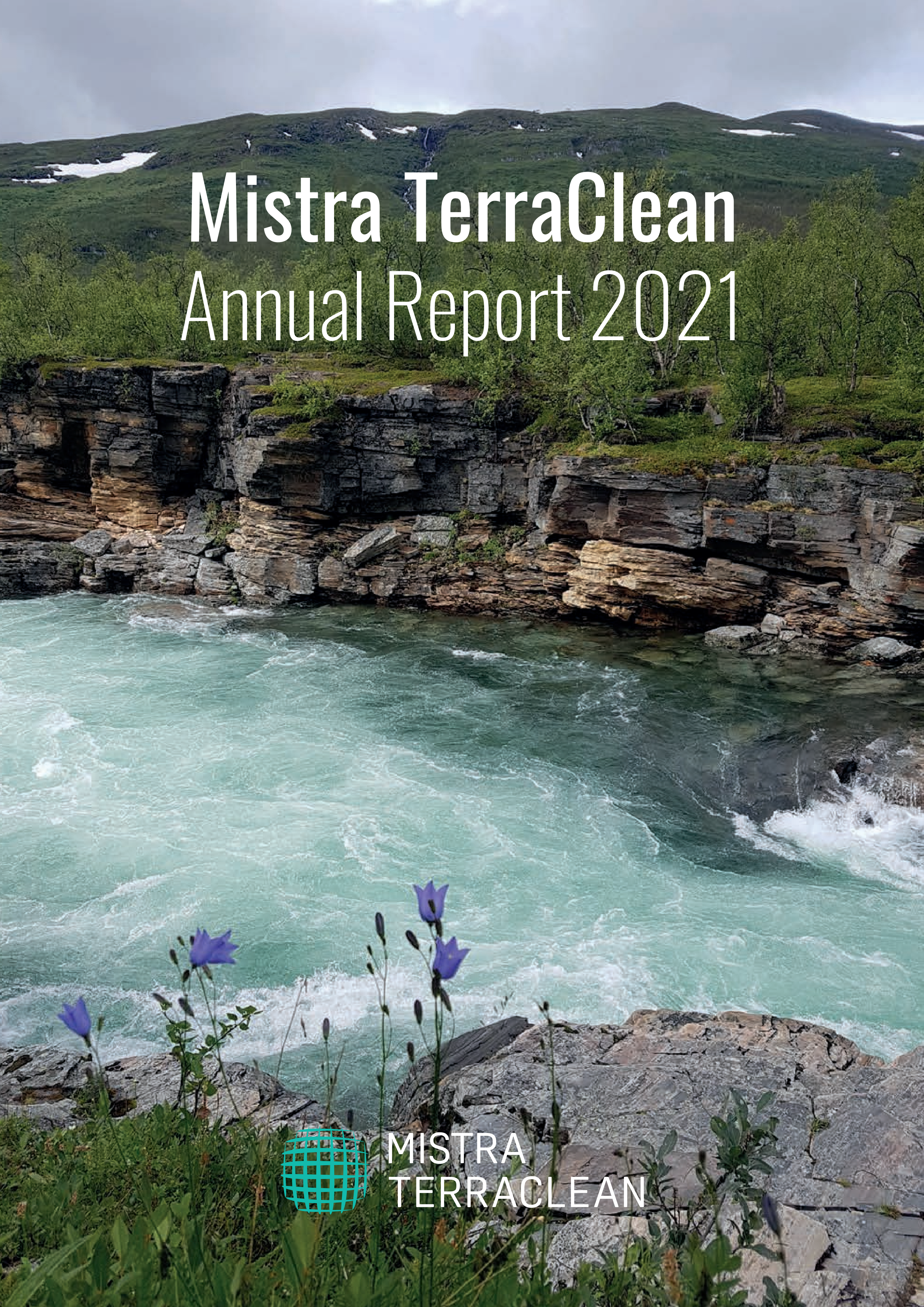
Mistra TerraClean
Annual Report 2021



MISTRA
TERRACLEAN

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Omslagsbild © Ulrica Edlund (Abisko nationalpark)

INTRODUCTION

It is delightful to be part of the success of the Mistra TerraClean program. The multidisciplinary approach combined with prominent scientific quality creates an effective research environment that enables the programme to address the sustainable challenges of today. The programme has accomplished a lot during this year, and I would like to thank everyone involved for the great work that you have done.

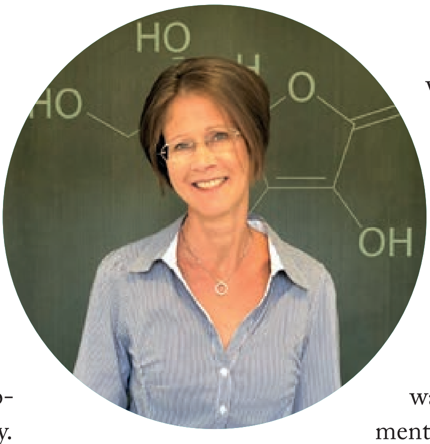
The MISTRA Fellow internship at WHO gave the programme the opportunity to get information and insights on one of the big issues that the programme is working to address, namely drinking water. The VA Award 2021, which is given to research that contributes to the water issue in Sweden, is another great acknowledgment of the importance and relevance of this programme. All this could not have been achieved without the devoted team that is involved in Mistra TerraClean and I am very impressed by your work.

I would also like to give an extra recognition to the excellent programme director, professor Ulrica Edlund. I very much look forward to continuing the work in this important and very relevant program.

Great work everyone! Thank you!

Katja Pettersson Sjöström

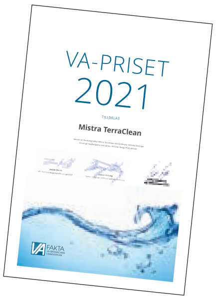
EXECUTIVE SUMMARY



I look back at 2021 with a strong sense of gratitude to be a part of such a competent and amazing team as Mistra TerraClean. The Mistra TerraClean programme has established a research and development platform to bring forward "smart" material chemistry and application device innovations directed at remediation of problematic chemical exposures in society. Many interdisciplinary collaborations have been established within the programme, which accelerates the progress and enables us to address complex research questions. Synergy effects are research results that no partner would have reached alone, but that were enabled by the establishment of our Mistra-funded consortium. The total impact is higher than the sum of all individual contributions.

The many highlights of 2021 include the development of functional activated carbons, lignocellulosic membranes, electrochemical sensors printed into membranes, cellulose aerogels for gas separation, and photocatalytic papers for removal of NOx from air. A laboratory study combined with a pilot-scale device at Hammarby Sjöstadsverk demonstrated that per- and polyfluoroalkyl substances (PFAS) can be efficiently captured from drinking water with new technology. According to the Mistra TerraClean tiered approach, the PFAS case study went hand-in-hand with a life cycle assessment, where environmental performance (including ecotoxicological and human health aspects) of the new technology was compared with scenarios describing the more conventional techniques. Mistra's generous program 'Mistra Fellow' enabled one of our team members to do an internship at the World Health Organization in Geneva, acquiring knowledge that will benefit not only Mistra TerraClean but the water quality stakeholder community at large.

We are immensely proud of winning the VA award for 2021. The VA award is presented by the trade organization VA-Fakta to municipalities, companies, research initiatives, or individuals who work to the benefit of better water quality and management in Sweden.


VA-PRISET
2021
Mistra TerraClean

"The approach and results in Mistra TerraClean, to purify the Swedish drinking water and to solve the global water crisis, are fascinating."
Hampe Moberg, VA-Fakta

In 2021, we reached the milestone of four years in practice. Granted an additional 57 million in funding from Mistra, we kicked off our next four-year phase in October. The knowledge and techniques generated within our programme since the start in 2017 will be carried over and help us expand on our goals and bring on more materials and test for capture in more environments with more stakeholders in the next years to come. We thank Mistra for the trust invested in us and accelerate into the new phase with an ambition to generate new knowledge of great value.

A heartfelt thank you to our board and Mistra for deeply appreciated support and guidance on our quest. A likewise wholehearted thank you to partners and supporters of Mistra TerraClean for your contributions: expertise, funding, dedication, and the collaborative spirit that enables a transdisciplinary research programme to advance far beyond the borders of each discipline.

Ulrica Edlund, February 2022

MISTRA FELLOW – AN OPPORTUNITY FOR DEEPER INSIGHTS

Johan Strandberg, researcher with Mistra TerraClean, has worked for the World Health Organization (WHO) as a Mistra Fellow for a year.

The idea was to have one year on site at the WHO headquarters in Geneva. It turned out to be one year in front of the computer in Sweden. The pandemic really put a spoke in the wheel for Johan Strandberg's exchange as a Mistra Fellow; he is researcher at IVL Swedish Environmental Research Institute and member of the Mistra TerraClean research project. However, the exchange still led to important work and experiences.

Johan Strandberg works with potable water as part of Mistra TerraClean. As a Mistra Fellow, he has been part of the WHO team on the quality of drinking water, which has two employees on site in Geneva and two consultants who work remotely. The working group is responsible for the publication of the WHO standard for drinking water quality and is part of the organisation's unit for water and sanitation.

"The drinking water standards are used globally, as a reference for drinking water quality, and we have worked on the most recent edition, which will be published soon."

Pathogens and lead in drinking water

As part of the work on the standards, Johan Strandberg has worked on coordinating a compilation of the available knowledge about pathogens (microorganisms that cause disease) in drinking water, as a series of factsheets.

