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EmpaNews

Magazine for Research and Innovation
Volume 11 / Issue 39 / January 2013

Fuss and Fumes

EMPA
Materials Science & Technology

More than just fuss and fumes

Toxic decay products
Car cooling agent is harming the environment 04

Even though these are both intensely studied at Empa. To be more precise: noise and airborne pollution and the sources thereof, and how to avoid or reduce them. Both are problems that are becoming increasingly important. Because high-density housing, mixed usage of entire neighbourhoods and an ever denser siting of the entire country are continuously pushing (annoying) noise levels, at least in urban regions. And to be blunt: noise sucks.

In order to suppress this noise we first need reliable information about where, when and how much noise is occurring. Empa researchers use facilities such as comprehensive 3D computer models and simulations for this purpose. The resulting noise maps then reveal where it is loudest in Switzerland (see page 14), i.e. where the situation is most critical.

It is also evident that Swiss cities such as Zurich and Geneva – which (apart from the noise) are attractive and trendy – are anything but peaceful oases. Any area where large numbers of people live and work together, use transport and build houses and roads is bound to be noisy every now and so often. The head of Empa's "Acoustics/Noise Control" laboratory who lives in an area affected by aircraft noise and myself, having lived at Rosengartenstrasse for several years when it was still the main transit route through Zurich, can tell you a thing or two about that.

However, besides noise, our quality of life is also being affected by greenhouse gases and other airborne pollutants. Empa researchers are examining their spread in the atmosphere with highly sensitive self-developed analytical instruments and computer models. This allows us on the one hand to discover who is emitting how much "filth" (at least at regional levels within Europe); on the other hand, said technologies can also be used for alternative purposes such as detecting aerosols leaking from tin cans (see page 8).

At the end of the day, all our research and development efforts have one common goal: to pave the way for a sustainable future thanks to innovative, resource-saving technologies and materials.

Speaking of which – on a more personal note: our valued readers can now also conserve resources in the form of paper by reading EmpaNews on their iPad – thereby enjoying numerous extra benefits such as multimedia features. Give it a try by simply searching for "EmpaNews" in the iTunes store and subscribing to it (free of charge, of course). In German or English.

Enjoy reading the current issue of EmpaNews!

Michael Hagmann
Head Communications

Cover

A Qantas Boeing B747 on its approach (picture: wikimedia.org) – an extremely drastic example of the problems that occur when transportation routes are close to residential areas. Empa examines noise sources and propagation and traces the routes taken by airborne pollutants.

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Imprint

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Published quarterly

ISSN 1662-7768

Acid from automotive air conditioning

R-1234yf, the new cooling agent for automotive air conditioning systems, is not just easily combustible – in the atmosphere it also decomposes into trifluoroacetic acid, an extremely persisting plant toxin. Empa researchers have calculated how much of this substance is coming down where.

TEXT: Rainer Klose / PICTURES: Empa

Atmospheric scientist Stephan Henne checks the rain collectors on the Empa campus. The samples also contain traces of trifluoroacetic acid – a toxin that originates from car air conditioning systems. For Henne systematic monitoring of this substance would be desirable.

Is the new cooling agent an advantage or a drawback? Ultimately, this is the question that should be addressed before vehicle manufacturers decide to use R-1234yf in automotive air conditioning systems. Because tiny amounts of the chemical "escape" again at some stage. All A/C systems have leaks somewhere – and this is how, over time, considerable amounts of R-1234yf are gradually being distributed throughout the environment by the global vehicle fleet.

A toxic acid

There is nothing particularly mysterious about the substance in question. The coolant known as R-1234yf is tetrafluoropropene, a simple molecule consisting of hydrogen, carbon and fluorine with the chemical formula $H_2C = CF\text{-}CF_3$. The benefit of this substance: when it escapes from the A/C system it decomposes in the air within ten days. Unlike its predecessor, it makes much less of a contribution to the greenhouse effect, and it is harmless to the ozone layer. The disadvantage: its decomposition results in trifluoroacetic acid (chemical formula $CF_2\text{-}COOH$), an extremely stable molecule that is not broken down in nature. The acid accumulates almost permanently in soil, water and organisms. It is also toxic to plants, particularly some types of algae.

What happened before

This bears the question: who would want to introduce such a substance, and why? A brief look into the past provides the answer: in the mid-1980s a hole was discovered in the ozone layer above Antarctica, and so-called CFC's (chlorofluorocarbons) were said to be the cause. In September 1987, the global community agreed to ban the production of such chemicals in the Montreal Protocol, signed by almost 200 nations.

Hydrochlorofluorocarbons (HFC's) were introduced as their replacement – such as R134a (tetrafluoroethane), which has been used in automotive A/C systems since then. It has no damaging effect on the ozone

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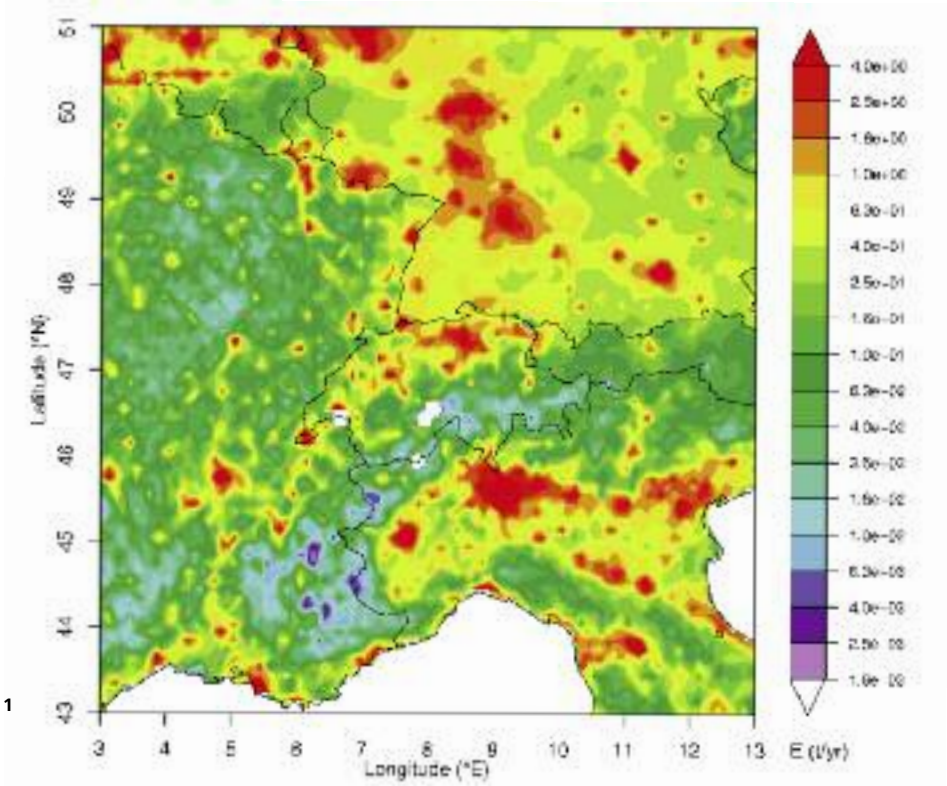

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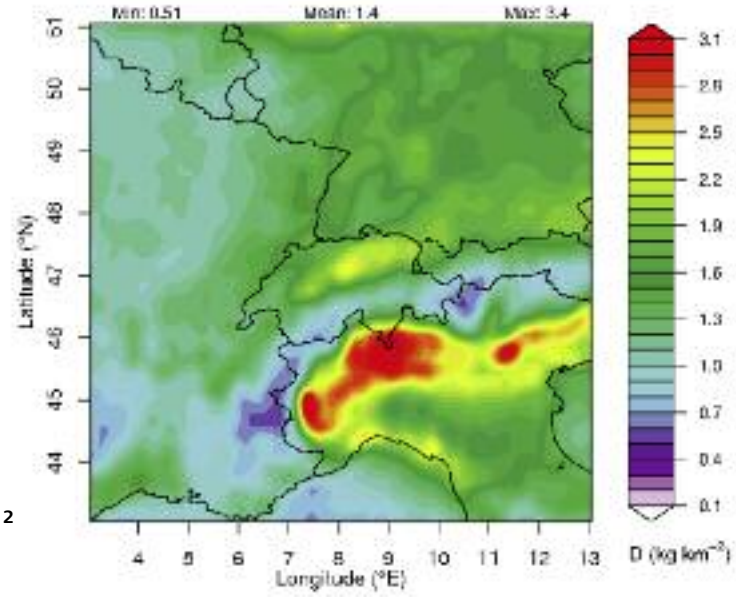


2

A/C cooling agent R-1234yf will be mandatory for new cars from 2013 onwards.

