wetsus
european centre of excellence
for sustainable water technology

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Editorial

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Clean and safe water is a key right for all living organisms. Development and application of technologies are instrumental in providing clean and healthy water, as Jelle Hannema of Vitens explains in this issue of S&T. The Wetsus research-pillar Healthy Environment offers innovative technologies and solutions to ensure this goal. Healthy environment is about providing a sustainable water cycle, and Wetsus is active all around this chain, providing safety assessments and solutions.

Further in this issue, recent publications. Sandra Drusová developed special fibers that better assess flows in water wells, thereby safeguarding these critical sources for our drinking water. The work of Caspar Geelen in Smart Water Grids contributes to the safe transport of drinking water, since he can predict the best place to place sensors to monitor pipe bursts. Antoine Karengera and his nematode worms of the Genomics theme ensure we have proper ways to measure the health risk of hydrophilic contaminants in water. Safety that is also checked by Edwin Ross, who makes clever use of combinations of data in the Sensoring theme to measure adverse effects of chlorination. Ultimately, the smarter we are in innovations in the water cycle, the lower the problems at the start of the cycle will be, ensuring clean water for all.

Science as a societal responsibility

Jelle Hannema MSc, CEO of Vitens, about his view on research for a better future for Vitens, science, and the world

“If you talk about water, you talk about sustainability,” says Vitens CEO Jelle Hannema MSc, “once you’ve seen what is happening all over the world: seeing rivers turned purple or blue depending on which color they use to dye T-shirts, seeing people still turn ill from drinking water, you understand the incredible importance of science.

Mr. Hannema, both as chief executive of Vitens and as member of the Wetsus supervisory board, emphasizes how research and innovation are the way forward. Especially in the water sector. Especially as a company. “We use research as a tool, driven by our mentality to be efficient, to be sustainable, to best serve our customers, and complete societal responsibility. We strive to have a positive impact on nature and humankind. That’s why we feel responsible for water availability and why we want to do as much as possible to be a sustainable drinking water company. Research & innovation is essential to that.

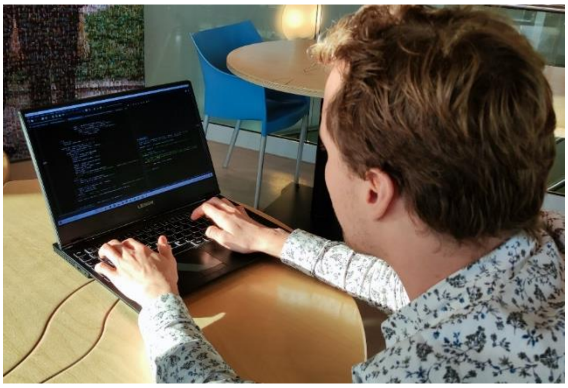
“There is still so much to learn and to win, from science. If we want to be a better world, we need the sciences for that. I’m genuinely convinced about that,” Mr. Hannema states. “And it is easy to praise without giving, but – especially in politics – this appraisal must be replaced by funding. We must understand that not every hypothesis leads to a fleshed-out innovation, but that’s why there should be enough money around. So it hurts me to see that Wetsus still has not been granted continuous financing. We need marketplaces, not ivory towers; agoras like Wetsus to stimulate interaction between knowledge providers and requesters.”

In the field of (digital) monitoring, innovation and research are already proving fruitful. Hannema: “Using intelligent systems, it’s not only the innovation that is helping us forward. It gives our customers better insight into their water use and global footprint, and it gives us a challenge to really understand the process behind it. Vitens likes to think pragmatically, but we need scientists to develop ideas, then our experts can put them into practice. That’s why we appreciate the data scientist working for Vitens, but also the innovations from all our partners.”

One promising fruit that dropped from the grafted Vitens-Wetsus tree is the pipe inspection robot. “We saw the value of this innovation,” Hannema says,” even if we need to develop it further. There is much to gain. We have a drinking water network of 50 thousand kilometers, and we’re pretty much blind as to the state of the ducts. Vitens has to prevent leaks. And above that all, we need to keep improving, for the world, for the customer. I am delighted to have the honor to lead such an organization.”