"It is an incredibly comprehensive review process and I am in contact with experts around the world who check the factsheets."

He has also been responsible for a "technical brief" about lead. He explains that this is an important issue in both high and low-income countries. Pipes and drilled wells cause lead to enter drinking water supplies, so there is a demand from authorities who want facts and guidance from the WHO on what to do if lead is detected.

"It has been a challenging work, as the final product had to be short but still contain all the information. It must be easily understandable, but include all the latest research. Fourteen versions later, it's pretty much finished – and I've discussed it with numerous experts. It is going to be a reference standard, which is fun. Now we have a partnership with UNICEF and other aid organisations that work with water issues, and a global campaign for stakeholders with a shared agenda for drinking water is in the works."

"Fantastic but depressing"

He says that the WHO has an important function for countries that do not have strong public administration, and that many countries use the information it develops. The documentation is well developed, with a great deal of hard work behind it.

At the same time, he finds it difficult to see a direct link between work at the WHO and the Mistra TerraClean research programme, which works on developing intelligent, safe materials and technologies for eliminating contaminants in air, water and soil.

"From one perspective, the exchange has been fantastic. But looking through 'Mistra TerraClean glasses', it has also been depressing. Two billion people drink water contaminated with faeces and two million children die every year from diarrhoea caused by waterborne pathogens. The sanitation guidelines we write at the WHO are far removed from the advanced cleaning technologies we work with in Mistra TerraClean. There, we work with really amazing things such as activated carbon and nanocellulose, but these are luxury materials in a global context."

Despite Johan Strandberg having worked with water issues in both India and China, the global problems with potable water have made a great impression on him. In many countries, the choice is to drink contaminated water or not to drink water at all.

In Mistra TerracClean, which is now entering its second phase, with another four years of research, Johan Strandberg will work on the problem of heavy metals in drinking water. He has received a small grant from the WHO to conclude his work on lead and is now in discussions with them about additional work. The exchange has also provided insights into how work and processes are managed at large organisations. Despite the organisation being an important global player, it has small resources, according to Johan Strandberg.

"Many people who work for the WHO do so for free, to do something good. However, there is a global need for their guidelines, and standards, and I still feel that there is more to do in the area of potable water in emergency situations. Not least, climate change will have a huge impact on the availability of drinking water in many countries, says Johan Strandberg."

Text: Jessica Bergh, Mistra

Mistra Fellows Programme

- Allows Mistra's research programmes to give researchers the opportunity to work at an organisation in another country, or to host researchers and experts from other organisations.
- The purpose is to build partnerships and increase knowledge exchange, during and after the exchange.
- The maximum amount per person is one million Swedish kronor and the placement can last up to a year.

MISTRA TERRACLEAN, PHASE I

WORK PACKAGE 1

MATERIALS DEVELOPMENT AND STRUCTURE

WP 1 Leader: Niklas Hedin (SU Stockholm University)

WP 1 deals with identifying and developing functionalized materials that are structurally or chemically tailored for use as filters, membranes, and adsorbents. Key questions involve synthesis, refining, functionalization, characterization, and structuring of functionally enhanced natural and engineered porous materials.

A vital question is how to integrate stimuli-responsive functions through targeted chemical functionalization and/or structuring. The responsive functions will relate to induced changes from different fields or adaptive chemistries. The major challenge of WP 1 is to develop, combine, and integrate materials with such stimuli-responsive functions that simultaneously fulfil the general and specific goals of Mistra TerraClean — being smart, safe, and sustainable. Such new and smart material-based solutions can capture selective emissions from air and water under adaptive control and monitoring. For materials for smart water purification, we have a set of specific aims. First, at least one developed smart material will withstand 30–50 bar of working pressures. Also, stimuli-responsive films will be made that manage biofilms (antifouling) and can remove chosen ions/molecules with better performance regarding the selectivity and capacity than presently available materials. It is also important to secure the IP rights for these films.

We target the removal of heavy metals, arsenic, humic acid, and medical waste. For materials for smart air purification, the aims are that they should be able to be integrated into filters to have minimum flow resistance and be able to remove gas (e. g. CO_2, NOx, SOx) and particles through electrical potentials, various chemistry, and photocatalysis. We have included studies of both established materials that can be tuned and optimized towards the intended applications, but also exploratory work towards the synthesis and integration of new smart materials into the filters. The studies towards new materials are integrated with the aligned tasks of Mistra TerraClean.

Results and achievements

WP 1 operated with seven separate tasks and some results and achievements are highlighted here. The activities are reported in relation to the different tasks.

1.1 Materials for removal of heavy metal ions

Materials for selective adsorption of heavy metal ions have been investigated as well as modification of activated carbon for enhancement of capacitive device performance. Researchers at UU have tested mesoporous magnesium carbonate (MMC) and surface-modified variations. These MMCs have been studied for numerous applications and several papers have been published on the topic. At KTH, work has been performed in relation to the electrodes of the capacitive deionization (CDI) devices. The work has also resulted in several publications and ready-to-publish manuscript.

FIGURE 1. Mesoporous magnesium carbonate as a dye adsorption material.

1.2 Synthesis of up-scaled surface modified mesoporous magnesium carbonate for pilot testing for water purification, including heavy metal/arsenic removal, and for gas purification

Work is progressing.

1.3 Surface modification of cellulose versions and hybrids with hemicellulose

Many studies have been performed on, for example, the chemical modification of cellulose nanocrystals (CNCs). The hybrids have been tested for heavy metal removal and non-fouling and antibacterial properties (Fig. 2).

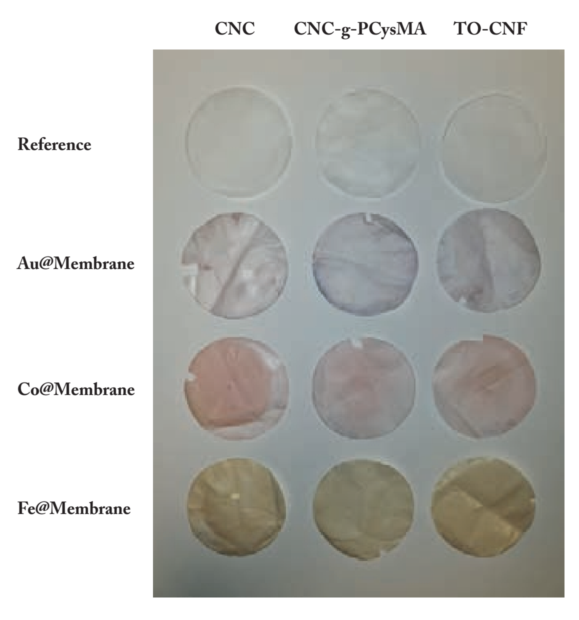


FIGURE 2. Cellulose membranes before and after adsorption of heavy metals.

1.4 Self-organized wet-stable nanocellulose functionalized aerogels

The team at KTH has studied materials and approaches to derive materials that are efficient materials for water purification. They have explored the use of aerogels (Fig. 3), including shapeable and wet-stable aerogels based on cellulose nanofibrils (CNFs). The initial work has been focused on specific surface modification techniques, using a molecular layer-by-layer (m-LBL) technique which allows for a precise deposition of thin films on the aerogels. In the continuation of the project, composites of CNFs and amyloid nanofibrils have been prepared to create new specific materials for adsorption of dyes and metal ions.

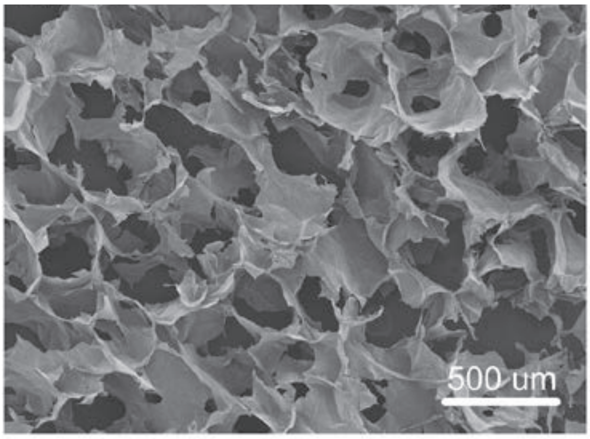


FIGURE 3. The interior of a microporous covalently crosslinked cellulose aerogel.

1.5 Activated carbons and porous polymers derived from relevant biomass and waste. Refined hydrochars

Several types of biomass have been studied for the derivation of activated carbons, and porous polymers have been derived in the team at SU, (Fig. 4). Several exchange PhD students have been involved in the studies and one paper has been published and a few others are in a manuscript form.

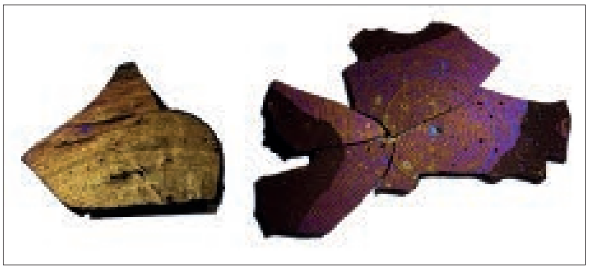


FIGURE 4. A combination of thin film hydrochars (golden and blue) attached to the spherical hydrochars(black) prepared by hydrothermal carbonization of glucose and iron(II)sulfate.

