas-phase fraction of exhausts and oxidize it with ozone (up to 60 ppm) at residence times of about 10 seconds. Figure 3 displays an example of secondary aerosol emissions (g/lit-fuel) during cold and hot WLTC. In conclusion, the secondary aerosol released per liter of fuel is several orders of magnitude lower than what has been observed in wood burning experiments.
novatlantis
Sustainability at the ETH Domain – Promotion of Transdisciplinary Science

Scope of activities

novatlantis – Sustainability in the ETH Domain – is the interface between research (ETH Zurich, EPFL, PSI, WSL, Empa and Eawag) on the one hand and industry, society and the public sector on the other. The aim is to contribute towards the sustainable development of our society whilst taking the ecological, economic and social dimensions of sustainability into account. Broad-based pilot projects are used to promote the transfer of the latest research results for the sustainable development of cities, municipalities and regions. The basis for this is the initiation of transdisciplinary projects in close collaboration with scientists from the ETH Domain, other research institutions and companies as well as with authorities at municipal, cantonal and national level.

The main points in brief

In terms of personnel, the 2015 financial year was characterized by more new additions to the novatlantis team. Regina Flury von Arx, agronomist and spatial planner at NDS ETH, took over various tasks in Zukunftsregion Novatlantis Argovia as a project manager. Cornelia Moser, a business economist with a master’s degree in Strategic Environmental Management and Policies, joined the team as a project manager for energy and mobility.

The major milestones in the 2015 financial year were the activities and projects in Zukunftsrregion Novatlantis Argovia and the practical lab for the 2000-watt society in the pilot region Basel. The two novatlantis construction forums on «City Vision 2050» attracted great interest, integrating contributions from the Swiss Competence Centers for Energy Research (SCCER) for the first time. In Lucerne, the construction forum was again held in collaboration with the Lucerne University of Applied Sciences and Arts and the Canton of Lucerne, and highlighted the topic «Buildings and areas of the future». The Zurich-based construction forum focused on the interplay between «People, buildings and sustainability».

novatlantis continued to step up its networking and PR work. novatlantis is now a network partner to Öko-Kompass – the environmental consultancy agency for small and medium-sized enterprises (SME) in the City of Zurich – and will act as patron for «Research and science» at the 2016 brennet Status Seminar.

Regina Flury has been responsible as a project manager for various tasks in Zukunftsrregion Novatlantis Argovia, including interviews and data processing for potential analysis in the municipalities and the Energy Accounting project. She developed a stepping stone concept for Zukunftsrregion Novatlantis Argovia and acts as webmaster for the novatlantis homepage.

A bigger novatlantis team

novatlantis added new members to its team in the 2015 financial year, Regina Flury von Arx and Cornelia Moser.

Since March 2015, Regina Flury has been responsible as a project manager for various tasks in Zukunftsrregion Novatlantis Argovia, including interviews and data processing for potential analysis in the municipalities and the Energy Accounting project. She developed a stepping stone concept for Zukunftsrregion Novatlantis Argovia and acts as webmaster for the novatlantis homepage.

Regina Flury studied Agronomy at the Swiss Federal Institute of Technology in Zurich. After a year of postgraduate studies in the USA, she worked as a research associate in the International Affairs Office of the Swiss Farmers’ Union, focusing on the topics of GATT and EEA negotiations. After training as a spatial planner at NDS ETH, she worked at the Coordinating Office for Environmental Protection in the Canton of Bern Department of Construction, Transport and Energy, where she dealt with matters relating to tourism, agriculture and materials extraction. As head of the specialist environmen-
tal office for the town of Olten, she was responsible for the areas of «Energiestadt» (energy town), energy consulting, mobility, combustion control, nature and environmental education. In the Urban Development department, she carried out projects to engage with and mobilise the residents in the neighborhood.

Cornelia Moser joined novatlantis as a project manager in September 2015. She studied Business Economics and has a master’s degree in Strategic Environmental Management & Policies. Thanks to several years of experience in the private sector and in federal administration, she can perfectly complement the sustainability competency of novatlantis. Cornelia Moser contributes her theoretical and practical knowledge of interdisciplinary project work as well as her expert knowledge in the fields of energy and mobility in particular. She primarily manages projects within the framework of the pilot region Basel, but is also involved in the further development of Zukunftsregion Novatlantis Argovia and in establishing other novatlantis activities.

Dr. Anna Roschewitz is still the Managing Director at novatlantis, and Agnieszka Hamburger is responsible for accounting. The Paul Scherrer Institute is the leading house for novatlantis.

Zukunftsregion Novatlantis Argovia

Zukunftsregion Novatlantis Argovia (ZURA) was founded in 2013. It stems from a joint initiative of the Canton of Aargau, the energy suppliers IBAarau AG, Regionalwerke AG Baden and AEW Energie as well as «novatlantis – Sustainability in the ETH Domain».

In collaboration with the municipalities in the Canton of Aargau, Zukunftsregion Novatlantis Argovia is looking to make a contribution towards the transition in energy policy, especially in the fields of energy, mobility and buildings. The partners realize pilot projects and encourage dialogue within the network of municipalities. They help disseminate knowledge and experience in energy and efficiency-related topics throughout the region.

The partners regard Zukunftsregion Novatlantis Argovia as a practical laboratory for sustainability. New and established research results and technologies should rapidly find an application, tailored to the individual parameters and needs in the cities and municipalities.