1
Large map: the Empa simulation shows where particularly large quantities of the substance have escaped into the atmosphere: the metropolitan areas of Stuttgart, Zurich, Geneva and Milan are clear to see.

2
Small map: R-1234yf decomposes into trifluoroacetic acid, an indestructible plant toxin. In precipitation it gets back to the ground. With up to three kilograms per square metre Northern Italy and the canton of Tessin are particularly affected.

layer – but staggering potential as greenhouse gas. It has a GWP value ("Global Warming Potential") of 1430 – i.e. its greenhouse effect is 1430 times higher than the one of the carbon dioxide, CO_2. The EU intervened, and the substance was banned for use in automotive A/C systems. After some lengthy delays, the ban has come into force on December 31, 2012. From this day on, no new vehicle model with this cooling agent will be permitted in the EU.

The automotive industry searched for and found another replacement: R-1234yf – the aforementioned tetrafluoropropene. It doesn't damage the ozone layer, it has little greenhouse effect (GWP = 4) – but unfortunately is not exactly harmless. In an extreme case tetrafluoropropene is flammable: if it is sprayed directly onto a hot exhaust, it can ignite. If this occurs, toxic and caustic hydrogen fluoride (HF) is released, which has led to protests from Fire Brigade unions and motoring organisations. To date, only Daimler has refrained from its introduction. All other car manufacturers are hanging on to R-1234yf.

Empa comes into play

So how damaging really is a substance that can escape from millions of automotive A/C systems and then turns into trifluoroacetic acid? Where does it go in the atmosphere, and where is it rained down again? Is the environment affected? Stephan Henne and Stefan Reimann, two atmospheric scientists from Empa, started calculating.

To date, about 25,000 tons per year of the old R-134a cooling agent have been released into the atmosphere in Europe. The researchers calculated that each year be-

tween 11,000 and 19,000 tons of the new R-1234yf will escape into the atmosphere by 2020, taking improvements in the sealing and efficiency of the A/C systems and an increase in the number of vehicles into account. This creates an equal amount of trifluoroacetic acid – i.e. about 19,000 tons, which is washed out again in Europe over the course of the year.

Henne and Reimann ran two different calculation programs on Empa's high-performance computer: Flexpart, a so-called Lagrangian model, which had already been used to calculate the volcanic ash cloud from the Eyjafjällajökull eruption in 2010. In the model, R-1234yf emissions were assigned to individual air packages, which then moved through the model atmosphere. Empa extended the model with simplified chemistry, which describes the conversion of the substance into trifluoroacetic acid and how it is washed out by rain. The atmospheric chemistry model from the University of Bristol, CRI-STOCHEM, was used as the second model. In this case the atmosphere is simulated in more detail, but the transportation of the molecules is calculated using a somewhat less sophisticated model. Both programs calculated the pollutant's concentrations in the air and in rain over an entire year, in order to detect seasonal differences.

More trifluoroacetic acid in the Southern Alps

The result can be seen on the coloured maps (left): R-1234yf mainly gets into the air where a lot of cars are driving (and parking). The metropolitan areas of Zurich, Stuttgart, Geneva and Milan are clearly recognisable in the simulation. The quantities of trifluoroacetic acid that are rained down during the course of the year are greatest south of the Alps, through northern Italy and in the canton of Tessin. However, the highest concentrations in the rainwater occur in locations where it rains less often, allowing trifluoroacetic acid to first accumulate in the air. This is on the lee side of the Alps, west of Turin, and also at the east coast of Italy, the south-west of the Czech Republic and in some areas of North Africa.

So how dangerous are the expected concentrations? There is no need to panic, says Henne. Although the concentration of trifluoroacetic acid in surface water is already at a detectable level and would increase further due to the introduction of R-1234yf, it is currently still a hundred times lower than the threshold that would harm the most sensitive fresh water algae. Exact data about earlier concentrations is, however, lacking. "We should start systematically monitoring the concentration of trifluoroacetic acid in rainwater, streams, lakes and the sea in the near future", recommends Henne.

And we should consider the advantages and drawbacks of the new cooling agent. Especially given that an effective and cheap alternative has long since been available – namely CO_2. This gas, which occurs in large quantities in exhaust, can also be used as a coolant. The A/C system would only have to be somewhat bigger and stronger. The reason why car manufacturers are not tackling this straightforward technical development remains a mystery as far as atmospheric scientists are concerned. //

Aerosol cans are really something. In order to spray hairspray, paint or shaving foam, the pressurised container often contains a highly explosive mixture of propane and butane as propellant. In order to prevent accidents from occurring during transport or at the customer's, each individual can is painstakingly checked for leaks in a water bath during manufacture. Rising bubbles indicate which spray cans may not be allowed to leave the factory. However, this process is time- and energy-consuming: the water must be heated to 50 degrees C and purified after each test, and the cans also have to be dried afterwards. Wilco, a specialist for leak testing machines based in Wohlen in the canton of Aargau, was looking for new, commercially competitive technology that can detect the propane-butane mixture that is used in aerosol cans within fractions of a second. The goal: the new equipment should not just detect leaks faster, but also be more compact than the traditional water bath and be capable of inspecting at least 500 cans per minute.

1

The Aerosol Sniffer

The minutest traces of airborne pollutant can be detected using quantum cascade lasers. This technology is also suitable for industrial use. It could, for instance, be used to "sniff out" propellants escaping from defective aerosol cans within fractions of a second. Together with an industrial partner, Empa has developed an analytic device that can prevent leaky spray cans from leaving the factory.

TEXT: Martina Peter / PICTURES: Empa

Quantum cascade lasers are also suitable for use in industry

"This project was extremely exciting for us," says Lukas Emmenegger, head of Empa's "Air Pollution/Environmental Technology" laboratory. "It was an almost perfect opportunity to prove that our gas analysis system using quantum cascade lasers, with which we successfully detected CO_2 on the Jungfraujoch several years ago and decrypted its isotope signature, can also be used profitably in industry".

Whereas the objective on the Jungfraujoch was to make an accurate distinction between the different isotopes, the new aerosol sniffer will "only" have to detect traces of propane and butane. However, the system must be lightning fast and extremely sensitive. The new device, containing a semiconductor laser in the mid-infrared range, should be able to detect escaping gas in the ppm range (i.e. one molecule of the propellant per one million air molecules) in less than a tenth of a second. The specification from Empa's industrial partner also stipulates that it must do this more cheaply than the current measuring devices.

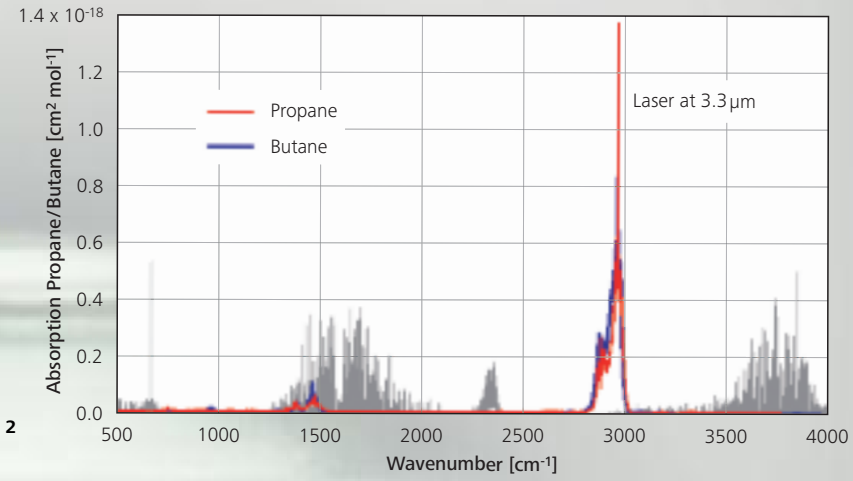
Supported by the National Centre of Competence in Research (NCCR) "Quantum Photonics", Empa and Wilco constructed a test facility that by far surpasses initial expectations. Its centrepiece is an innovative Fabry-Pérot quantum cascade laser that had been developed at the ETH Zurich only in March 2012. In comparison to the laser diodes that are used in telecommunications, for example, the quantum cascade laser produces light with a wavelength of 3 micrometres, ideal for detecting propane and butane.