Smart Water Grids theme

Using observability models to calculate ideal sensor placement: Observability Gramians



Enormous complicated drinking water networks are operated without precisely knowing what is happening below the surface. Caspar Geelen developed a new model that aids in the optimal placement of sensors to obtain insight in these underground dynamics and help detect leaks. It is faster, cheaper, and has more capabilities than the current standard.

Drinking water pipes spent decades underground serving their purpose. Not only are large amounts of water lost if they break, these water floods can cause massive damage to other infrastructure – such as roads, electricity or gas networks. Figuring out which pipe to replace and when replacement is prudent is costly – time and money-wise. Yet, until now, few alternatives have been in place.

Physical monitoring options are limited and hard to execute, so network managers rely on collected data and network models to detect leakages. In order to make this possible, water companies rely on real-time flow and pressure sensors installed throughout the network. Where to place these sensors for the best results, remains challenging, as the number of parameters to track is immense and thus requires daft amounts of computing power. Due to the fundamental structure of current standard methods, further parameter reduction is not viable. So, Ph.D. candidate of the Smart Water Grids theme, Caspar Geelen, developed a better way.

Geelen designed an efficient observability-based model that can quickly calculate ideal sensor placement in complex networks. This new knowledge, together with his research on leak detection using existing sensors, aids in further digitalization of the water sector and has never-before-seen capabilities regarding improving the hydraulic network models and working towards digital twins, as well as the detection of water hammers: sudden pressure increases that can cause leaks.

The veins of a leaf

Drinking water networks span enormous areas, all under the control of a few sensors that cannot keep up with modern measurement requirements. The systems – district metering areas – usually stretch from the main inlet to end users. "Like the veins of a leaf," Geelen explains, "starting large and branching out - increasingly smaller in every direction. Even though the number of sensors in this webbing of ducts increases with residential smart sensors, networks are tough to monitor. "The number of pipe connections is so large that you cannot possibly measure every corner of the network."

And the occasional measurement is not sufficient to monitor the entire vast closed-off tubing system, so nowadays, hydraulic models are used to calculate the flows and pressure for all unsensored spots.

And these systems do their job, but they have to take into account many parameters and accompanying uncertainties that add up, thus, requiring extensive computing power. "It's a great solution," Geelen says, "but we need better models to reduce the high uncertainty involved." Current systems take all into account, from flow rate to pressure resistance. The current Hydraulic water transport models do a marvelous job, yet still lack in speed and capabilities.

Simpler and smarter

So Geelen made a cheaper and less computing-intensive model that focus on increasing our insight in these hidden pipes, as well as the traditional leak-preventing capabilities. "We developed a model using systems and control theory. We do clever calculations using so-called observability Gramians, mathematical matrices that contain intrinsic information about the distribution system.

The scientist mapped out the network in terms of connections and junctions. Starting small but increasing in size as the model turned out to be effective. Without actually having to digitally simulate network flows and pressures, ideal sensor locations can be identified purely based on pipe characteristics, such as friction, conductivity, and resistance.

The use of fluid calculations and parameters drastically decreases the number of steps to calculate. "We still have to rely on an iterative approach, but with fewer parameters, the system becomes a lot quicker while still retaining its function as a digital copy of the water network," Geelen says. All the while, it calculates the ideal placement for more sensors to ever increase the realism of the model.

And this way, the model has more advantages too. Current methods do not always take pressure dynamics into account when determining sensor placement. However, detection of sudden pressure changes, or water hammers, is essential for burst detection, and therefore these dynamics should be taken into account when looking for the best sensor.

Merely the beginnings
Not only is the model crucial for sensor placement, defining effective locations for actuators also belongs to the system's capabilities. Pumps, valves, and pistons can be fitted on the most reliable spot, helping to further reduce the costs required for district metering areas.

We can expect even more in the future. Geelen: "This paper is only a proof of concept. We foresee many additional applications for this new framework."