After conducting a potential analysis in 20 interested municipalities in a bottom-up approach in 2014, the results revealed that the datasets for the determination of relevant key figures in the municipalities are very different. Moreover, it was found that key qualified and quantified figures on the expansion potential of renewable energy sources are often lacking. For a uniform calculation of an energy and carbon footprint per municipality, the collection of data would have to be developed further for the majority of the municipalities.

ZURA made progress in various different areas in the 2015 financial year. For example, two further municipalities, Wettingen and Stetten, announced their commitment to the Zukunftsregion concept. As new members, they benefit from the potential analysis in the form of a hotspot matrix as well as the corresponding figures. At an organizational level, Wolfgang Reisner from Stetten town council joined the steering group as a representative of a smaller municipality. The project team received support from the larger novatlantis team and also added a new member, Sabine Wirthner (IBAarau).

Pi lot projects of Zukunftsregion Novatlantis Argovia

The pilot projects were progressed further. The «Forum», conceived as a series of annual events, took place for the first time in July. Fourteen municipalities discussed the topic «Energy balances for municipalities – specific advantages and best practice». Based on the positive feedback, there are plans to hold the Forum twice a year in future.
Potential analysis

The project «Potential analysis / Accounting for energy and buildings» uses existing software solutions (e.g. EnerCoach, Energie-Region) for energy accounting for public buildings and accounting for the comprehensive energy and CO₂ data for the municipality. This provides support to municipalities in monitoring and visualizing the data recorded. Potential analysis forms the basis for in-depth energy and climate policy decisions in the municipality. The objective is for each municipality to know its energy consumption, greenhouse gas emissions and its potential in the area of renewable energies.

As in the prior year, in 2015 the municipalities were contacted directly by the cantonal municipal advisors for the Canton of Aargau on behalf of Zukunftsregion and the individual procedures were agreed. The two municipalities of Wettingen and Stetten joined in potential analysis for the first time.

Biomass

Biomass is a valuable resource which can be used as material or to create energy. Today's disposal channels often only use biomass either as a material (composting) or to create energy (waste incineration, wood-fired systems). The aim is to use biomass both as a material and to create energy where possible. In the case of moist biomass (farmyard manure, cuttings etc.), this is already state of the art with the fermentation technology used to produce biogas. Realizing biogas projects will herald a change in existing disposal channels. As a result, there is a need for regional and sustainable solutions with the combined effort of the canton, the municipalities and the private sector (integrated solution). As part of the project «Biomass value flows», the information compiled in the municipalities led to the creation of a map of Aargau that shows the current recycling channels. Among others, the map shows potential in the «Suhrental» area as well as a good constellation for biomass recycling. Further clarification and discussions regarding setting up a biogas plant are taking place.

Community photovoltaic systems

The municipalities have roof surfaces that are well suited to renewable electricity generation. The project «Community photovoltaic systems» provides for a financing model by the residents where they get involved by means of an interest-free loan. Amortization of the investment is paid back using a fixed solar electricity share over 20 years – which benefits investors (price security, ecology) and the municipalities (financing). Basic materials for the project in the form of white-label documents – neutral, standardised documents – based on the successful suhrSOLAR model were produced with assistance from the Lucerne University of Applied Sciences and Arts. These documents are available to all interested municipalities free of charge. This prompted Stadtwerke Zofingen to create Zofinger Solarstrom, which is precisely such a public participation model. Other municipalities and public utilities are also planning to build these systems.

Mobility concept for areas

The interest of the municipalities in the project «Mobility concept for areas» was compared against existing national, cantonal and municipal offerings. It was found that the municipalities have an experienced partner for mobility concepts in the mobility platform aargauMOBIL, supported by the Canton of Aargau. The corresponding synergies are exploited and the municipalities interested receive professional advice from aargauMOBIL.

Needs-based and cost-saving mobility systems

Passenger transportation poses major challenges for many

Figure 1: The first forum of the Zukunftsregion Novatlantis Argovia was held in July 2015.
municipalities. Cost optimization, availability and special requirements are just some of those challenges. IT platforms and smartphone apps provide effective support in the planning and implementation of new approaches for sharing and car-sharing. The project «Needs-based and cost-saving mobility systems» involved drawing up the specific needs using dialogue with stakeholders and bringing the local partners together around a table. Based on the feedback from the stakeholders, an overarching project to coordinate mobility services was set up.

Three projects were postponed in the financial year because they did not promise to be successful for various reasons:

• As far as the project «Decentralised storage of electrical energy» is concerned, an analysis of different possibilities for use showed that currently there is a lack of uses for storage pilot projects as well as a lack of economic incentives for municipalities. Consequently the project was postponed, but these two points will be examined again in the coming years.
• The topic «Modernising in a protected townscape» originally met with interest amongst the municipalities. However, further clarification showed that this did not translate into specific modernisation plans for listed buildings owned by the municipality. As a result, the project was postponed until further notice.
• The project «100% renewable fuels» was also postponed, as the evaluation in the municipalities interested showed low chances of success. Thanks to a case study by ETH Zurich, however, it was possible to get important findings for the Aarau region in relation to electromobility and non-motorized transport. The case study for the lecture «Introduction to dealing with environmental systems» (EUUS) on the Environmental Sciences programme was carried out in collaboration with Zukunftsregion. Around 100 students worked in groups to prepare scientific, economic, legal or stakeholder analyses. The results were then compiled and used to create a systems analysis.

Stepping stones

In addition to the original projects continued in the prior year as part of ZURA, novatlantis developed the «ZURA-Trittsteine» (ZURA stepping stones) programme. This was in response to the fact that the municipalities in Zukunftsregion are very varied in terms of size, population, administrative resources, strategic and operational planning, implementation and controlling of energy and resource-saving measures.