The gas samples to be measured are sucked in and "bombarded" by a pulsating laser beam in a measuring cell. If certain molecules are present (in this case propane or butane) they absorb the laser light, which is picked up by the detector. The system issues the command to reject the leaking can in less than a tenth of a second.

Successful Prototype

"The tests were extremely successful, the prototype worked," rejoices Empa project leder Jana Jagerska. The device even manages to inspect up to 900 cans per minute. What's more, the "sniffer" only requires a fraction of the energy of the water bath method. And yet another bonus: the "Wilcomat" – as the instrument is termed – does not just detect traces of propane and butane but also tiny quantities of many other organic substances such as drugs and solvents.

Wilco has already filed a patent for the ultra-fast analytic device, and a first complete system is under construction. A prototype was exhibited at the Achema in Frankfurt am Main this summer, the world's biggest trade fair for chemical technology, environmental protection and biotechnology. Heino Prinz, the Research and Development Manager at Wilco AG, appreciates the collaboration with Empa. The complex question was tackled in a professional way thanks to excellent know-how and state-of-the-art technology. "With the Wilcomat AE/GD1 that has been developed by means of this cooperation, we now have a product that allows us to perform the testing required to meet the safety requirements for the aerosol can production process," says Prinz. //



2

1
Components of the aerosol sniffer are being presented at a trade fair. The first instrument is already being deployed.

2
Absorption spectrum of propane and butane when the gasses are "seen" in laser light of three micrometer wavelength. The process is based on this principle.

“Aircraft noise comes from above – like a cold shower”

The acoustics experts at Empa have been tackling noise prevention in Switzerland for a number of years. Nowadays this is mainly done using computer modelling, which allows experts to predict the noise level anywhere in the country, a method developed at Empa.

TEXT: Rainer Klose / PICTURES: Wikimedia.org

Kurt Eggenschwiler, head of the "Acoustics/Noise Control" laboratory at Empa, is anything but a dull collector of statistics. His work involves the human need for peace and quiet, and the noise that disturbs it. Psychology plays a part in this, and occasionally philosophy, too. EmpaNews asked him what his team is currently investigating. However, Eggenschwiler prefers to start the conversation with a question: "What is noise, actually?" – only to answer it himself: "Noise is undesirable sound."

By nature of its design, a country like Switzerland, with sparsely populated mountain regions and a mere 8 million inhabitants swarming around the lowlands, is bound to have a noise problem. There are arterial highways running through the settlement areas, there are civilian and military airports. This is bound to lead to never-ending disputes. Eggenschwiler and his team work in the midst of this conflict-laden area. The erstwhile noise measurements have long since been replaced by computer simulation. The noise map of the country (see pages 12 and 13) are no longer created on the basis of individual measuring points, but are calculated on a computer. Most of the methods for doing this were developed at Empa.

The complicated cases end up at Empa

"The majority of noise calculations for street and train noise," says Eggenschwiler, "are carried out by engineering offices nowadays." Calculation models such as sonROAD (for street noise), sonRAIL (for railway noise) and sonARMS (for shooting ranges and military noise) – all developed at Empa – are the basis for the Swiss noise database sonBASE, which is managed by the Federal Office for the Environment (FOEN).

"Only" very special cases end up at Empa: How much noise do parked railway carriages make at night? How can the noise emission of church bells be assessed? How much worse is a plane landing at night compared to a plane landing during the day? "In order to answer these questions, we cannot just measure the noise, we must assess its impact in cooperation with psychologists," says the Empa researcher. When setting regulatory thresholds for how much noise can be tolerated at any given location, the number of noise-afflicted people plays an important part. And some of the results are remarkable: "We have a large number of German immigrants here. Did you know that more Germans are affected by aircraft noise in Switzerland than in Germany?" He laughs.

But before it gets political, Eggenschwiler prefers to explain the difference between aircraft and road noise. He quickly draws a road on a piece of paper, then adds one, two, three rows of houses next to it. "A regular employee lives here." He points at the row right next to the road. "When he is promoted, he moves backwards, away from the road". The pen points at the second row, then the third. "And there, at the edge of the forest, is where his boss lives." The problem is, aircraft noise doesn't take social status into consideration. "It affects everyone. Suddenly and from above. Like a cold shower," says Eggenschwiler. When people living at the edge of the forest are affected, they will make themselves heard. And then politics has a problem.

«Musik wird oft nicht schön gefunden, weil sie stets mit Geräusch verbunden.»

(Wilhelm Busch, German poet and caricaturist, 1874)

Individual flights added up in the computer

Fortunately, aircraft noise pollution today can be clearly quantified, thanks to powerful mainframes. Empa uses the aircraft noise program FLULA. For each year Eggenschwiler and his colleagues obtain arrival and departure data from Zurich Airport, and then simulate each individual flight on Ipiaza, Empa's high-performance computer. Topography and population density are also taken into consideration. Finally, the researchers reduce the detailed results to a single figure: "How many people are affected? How many people are rudely awakened at night?" In other words, the basis for the Zurich Aircraft Noise Index, a project that would have been impossible twenty years ago.

The calculation of road and railway noise is even more detailed, considering even the effect of the weather on noise propagation. It is noisier during atmospheric inversion, and the wind direction also plays a part. The calculation even takes obstructions and reflections into account. Does a building block noise from a railway? Is noise muffled by a forest? Or is sound reflected and intensified when it encounters a house wall?

In future, the aircraft noise calculation method will undergo further refinement with the goal of also simulating low-noise departure and arrival procedures. The Federal Office of Civil Aviation (FOCA) recently mandated Empa with this task. //

What can you do if affected by noise?

Besides working on calculation and noise mitigating methods and technologies, Empa occasionally acts as a neutral expert. However, for the majority of disputes Kurt Eggenschwiler refers people to communal, cantonal and federal noise protection specialists in charge. Telephone numbers can be found at *www.laerm.ch*.

An interactive noise map of Switzerland, which can be zoomed in to the level of side streets, can be found at *map.bafu.admin.ch*

The simulated wind farm

What does a wind turbine at the edge of town look like – and above all: how much noise does it emit? Empa researchers are developing computer models that can simulate the characteristic sound of a wind turbine at its planned location. Colleagues at ETH Zurich are in charge of the visual simulation.

TEXT: Rainer Klose / PICTURES: Empa

Good evening. Welcome to today's noise forecast". With these words Empa researcher Kurt Heutschi will be able to welcome his audience in a few months once his research project will be completed. Heutschi is crossing the line, in a manner of speaking: the guild of acoustic experts has, so far, been mainly preoccupied with calculating the noise pollution (see page 8) – now they want to generate noise themselves. Specifically, the virtual noise of a wind turbine that doesn't yet exist.

The goal of the VisAsim project (Visual-Acoustic Simulation for Landscape Impact Assessment of Wind Farms) that is jointly being worked on by ETH Zurich and Empa is to create a realistic simulation of the visual and acoustic impact of a wind turbine. The rotating turbine will be displayed on a screen where even the blades of grass on the meadow will move. The observer will hear the operating noise of the wind farm from a Home Cinema Surround Sound System. The intention is to make it possible for local councils, investors, and also action groups and environmental activists to evaluate a wind farm even before it is approved.

Kurt Heutschi looks after the acoustic part – the visual simulation is being developed by the PLUS research group (Planning for Landscape and Urban Systems) at ETH Zurich. The project,

which is funded by the Swiss National Science Foundation, started in 2011 and will run through 2014. The first simulation video is already on Youtube (youtu.be/1tsHPnb5PzE) and shows an animated landscape with wind turbines. It is based on the CryEngine3 software, developed by the German computer game manufacturers Crytek.

For Heutschi and his colleague Reto Pieren things weren't quite as simple: synthesisers for machine noise do not yet exist. They had to build everything from scratch. First, they generate the emission signal, depending on turbine model and wind speed. Then the location of the listener is set, and the propagation of the sound is simulated. Is the wind turbine on a hill, or a level surface? Is the noise muffled by strips of forest or blocked by roofs? Finally, different weather conditions are considered. A quiet evening? A morning with thick ground fog? Or a strong breeze that drives the noise straight at the listener?

But it doesn't stop there: the impact of noise also depends on the background noise. "Wind turbines don't disturb anything like as much during strong winds," says Heutschi. "Bushes rustle, the corner of the house whistles. There's enough noise all around." However, the disturbance is particularly bad when the wind is moderate. The simulation must be particularly exact in this area. At the moment, the Empa team is working on simulating the edges of forests. Heutschi: "We differentiate between coniferous and deciduous forests – and also between summer and winter, of course." The simulation divides the edge of the forest into sections, 30 metres long, and simulates the noise as a point source – in order to keep the calculation simple.