1.6 Biomass-derived activated carbons and porous polymers with magnetic features

The team at SU has focused on the derivation of activated carbons from hydrothermally carbonized glucose. One paper is under revision that documents the derivation of colored hydrochars with luster. The use of a combined $FeCl_3$ and H_3PO_4 activation method to derive activated carbons modified by iron phosphates has been explored. Studies are performed with Camfil and RISE with activated carbons for the removal of certain volatile organic compounds.

Furthermore, there are ongoing studies on the use of FeS and FeSe within activated carbons to remove Pb and Cd from water in State of Azad Jammu and Kashmir (AJK) in Pakistan. Some of the health issues in AJK are related to Pb and Cd in drinking water.

1.7 Synthesis of zeotype materials suitable for biogas upgrading

At SU, we have studied how the archetypical zeolite A can be used to select CO_2 over gases such as N_2 and CH_4, which is relevant for the upgrading of biogas into fuel quality. A set of different zeolite A compositions with varying the Na-to-K ratio by ion-exchange of zeolite NaA and zeolite KA was prepared. For the resulting compositions, some differences concerning the gas-separation tendencies for zeolites prepared from NaA and from KA was observed, even with identical compositions.

WORK PACKAGE 2
SMART FILTER DESIGN AND VALIDATION

WP 2 Leader: Mats Sandberg (RISE)

Filter materials are considered smart if they respond to stimuli. Possibilities of utilizing the smartness of these materials, either to manipulate the accumulation properties or using the material as a sensor material, requires conduits for stimuli and sensor signals. This WP concerns building filter devices constructed to have conduits for signals and with materials responding electrically and optically to accumulation.

Many technologies developed in phase I of Mistra TerraClean reached maturity and produced important achievements. A zeolite-based filter paper was for example produced at pilot scale, in a cooperation between SU and RISE MoRe Research. Plenty of work concerned composites of cellulose and metal organic frameworks. A pilot-scale testing of CDI-technology, developed in task 2.6, was carried out in the consortium, and a life cycle assessment (LCA) of this technology was published during the year.

To build devices utilizing the smartness of materials is a key activity in WP 2, with the following tasks.

2.1 Sensory filter material and actuators development

A sensor-absorbent material aimed at heavy metal detection and absorption was scaled up and formed the base of an electrode coating composition. The material represents a new method for modifying porous carbon and has the property of chelating heavy metals, being redox active and distributed within electron tunneling distance of the conducting carbon framework. It can be produced at low cost.

2.2 Smart material filter design and manufacturing

Pilot-scale production cellulose-metal organic frameworks (MOFs) sheets using XPM-pilot at RISE MoRe.

The aim of this task was to produce large-scale celloluse-MOF sheets.

The method involves the in-situ synthesis of zeolitic imidazolate frameworks (ZIFs) as a MOF model using cellulose fibers (CF) and 2,2,6,6-tetramethyl-piperidine-1-oxyl (TEMPO)-mediated oxidized cellulose nanofibers (TOCNF, Fig. 5). The prepared materials, i.e., ZIF@CF and ZIF@TOCNF, were used as additives for the XPM method at MoRe (Fig. 6). The produced sheets are abbreviated as CelloZIF sheets. Different loading of 10, 20 and 30 wt.% was added to CF before processing with and without starch, 0.3 wt.%.

2.3 Photocatalyst materials. Photocatalytic fuel cells

The aim of this work was to show that expensive and noble metals typically used in photocatalytic fuel cells can be replaced with conducting polymer to reduce the cost and the environmental foot-print of photocatalytic fuel cells. Photocatalytic fuel cells (PCFC) utilize the combustion energy of pollutants being photocatalytically degraded to produce power, to drive sensors or higher loads (Fig. 7).

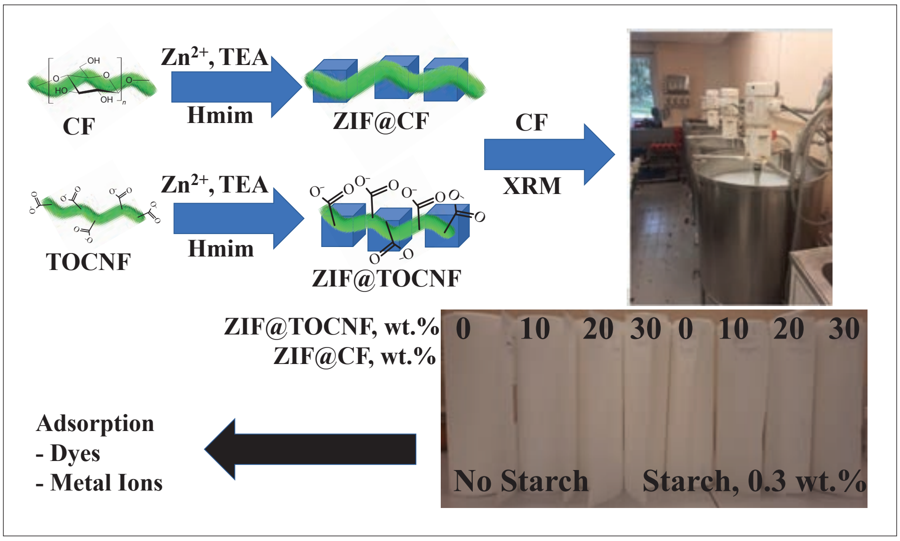


FIGURE 5.
Schematic representation for the large-scale fabrication of ZIF@CF and ZIF@TOCNF and their processing into sheets.

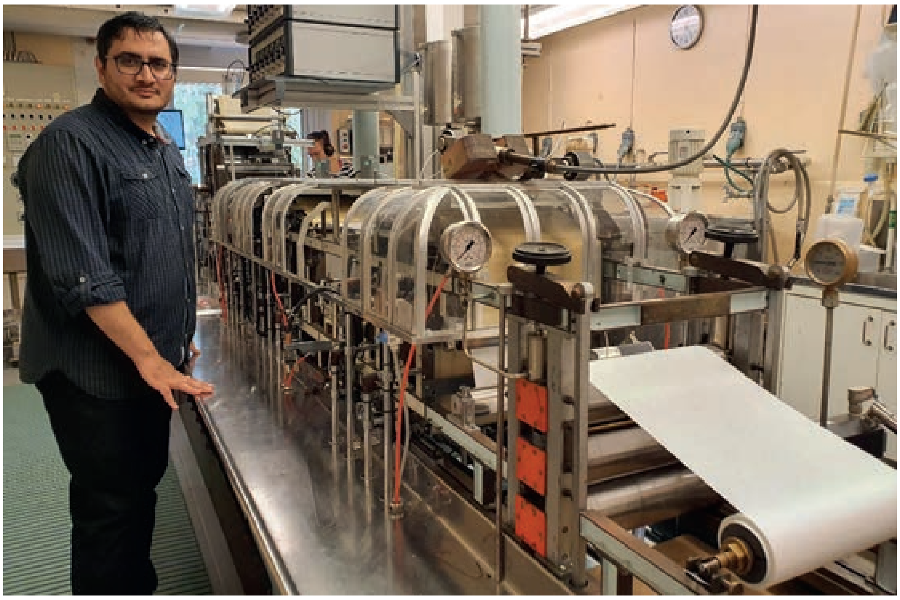


FIGURE 6.
Pilot scale production cellulose-metal organic framework filters on XPM at RISE MoRe Research.

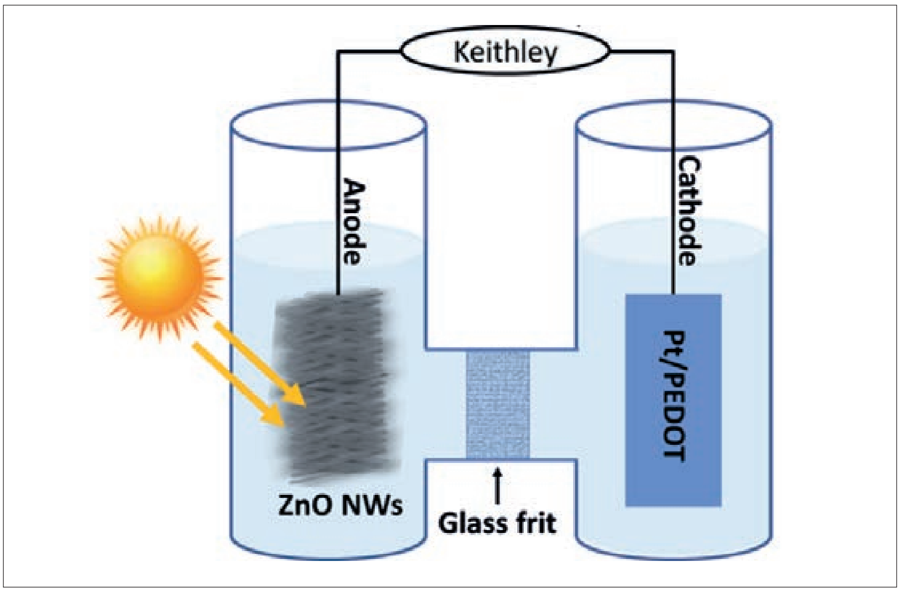


FIGURE 7.
Schematic representation of a photocatalytic fuel cell.