Complex projects such as «Biomass value flows» or «Needs-based and cost-saving mobility systems» make very high demands on the existing resources from public administration and politics, on the network and on the experience in the realization of planning projects. Such projects require an intensive preparation phase, often spanning several years, before they can be implemented.

The aim of the ZURA-Trittsteine (stepping stones) approach is to bridge this time gap with small but significant successes through the implementation of simple measures. Fast results are to be achieved by the coordinated implementation of simple measures that can be realized in the short term and have a far-reaching effect. To do this, tried-and-tested concepts will be adopted, synergies from ongoing funding programmes will be used and the experience of trusted partners will be built on.

A conscious decision has been made with the ZURA-Trittsteine programme to do without the complex introduction of new technological developments. This aims to ensure that projects and measures can be implemented in the municipalities with an appropriate use of resources that is tailored to the size of the municipality. The programme’s innovative power is based on the coordinated implementation of measures that will achieve tangible...
results in the municipalities. This will allow for economies of scale to be exploited and will lay the foundations for positive intrinsic momentum.

The stepping stone for 2016 is currently in the evaluation phase; initial exploratory talks have already taken place with potential partners.

**New project 2016: Gemeinde-Energie-Spiegel Argovia, GESA (Municipal Energy Level Argovia)**

A new project is being added to the Zukunftsregion portfolio for 2016. The project was developed by novatlantis and is managed by novatlantis: «Gemeinde-Energie-Spiegel Argovia» (Municipal Energy Level Argovia). The project is called GESA for short and it provides a meaningful extension to the existing projects, perfectly complementing the ZURA-Trittsteine (stepping stones) concept.

The background to the project is that the majority of the 213 municipalities in Aargau (approximately 182 or 85%) do not have any systematic recording of their energy and CO₂ data, neither at the public building nor at municipal level. Thus the challenge is to realize long-term, consistent and uniform monitoring of energy and CO₂ for the 213 municipalities and for the canton. To do this, the data must be mutually comparable and of high quality and thus suitable for aggregation. This is only possible by an offering at cantonal level that on the one hand offers added value for the municipalities and on the other hand provides the canton with the basis necessary to monitor the achievement of its own energy goals while at the same time supporting the various goals of the energy strategy (including energy planning).

To achieve this, the GESA pilot project comprises two sub-projects: «Datasets» and «Practical testing». The first sub-project, «Datasets», involves putting together an overview of the existing datasets and answering fundamental issues about the design of the project. The objective is to recognise and describe significant points relating to data collection, data storage and possible process design that are relevant for implementation. In the second sub-project, «Practical testing», the data model developed will be tested in four pilot municipalities. The results from these two sub-projects will serve to develop recommendations on how to proceed at municipal and cantonal level.

**Accompanying research on Zukunftsregion**

In line with its definition, Zukunftsregion Novatlantis Argovia focuses its activities on the Canton of Aargau. However, it is likely that important findings from the collaboration at municipal level and the Potential Analysis project in terms of handling energy and CO₂ data for public buildings or municipalities can be applied to other municipalities. This poses the question surrounding the overarching success factors of energy accounting for buildings and energy and CO₂ accounting in towns and municipalities. **novatlantis** has developed a concept for an accompanying research project to answer this question.

The project aims to examine the success factors for active participation of municipalities in programmes to promote sustainability and energy efficiency, such as «Zukunftsregion Novatlantis Argovia» or «Energiestadt», and to look in more detail at the requisite framework conditions for introducing and putting a value on energy and CO₂ accounting in towns and municipalities. The first step is to get an overview of the different accounting methods, how common they are at present and what role they play in municipal, cantonal and national energy and climate strategies. The second part will involve empirical accompanying research and will take the form of examining decision-making processes in favour of or against taking part in programmes as well as the implementation processes using the example of energy and CO₂ accounting in municipalities. The objective is to name and assess the benefits, accommodating factors or obstacles, additional expenses and costs as well as other stumbling blocks.

The empirical accompanying research will be geared to the processes in the municipalities. They will record energy consumption between the heating periods and ideally update them every year. An examination of the first data recorded and the first update will thus run over two years. Together with the basic and consolidation phases, the total project duration is three years and will...
lead to a closing report as well as a «Solutions for meaningful energy and CO₂ accounting for municipalities» toolkit with best practice examples for municipalities. With those tools and the in-depth knowledge of the leverage effects at municipal level, the project will contribute to enabling municipalities to better exploit their potential for achieving the objectives of Energy Strategy 2050.

This three-year accompanying research on ZURA will be funded by a foundation and will commence at the beginning of 2016.

Basel as a pilot region for the 2000-Watt society

More than ten years ago, novatlantis – Sustainability at the ETH Domain developed a visionary model of a sustainable energy future with the «2000-Watt Society». Pilot regions were sought that were willing to put the latest research results into practice. Conversely, these regions were also tasked to bring specific questions to the research institutes. The Canton of Basel-Stadt agreed to this collaboration. Thanks to a network of science, industry and public administration, a «practical laboratory for sustainability» with different pilot and demonstration projects in the fields of construction, mobility and spatial development took shape.

The Great Council approved various loans to the tune of CHF 3.9 million between 2003 and 2012 to initiate and promote «flagship projects». Thanks to these funds, a vast range of pilot and demonstration projects (P+D projects) were developed in the canton. The Great Council granted another loan of CHF 2.6 million for 2013 to 2016. As a result, the broad-based network that has been established between research institutes, companies and public administration in recent years can remain active.