Finally, the noise mixture is fine-tuned with the observer's location and played back using a surround sound system with five speakers. The observers will see the wind turbine on the screen and hear the individual noise components from where they would come from in reality.

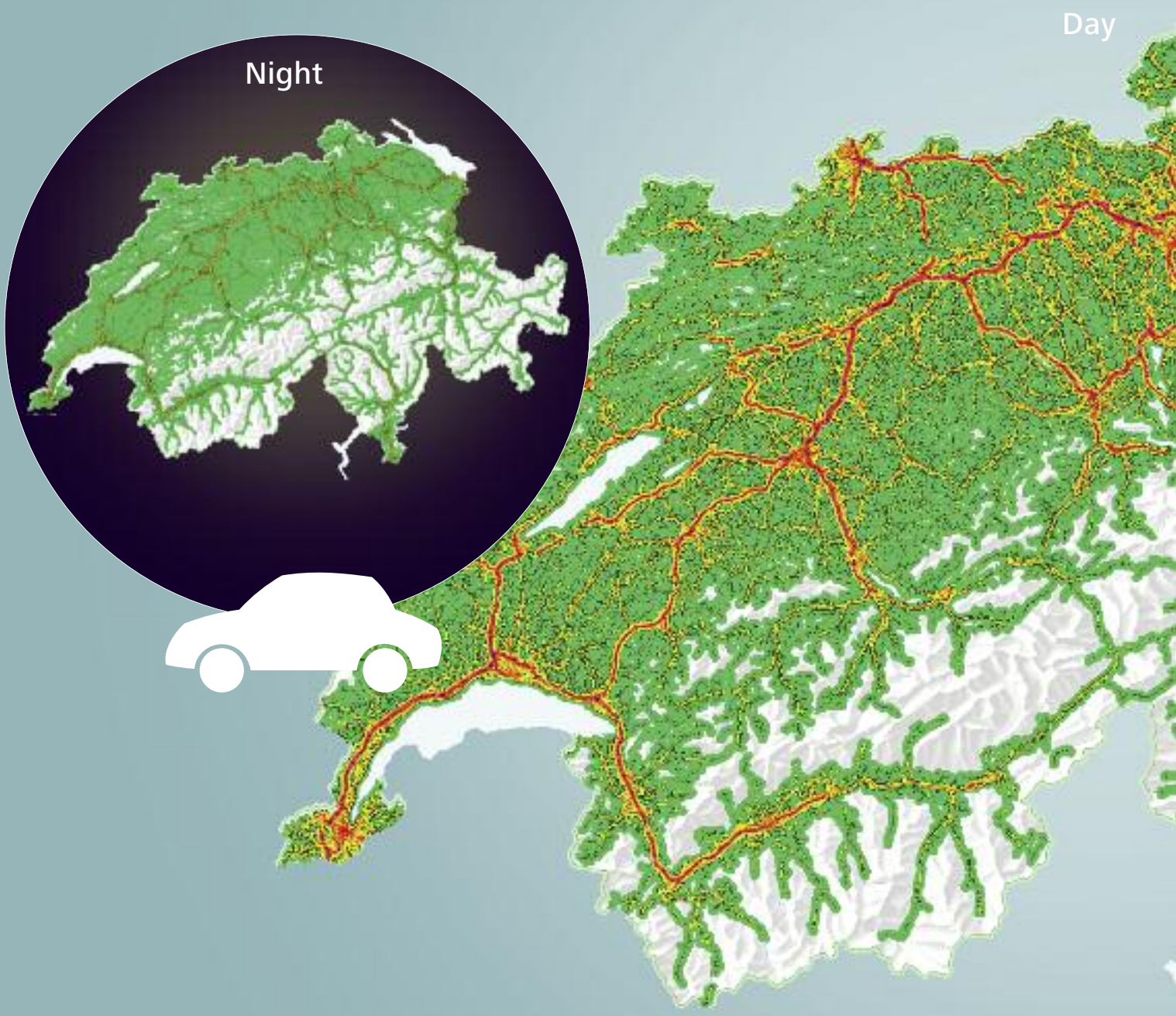
The "wind turbine home cinema" is still installed at Empa. But the simulation system will soon be moving to ETH Zurich, where test persons will compare the simulation with actual recordings. This feedback will give the method its final polish. //

Top: acoustic specialist Kurt Heutschi demonstrates the visual and acoustic simulation of a wind turbine to a group of test persons. Now it's a case of fine tuning: is everything realistic? Large picture on left: wind farms in the middle of a harbour area in Gothenburg.

Video:
Simulation film of the VisAsim project

An initial simulation film shows an animated landscape with wind turbines. Based on the CryEngine3 software from computer game manufacturer Crytek.

youtu.be/1tsHPnb5PzE
For Smartphone users: scan QR code (with the "Scanlife" app, for example)



Switzerland – not the quietest of countries

Cantonal roads and motorways run through Switzerland like blood vessels in the human body, supplying the country with people and materials. The large map shows noise pollution caused by traffic during the day – from 6am to 10pm, and the small map shows the levels during the night from 10pm to 6am. The motorways are clearly evident during the day, and there are also concentrations of noise in the metropolitan areas of Zurich, Basel, Berne and Geneva. It becomes quieter at night, even in the densely populated Mittelland area – the level is between 40 and 45 dB.

Aircraft noise problems only affect small parts of the country, but the effect is more severe. Only the airports in Zurich, Basel and Geneva are active from 10pm to 6am. The map shows the modified approach routes to Zurich airport during the night (status: 2008).

Source: "Lärmbelastung in der Schweiz – Ergebnisse des nationalen Lärmmonitorings SonBase. 2009".
PDF download available from *www.bafu.admin.ch/laerm/*

Emissions
In decibels (dB)

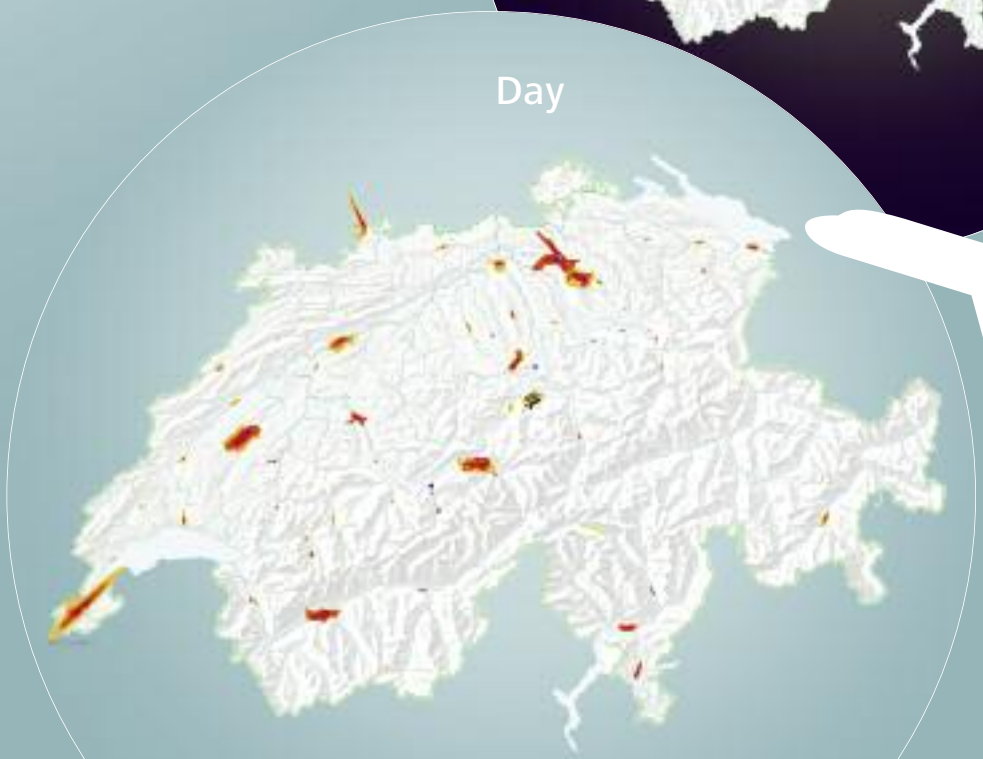
- ≥ 75
- 70 – 74.9
- 65 – 69.9
- 60 – 64.9
- 55 – 59.9
- 50 – 54.9
- 45 – 49.9
- 40 – 44.9
- < 40

Day: 6 – 22 hrs.
Night: 22 – 6 hrs.