Read more on this paper:
Geelen, C. V. C., Yntema, D. R., Molenaar, J., & Keesman, K. J. (2021). Optimal sensor placement in hydraulic conduit networks: A state-space approach. Water, 13(21), 3105. https://www.mdpi.com/2073-4441/13/21/3105/pdf

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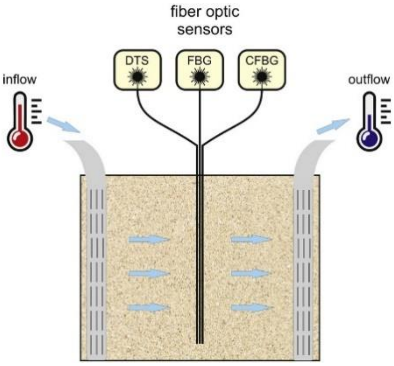
Groundwater technology theme

Temperature and pressure measuring in groundwater wells: fiber Bragg grating sensors



The state of groundwater wells remains an educated guess. Data gathering used to be laborious and inaccurate, but the time is ripe for change. Sandra Drusová developed a flexible, quick, and reliable sensing method that better substitutes several groundwater measuring applications.

In short:
Gathering data is essential to determine the state of groundwater wells and to run them proactively. Occasional flow measurements tell the longevity of the source in both storage and the flow of toxins to the well from neighboring grounds. The water temperature in such aquifers is not only a tell-tale sign of flow fluctuation but also relevant to the water used for geothermal energy storage.

Despite the possibilities of measuring flows inside the wells and probing for the temperature, information on the buried groundwater near wells is based on low-resolution models. Underground environments vary from layer to layer, and little is known due to insufficient field data. Information about soil structure, groundwater pressure, and temperature is estimated from a few sampling points. As a result, flows near wells are modeled from a portion of available data, and the interpretation of results relies on the gut feeling of experienced experts.

The water sector could greatly benefit from more data to optimally use groundwater wells and inform on dangerous contaminant flows that threaten consumers' health. That's why Ph.D. graduate in the groundwater theme, Sandra Drusová, developed a multi-purpose fiber-optic sensor with similar infrastructure to what already is in place.

Using fiber Bragg grating (FBG) sensors, she researched a customizable fiber optics cable that allows the user access to data on strain and temperature near drinking water wells. From this, she could extrapolate water pressure and temperature using machine learning methods.

Never-before-seen accuracy
As it is gathered now, one drilled spot – a borehole – corresponds to one data point. To get a spatial variation of data with depth, one needs to drill more boreholes up to different depths. Despite being possible, this quickly

increases costs for such an operation. Acquiring data requires regular measurements and sensor readouts, which is labor-intensive work. Real-time data reading possibilities are few, and they are hardly in place.
Fiber-optic sensors offer great possibilities for hydrogeology because they can provide real-time data with high spatial resolution. One fiber-optic cable can have multiple sampling points along the length. When fiber optic cables are buried in direct contact with soil, they cause minimal disturbance to the underground environment and provide many data points along its length.

So, Drusová innovated a sensing method she then compared to the current state of the art, yielding accuracy never seen before, perplexing cooperating geologists. “With our new sensors – fiber Bragg gratings – we used a set of already-existing sensors incorporated into a glass cable,” explains the young doctor. These sensors make use of light to determine the properties of the fiber and the environment where it’s placed. Drusová: “By sending light down the cable and looking at the frequency of the reflected light, we can say something on the strain and temperature of the fiber.”

The fundamental physical principle here is constructive interference. One FBG sensor is a periodic structure reflecting light. Multiple reflections from one sensor will constructively interfere if the frequency of the light corresponds to the period of the sensor. Changing the length of the fiber causes changes in the period of the sensor itself, and therefore the reflected frequency is different too.

“The frequency that bounces back to the detector differs with temperature and pressure changes in groundwater,” Drusová explains. For example, when we start pumping water from a well, we decrease water pressure in the ground. As a result, the soil compresses. Strain in a fiber optic cable tells us how much it was stretched or compressed with the surrounding soil.