In collaboration with the research institutes and in consultation with the Construction and Transport Department (BVD) and Industrielle Werke Basel (IWB), the Department of Economics, Social Affairs and Environment (WSU) in charge identified topics to be developed further in the pilot region. As P+D projects, they contribute towards the transfer of research and development into practice.

For the current period from 2013 to 2016, eleven projects were proposed in the topic areas of construction, renewable energies and vehicles. They are designed to highlight how Basel can continue on its path towards the 2000-Watt society. The Office for Environment and Energy, the FHNW’s Institute of Energy in Construction, novatlantis and Sustainserv GmbH are responsible for realizing the projects.

Projects in the fields of construction and renewable energies:
- Prefabricated Façade Modules
- High-Performance Insulating Plaster
- Solar Façades
- Network Optimization with Buildings
- Local Electricity Storage

Projects in the field of vehicles:
- Hydrogen Service Station for a small fleet of fuel-cell vehicles
- Hydrogen Admixture to Natural Gas
- Electromobility – public, battery-operated electric buses
- Natural Gas Hybrid – vehicle concept for various vehicle classes

Other projects:
- Local Energy Hub
- River Water Usage – Thermal Use of the Rhine

After the eleven projects were planned in more depth and their feasibility studied in 2013, seven of the projects were launched in the following year. Three existing pilot studies and the project «Prefabricated Façade Module» have still not started, as an investor is yet to be found.

The «Energiedrehscheibe» (Local Energy Hub) project led by novatlantis as part of the IDEAS4Cities initiative (Integration of Decentralized Energy Adaptive Systems for Cities) was continued in 2015 as planned – also thanks to the good collaboration with the project partner Industrielle Werke Basel IWB. The project provides for the creation of a cost-optimized model of the energy system in Basel that contains information on supply and demand right down to neighborhood level. The aim of the project is to simulate, based on the data available, different scenarios with centralised and decentralised energy production and storage and to examine aspects such as sustainability, costs, flexibility and modularity. Model vari-
ables include CO₂ levies, feed-in tariffs, renovation potential as well as fuel prices. A first basic model will be available in the spring of 2016. There are plans to use the data model to make recommendations for IWB and for the Canton of Basel-Stadt and if applicable to implement these recommendations in subsequent pilot projects.

In the case of the Hydrogen Service Station project managed by Sustainserv GmbH, novatlantis actively contacted project partners in the second half of 2015 to clarify whether there was demand for scientific accompanying research for the project alongside the infrastructure project. Initial feedback showed that topics such as community acceptance and participation, environmental and economic aspects or the analysis of energy chains using a real-life example could be interesting research topics for researchers at PSI, Empa and other research organizations contacted. It is also necessary to clarify to what extent a collaboration with the existing hydrogen projects at PSI («Energy System Integration Platform») and at Empa («Move» Platform) might make sense. Preliminary clarification has been concluded, but delays in the infrastructure project have meant that the accompanying research has not yet started. In-depth clarification for carrying out the accompanying research will commence as soon as there is a specific timeframe for implementation of the infrastructure project.

Series of events – the novatlantis construction forum «City Vision 2050»

The novatlantis Construction Forum – Platform for Sustainable Construction – is a series of events where the latest developments from the university sector and from sustainable building in practice are presented and discussed. It is geared towards those responsible for the real estate portfolios of private and institutional investors, pension funds, authorities, building contractors and architecture and planning firms.

The novatlantis construction forums on «City Vision 2050» met with great interest. In Lucerne, the construction forum was again held in collaboration with the Lucerne University of Applied Sciences and Arts and the Canton of Lucerne, where the topic was «Buildings and areas of the future». The Zurich-based construction forum focused on the interplay between «People, buildings and sustainability». Poster and product exhibitions in the form of innovation drinks receptions promoted the knowledge transfer from research to practice and offered welcome opportunities for networking. With the active participation of two Swiss Competence Centers for Energy Research (SCCER) in the two construction forums, it was also possible to contribute to the transfer of knowledge and technology.

The talks, posters and photographs at the construction forums can be downloaded from www.novatlantis.ch. novatlantis also reports on every event in the form of brief articles published in journals and on the homepage. Various sponsors from the private and public sectors provided financial support to the novatlantis construction forums.
**novatlantis**

**Sustainability at the ETH Domain – Promotion of Transdisciplinary Science**

**novatlantis construction forum Lucerne: Sustainable energy concepts as success factors for buildings and areas of the future**

January 2015 marked the second occasion of a *novatlantis* construction forum held in Lucerne in collaboration with the Lucerne University of Applied Sciences and Arts and the Canton of Lucerne. The topic, «Buildings and areas of the future», met with a great deal of interest from the specialist audience and resulted in a sold-out event. The three partner institutions will also continue their collaboration in 2016 and plan to establish the *novatlantis* construction forum Lucerne as an annual series of events.

The *novatlantis* construction forum Lucerne examined the question of how sustainable energy concepts can become success factors for buildings and areas of the future. The event centred on talks by different stakeholders who presented technical and organizational approaches to specific projects from the perspective of politicians, the public administration, the private sector and research. SCCER Heat & Electricity Storage was also presented at the event. An attractive innovation drinks reception with posters and exhibitions from research and practice as well as a podium discussion rounded off the occasion.

At the end of August 2015, more than 100 experts convened for the *novatlantis* construction forum Zurich at ETH Zurich, which has been firmly established for several years now. They focused on the question of how sustainable urban and neighborhood development can be realized together with the residents. The talks and discussions examined the main issue of how to succeed in creating buildings that are future-proof and that appeal to people at the same time. It became clear that much communication is needed in order to do this. In a brief presentation, SCCER Future Energy Efficient Buildings & Districts (FEEB&D) was introduced.