In comparison
Rustling leaves: 25 – 30 dB
Quiet house: 35 – 45 dB
Normal discussion: 50 dB
Frequent wakening during the night from 60 dB

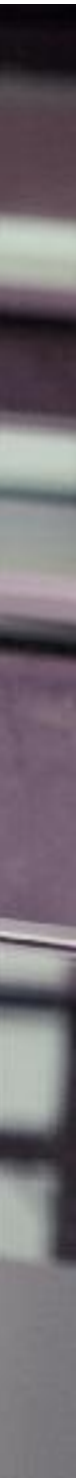
Website:
How loud is it in your area? Zoomable noise map from the Federal Office for the Environment

map.bafu.admin.ch
For Smartphone users: scan QR code (with the "Scanlife" app, for example)



«There is a great potential in US research experience with

combining European and the culture of this country.»



Chemist and nanocrystal expert Maksym Kovalenko is in the process of establishing his workgroup at Empa. He talked to EmpaNews about his return to Europe after several years in the US, the inner life of future lithium ion batteries – and his "welcoming marathon" in Switzerland.

INTERVIEW: Rainer Klose / PICTURES: Empa

I have taken a peek at your CV: You were born in the Ukraine, did your Ph.D. in Linz and held research positions in Berkeley and Chicago. What brought you to Switzerland?

Well, to be honest: if you draw up five criteria to determine where you want to do research and live, in my opinion, Switzerland is the only country that holds a top ranking in every discipline. I also had offers from the US and from Germany but when you compare the locations, you quickly realise that Switzerland simply has no disadvantages. For example, I had a few offers from US universities that were on a similar level, but I found the quality of life there to be lower. Moreover, I am quite familiar with the European way of doing research, due to my doctoral studies in Austria.

What do you mean? Is it not the same all over the world?

As a scientist in Switzerland and Germany you can pursue a longer term strategy than in the US. Over there, they are mainly interested in quick wins – and there sometimes is a tendency to hype your successes, i.e. to "oversell" them. A lot of showbiz going on over there.

What is the reason for that?

It's the way of funding research. In order to obtain funds, you have to keep proving how unique your work is – even though that is not always the case. You can be much more honest here in Europe. However, I can't deny that things are extremely dynamic in the US. But that's precisely what makes strategic research more difficult in the States.

Grant for nanocrystal research

The European Research Council (ERC) recently awarded the "ERC Starting Grants" for the fifth time. One of the prize winners was Maksym Kovalenko (30), professor at the Laboratory for Inorganic Chemistry at ETH Zurich and group leader at Empa. The 1.8 million Franc grant will allow him to quickly establish his own team.

Already in his studies Kovalenko, who was born in the Ukraine, specialised in nanotechnology, he obtained his doctorate in Linz and then worked as a postdoc at the University of Chicago before joining Empa and ETH Zurich as an assistant professor. Kovalenko is investigating so-called nanocrystals. These have unique properties, but in order to use them for new technologies it must first be possible to integrate nanocrystals in other nanocrystalline solids. In his ERC project Kovalenko wants to better understand and control, amongst other things, the surface chemistry of nanocrystals.

>>

Your research topics are fairly basic – meaning that things will not be appearing in our daily lives within the next ten years or so.

We pursue both aspects. On the one hand, we carry out curiosity-driven research in order to understand basic processes; but we will also be investigating things that are of interest to industry such as lithium ion batteries. This is an extremely interesting and important topic. A topic that I have not worked on before, by the way. This is where the strategic element that I mentioned before comes in.

What happens when you start to work in a completely new field? Do things start to work out straight away?

Oh yes! During our initial investigations it emerged that some methods that we developed to manufacture other materials were perfectly suitable for the use in lithium ion batteries. We were therefore able to tie in with our experiences in other areas in an extremely efficient way.

What exactly are these methods? Can you explain them?

They are ways of producing nanocrystals that are extremely small and yet uniform. A great deal of modern battery research involves the use of extremely fine particles, and mixtures thereof, that are becoming increasingly complex.

How large are these crystals, and what makes them so interesting?

These nanocrystals can be the size of molecules, i.e. just a few nanometers, up to 100 nanometers. The most interesting ones are those that are smaller than 20 nanometers. The surface is extremely large in comparison to the volume – and surface and quantum effects start to occur; we refer to them as "quantum dots". Our research is particularly focused on chemistry that occurs on surfaces. There are many different kinds of interactions: there are layers that wrap the crystallite in a protective "skin" of sorts, and there are other layers that foster and accelerate chemical reactions. That is extremely important but often also very difficult to understand.

That sounds like a completely new type of chemistry. Totally different from what I was taught 25 years ago. Is the chemistry of the 20th century outdated?

These nanocrystallites have been known for decades. They were then referred to as colloidal dispersions or systems. However, new tools are now available for examining these materials closely. Back in those days they were "blind" to a certain extent – and could not yet recognise many of the properties of these nanocrystals. Not only have the chemists become smarter, but they also can "see" much better nowadays. We can now explain how a material's macroscopic properties arise from its nanostructure.

What do these nanocrystals that you are interested in consist of?

On the one hand, we work with semiconductor materials such as gallium arsenide, on the other hand with tin – a metal that is extremely cheap and available in large quantities. It is used as coating on every can. But is can also be found in lithium ion batteries, where it could play an important part in the future.

How big is your team at the moment, and how will it fit into Empa's research portfolio?

At present, my group consists of three Ph.D. students and three postdocs. Next year, we hope to be up to a total of ten to twelve scientists. I am already collaborating closely with several other Empa labs, e.g. the Electron Microscopy Center. And initial projects are already in the pipeline together with Ayodhya Tiwari who is researching flexible solar cells. These will be starting in 2013.

«Modern battery research involves the use of extremely fine particles, and mixtures thereof, that are becoming increasingly complex.»

How will you divide your team between the research facilities at Empa and ETH Zurich? And how will you split yourself?

As far as the lab work is concerned the matter is clear: complex chemical syntheses are conducted at ETH Zurich, many other syntheses, analyzes and tests are carried out at Empa. It will be my job to become familiar with both campuses in the coming year. I really want to belong to both communities and not just be a visitor. In order to network myself scientifically, I would like to get to know as many of my colleagues as possible in the near future. This will not be easy – I have counted them. The Department of Chemistry and Applied Biosciences at ETH Zurich is about the size of Empa. There are 50 chemistry professors at ETH. Here at Empa, there are about 50 group leaders. This represents a good opportunity for me to hatch some useful ideas in both institutes.

Plenty to do for you.

Correct. Even if I meet a new colleague every third day, it will take me the whole of next year. (laughs) //

HITTEC – a turbo-charger for fuel cells

Waste heat from a fuel cell can also be converted into electricity. In the HITTEC project, Empa researchers are collaborating with Hexis AG to develop a thermoelectric converter that increases the efficiency of fuel cells: this should make them provide up to 10 percent more power. However, suitable materials that meet the wide range of requirements first need to be developed.

TEXT: Martina Peter / PICTURES: Empa

When a solid oxide fuel cell (SOFC) converts chemically bound energy into electrical power, temperatures of up to 900 degrees C occur. This waste heat is currently only used for domestic hot water. Andre Heel, chemical engineer and research coordinator of the strategic partnership between Empa and Hexis AG, wants to do something entirely different: he would like to recover valuable electricity from the (waste) heat using thermoelectric converters. “This does not just increase the efficiency of the fuel cell system”, says Heel. “Highly-efficient energy conversion technology also helps to conserve our fossil and renewable energy resources in the most effective way”.

Under Heel’s management, Empa started the four-year HITTEC project together with Hexis. It is devoted to the further development and optimisation of materials for thermoelectric converters (TECs). The new materials will then be integrated in SOFCs in the next step.