2.4 Identification of applications and scalability issues

Gas separation studies with focus on materials based on cellulose aerogel hybrids is an ongoing collaboration between Camfil, KTH and RISE. Molecular adsorption of acidic gas (SO_2) from air is improved by modification of the cellulose aerogel hybrids, containing MOFs (here zeolitic imidazolate framework-8 (ZIF-8)), followed by deposition of a thin organic layer with basic amine functional groups, introduced using plasma technology (Fig. 8). Through plasma surface modification different reactive species created in the plasma are allowed to react with the surface. Depending on the gas or vapor used, the interactions result in a chemical modification of the surface or a deposition of a thin organic or inorganic layer. In this project the thin organic layer was applied by plasma polymerization.

2.5 Benchmarking of filter material smartness

A filter cartridge with fittings for optical fiber bundles was constructed. This device enables direct optical monitoring of filters during filtering operation. Due to problems of baseline variations, we could not produce reliable spectra during operation. The device will be used in phase II of Mistra TerraClean for monitoring accumulation of micro-organisms by fluorescence methods.

2.6 Active capacitive deionization device

Fundamentally capacitive deionization (CDI) works on "capacitive ion storage", a phenomenon where in response to energy applied as voltage or current across CDI electrodes, ions of salt are accumulated and stored capacitively as electrical double layers (EDL) at the surfaces of CDI electrodes (similar to a capacitor or battery). Since the accumulation of ions is dominated by physical phenomena (no chemical reaction), it is a reversible process with systems based on CDI technology being characterized by low energy requirements, reduced maintenance and a long service life. With an aim to enhancing supercapacitor water purification with artificial intelligence several models including a dynamic Langmuir model useful for the prediction of how the effluent concentration in a continuous-mode constant-voltage operation varies with time, as well as how it depends on the flow rate, applied voltage, and inlet ion concentration, prediction and enhanced ion selectivity in multi-ion were developed within this work package that are now available as open source software programs.[1,2,3]

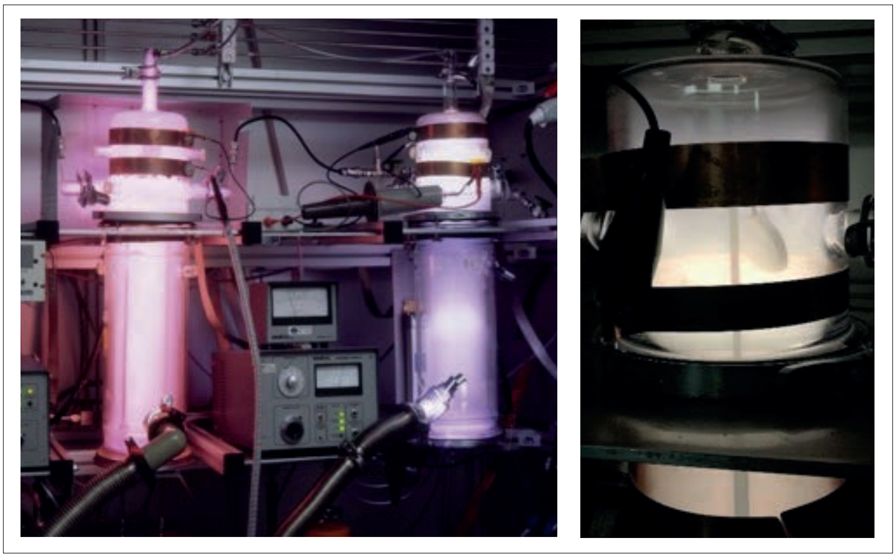


FIGURE 8.
Plasma modification at RISE was used to change the surface chemistry of the MOF-containing cellulose aerogel discs. The two photos show, (left) two plasma reactors available for surface modification, and (right) the cellulose discs during plasma polymerization to deposit a thin organic layer.

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[1] https://doi.org/10.1021/acs.jpca.9b05503

[2] http://dx.doi.org/10.1021/acs.langmuir.9b03571

[3] https://doi.org/10.1021/acs.langmuir.0c00982

WORK PACKAGE 3
APPLICATION PLATFORM

WP 3 Leader: Henrik Kloo (IVL Swedish Environmental Research Institute)

Environmental problems have been identified at industrial partners and the intention is that Mistra TerraClean will provide promising solutions with the potential to show improved functionality and economy compared to existing methods. In WP 2, tests on PFAS removal were performed with a CDI device and showed promising results. Based on this, a separate project on PFAS removal with a CDI pilot plant designed by Stockholm Water Technology (SWT) was initiated. The applicability and scalability as well as the prospect for cost level on the various adsorption and absorption materials from WP 1 were reviewed. The result of this will be used for future case studies and are implemented in case descriptions in the application for Mistra TerraClean phase II.

Results and achievements

The lab-scale trials were performed by KTH using a CDI module and synthetic solutions of perfluorooctanesulfonic acid (PFOS) and perfluorooctanoic acid (PFOA). The pilot-scale tests were performed by SWT and IVL at Hammarby Sjöstadsverk using a pilot system developed and built by SWT (Fig. 9). The pilot was operated with water that had a composition similar to that of groundwater in Uppsala (PFAS concentration 120-160 ng/L including both short- and long-chain PFAS).

The lab-scale experiments provided a better understanding of underlying principles for PFAS removal by the CDI technology, which can enable further optimization of the technology in a large scale. Among the scientific questions studied by lab-scale experiments was the influence of the water composition on the process performance, influence of pH,

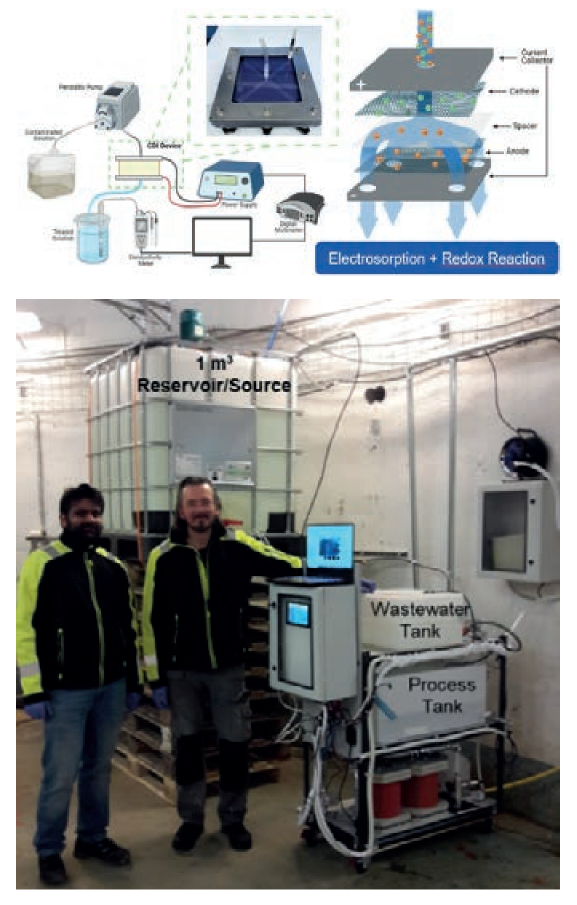

FIGURE 9. CDI-modules used in the tests: left – lab scale device; right – pilot-scale plant with two CORE® CDI modules.

influence of applied voltage, regeneration degree and the mechanisms for PFAS degradation.

An interesting conclusion from the lab-scale trials was that the removal rate/efficiency of PFOA removal was considerably increased in the presence of PFOS. pH was found to influence the process and slightly better removal efficiency was achieved at a lower pH (pH 6). However, the removed PFAS at this pH was mostly found in the regeneration solution, meaning that the removal was mainly attributed to electrosorption and to a lesser extent to degradation. At pH 8 the removal of PFAS was lower, but the removed PFAS were degraded to a higher extent comparing to the degradation at pH 6.

Several voltages were applied to study the degradation process. No substantial increase in removal rates were observed for voltages above 3.0 V. Since it is known from previous studies that degradation of electrodes is higher at higher voltages, it was recommended to limit the applied voltage to 3.0 V in the pilot-scale trials.

To keep a high removal efficiency of the CDI process during extended time an efficient regeneration of the sorbed pollutants is required. Regeneration of the electrodes was tested in lab-scale trials by short-circuiting the electrodes. However, it was found that this type of regeneration was not efficient for complete desorption, as indicated by further PFAS desorption when organic solvent was applied. This led to the recommendation of use of reversed voltage pulsing as a more efficient means of regeneration, which was tested during the pilot-scale trials.

To confirm that the deficit in PFAS mass balance is due to a complete mineralisation and not a partial degradation of PFOA and PFOS, the samples of the treated water and produced concentrate were further analysed for traditional short-chain PFAS (PFAS 11) and for possible degradation products due to incomplete defluorination of PFAS. No degradation products were however found in the treated spiked water samples in considerable concentration, which suggests that the mineralisation of the missing PFOA and PFOS is complete. This was further confirmed by organic fluorine analysis which showed that the remaining PFOS and PFOA in the samples were the only fluorocarbons present in the samples in considerable concentrations.