In the accompanying exhibition, the City of Zurich presented two specific offerings, thus demonstrating how dialogue with the users of buildings can work: The authorities use an «energy coaching» service to target building contractors and companies and encourage them to increase energy efficiency in construction and renovation. «Öko-Kompass» is an advisory offering for SMEs that want to get information directly at their own location concerning specifically what they can do for the environment while at the same time saving money. Around 600 firms in the City of Zurich have already made use of this advisory service.
Network and PR work

novatlantis stepped up its networking and PR work in the financial year. novatlantis is now a network partner of Öko-Kompass – the environmental consultancy agency for SMEs in the City of Zurich – and will act as patron for «Research and Science» at the 2016 brenet Status Seminar. By taking part in the online Advent Calendar on Sustainable Development 2015, where novatlantis designed what is behind the door on 14th of December, and sponsoring the sharing DVD «The Human Scale» on sustainable urban living, novatlantis succeeded in reaching out to further target groups.

novatlantis as a network partner to Öko-Kompass

novatlantis is the new network partner of Öko-Kompass, the environmental consultancy agency for SMEs in the City of Zurich. One reason for this is that the undertakings from the energy, finance and construction sector complement novatlantis’ network perfectly. Secondly, a broader application of Öko-Kompass is planned, and an SME advisory service could also be of interest to Zukunftsregion Novatlanits Argovia.

Based on the motto «Good for the environment, good for business», the City of Zurich has been offering environmental advice that is specially tailored to small and medium-sized enterprises since 2009 in the form of the Öko-Kompass («eco compass»). Specialists come on site to show how companies can save resources, leverage efficiency potential and reduce operating costs.

The Öko-Kompass achieved memorable success in the financial year, winning 2nd place in the «Excellence Publique» prize in the category for Intelligent Saving. This national competition is held annually by the Swiss Society of Administrative Sciences (SSAS) and awards innovation in public administration.

Patronage of «Research and Science» at the brenet Status Seminar

On September 8 and 9, 2016, the Building and Renewable Energies Network of Technology (brenet) will hold the 19th Status Seminar at ETH Zurich. Findings by Swiss-based researchers and innovations in the area of buildings and settlements with a focus on energy and environmental topics will be presented and discussed. The conference is designed for specialists from industry, research and the authorities as well as engineering and architecture firms. novatlantis has assumed the patronage of «Research and Science» for this important event.

Online advent calendar on sustainable development 2015

On 24 different days in December, the online Advent Calendar on Sustainable Development 2015 showcases innovative projects and specific initiatives for promoting responsible business and action.

Live chats with dedicated personalities from the fields of business, politics and science invite the public to get involved. A current book related to the topic of the day is presented each day. In the «Tips for Kids» area, children
and families can get inspiration for trips, games and things to make. With a little luck, the participants in the daily quiz can win selected sustainable gifts. The central topics in 2015 include new approaches in the circular economy, contributions on the transition in energy policy and on the Climate Conference in Paris as well as the inclusion of people whose access to the labour market is impeded for various reasons.

Novatlantis designed what is behind the door on 14th December 2015 with information about our sustainability platform, the next Construction Forum on the topic of «City Vision 2050 – building and mobility» in January 2016 in Lucerne as well as the projects in our focus regions «Pilot Region Basel» and «Zukunftsregion Novatlantis Argovia».

Sharing DVD «The Human Scale»

Last year, Novatlantis entered into a partnership with the association «Films for the Earth» for the national film festival with the aim of disseminating knowledge and raising awareness of sustainability issues. Following on from that, Novatlantis sponsored the sharing DVD «The Human Scale» in the 2015 financial year. This impressive plea for a greener, calmer and more human city focuses on sustainable urban living for human beings, making it the perfect give-away for the Construction Forums on «City Vision 2050» and for various projects in the two focus regions.

Figure 7: A Chinese sports field, a glance in the trailer of the film «The Human Scale».
Register
## List of Finalized Projects

### Mobility

<table>
<thead>
<tr>
<th>Year</th>
<th>Project Code</th>
<th>Project Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>2006–2009</td>
<td>CEMTEC</td>
<td>Computational Engineering of Multi-Scale Transport in Small-Scale Surface Based Energy Conversion</td>
</tr>
<tr>
<td>2006–2009</td>
<td>HY_Change</td>
<td>Transition to Hydrogen Based Transportation – Challenges and Opportunities</td>
</tr>
<tr>
<td>2006–2009</td>
<td>TransEngTesting</td>
<td>Transient Heavy Duty Engine Facility for Engine up to 4000 Nm Peak Torque</td>
</tr>
<tr>
<td>2006–2010</td>
<td>CELaDE</td>
<td>Clean and Efficient Large Diesel Engines</td>
</tr>
<tr>
<td>2006–2010</td>
<td>LERF</td>
<td>Large Engine Research Facility</td>
</tr>
<tr>
<td>2006–2010</td>
<td>NEADS</td>
<td>Next Generation Exhaust Aftertreatment for Diesel Propulsion Systems</td>
</tr>
<tr>
<td>2006–2013</td>
<td>hy.muve</td>
<td>Hydrogen Driven Municipal Vehicle</td>
</tr>
<tr>
<td>2010–2013</td>
<td>Cohyb</td>
<td>Customized Hybrid Powertrains Methodology for Definition of Optimized Hybrid Powertrains for Specific Drive-Cycles</td>
</tr>
<tr>
<td>2010–2014</td>
<td>NADIP</td>
<td>NO\textsubscript{x} Abatement in Diesels</td>
</tr>
<tr>
<td>2010–2014</td>
<td>THELMA</td>
<td>Technology-Centered Electric Mobility Assessment</td>
</tr>
<tr>
<td>2012–2015</td>
<td>DuraCAT</td>
<td>Highly Durable Oxide-based Catalysts for Polymer Electrolyte Fuel Cells</td>
</tr>
<tr>
<td>2012–2015</td>
<td>CatPor</td>
<td>Catalysis in Porous Media for Automotive Applications</td>
</tr>
<tr>
<td>2012–2015</td>
<td>NO\textsubscript{x} Reductions</td>
<td>In-Cylinder Emission Reduction in Large Diesel Engines</td>
</tr>
</tbody>
</table>