Thermoelectric converters for high temperatures

TECs are already commercially available. They are “stuck” to the heat-emitting walls of engines or furnaces like band-aids. The modules consist of a semiconductor material with p-type and n-type doping. If there is a temperatures difference between the two sides, an electric current is produced. At an atomic level, this means that

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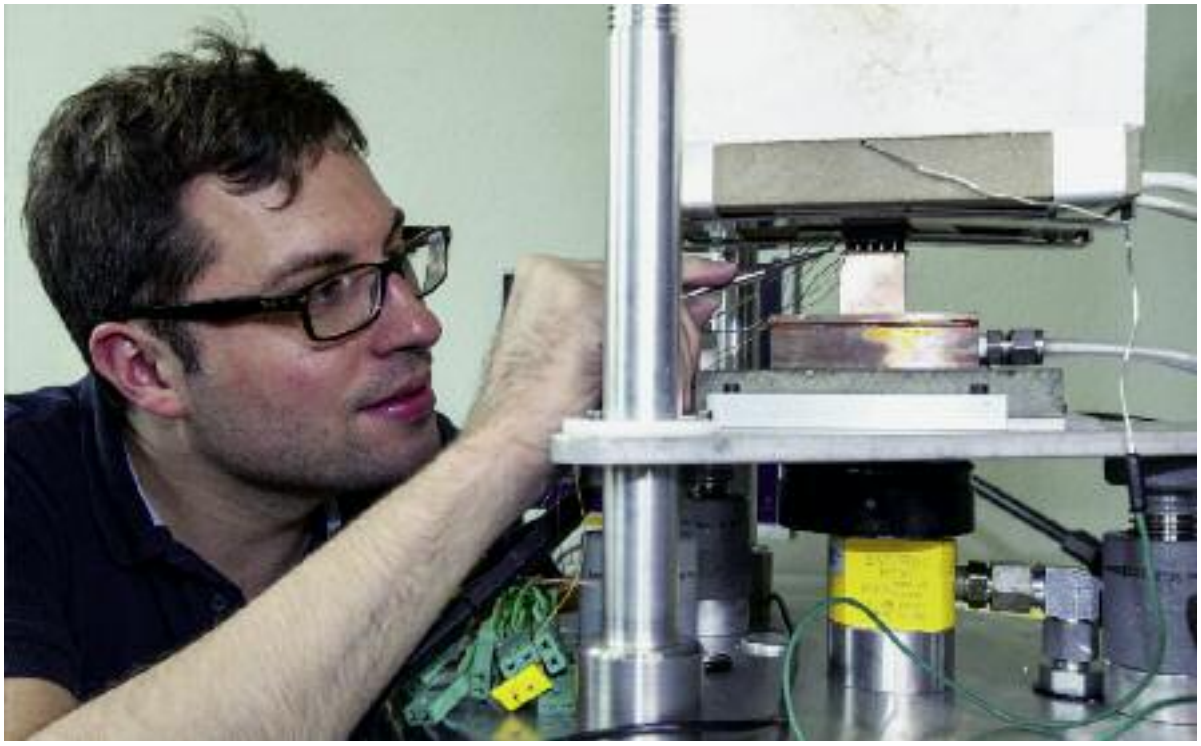


1
Philipp Thiel brings a prototype of the HITTEC thermo-converter to the test bench.

2
The internals of a high-temperature solid oxide fuel cell (SOFC). Thermo-converters will convert the heat lost from SOFCs into electricity.

there is more movement in the freely moving electrons at the warm side than at the cold side because they have more energy. Since each system attempts to achieve the most favourable condition with regard to energy, the electrons therefore move from the warm to the cold side. The resulting "migration" of the electrons can be used to generate electricity.

However, 300 degrees C is the upper limit for the latest generation of TEC modules. Converter materials that can withstand temperatures of up to 600 degrees higher do not exist. At least not yet. However, novel High Temperature Thermoelectric Converters (HITTECs) will have to be more than just temperature resistant: "They will even have to combine several conflicting properties", explains Heel. For example, they will have to be electrically conductive like metals, have a high degree of thermoelectric power like semiconductors, and may only conduct little heat, like insulators.

For this reason, it is first and foremost a matter of finding good compromises in the material properties. Only those materials whose chemical composition hints at a high efficiency will be short-listed.

Perovskite-type metal oxides have proven to be ideal candidates (see box 1). The team of Anke Weidenkaff, head of Empa's "Solid State Chemistry and Catalysis" laboratory and professor of chemistry and biochemistry at the University of Berne, has set its sights on these materials because they are chemically and thermally stable, non-toxic and can be manufactured in large quantities at low cost. They are also conductive and have good thermoelectric properties. "These oxides are extremely stable in air, and are therefore suitable for applications at temperatures of up to 1000 degrees C", explains Weidenkaff.

The "HITTEC" project

The "HITTEC" project (Integration of high temperature thermoelectric converter for electricity generation in a solid oxide fuel cell system)

Partners
- Empa, Laboratory of Solid State Chemistry and Catalysis
- EPF Lausanne, Laboratory of Physics of Complex Matter
- Zurich University of Applied Sciences, Institute of Computational Physics
- ETH Zürich, Institute for Theoretical Physics
- Centre National de la Recherche Scientifique, Laboratoire de Cristallographie et Science des Materiaux)
- Hexis AG

Funding
- Competence Centre Energy and Mobility (CCEM)
- Swiss Federal Office of Energy

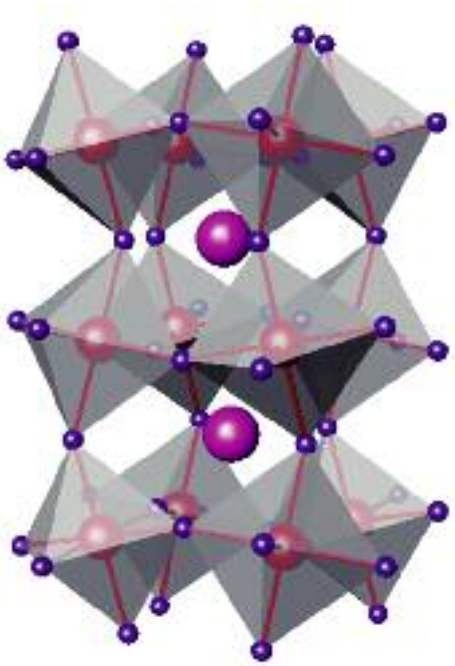
The **Swiss Thermoelectric Society** has its headquarters at Empa. Its members are regularly informed about developments, courses and projects in the field of thermoelectricity and invited to events. *http://thermoelectric.ch*

Video:
Thermo-electrical converter
(German language)

youtu.be/wj2BNbTn5jU
For Smartphone users: scan QR code
(with the "Scanlife" app, for example)

Perovskite-like metal oxides

Perovskite-type metal oxides are compounds with the chemical formula of ABO_3 – whereby A and B stand for transitional metals, and O is Oxygen. Due to their high temperature, pressure and oxidation stability, they can be used in many different areas and non-hazardous. In a naturally-occurring perovskite, A is calcium and B is titanium, for example. Thanks to its flexible but stable crystal structure, the chemical composition of the perovskite can vary considerably. By specifically substituting the metal ions, but also the oxygen, the physical properties of the materials can be optimised, i.e. their magnetic behaviour, their electrical and thermal conductivity, their colour and much more. The goal is to take low-cost and environmentally friendly elements and synthesise new materials for various applications. Besides being used as thermoelectrics and in fuel cells, perovskites are also suitable for rechargeable batteries in electric vehicles and catalytic converters, to name but a few devices.



Lab work

One of her PhD students, Philipp Thiel, is currently dealing with the material aspects of the metal oxides, poring over literature, busying himself with theories and looking for material compositions, with which the required characteristics can be achieved. During preparatory work, Weidenkaff's team identified compounds made from calcium manganate that had been substituted with tungsten as being particularly promising. Synthesised from nanoparticles, Thiel now compresses and sinters perowskite in as pure a form as possible. He characterises powder samples and compressed, round disks in the Empa laboratory using a wide variety of methods; he checks the thermal conductivity using differential calorimetry, determines the electric conductivity and examines their temperature conductivity in the laser flash absorption machine.

He is assisted by physicist Gesine Saucke, whose PhD thesis also deals with the development of TECs that are stable at high temperatures. She is working on a project that has been co-funded by the Swiss Federal Office of Energy. In this project, the plan is to utilise waste heat from the foundry melting furnaces of industrial partner VonRoll Casting.

Empa has developed a new type of measuring system, especially for HITTECs, that can subject the HITTEC modules to extremely high temperatures. Any soft spot will soon become evident. "However, we will have to come up with something for the solder points that connect the newly developed material to the wiring", says Thiel. Normal solder will melt at these temperatures.