Removal of PFAS by CDI in a larger scale showed to be more complicated than anticipated in the beginning of the project and required significant amount of testing of different operational conditions and flow patterns within the unit in batch tests. The tests performed in the pilot scale included several periods where different operational conditions were tested, both in batch mode and in continuous operation. During the continuous operation period the pilot was run at a voltage of 2.0 V, a treatment time of 60 min and a short reverse voltage pulsing during the regeneration phase. The system showed good performance from the beginning of the period until at least 6 000 L of contaminated water was treated reaching PFAS 11 removal of 90 %. Even after treatment of 12 000 L of water (7 weeks of operation) the PFAS-removal of the system was sufficient to reduce the PFAS concentration under the legal limit (reduction from 120 ng/L to 81 ng/L).

A stable PFAS removal needs to be demonstrated if the technology is to be applied in large scale. However, the technology showed a good promise to be optimized for continuous and better removal of PFAS through modification and optimization of the system and control processes which were not evaluated in this pilot application.

> “The panel was impressed by the close integration of business stakeholders into Mistra TerraClean in phase I.”
>
> Evaluation Panel Report, May 2021

WORK PACKAGE 4

HUMAN AND ENVIRONMENTAL SAFETY, LIFE CYCLE ASSESSMENT, SCIENCE AND SOCIETY

WP 4 Leader: Ian Cotgreave (RISE)

WP 4 provides toxicological input into various aspects of the projects integrated delivery of smart, flexible and effective filtration materials, fit for manufacture and testing in various societal situations.

LCA of potential environmental impacts and a risk assessment of hazards to humans and the ambient environment support the design and interpretation of results from material development and the case study, in relation to national standards and future environmental aims. The work also covered transmission of the results of the project and consequences of these to various stakeholder groups in society, including policy makers, regulatory authorities, industrial sectors and the general public. This to ensure maximal coordinated impact of the consortium work on Sweden's future industrial and environmental development, and the perpetuation of the consortium structure as a national resource for the area.

Results and achievements

In WP 4, the major task during 2021 was the LCA and life cycle costing (LCC) as part of the major case study in the programme. In this case study a new process for the mitigation of PFAS contaminated water by application of low-voltage electrochemical treatment by capacitive deionisation (CDI) was assessed.

The process of CDI was studied in both lab- and pilot scale. The lab-scale experiments were aimed to study the underlying mechanism of PFAS reduction through electrosorption and electrochemical degradation of PFAS. The experiments were performed using pure solutions of PFAS in deionized water which gave possibility to track the conversion of PFOS and PFOA to other species and to analyse the degradation products form the PFAS decomposition.

The aim of the pilot-scale experiments was to simulate treatment of drinking water polluted with relevant concentrations of PFAS. The experiments were performed both as batch short-term experiments performed at different operation conditions and as continuous experiments aiming to study performance of the process during long-term water treatment. The process performance was continuously monitored by chemical analyses and logging of process parameters, which was further used for conduction the LCA and LCC.

In the case study LCA and LCC were conducted to support further optimization of the CDI for this application. In a dialogue with KTH and SWT, a life cycle inventory for the manufacture and operation of the CDI in a capacity and size suitable for pilot studies was derived. In a prospective scenario this system model was scaled up, based on learnings from the pilot. As a reference scenario for established technology, based on literature data for a full-size application, the conventional water treatment using granulated activated carbon (GAC) was modelled. Characterization of potential toxicity and ecotoxicity impacts across the life cycle of the device was made possible by the inclusion of a system model in the novel method ProScale and calculation of new per- and polyfluoroalkyl substances (PFAS) characterization factors. Life cycle impact assessment (LCIA) was focussed on climate change and (eco)toxicity indicators. A broader set of indicators were investigated with a screening approach based on normalized results (person equivalents) for the recommended environmental footprint categories. An LCC was conducted based on inventory of energy demand and relevant costs associated with the CDI device and reference GAC scenario over their respective life cycles.

LCA (Fig. 10) results indicated that, in pilot scale, energy use during operation is an important source of potential environmental impacts for the CDI for the indicators climate change, indirect human toxicity in the non-cancer effects category and ecotoxicity, while the manufacturing life cycle stage has important contributions for indicators indirect human toxicity in the carcinogenicity effects category and direct toxicity effects. At pilot scale system auxiliary materials had a large contribution to the accumulated impact scores, but it was shown that in a larger scale system their importance would be drastically reduced in relation to core module components. Quantification of potential impacts from PFAS emissions with the treated water, when the treatment goal is set to 85 ng/L (sum PFAS-11), indicate that potential impacts from the emitted water could still be, in relation to device manufacture and operation, an important contributor to overall potential impacts (indicator human toxicity, non-cancer effects). Thus, illustrating the relevance of the water treatment but also highlighting the great potential from in situ PFAS destruction.

Relating the prospective large-scale scenario to the scenario of the established GAC treatment was found challenging due to differences in scale. The evaluation was still able to highlight areas with possibility to improve the system further to strengthen its competitiveness with conventional techniques.

The LCC analysis was equally challenged by the differences in scales between the systems. It was concluded that if further technology development leads to enhanced PFAS degradation during the treatment with only trace amounts of PFAS remaining in the concentrate, this would positively influence the outcome of LCC, since treatment of the concentrate is currently a major cost component. Furthermore, it is possible that the CDI system is more cost-effective for treatment of more challenging water streams containing both PFAS and other pollutants.

In conclusion, LCA and LCC results proved already during pilot operations to be relevant guidance in the further development of the CDI for treatment of PFAS contaminated water. In future research and further development new knowledge gained can be incorporated into the systems models in a tiered approach to further support the development of smart solutions for water and air purification.

During 2021 the phase I work with societal stakeholder groups was evaluated and a new structure was developed for phase II. An analysis was made based on interviews with researchers in the program, companies and contacts taken with authorities. A closer collaboration with Mistra SafeChem on societal outreach was achieved and will become visible in 2022.

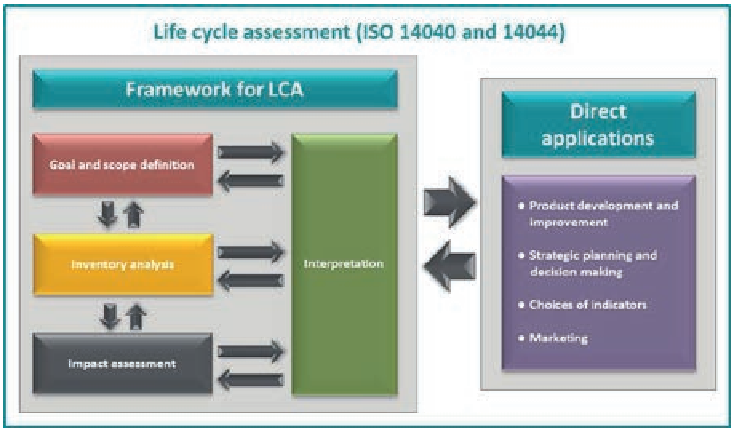

FIGURE 10. Schematic presentation of the LCA procedure.

(Source: Standard document ISO 14040-44.)

WORK PACKAGE 5
MANAGEMENT, IP HANDLING AND COMMUNICATION

WP 5 Leader: Ulrica Edlund (KTH Kungliga Tekniska Högskolan)

WP 5 includes setting up the administrative routines and carrying out activities to ensure that all partners fully understand their role and are committed to the program. It implements routines for communication, document exchange, technical and economic progress reporting, to assure that resources allocated for research, development and outreaching objectives are properly utilized.

All management work is carried out within this WP assuring deliverables, prototypes and demonstrations and communication with stakeholders are on time within the given budget. WP 5 facilitates an effective cooperation and communication between the different WPs.

Results and achievements

Work within WP 5 was throughout the programme devoted to facilitating the progression of activities in all aspects. The year 2021 started – and continued – during a pandemic that to some extent challenged progression, not in the least by limiting our access to laboratories, industrial sites, and tests beds. Social distancing presented challenges to uphold communication and outreach. Lessons learned from the pandemic have made us better prepared for future pandemic impacts and how to adapt accordingly. Even in these pressing times, all partners continued to deliver, uphold fruitful collaborations, and contribute to the transdisciplinary knowledge-transfer that is key to addressing and succeeding in solving complex challenges.

The Royal Academy of Engineering Sciences, IVA, managed a project on Sustainable water supply management and strategies in urban environments, aiming to map Swedish challenges, opportunities and elaborate an action plan for the future, *Hållbar vattenförsörjning*. Prof. Edlund served as a working group member at IVA throughout the project in 2020-2021, contributed to the final report released in 2021, and presented some findings at a public webinar in February 2021.

A journey from phase I to phase II

The year 2021 was the year when the four-year term and funding originally granted by Mistra reached an end. Convinced that the goals and activities of Mistra TerraClean are still of immediate value, and encouraged by the important results so far, we set out to evaluate the programme and apply for a continuation of four years, a second phase.

A series of consortium and steering group meetings all contributed to self-evaluation and analysis of the performance of the programme and the consortium. This valuable exercise helped us identify weaknesses and strengths and devise a strategy and plan for phase II: to build on the strength achieved in phase I and constructively handle the weaker parts. We also identified the need for some new collaborations to level up and embark on new challenges and connect with new partners.

An evaluation report and a full proposal for continued research were prepared in intense efforts and impressive collaboration from the entire consortium and submitted to Mistra in March 2021. An evaluation process, involving an external expert panel, provided excellent feedback.

Phase I started largely from low TRL levels which has influenced the structure of the case portfolio. During phase I, a gap of supplied and required TRLs levels was identified. In phase II, this gap is addressed and bridged with a new working structure with elaborated case packages.