### Electricity

<table>
<thead>
<tr>
<th>Year</th>
<th>Project Code</th>
<th>Project Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>2006–2010</td>
<td>ONEBAT (1 + 2)</td>
<td>Battery Replacement Using Miniaturized Solid Oxide Fuel Cell</td>
</tr>
<tr>
<td>2006–2010</td>
<td>PHITEM</td>
<td>Platform for High Temperature Materials</td>
</tr>
<tr>
<td>2007–2010</td>
<td>ThinPV</td>
<td>Cost Efficient Thin Film Photovoltaics for Future Electricity Generation</td>
</tr>
<tr>
<td>2008–2010</td>
<td>GTCO\textsubscript{2}</td>
<td>Technologies for Gas Turbine Power Generation with CO\textsubscript{2} Mitigation</td>
</tr>
<tr>
<td>2012–2015</td>
<td>Hydronet 2</td>
<td></td>
</tr>
</tbody>
</table>
### List of Finalized Projects

#### 2008–2012  
**CARMA**  
Carbon Dioxide Management in Power Generation

#### 2011–2012  
**Battery Test Bench**  
Acquisition of Automated Cell and Battery Test Stations

#### 2008–2013  
**PINE**  
Platform for Innovative Nuclear Fuels

#### 2010–2013  
**DURSOL**  
Exploring and Improving Durability of Thin Film Solar Cells

#### 2011–2013  
**SwissKitePower**  
Novel Wind Energy Extraction Technology

#### 2012–2015  
**MeAWaT**  
Methods of Advanced Waste Treatment

#### 2012–2015  
**HITTEC**  
High Temperature Thermoelectric Converter for Electricity Generation in a SOFC System

#### 2012–2015  
**FAMSADI**  
Swiss High Energy Density Batteries – From Advanced Materials to a Safe Device

#### Heat and Building

#### 2006–2010  
**ccem-house2000**  
Innovative Building Technologies for the 2000 Watt Society

#### 2006–2011  
**ccem-retrofit**  
Advanced Energy Efficient Renovation of Buildings

#### 2008–2012  
**AQUASAR**  
Direct Re-Use of Waste Heat from Liquid-Cooled Supercomputers

#### 2009–2012  
**SuRHIB**  
Sustainable Renovation of Historical Buildings

#### 2010–2013  
**ARCHINSOLAR**  
Unique and Innovative Solution of Thin Silicon-Film Modules Building-Integration

#### Fuels

#### 2007–2010  
**2ndGeneration Biogas (1 + 2)**  
New Pathways to Efficient Use of Biomass for Power and Transportation

#### 2007–2010  
**WoodGas-SOFC**  
Integrated Biomass – Solid Oxide Fuel Cell Cogeneration

#### 2009–2012  
**ARRMAT**  
Attrition Resistant Reactive Bed Materials in Fluidised Beds

#### 2013–2015  
**ARRMATplus**

#### 2011–2014  
**WoodGas-SOFC II**  
Integrated Biomass – Solid Oxide Fuel Cell Cogeneration

#### 2010–2015  
**Syngas Diagnosis**  
Online Diagnostics for Performance Assessment of Biomass Gasification Processes

#### 2010–2015  
**SunChem**  
Bio-Synthetic Natural Gas from Microalgae
## List of Finalized Projects

<table>
<thead>
<tr>
<th>Year</th>
<th>Program</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2012–2015</td>
<td>HyTech</td>
<td>Sustainable Hydrogen Utilization</td>
</tr>
<tr>
<td>2012–2015</td>
<td>Solar Fuels</td>
<td>Solar Thermochemical Production of Fuels from CO$_2$ and H$_2$O Using Ceria Redox Reactions</td>
</tr>
</tbody>
</table>

**Education** 2008–2013 MOSUM Mobility Support for Master’s in Nuclear Engineering
Scientific Project Partners and Financing Institutions

Research institutes of the ETH Domain
- ETH Zurich (ETHZ)
- EPF Lausanne (EPFL)
- Paul Scherrer Institute (PSI)
- Materials Science and Technology (Empa)
- Swiss Federal Institute for Forest, Snow and Landscape Research (WSL)
- Swiss Federal Institute of Aquatic Science and Technology (Eawag)

Universities and other research institutions
- University of Bern
- University of Neuchâtel
- Federal Office of Meteorology and Climatology (MeteoSwiss)
- Institute of Modern Physics, Chinese Academy of Sciences
- Centre Suisse d’Electronique et de Microélectronique (CSEM)
- Chalmers University of Technology, Gothenburg, Sweden
- Centre National de la Recherche Scientifique (CNRS), Caen, France
- Biomass Technology Group BV (BTG), Enschede, Netherlands
- Universidade Estadual de Campinas (Unicamp), Campinas, Brasil