“Geologists at first couldn’t believe we were able to detect minor shifts in ground movements as a result of altering flows,” the scientist explains. “The resolution of our new method alone, being on a micrometer-scale versus current centimeter to meter scale, already gives a lot more insight.”

Insights from the lab

In their latest paper, Drusová and a fellow theme researcher Wiecher Bakx compared three different fiber optic sensors. One of them was Distributed temperature sensing – DTS – the current gold standard concerning fiber optic temperature sensing in hydrogeology.

They did so by recreating a controlled groundwater environment on a lab scale. This allowed the researchers to gain valuable insights on how to calibrate the fibers, their resolution, and how much the cable packaging choice influences the measurement — concluding that FBG sensors allow for much more customizability and thus flexibility for several measuring methods.

Harnessing expertise

Drusová’s research has cast light on groundwater movement and reflects the use of fiber optics within the field. She has shown that optical fibers can do far more than connect the world via the internet; they can offer temperature and pressure data simultaneously.

As a result of her work, a new Ph.D. position has opened in the latest recruitment call EMPOWER. “We developed a testbed for the next researcher, allowing data analysis from a controlled environment.” Essential steps towards further method developments in the groundwater sector and harnessing the knowledge of experts in the scientific method, is something we can certainly expect from Drusová’s successor.

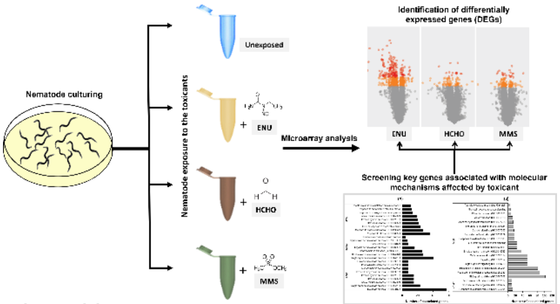
Read more on these papers:

Development:
Drusová, S., Wagterveld, R. M., Keesman, K. J., & Offerhaus, H. L. (2020). Temperature and Consolidation Sensing Near Drinking Water Wells Using Fiber Bragg Grating Sensors. In Water (Vol. 12, Issue 12, p. 3572). MDPI AG. https://doi.org/10.3390/w12123572

Comparison:
Drusová, S., Bakx, W., Doornenbal, P. J., Wagterveld, R. M., Bense, V. F., & Offerhaus, H. L. (2021). Comparison of three types of fiber optic sensors for temperature monitoring in a groundwater flow simulator. Sensors and Actuators. A, Physical, 331(112682), 112682. https://doi.org/10.1016/j.sna.2021.112682

Genomics-based water quality monitoring theme

Using nematode’s RNA to measure toxins: a transcription-based bioanalytical tool



A multitude of waterborne chemical substances and their degradation byproducts may threaten the environment and human health. Due to the broad range and low concentrations, these compounds may go undetected or require a specific set of more advanced analytical techniques. Antoine Karengera developed a bioassay based on differential mRNA expression in the nematode Caenorhabditis elegans to detect toxic potencies of chemical contaminants.

In short:
To make drinking water accessible, a comprehensive set of parameters should be screened for. First and foremost, no toxins should creep through the system. Though, this is quite the task as concentrations of dangerous compounds can be immeasurably low. Yet still, they can cause a risk by accumulation in higher organisms or because their metabolites are more toxic.

Water is currently assessed through a series of chemical analysis methods mostly specific to a limited number of compounds, and the detection limits can pose challenges. And further difficulty lies in the fact that some of these toxins are hydrophilic and thus hard to extract. Therefore, a Ph.D. candidate in the theme of genomics-based water quality monitoring, Antoine Karengera, developed a bioassay capable of detecting biologically active chemicals.

Karengera studied the effects of hydrophilic compounds on the genetic make-up of the nematode *C. elegans*. Using a set of model compounds, he identified gene transcripts – RNA copies – that respond specifically to the tested toxicants in a concentration-dependent manner. This tool can determine and predict the toxic potencies of water contaminants.