Thermal converter integrated in the fuel cell

But the materials scientists aim even higher: "We do not just stick our converters onto the fuel cell", explains Weidenkaff. On the contrary, the Empa researchers want to combine fuel cell and converter and construct a unique new system. "A crazy idea", as Anke Weidenkaff admits, because her idea makes the project even more complicated. The thermoconverter is going to be directly attached to one of the electrodes, i.e. right at the point where the chemical reaction of the fuel cell is going to take place. Weidenkaff sees a huge opportunity in the similarity of the used materials: the conductor system made from high-temperature ceramics in the SOFC consists of similar materials to the perovskite-type metal oxides for the HITTECs.

In order to achieve this ambitious goal a wide range of know-how is required, which is provided by fellow scientists from the Zurich University of Applied Sciences, EPF Lausanne and ETH Zurich. These partners look after the design of modules and materials, and specify the best way to accommodate the materials in the SOFC. They will then collaborate with Hexis to build first prototypes. According to an estimate by HITTEC project leader Heel, SOFC systems could increase output by 10 percent using the converters. //

Increasing electricity prices? Keep cool!

The head office of IBM Switzerland in Altstetten is equipped with a sophisticated air conditioning system. IT student Sutharshini Rasathurai collaborated with Empa and IBM to examine how this system can operate more cost-effectively. The tool she used was "Smart Grid Demand Shaping", an intelligent power grid that determines its requirements on the basis of the current demand and the price of electricity.

TEXT: Marco Peter / GRAPHIC: Empa / PICTURE: IBM

When you walk into the headquarters of IBM Switzerland in Altstetten, you find yourself in a large lobby. Your steps echo long and loud on the stone floor, whilst your eyes search in vain for irregularities in the sea of rectangular shapes. With its simple, monolithic structures the hall is a reflection of the entire building, and leads you to surmise that this is something special. 1250 workplaces are distributed on up to 13 floors.

A well thought-out A/C system

A large building is accompanied by the major challenge of providing a working climate that is both pleasant for people and practicable for the machinery. The core of the A/C system at IBM consists of three so-called "chillers", which fill two 13,000 litre tanks with water of 11 to 12 degrees C and thus charge them with cooling energy in a similar way to a battery. The cold water is led into the offices, server rooms and ventilation via a closed network of pipes, where it cools the air. The warmed-up water is returned to the chillers. These cool the water down again, producing waste heat, which is stored in warm water tanks at about 38 degrees C and used for heating. Extra heat can also be generated by two gas boilers.

If heat exchange is needed somewhere in the building because the temperature of a room needs to be corrected, the A/C system checks whether it can carry out the exchange using stored energy from the warm or cold water tanks. If this is not possible, cooling units or gas boilers switch themselves on automatically depending on requirements. This also happens if the cold water tank drops below a minimum level of 75%. Remarkable: energy consumption is twice as high in summer than in winter.

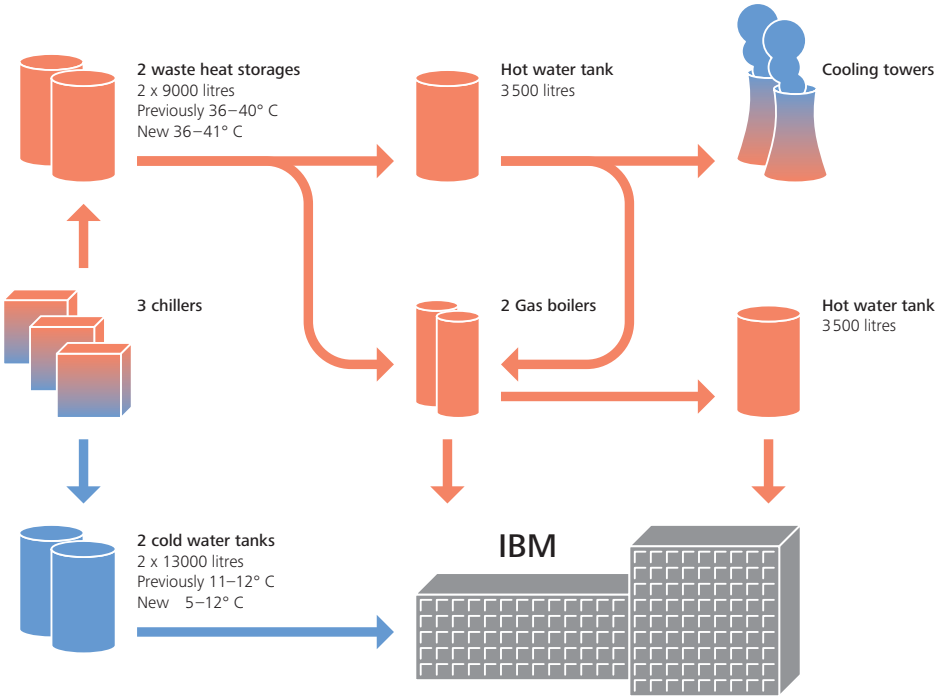
System optimised by IT student

The biggest power consumer, the three chillers, switch themselves on automatically at any time, regardless of whether electricity is expensive (day rate) or cheap (at night). IBM SmartGrid researcher Dieter Gantenbein spotted the problem and recommended it as the subject of a Master's thesis. IBM Switzerland factory student Sutharshini Rasathurai from the University of Zurich got to work. The money-saving idea: operating costs could be reduced if the chillers were only switched on during nightshifts. In her Master's thesis she examined how this idea can be implemented. Her supervisor was Lorenz Hilty, Professor of Informatics and Sustainability at the University of Zurich and Empa scientist in the "Technology and Society" laboratory.

Of course, Rasathurai was not able to simply march into the equipment rooms in Altstetten, fiddle around with the controllers and watch what happened. She simulated the entire A/C system on the computer and was therefore able to manipulate it and observe the effects. "If the cooling units are only to run at night, it must be possible to cover the daytime demand from the tanks. At present, however, they do not have sufficient capacity", says the student.

Cold water reserves cover the cooling requirement

In an initial scenario she therefore lowered the temperature in the cold water tanks to 5 to 12 degrees C instead of 11 to 12 degrees C; this increased the amount of storable cooling energy in the tanks sevenfold. If the amount of stored cold water was still insufficient, the units are switched on independently of the electricity price. In order to avoid this, the student raised the minimum charge status setting of the cold water tanks to 95% and also increased the capacity, with which the tanks are filled in the summer months. With these changes the A/C system now draws on



Air conditioning system in the Swiss IBM head office: 25 per cent less energy consumption without structural changes.
Right: IBM Switzerland head office in Altstetten.

its reserves during working hours; as soon as Energiewerke Zürich (the local power company) provides energy at cheaper rates, the chillers come on and cool the cold water tanks down again until they are fully charged. According to the computer model these adaptations would cut costs by 10% in winter and 17% in summer.

More savings thanks to dynamic electricity prices

Electrical energy is traded like oil or steel. The prices change on an hourly basis depending on supply and demand. However, end consumers do not have access to these wholesale prices. Rasathurai designed a second scenario, in which she assumed that IBM could purchase electricity at these dynamic prices, and the system would receive price quotes up to 34 hours in advance from the European Energy Exchange AG in Leipzig. In this simulation the chillers always first compare the current electricity price to that of the coming hours before they switch themselves on. Once the most favourable time has been determined, they shift the charging process. With such a dynamic pricing system savings of up to 31% would be possible in summer, Rasathurai calculated.

Not just cheaper but also more efficient

The surprise was even greater when the simulation revealed something else: the new system does not only operate with cheaper electricity but it also consumes about a quarter less. “This is because the chillers and the gas boiler are not switched on as often with the improved emptying and filling rhythm of the tanks”, says Hilty. And if so, they generate exactly the amount of energy that is needed.

The study has revealed a substantial saving potential thanks to Smart Grid Demand Shaping in A/C systems that can be achieved without any structural measures whatsoever. Hilty is very keen on recruiting further students to continue Rasathurai’s work, since: “If we examine the flows of waste heat in more detail and refine the advance calculation of the electricity prices, even more money can be saved”, he is convinced. At the moment this is still theory, but in a few years the new technology will be ready for use in domestic utilities management systems. //

IT starting signal for an energy-efficient future

Lorenz Hilty, Empa scientist and professor of Informatics and Sustainability at the University of Zurich, outlines his vision for intelligently controlled energy consumption. The idea is to use the "ICT for Sustainability" (ICT4S) conference organised by Hilty in February in Zurich as the starting signal.