Universities of applied sciences (UAS)
- Fachhochschule Nordwestschweiz (FHNW)
- Hochschule Luzern – Technik und Architektur (HSLU)
- Hochschule für Technik Rapperswil (HSR)
- Zürcher Hochschule für Angewandte Wissenschaften (ZHAW)
- Berner Fachhochschule Technik und Informatik (BFH-TI)
- Scuola universitaria professionale della Svizzera italiana (SUPSI)
- Haute Ecole Spécialisée de Suisse Occidentale (HES-SO)

Financing institutions
- Swiss Confederation’s Innovation Promotion Agency (CTI) / Förderagentur für Innovation des Bundes (KTI)
- Swiss Federal Office of Energy (SFOE) / Bundesamt für Energie (BFE)
- Federal Office for the Environment (FOEN) / Bundesamt für Umwelt (BAFU)
- swisselectric research (a section of swisselectric, an organization of Swiss electricity grid companies)
- Competence Center Environment and Sustainability (CCES)
- Service Industriel de Genève (SIG)
- Verband Schweizerischer Elektrizitätsunternehmen (VSE)
Appendix
Presentations

CCEM – Competence Center for Energy and Mobility


NOx Reductions – In-Cylinder Emission Reduction in Large Diesel Engines


DuraCAT – Highly Durable Oxide-based Catalysts for Polymer Electrolyte Fuel Cells

- Binninger T. et al., «Electronic Interactions between Pt Nanoparticles and Metal-Oxide Support». Science and Technology Facilities Council (STFC, UK) Early Career Researchers Conference, Abingdon, UK, March 18, 2015.
- Binninger T. et al., «In Situ Small-Angle X-Ray Scattering for the Analysis of Electrochemical Degradation of Metal Oxide Supported Pt Nanoparticles». 227th Meeting of The Electrochemical Society (ECS), Chicago, USA, May 24, 2015.
Appendix

Presentations


HITTEC – High Temperature Thermoelectric Converter for Electricity Generation in a SOFEC System


Connect PV – Conductive Transparent Electrodes: a Competence Cluster for Highly Efficient Thin Film Photovoltaics


ADMIST – Advanced Understanding of Micro Structures in Fuel Cells and Batteries through X-ray Imaging


TeKaF – Temperature Dependent Ampacity Limit Modelling of Overhead Power Lines

- Rodriguez J., Buehlmann P.B., Franck C.M., «Thermal-mechanical behavior of Aldrey overhead line conductors and clamps up to their thermal limit». Le réseau électrique de demain, SwissTech Convention Center, EPF Lausanne, Mai 21 2015.
Presentations


Geotherm 2 – Geothermal Reservoir Processes: Towards the Implementation of Research into the Creation and Sustainable Use of Enhanced Geothermal Systems

- Jenny P., Deb R., «Phase Transition and Reverse Pumping During Flow Induced Shear Failure». SIAM Geoscience Conference, 29 June – 2 July, 2015, Stanford, California, USA.
- Karvounis D.C., Wiemer S., «Monte Carlo Simulations of EGS Stimulation Phase with a 3-D Hybrid Model». 1st Schatzalp Workshop on Induced Seismicity, March 10–13, 2015, Davos, Switzerland.
- Moret S., Gerber L., Ambiard F., Peduzzi E., Maréchal F., «Geothermal Energy and Biomass Integration in Urban Systems: a Case Study». 40th Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, USA.
- Valley B., «2015. Stimulation and zonal isolation working group, overview of current activities in Switzerland». IPGT Joint Steering Committee and Working Groups Workshops, April 19, 2015, Melbourne, Australia.
Appendix

Presentations

- Valley, B., Moen M., Evans K.F., «Physical linkage between power-law scaling relations for stress, microseismicity (b-value) and fracture length distributions». Project Image meeting, March 26,– 27, 2015, Potsdam, Germany.
- Ziegler M., «Induced seismicity during deep tunneling and EGS well stimulation in Switzerland». ICDP WORKSHOP (Drilling into Seismogenic zones of M2.0 – 5.5 earthquakes in South African gold mines), October 31 – November 3, 2015, Potchefstroom, South Africa.

MeAWaT – Methods of Advanced Waste Treatment


ISCHESS – Integration of Stochastic Renewables in the Swiss Electricity Supply System


IDEAs4cities – Integration of Decentralized Energy Adaptive Systems for cities

- Evins R., Orehounig K. Dorer V., «Integrated urban energy modelling approaches to support the Swiss Energiewende 2050». CISBAT 2015, Lausanne (Switzerland), September 2015.
- Mavromatidis G., Orehounig K., Carmeliet J., «Climate change impact on the design of urban energy systems». CISBAT 2015, Lausanne (Switzerland), September 2015.
Presentations


SECURE – Synergistic Energy and Comfort through Urban Resource Effectiveness


- Upadhyay G., Mauree D., Kaempf J., Scartezzini J., «Evapotranspiration model to evaluate the cooling potential in urban areas – a case study in Switzerland». 14th International Conference of the International Building Performance Simulation Association, Hyderabad, India, December 7–9, 2015 (accepted for the final presentation).
Appendix

Presentations


Syngas Diagnosis – Online Diagnostics for Performance Assessment of Biomass Gasification Processes


OPTIWARES – OPTImization of the Use of Wood as a Renewable Energy Source


Solar Fuels – Solar Thermochemical Production of Fuels from CO₂ and H₂O Using Ceria Redox Reactions

