**Hot on the heels of cement’s formulae**

**Bridges, houses, dams – for decades, cement has been a permanent feature of our urban environment. What is deemed a robust and lasting material, however, is actually fragile and highly complex on the inside. Barbara Lothenbach understands the building material right down to every last detail – and how it opens up fabulous new possibilities. The Empa researcher was recently elected a Distinguished Senior Researcher in recognition of her many years of outstanding research in cement chemistry.**

When we talk about cement, it is usually about its mass, stability and wealth of possible applications. Very few associate the gray building material with the term “environment”. Cue Barbara Lothenbach, a researcher from Empa’s Concrete/Construction Chemistry laboratory. For her, cement is more than just a run-of-the-mill construction material. Apart from anything else, it can be optimized – both as a material and ecologically. After all, between five and eight percent of the global CO2 emissions can be attributed to the production of cement. “The most commonly used cement, Portland cement, is made of lime marl, a mixture of chalk and clay, and produced in a combustion process at approximately 1,450°C,” explains Lothenbach. This produces ‘cement clinker’, which is then ground up and mixed with plaster. And limestone contains large quantities of bound CO2, which escapes into the atmosphere during combustion. However, it is exactly the calcium oxide contained in limestone that gives Portland cement many of its excellent properties.

An environmental chemist by trade, Lothenbach is thus particularly interested in how emissions might be curbed, for instance by replacing cement clinker with alternative materials, such as fly ash from coal burning or slag from the iron smelting furnace. However, fly ash and slag contain far more aluminum than Portland cement, which reduces the cement’s solidity and durability. Moreover, different types of cement react very differently to environmental influences such as water, wind, temperature or – in tunnel construction, for instance – the composition of the groundwater. “The better we understand these relationships on a chemical level,” explains Lothenbach, “the more efficiently and above all ecologically we will be able to produce cement and use it in practice, such as cement with a higher proportion of fly ash, slag or other promising materials like calcined clay or even unburnt limestone.”

But even if new types of cement display good solidity and durability, the road to their practical application is long and requires sound proof that these new materials are capable of withstanding any influence. After all, what engineer wants to build a bridge with materials, for which there are no empirical values? While industry can look back on more than a century of experience with Portland cement, our knowledge of such new materials needs to be expanded further, especially when it comes to their long-term behavior.

Chemistry and especially the simulation of chemical reactions on the computer can help exclude certain compositions with unsuitable properties from the outset and make predictions on how the cement will behave in different situations and over a period of several years. To this end, Lothenbach uses a giant database that contains the behavior and mutual interactions of countless chemical components. She varies the mixture on the computer and can then use a simulation to calculate how different mixtures will behave under real conditions. For this to work, however, it is vital to know the properties of all the possible cement components in detail and how they interact with each other – knowledge that Lothenbach has acquired during years of research at Empa and that made her one of the world’s leading researchers in cement chemistry.

Industry is also actively looking for other substitute materials besides fly ash and slag. In particular, cements based on calcium sulfoaluminates are in the pipeline. The resulting cement has definite advantages: compared to Portland cement, it requires less limestone in the production phase and is burned at temperatures that are approximately 200°C lower, which reduces the CO2 emissions. If the composition is wrong, however, the cement can expand in volume, which may cause cracking in a structure, as Lothenbach explains. Not only does she conduct basic research with her team; she and her colleagues also collaborate regularly with industrial partners who would like to optimize their product or use it to tackle certain problems. One of these industrial projects focuses on magnesium phosphate cement, which can be used as repair mortar on the one hand, but also as a food additive, in dentistry and as bone substitute.

**Finishing touch for large structures**

So cement is not just cement. Whether it can be used in bridges, houses, dams, subterranean sewers or to stabilize nuclear waste disposal sites, however, is ultimately all pure chemistry. It is just that you don’t immediately think of the smallest components in concrete responsible for its sturdiness when you see a massive highway bridge. “We also have concrete mixers here in our research lab, of course,” explains Lothenbach. “But my team doesn’t have anything to do with them directly.” Instead, her work takes place in the lab – in small test tubes and with samples on a gram scale – and on the computer, where she makes predictions with the aid of simulation programs before checking them in lab tests.

This interplay between lab research and computer simulation carries numerous advantages. By comparing the results of the simulations with lab tests, Lothenbach can keep improving the reliability and validity of the database. The lab tests, on the other hand, give the scientist more leeway when it comes to evaluating the viability of new mixtures or new combinations for industry. “The computer simulations benefit from our lab experience and vice versa,” says Lothenbach.

Besides a mixture of empirical (lab) research and virtual simulation, the exchange between industrial projects and basic research is also what Lothenbach particular cherishes about her job. “This makes working at Empa incredibly varied.” Which is in stark contrast to her first impression as a student at the start of her biology degree in Zurich: she had to learn how to skewer insects with pins so they could be catalogued, for instance. “I realized the biology degree was – at least back then – too restricted to the systematics of the living natural world instead of examining topics like ecology and environmental protection.” She wanted to get to the bottom of things, understand them and then alter them so they benefit the environment. Consequently, after a year, she switched to environmental chemistry and has never looked back.

**A garden blooming with knowledge**

Although her professional passion is now cement, she has not forgotten her love of soil, plants and other living organisms. Her main hobby is her garden, where from time to time the scientist in her also bursts through. For instance, she regularly draws up plans of which plants she has planted where and in which year to guarantee a good yield – much like our ancestors, who always rotated crops between different fields. Like novel cement components, plants do not always make happy cohabitants. “Some plants are good neighbors, others have to be planted far apart. One might like dry soil, another enjoy the shade and moisture,” says Lothenbach.

And external influences are to cement what snails are to garden plants – whether it be sulfate in the San Bernardino Tunnel or in the groundwater, which wears away the cement pipes. “In my garden, I have to know where the snails are and use hardy plants there.” By the same token, cement needs to measure up to the demands of its respective environment. In other words, the basic recipe for the cement mixture has to be adapted to the external influences.

In other words, the awarded researcher – incidentally, only one of three Distinguished Senior Researchers at Empa – did not escape insects on pins entirely. With the difference that she not only knows the individual chemical components of “her” cement systematically inside and out, but can also use them accordingly to tweak certain processes and properties for the better. While she cannot influence the color of her potatoes as she likes, for instance, she can make their surroundings as ideal as possible. In the case of cement, on the other hand, it is the exact opposite: she can alter the cement mixture so that it adapts perfectly to a particular environment.

With her broad range of knowledge in this field, she has been a key contact for experts from industry and research for a number of years. This is also thanks to good collaboration with other experts in the department and the excellent research infrastructure at Empa and in Switzerland. Technical advancements enable Lothenbach to keep expanding her expertise and pave the way for other future and, where possible, more efficient and ecological methods to produce and process cement. After all, the same ultimately goes for cement and the plants in her garden: the chemistry needs to be just right.

<https://www.youtube.com/watch?v=L4OLBNXMdHk>