Phase I provided an in-depth survey of the scientific, technical and industrial landscape and resulted in more knowledge about hot-spots and knowledge gaps. As a result, we established relationships around identified areas of mutual interest, and several new partners expressed an interest to join phase II.

The consortium gathered competences from a range of different areas, including chemistry, material physics, membrane technology, environmental analysis, toxicology, fluidics, and from different sectors: academy, research institutes, and industry. Phase I fostered knowledge transfer and cross-disciplinary learning, for instance by cross-sectional learning seminars and study visits for all consortium members. We will carry over this activity to the next phase.

The proposed continuation of Mistra TerraClean builds on lessons learned during the first stage and provides a coordinated, transdisciplinary, and highly skilled set of competences to address current and upcoming challenges in the complex landscape of air and water purification. Generated materials and research results have shown us what we can do and how we can progress.

Our proposed plan for a second phase was to expand to address new challenges and tasks and we identified competences and actors that we wanted to add to the consortium.

In June 2021, the board of Mistra decided to grant Mistra TerraClean 57 million SEK for a continuation until September 2025. The decision spurred an intense preparation process crowned by kick-off of phase II in October 2021.

> “The panel concludes that the Mistra TerraClean programme can be expected to uphold a high standard of academic achievements in phase II. The second phase follows seamlessly from the work packages and developments in phase I. It has the potential to generate additional new knowledge of great societal value.”

Evaluation Panel Report, May 2021

MISTRA TERRACLEAN, PHASE II

STRUCTURE OF THE PROGRAM

Phase II of Mistra TerraClean will run from 2021 to 2025 with a new working structure and with elaborated case packages.

Given all the expertise and materials developed in phase I, we can address both continued and new challenges in phase II. With new challenges, an extended network, and an increasing attention in the potential of Mistra TerraClean has attracted attention from many companies. In phase II, we are adding on several new partners to strengthen our ability to address current and future needs.

There is an immense need for new technologies and efficient solutions for clean air and water and we cannot possibly address them all. We have chosen six areas of prime concern where our smart material hub for environmental solutions can add value, and where Mistra TerraClean expertise could meet the needs. These areas are denoted Case Study Packages, CSPs, and include several activities on different technology readiness levels (TRL), where materials and devices are evaluated and developed in collaboration with stakeholders for specific contaminants (Fig. 11). Selection criteria for the CSP topics were value to users, the advantage of smartness, energy and resource consumption, TRL and generality.

The case topics are well motivated and responds to the needs of today while being pro-active for those of tomorrow. Mistra TerraClean I has surveyed the area, built a firm foundation and implemented an interdisciplinary competence hub. Mistra TerraClean II is about levelling-up.

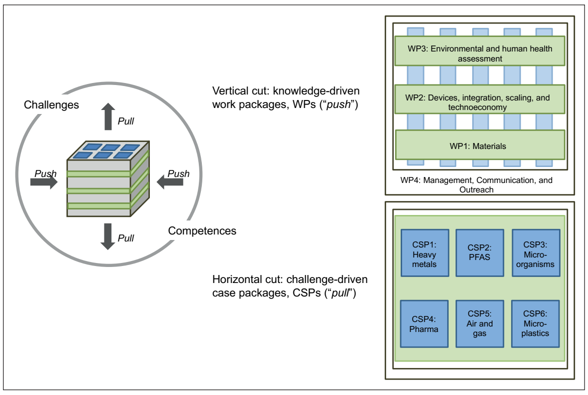

FIGURE 11.
The push-pull driven structure of Mistra TerraClean II.

> "The proposed work plan of phase II continues the ambitious programme with the aim of addressing not only current, but also up-coming challenges in the complex landscape of air and water purification. The panel acknowledges the proposed restructuring of the programme organization in challenge-driven case packages that focus on removal of special classes of pollutants and crosscut the knowledge-driven work"
>
> Evaluation Panel Report, May 202

VOICES FROM CONSORTIUM PARTNERS

Peter Gruvstedt, Manager, Wastewater treatment plant, Astra Zeneca

Why are you engaged in the Mistra TerraClean II?

Environmental protection is one of AstraZeneca's sustainability priorities, under which some of the focus areas are waste management, greenhouse gas reduction, water stewardship and pharmaceuticals in the environment.

All these areas are aspects that the Mistra TerraClean program focus on. The set up with partners from different universities, research institutes and different innovative companies makes a perfect platform for using each other's experience and expertise.

Our wastewater plant in Södertälje was built and optimized 25 years ago, for treating the process wastewater generated at our sites. In the case studies that we contribute with, we are investigating alternative techniques for removing pharmaceutical residues in our effluent water. The aim is to further improve our existing processes.

What are the benefits of joining a consortium, for a company of your size and kind of business?

The best way of addressing and solving complex problems is to collaborate with others. We have good knowledge when it comes to our unique conditions, and the characteristics of our process wastewater. However, we are no experts in developing new techniques for water treatment. So basically, we have a challenge, and the other partners have solutions and expertise that we can benefit from.

What do you expect from being a partner in Mistra TerraClean II?

Evaluating new techniques that potentially could improve our process – and our knowledge for future technology selection.

Provide real cases that can help the innovative companies evaluate and improve their current techniques or test and receive results from new application areas.

Personal development for us involved – both through collaboration and learning from all experts involved, but also through all the workshops and seminars arranged within the program.

What will be the ideal result from Mistra TerraClean II?

A wider knowledge of suitable techniques. Hopefully we find a technique that is scalable, more efficient, more predictable, and even more sustainable.

What, and how, do you plan to contribute to the program?

We will be contributing with different case studies for removing pharmaceuticals from our process wastewater. The proposed case studies focus on removal and destruction of potentially harmful organic chemicals from process wastewater.

We will be working together with Stockholm Water Technology, Radma Carbon and Axolot, RISE and KTH. Different techniques will be tested, optimized, and scaled up. From lab scale to on-site pilot tests at our unique wastewater treatment plant.

Zhaleh Atoufi, PhD Student, KTH

How does your work address the societal challenges of clean air and water?

Water contamination with inorganic and organic pollutants is a severe environmental issue. Hence, it is crucial to develop effective techniques for robust water purification. My research activities focus on preparing cellulose-based aerogels for removal of different contaminants including organic solvents, heavy metals and dyes from water. Considering the importance of sustainability and using natural renewable resources, and since around 69% of Sweden is covered by forest, it would be a great opportunity to form efficient cellulose-based adsorbents for water purification.

What is it like to be a PhD student in a large and multidisciplinary program?

It´s been indeed a great opportunity for me to be part of Mistra TerraClean program where both industry and academic partners contribute. Collaborating with industry gave me insight on the practical challenges that companies are dealing with and the requirements that a novel filter or adsorbent must have to be scaled up. In addition, collaborating with academic partners who have experience at different research areas improved my knowledge and wisdom.

In what way does the network contribute to additional dimensions in the work?

The network contributes in two ways: generation of the knowledge and its application. Although there have been various studies in this field, the network empowered me to generate a knowledge that is both practically and theoretically valuable. The combination of these two features enables societal and scientific stakeholders to provide sustainable and applicable solutions to air and water pollutant problems.

Emil Vestman, CDO, Mimbly

Why are you engaged in the Mistra TerraClean II?

We are engaged in the program to contribute to microplastic free laundry to the highest degree possible. Its one of our core values as a company and being a part of the MistraTerraClean allows us to talk to experts in the field and contribute to new solutions tackling this problem.

What are the benefits joining a consortium for a company of your size and kind of business?

We get a much broader view on the issue, potential solutions and increase the chances of creating a truly sustainable solution that is aligned with our goals as a company.

What do you expect from being a partner in Mistra TerraClean phase II?

We expect to get insights from experts in the field of microplastics, filtration and materials science.

What will be the ideal result from Mistra TerraClean phase II?

The ideal result from this project for us would be that we get a better understanding of the complex nature of this issue and that we can develop solutions to the problem during the program.

What, and how, do you plan to contribute to the program?

We plan to contribute to the program by sharing real life experiences from filtering microplastics on the field, and contribute with water samples, test benches and anything that is related to end usage of filtering micro plastics from laundry.

WORK PACKAGE 1
MATERIALS

WP 1 Leader: Niklas Hedin (SU)

Key questions and scope

New materials are synthesized and functionalized for the six CSPs with their targeted applications. Materials with targeted functions are provided for the different cases, i. e. heavy metals, pharmaceuticals and related molecules, VOCs and PFAS removal from water, microorganisms and fouling, microplastics and gas purification in relation to, for example, CO_2 removal.

All the tasks involve efforts that make the materials either adaptive, responsive, or interactive, preparing for integration in devices in WP 2 and in the CSPs.

Progress and achievements during 2021

WP 1 is in phase II arranged in five tasks and many of the activities have a seamless transition from phase I.

1.1 Carbonates, hydroxides, and related compounds

UU is continuing with the development of carbonate, hydroxides, oxides, and related compounds. The development of normal framework porous materials together in composite and as a stand-alone sorbent for gas purification has now started.

1.2 Carbon-based smart materials

Activities are ongoing with, for example, the studies of amine-modified carbons for CO_2 capture in relation to CSP 5. Also, activated carbons are being derived for the use in CSP 5 for the removal of volatile organic compounds, which is of interest for Camfil and RISE.