- Rothensteiner M., Bonk A., Emerich H., van Bokhoven J.A., «In situ X-ray Absorption Spectroscopy of CeO.5Zr0.5O2-d at 1773 K». Poster, Fall Meeting of the Swiss Chemical Society, Catalysis Engineering and Technology Poster Session, EPFL Lausanne, 4.9.2015.
Presentations

- Bonk A., Maier A.C., Schlupp M.V.F., Burnat D., Battaglia C., Vogt U.F., „Ceria-based Ceramic Foams for Solar Thermochemical Redox Reactions“. 90th DKG Annual Conference & Symposium on High-Performance Ceramics, Bayreuth (Germany), 15.03.–19.03.2015.
Appendix

Presentations


GasOMeP – Gasoline Vehicle Emission Control for Organic, Metallic and Particulate Non-Legislative Pollutants

Publications

NOx Reductions – In-Cylinder Emission Reduction in Large Diesel Engines


CatPor – Catalysis in Porous Media for Automotive Applications


DuraCAT – Highly Durable Oxide-based Catalysts for Polymer Electrolyte Fuel Cells

- Binninger T., Schmidt T.J., Kramer D., «Electronic metal–support interactions as novel design paradigm for catalytic materials». Submitted.
HITTEC – High Temperature Thermoelectric Converter for Electricity Generation in a SOFEC System


Connect PV – Conductive Transparent Electrodes: a Competence Cluster for Highly Efficient Thin Film Photovoltaics


ADMIST – Advanced Understanding of Micro Structures in Fuel Cells and Batteries through X-ray Imaging

• Pietsch P., Hess M., Ludwig W., Elier J., Wood C., «Combining operando synchrotron X-ray tomographic microscopy and scanning X-ray diffraction to study lithium ion batteries», (Submitted)
• Pietsch P., Westhoff D., Feinauer F., Elier J., Marone F., Stampanoni M., Schmidt V., Wood V., «Operando X-ray tomographic microscopy on lithium ion battery graphite electrodes», (Submitted)

TeKaF – Temperature Dependent Ampacity Limit Modelling of Overhead Power Lines

Appendix

For full list of presentations, publications and patents since 2006 see website www.ccem.ch.

• peer reviewed papers
• other papers

HydroNet 2 – Modern Methodologies for the Design, Manufacturing and Operation of Pumped Storage Power Plants


Geotherm 2 – Geothermal Reservoir Processes: Towards the Implementation of Research into the Creation and Sustainable Use of Enhanced Geothermal Systems


MeAWaT – Methods of Advanced Waste Treatment

For full list of presentations, publications and patents since 2006 see website www.ccem.ch.

Peer reviewed papers:


Other papers:


Publications


SLIB – All Solid State Li-Ion Batteries based on New Ceramic Li-Ion Electrolytes


ISCHESS – Integration of Stochastic Renewables in the Swiss Electricity Supply System


IDEAS4cities – Integration of Decentralized Energy Adaptive Systems for cities


SECURE – Synergistic Energy and Comfort through Urban Resource Effectiveness


Publications


ARRMAT – ARRMATplus – Attrition Resistant Fluidized-Bed Materials and Methanation Catalysts


OPTIWARES – OPTImization of the Use of Wood as a Renewable Energy Source


RENERG2 – Renewable Energies in Future Energy Supply


SCHE-dual – Stable and Clean High-Efficiency Diesel and Dual-Fuel Combustion


Solar Fuels – Solar Thermochemical Production of Fuels from CO2 and H2O Using Ceria Redox Reactions


Appendix

Publications


Hy-Form – Formic Acid – Chemical Storage of Electrical Energy and On-Site Hydrogen Production for Use in PEM Fuel Cells


HyTech – Sustainable Hydrogen Utilization


For full list of presentations, publications and patents since 2006 see website www.ccem.ch.

- peer reviewed papers
- other papers
For full list of presentations, publications and patents since 2006 see website www.ccem.ch.

CCEM – Competence Center for Energy and Mobility


UFCEV – Ultra-Fast Charging of Electric Vehicles


DuraCAT – Highly Durable Oxide-based Catalysts for Polymer Electrolyte Fuel Cells


FAMSADI – Swiss High Energy Density Batteries – From Advanced Materials to a Safe Device


RENERG – Renewable Energies in Future Energy Supply


SuRHiB – Sustainable Renovation of Historical Buildings

- Stahl Th., Zimmermann M., Brunner S., Koebel M., European patent 2013 for aerogel Render (under preparation).
- Stahl Th., Zimmermann M., Brunner S., Koebel M., Empa license agreement with industry partner Fixit for aerogel Render, 2012.

SunChem – Bio-Synthetic Natural Gas from Microalgae


ARCHINSOLAR – Unique and Innovative Solution of Silicon Thin-Film Modules for Building-Integration

Patents


Contact

Competence Center Energy and Mobility CCEM
c/o Paul Scherrer Institute
5232 Villigen PSI, Switzerland

Phone: +41 56 310 2792
Fax: +41 56 310 4416
E-mail: ccem@psi.ch
Internet: www.ccem.ch

Urs Elber, Managing Director
Phone: +41 56 310 5733
E-mail: urs.elber@psi.ch

novatlantis – sustainability at the ETH domain
c/o Paul Scherrer Institute
5232 Villigen PSI, Switzerland

Phone: +41 56 310 2792
Fax: +41 56 310 4416
E-mail: info@novatlantis.ch
Internet: www.novatlantis.ch

Dr. Anna Roschewitz, Managing Director
Phone: +41 56 310 5078
E-mail: anna.roschewitz@novatlantis.ch