Invisible threats

Invisible threats lurk in our water sources. Yet-to-be-determined compounds float about, causing potential harm to the consumer. They go undetected due to several stacking factors: low concentrations – making them hard to detect, harmlessness in parent form – only once broken down they form a toxic molecule, and extraction difficulties – as the compounds do excellent dissolving in water and thus are hard to pull from it. Add on top of that, that each compound – or at least a class of molecules – needs a specific analysis method test to determine their potential risk, and you have the perfect recipe for unwanted compounds slipping through the cracks of detection systems.

And maybe because of these difficulties, few chemical tests are currently available. But a growing concern are hydrophilic contaminants in water, as they are challenging to detect. “That’s why we need a bioassay that can determine whether the possibly present pollutants in water sources do or do not pose a risk,” explains Karengera, “our recently published work explains the concept of this bioassay method.”

Toxic fingerprints

The solution to the aforementioned challenges in water quality monitoring is to use a well-known invertebrate: the nematode *C. elegans.* This little worm can function as a biosensor that tells us whether the pollutants present in water might pose harm to consumers. Upon exposure, it makes RNA transcripts of part of its DNA to synthesise proteins than can deal with the situation. These gene expression patterns could also be used as biological markers to indicate the presence of chemical compounds.

“We grew the nematodes at the fourth larval (L4) stage, and we treated them with model compounds dissolved in water. These compounds were selected based on their well-known mode of toxicity, mainly related to the direct DNA damage – or genotoxicity,” Karengera explains. “Differential gene expression analysis in nematodes revealed the genes whose transcription levels changed after chemical exposure.”

The studied toxicants were expected to induce differential expression of the genes that participate in maintaining DNA integrity. But, this hypothesis was proven false. “Surprisingly, we didn’t detect any changes in expression of DNA damage response genes,” Karengera says, “once we mapped out more, we could see a complex pattern emerging depending on the model compound. Like a fingerprint per compound class.

A large part of the study was dedicated to designing experimental protocols to investigate the transcriptome response of nematode to DNA-damaging model chemicals in a watery medium. Karengera: “This has never been done before. That made the study exciting but required the bulk of the work. It immensely helped to have people from all disciplines and fields around, and learn from their insights.

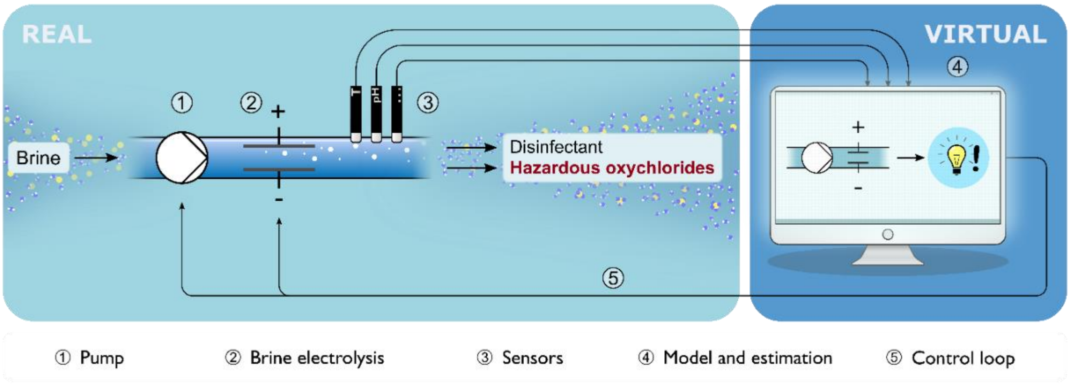
Large-scale and cross-checkable
Shortly, we can see more fruits of Antoine's labor. "We've got this fascinating paper coming up in which we detail the system for indirect-acting toxins." That are first metabolized. "And even more on how to apply the system in a large bioassay that is not only compound-class specific but cross-checkable. That way, we can learn from different disciplines and accelerate the study of all water-based toxins."