1.3 Lignocellulosic materials

The activities are large and different materials are derived and being studied.

1.4 Chemically modified materials

This chemistry-oriented task supplies materials and knowledge for several of the CSPs and the activities are ongoing.

1.5 Characterization platform

The task is dedicated to characterizing the sorbent materials developed and validate their selectivity and ability to capture metal ions, molecular species, etc., either after or in situ, either during molecular adsorption tests or catalysis. The techniques of relevance are many and this task is to facilitate the information of use of the various materials characterization equipment at the involved partners' sites.

WORK PACKAGE 2
DEVICES, INTEGRATION, SCALING AND TECHNOECONOMY

WP 2 Leader: Mats Sandberg (RISE)

Key questions and scope

Technoeconomy, scaling, integration and interactions are key elements in WP 2. At the molecular level, interactions between absorbent materials and stimuli forms the cornerstone of smart filter materials and sensor absorbents. At the device level, filter devices are provided with conduits for stimuli to access materials and enable smart operation. At the organizational level, work on scaling and technoeconomy is to link industrial needs and regulatory processes with targets for the materials development.

PFAS-sensor concepts are to be developed in WP 2, as well as work on other sensor technologies for CSP needs. Methodologies in materials development are increasingly supported by robotization and machine learning. Possibilities of using automatable or robotized tools to manufacture and evaluate filter and sensor materials, and potentially applying machine learning support in evaluation and development of materials, should be utilized to the extent possible.

Progress and achievements during 2021

Most of the activities October to December 2021 were start-up activities.

Planning and organization

WP 2 has scheduled monthly on-line meetings for the spring 2022. These are planned to be themed on the six CSP's one per monthly WP-meeting. One purpose of this is to link up the WP with the CSPs and to understand the technology needs of interest to WP 2. Another purpose is to bring in the "pull-side" perspective in the CSP and WP work, that is, the commercialization and scaling perspective by shedding light on industrial needs, potential markets etc..

Connecting activites in WP 2 with WP 3 was discussed and planned.

Task 2.3 can be considered a first milestone for materials and devices developed in Mistra TerraClean. To facilitate the processes of materials evaluation, WP will setup a list of materials coming out from the project and from WP 1.

Task 2.1 Connected filter devices and integration

During 2021, the activites in task 2.1 were limited to planning and literature surveys on sensor needs. The planning concerns mapping if sensor needs for the CSP's and the device types intended for use and development during phase II of the programme. As we anticipate that developing sensors for PFAS will be the most difficult and badly needed challenge in this task, the Mistra TerraClean Seminars series started in 2021 with a seminar on electrochemical PFAS sensors.

Task 2.2 Sensors and sensor materials

The need for high throughput experiments in the development and evaluation on materials is widely recognized and materials laboratories around the world are gradually robotized. High throughput testing is essential when many tests need to be carried out on a large number of materials. Mistra TerraClean is a response to a call do develop smart materials, and therefore an endeavor expected to produce many materials with a range of filter applications.

Further, the consortium is to evaluate the smart materials for filter and sensor functions, a task that require determination of many absorbent and sensor parameters by test series for each materials candidate under evaluation. The sheer number of tests for each material needed for the evaluation process translates into an overwhelming experimental task. For this reason, we explore robotized and high throughput methods for smart materials evaluation.

Arrays of electrochemical cells for robotized testing of sensor-absorbents. Smart materials are defined as materials responding to external stimuli, and to the extent the stimuli is in the form of electrons and potential, development of the electronic smart material, the task of evaluation is similar to the task of development of electrodes. Electron responding smart filter materials constitute electrochemically responding sensor absorbents where evaluation methods are similar to that of electrodes. To this end, we have designed arrays of printed electrochemical cells for robotic handling and robotic dispensing of test solutions and robotic deposition of smart materials.

More specifically, the arrays of the electrochemical (EC) cells are designed to fit within the size of 96-well plates, such as used in enzyme-linked immu-

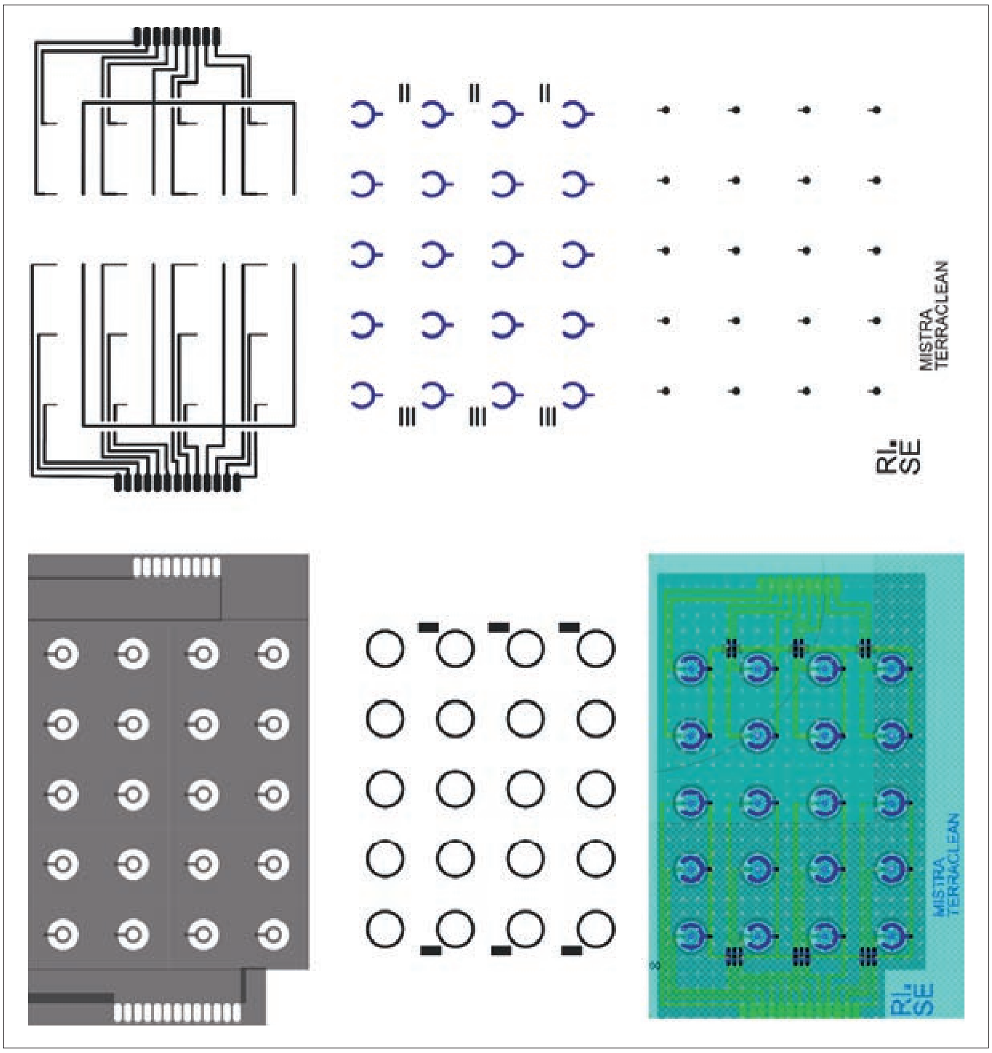

FIGURE 12. CAD-layout and layers for a screen-printed array of electrochemical sensors for robotized characterization of sensor-absorbent electrode materials.

nosorbent assay (ELISA) tests, and the EC cells are in register with the 96-well positions (Fig. 12). To simplify the design, we have opted for plates with 19 EC cell wells (where number 20 is replaced with a grip for robotic handling). The cells are constructed as two-electrode cell with a working electrode and a larger counter-reference electrode.

Three structures are printed on each substrate sheet. Two are designed to be contacted from the top of the plates and one designed for bottom contacting. Top contacting is simpler to realize in a first round of tests, while the bottom contacted structure is simpler to handle and contact. In one cell of the top-contacted structures, the two-cell structure is replaced with a transistor structure. This is mainly to demonstrate the possibilities with the home-made design. Further, sensors constructed as electrochemical transistors can exhibit higher sensitivity than sensors built as normal two- or three electrode cells.

There are two main use-modes of the EC-cell plate. In one mode the material under test is screen printed during plate manufacturing. The material under test is then dispensed onto the cell to from an array of different test solutions. In the other mode, the active sensor material is deposited onto electrochemically inactive electrode materials with a dispensing robot. After drying, the modified electrodes are tested against one or more test solutions.

In addition to the plates, a measurement platform has been designed, where the plate is to be placed and contacted for measurements. The platform is designed to fit into the Proteus robotized test setup at RISE. These designs were finished during 2021 in Mistra TerraClean phase II and screen-printing patterns are being manufactured.

Task 2.3 Materials mapping

Compilation of scalability, technoeconomical, and performance evaluation of materials developed in WP 1 and devices (rolling report) was started. Some WP and CSP leaders as well as selected researchers have been contacted, and material developed in the project was compiled in a document. The document has connected material, applications and as much as possible on references (articles and reports). A timetable was established to include WP 3 in the rolling report and focus on new materials for evaluation.

FIGURE 13. Consortium meeting at KTH, October 2021.