INTERVIEW: Rainer Klose / PICTURES: Empa

Mr. Hilty, you are currently preparing the ICT4S Conference – the first of its kind. Do we really need another sustainability conference?

Lorenz Hilty: Digitalisation has been rapidly changing society for at least 20 years. However, the awareness that this potential for change could also be used to accelerate sustainable development does not yet exist. For example, could we achieve the energy turnaround with the help of ICT? The basic theory behind this conference is that it won't happen on its own. Advances in ICT will not automatically lead society into a sustainable future. But it is possible to use it for this purpose.

Isn't it true that the debates have gone on independently of each other so far – on the one hand the debate about technological advances in ICT, and on the other hand the sustainability debate?

They are no longer completely isolated. The discussion about "Green IT" has been going on for some years now. People have realised that IT has something to do with protecting the environment and matters concerning energy. We now want to take the topic a step further to the general question of whether we can we achieve a more resourceful and sustainable daily life by means of smarter processes and intelligent control and regulation.

Does this mean that there is more to the concept of "Green IT"? Until now, I have only associated this catchphrase with semiconductor technology, which is less damaging to the environment.

That is where it all began. Some interesting questions were already on the table, such as: how much power is consumed by the Internet? Or: how can we make our entire office communication more energy-efficient? But then the IT industry noticed that we were talking about approx. 2% of global energy consumption. If we wish to achieve something we must think about how to reduce the remaining 98%, such as heating more intelligently or optimising traffic. We must create structures that can provide a new solution for the interaction of information processing, mobility and supply with goods and energy.

Until now is has only been possible to control power consumption at short notice: as soon as a load occurs, someone turns a wheel in the power station and increases output. How can this be changed? How can we anticipate power consumption?

You can look at both sides and carry out "demand shaping", for instance. In order to do this I construct a device in such a way that it can decide for itself: I don't need the energy right now but can instead connect up later. I would thus avoid peak loads and only consume power when there is less demand. The coordination of such devices can be linked with a market mechanism that makes energy expensive when demand is higher – in other words, dynamic energy prices. However, a prerequisite for this is that the shortage signals are made available in the system, in other words introduce new information flows. Such a thing is then known as a "Smart Grid".

How can a "Smart Grid" help to save energy?

The meaning of this approach is only really coming into effect now, because we want to use many more renewable energy sources in the future. Of these sources, only hydroelectricity is easy to control, but is essentially exhausted in Switzerland. In comparison, solar and wind power are difficult to adjust – these have to be "harvested" when they occur. This means that in future there will be bigger fluctuations at the energy supply end, something that would seriously intensify the coordination problem between supply and demand. This is where IT must – and can – help. The system that we need in the future must estimate in advance where energy supply and demand exists, so that the energy flow can be managed accordingly.

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On a personal note…

Lorenz Hilty is a scientist at Empa's "Technology and Society" laboratory and professor of Informatics and Sustainability at the Department of Informatics of the University of Zurich. He develops IT applications that contribute to achieving sustainable development. His research area also includes social discourse by means of new technology.

Are there already precursors to this development?

Yes, particularly in IT. Computer centres require ever-increasing amounts of electricity. The computing load can be shifted by means of Cloud Computing if energy is scarce somewhere in the world. Information is easier to transport around the world than energy nowadays. This means that I can move a calculation task from Europe to Alaska or Australia, for example, if energy from renewable sources is currently available there. And the customer is not even aware of this.

However, it is not just data that is moving around the world but also people and goods. Is it also possible to organise physical transportation in a better way with the help of IT?

Yes, IT-based concepts for this exist as well. For example, people can carry small devices such as smartphones that will identify them and allow them to use transport services. I can get into a taxi or a train. I can hire a car-sharing car or a bike. And all of these mobility options that I can freely combine come at a price. This price can depend on current demand – during a traffic jam I will pay more for using the roads; the tram will cost more during rush hours and the last available bike will cost more to rent. Everyone who can manage it would then avoid travelling at peak times. Even in a system such as this (a type of "Smart Grid" for personal travel) I would need a shortage signal, that would be relayed quickly within the system. I would need skills from the ICT area. Cheap and efficient technologies already exist that can solve these problems.

In this future, people with low incomes such as poor pensioners will have to reschedule their activities for off-peak times and during the night. That leaves the question: is that what society wants?

At our ICT4S conference, the question of desirability will also be raised. We have invited social scientists from countries like Sweden, among others, who are experimenting with "Smart Cities" in an area south of Stockholm. They have already noticed that even the most forward-looking plans are regularly being overtaken by technological developments. This means that governmental planning of such structures is much slower than technical progress. We must therefore create "Smart Cities" as a dynamic system. A "Smart City" must continuously reinvent itself if it wants to function efficiently.

Such a high-speed development may require a different form of government. Can we accomplish this in a democratic society with all of its objection rights?

That could indeed mean that the governance structures would have to be different by allowing more self-organisation, for example. We have contributions at the conference that deal with issues like these.

It hardly sounds like a walk in the park. Are you expecting political opposition?

It is there already. Take the example of "Smart Grids". Anyone who seeks to enforce such a thing will encounter opposition from the power industry, where old monopolies are being defended in some cases. It is socially and economically extremely complex. The only way to move forward in the area is via large-scale experiments and case studies, in my opinion. We can only learn about this new world by means of "trial and error". We have to choose regions where we can experiment – i.e. set up a "Smart Grid" or design a "Smart City". Even if it doesn't bring the expected advantages for the pilot region, experience can be gained. And we can develop a culture around this structure.

How can I convince the population to go along with this?

The idea of "persuasive computing" would be suitable for this task – these are systems that convince people to behave in an energy-saving way, for example. For instance, it would help if you could calculate eco-balances in real time on your mobile phone.

The conference

The conference: The first international "ICT for Sustainability" (ICT4S) conference is taking place at the ETH Zurich from February 14 – 16, 2013. It is all to do with having better control of energy and resource consumption by means of intelligent IT systems and better use of renewable energy sources, and the question of whether goods can be replaced by services. 42 speakers from 27 countries and five continents will be devising the IT use of the future and discussing the effects thereof. The opening of the conference on February 13, is accompanied by a series of public lectures, e.g. a crash course in "Green IT".

Public workshop: On Saturday, February 16, the Swiss Federal Office of Communications (OFCOM) and the Federal Office for Spatial Development (ARE) are organising a public workshop at the ETH Zurich. How can new links be established in Switzerland between today's emerging information society and the desired sustainability? Entry is free of charge. Register at *www.ict4s.org*

Zürich Greenhackathon: The "Zurich Greenhackathon" is taking place in the run-up to the conference on Tuesday, February 12, 2013. The participants are given 24 hours, in which to program software for a purpose that benefits sustainability. Registration and information at *zurich.greenhackathon.com*

Now, is it better to read the news in a printed newspaper or on your iPad? In Zurich, there is already a start-up company that provides cooking recipes for downloading and has calculated a detailed eco-balance for each one. This is a start. After all, psychology tells us that human behaviour can only be influenced by providing information in real time without patronizing. The sooner, the better.

The ICT4S conference is intended to be the starting signal for this type of research. What kind of people will I meet at the conference? What is on the agenda?

On the one hand, we have the classic "Green IT" topics; among all the visions, these must not be forgotten. The question is: how can we reduce the energy requirements of computer centres, and how can we minimise e-waste? Then there will be sessions on the subject of "Smart Cities" and "Smart Buildings". Here we will be discussing our living environment: we will be talking about houses that know when the residents are not at home and control their energy consumption accordingly. In another session, the topic is resource management such as smart water management. However, our conference is of an extremely interdisciplinary nature for a good reason – humanities and social sciences will also be represented. Because it would be naïve to believe that sustainability can only be achieved using technical measures. It is never the technical system alone that has an effect, but the people that use it. //

If you could call up eco-balances on your mobile in real time, it would significantly increase your energy awareness, says Lorenz Hilty. Ecological decisions could thus be made quickly: Should I watch the football match on the plasma TV, or drive to the stadium by car? Does downloading a film in HD use up as much energy as blow-drying your hair?

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February 14 – 16, 2013
ICT for sustainability
The challenge of making it real (ICT4S Conference)
ETH, Zürich

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Technology Briefing
Empa, Dübendorf

5. März 2013
Materialbearbeitung mit Laser
Kurs für Firmenchefs, Produktionsleiterinnen, Ingenieure
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6. März 2013
Löten
Kurs für Interessierte aus Praxis und Produktion
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7. März 2013
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