Read more on this paper:
Karengera, A., Bao, C., Riksen, J. A. G., van Veelen, H. P. J., Sterken, M. G., Kammenga, J. E., Murk, A. J., & Dinkla, I. J. T. (2021). Development of a transcription-based bioanalytical tool to quantify the toxic potencies of hydrophilic compounds in water using the nematode Caenorhabditis elegans. In Ecotoxicology and Environmental Safety (Vol. 227, p. 112923). Elsevier BV. https://doi.org/10.1016/j.ecoenv.2021.112923

Sensoring theme: sneak peek

Ensuring safe drinking water: real-time chlorate detection with sensor data fusion

Free chlorine guards a large part of Europe's drinking water but possibly harms us too. Learn how Edwin Ross secures our health while saving time and money as he counts immeasurable ions in real-time by fusing chemistry, sensors, and computer models.



The drinking water of a large part of the European states is pathogen-free because of the addition of a wondrous additive called free chlorine. This powerful oxidizer rips through all tiny life that gets in its way.

But more recently, the byproducts that come with the production of free chlorine have been suspected of harming human health. The so-called oxychloride ions have raised red flags for their consequences on unborn and developing children. They are thought to be developmentally neurotoxic. As a result, the EU has just imposed restrictions on the concentration of chlorate - ClO_3^- - in drinking water.

With no quick and reliable method, water producers rely on sampling: a laborious and costly process that is just too slow. At current speeds, it is hard to catch faulty batches before considerable amounts of dangerous drinking water are wastefully and riskily produced.

That is until Ph.D. candidate in the Sensoring theme, Edwin Ross, successfully fused sensors and chemical models to measure the minute concentrations of chlorate on a lab scale, just using pH meters, thermometers, and modeling software.

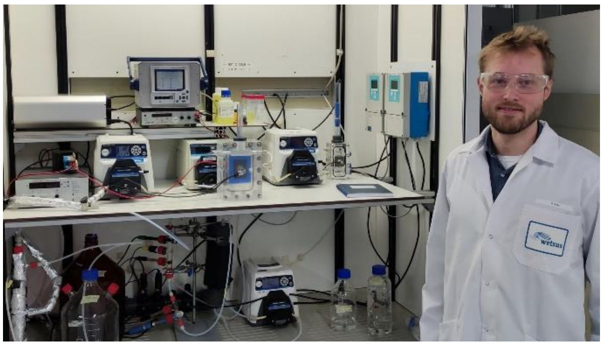
Hybrid approach
"Chlorate is notoriously hard to measure," Ross starts to explain, "the concentrations of it in the generation of drinking water are tiny, and no passive observation highlights it." So, he tackled the impossible by scouting a different route.

In order to use free chlorine, the current standard is first to form hypochlorite, with just salty water and electricity; Ross: "a process called electrochlorination." Unlike chlorate, hypochlorite – ClO^- - is easily detectable. By simply measuring UVA light and taking the absorbance, you get the ClO^- concentration.

"If you could uncover the relationship between the rate of hypochlorite formation and chlorate formation at a set of parameters, you will have found a method to measure the latter ion concentration in real-time," tells the scientist. So that is what he has been working on.

But just modeling the formation rate for the pathogen-killing particle is not enough. Ross: “electrochlorination is incredibly complex. The amount of parameters to control at the electrodes is immense.” So, he opted for a hybrid approach.

“With sensor data fusion, we can predict the rate of chlorate formation based on the measured pH and temperature, next to the hypochlorite concentration, of course, and coupling this to a chemical computer model. I can’t inform you on any details, though, as the paper describing this is in its reviewing phase.”



A viable future

But Ross happily discusses the flourishing nature of the project: “It is yet to be perfected, as we still need to take the occasional measurement to re-fit the data to the model, but the technique has proven its viability through comparisons of sample analysis to our model.”

Once asked about the current state of his research, Ross gives little away apart from grinningly stating that his problem-solving skills have certainly increased. To be continued…