WORK PACKAGE 3
ENVIRONMENTAL AND HUMAN HEALTH ASSESSMENT

WP 3 Leader: Hanna Holmquist (IVL)

Key questions and scope

WP 3 will provide ecotoxicity and human health related toxicity input into various aspects of the projects integrated delivery of smart, flexible and effective filtration materials, fit for manufacture and testing in various societal situations. LCA of potential environmental impacts and a risk assessment of hazards to humans and the ambient environment will be performed and documented. The work will also support the design and interpretation of results from a variety of case studies, addressing individual issues of environmental pollution and human safety, in relation to national standards and future environmental aims.

The life cycle perspective in phase II includes screening LCAs or further simplified approaches, but also more extensive LCA studies, including economic and toxicological effects and a cradle-to-grave perspective (Fig. 14).

Progress and achievements during 2021

WP 3 activities were focused on establishing a team of experts from the involved partners, IVL, RISE, RISE-IVF and SLU. Current plans for research activities in the respective tasks are focussed on establishing a "test case" for trimming procedures and on continuation of LCA-based studies from phase I. Interactions with other WPs and CSPs have been initiated. Initial risk mitigation plans for each CSP are in progress.

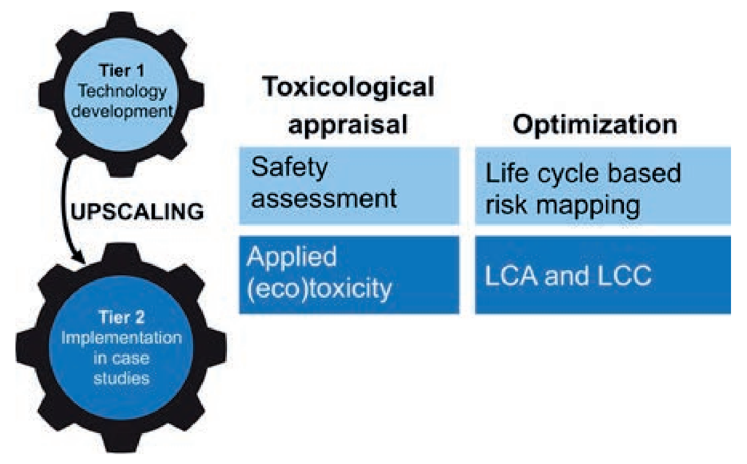

FIGURE 14. Different tools suggested for the appraisal processes.

WORK PACKAGE 4
MANAGEMENT, COMMUNICATION AND OUTREACH

WP 4 Leader: Ulrica Edlund (KTH)

Key questions and scope

WP 4 is crucial to the progress and success of the programme. All management work is carried out within this WP assuring deliverables, prototypes, and demonstrations are on time within the given budget. Key aims are to:

- Follow-up and support day-to-day operation, organizing programme functions and meetings.
- Establish efficient coordination and communication between partners
- Follow up progress and take necessary actions to assure that programme results are reached within budget; deliverables and milestones.
- Manage financial and administrative aspects of the programme.

Progress and achievements during 2021

WP 4 was instrumental in implementing phase II and, with as little lag time as possible, facilitate the transition from phase I to phase II: a seamless transition of tasks carried over from phase I and initiation and ramping up of new work activities. A consortium agreement was prepared and signed by all partners. A steering group was established, and a monthly meeting scheme was set up.

A kick-off consortium meeting was held in October 2021, at a time when restrictions caused by the pandemic still allowed for in-person meetings (Fig. 13). In a hybrid virtual and in-person event hosted by KTH, we welcomed all partners to Mistra TerraClean phase II and devised a roadmap for immediate action.

Phase II is planned to strengthen the attention to interaction with the broader community and authorities. Planning for case-oriented outreach activities started in late 2021, first with a seminar series (all digital if the pandemic situation does not improve) with industry and authorities to stimulate dialogue on where best available technologies are today and how Mistra TerraClean research can supply and fit in the development to more effective cleaning, as well as what current obstacles exist toward better technology.

The plan for outreach with public seminars and collaboration with authorities on new technology was launched and seminars for 2022 was decided: one seminar about EUs Industrial Emissions Directive and one about EU Chemical Strategy in collaboration with Mistra SafeChem.

CASE PACKAGE 1:
HEAVY METALS

Case Package Leader: Johan Strandberg (IVL)

Key questions and scope

CSP 1 is addressing the treatment of several types of water streams in mining and former mining operations, and the removal of heavy metals (Fig. 15). The methods addressed may also be applicable for the treatment of other waters contaminated by heavy metals, e.g. leachate water or contaminated storm water. Metal-enriched, acidic mine drainage (AMD) can be a threat to natural waters and might require treatment before it can be released to a recipient. The scope of this case package is to find new methods with higher efficiency, less waste and lower cost than the methods available today.

Progress and achievements during 2021

Work was initiated in January 2022, devoting the first two quarters of 2022 to establishing baselines concerning emissions of heavy metals from the three cases in the package. The baseline descriptions will be used to match the materials developed in the program.

FIGURE 15. Water effluents from mining sites are treated for the capture of heavy metals.

CASE PACKAGE 2: PFAS, POPS AND INDUSTRIAL WATER

Case Package Leader: Tove Mallin (RISE)

Key questions and scope

Persistent organic pollutants (PoPs), exemplified by PFAS, continue to present enormous problems to society and industry in terms of remediation of a wide variety of water sources. The PFAS problem is still high on the agenda for the EU in terms of restriction and/or regulation of use and need for remediation.

A cluster of case studies has been assembled which probe a variety of situations where contaminations, e. g. by PoPs, may occur, due to a variety of industrial activities. These cases, in general, utilize either the relatively high TRL material/device combination already tested in the programme, or explore the use of other materials with remediation potential from the extensive Mistra TerraClean material library. Since the remediation technology development is moving forward rapidly, constantly providing new materials and techniques, exploration of other smart materials may be added along the progress of the programme, either from additional industrial partners or from the Mistra TerraClean material library.

The technologies will be tested to an initial proof of concept (PoC) within the Mistra TerraClean in lab-scale, with the possibility to longer time period testing and/or scale-up, depending on the interest from the problem owners and possibility of additional external financing.

Progress and achievements during 2021

Two challenges were identified initially, PFAS contaminated water resulting from fire training activities and slop water resulting from oil drilling activities. It was decided to divide the work into the two different cases and separate meetings will be held in the SAAB case and the SKF case, respectively.

In the SKF case, tests with the CDI technology (SWT) are planned. In the SAAB case, tests with the CDI technology (SWT) and magnetic carbon (Radma carbon) are planned.

In addition, a meeting between Alfa Laval, RISE and IVL has been held. The membranes from Alfa Laval that will be tested for PFAS removal are right now on a lower TRL than the other solutions in the SAAB case. An initial test will be performed on tap water spiked with PFAS preferably early in 2022. IVL will perform the tests on their site and Alfa Laval will provide the membranes. IVL will provide a testing plan.

Interactions have mostly been with WP 3, Task 3.1 – Risk Mitigation Plan (RMP). A RMP for this CSP will be created, identifying and mitigating relevant risks for human health and the environment.

CASE PACKAGE 3: MICROORGANISMS AND FOULING

Case Package Leader: Ian Cotgreave (RISE)

Key questions and scope

The development and maintenance of effective, closed water delivery systems is area of utmost importance. One of the continual problems associated with clean drinking water supply is the area of biofouling. A slight biofilm on the surface of pipes in water supply is generally regarded as positive if mainly benign bacteria are present. However, the formation of biofilms with presence of pathogenic microorganisms in the water flow and blocking effects constitute problems. Similarly, in the wake of the corona pandemic, increasing focus is being placed on removal of microorganisms from circulatory air supplies in, for example, public buildings. Therefore, there is an urgent need to devise new air filtration techniques that are more effective and sustainable, and by 2022 addressing the problems of biofouling and lack of regenerability which exist with current approaches.

Two cases will be driven by the programme in this area, one in closed water loop biofouling and one in air filtration biofouling.

Progress and achievements during 2021

Progress regarding both the air- and water-borne biofouling cases has been slow. This has been due to restrictions in carrying out site visits at Uponor and Camfil. However, the following progress for each can be reported for 2021:

Concerning air-borne biofouling, a project group consisting of RISE and Camfil has been established where initial exchanges have centred around practical details of test rig design were discussed, ideas for sensor monitoring aired, and bacteriological approaches defined to some extent. The group now must move this into a planning stage, with definition of practical details, division of labour and use of resources. When it comes to water-borne biofouling, a project group has been established consisting of SU, Alfa Laval, KTH, SWT, Uponor and RISE. Initial exchange of high-level ideas has been performed, particularly in the area of chemical modification of cross-linked polyethylene (PEX) piping for biofilm prevention.

Discussions around the use of Alfa Laval and SWT approaches to removal of bacteria from water streams during hammer effects have begun. Discussions have been carried out around the use of standard bioreactors at RISE for initial studies on biofouling, including which bacterial species would be relevant.

The group now must move this into a planning stage, with definition of practical details, division of labour and use of resources. Initial discussion on the inclusion of fibre-optic, fluorescence-based detection/sensing in water flows and on pipe surfaces have begun with RISE.

CASE PACKAGE 4: PHARMA

Case package leader: Ian Cotgreave (RISE)

Key questions and scope

In addition to the normal solvent and solute wastes generally emitted from chemical plants, chemical processes involved in pharmaceutical production generate large amounts of active pharmaceutical ingredients (APIs), as well as potentially bioactive intermediates, which may potentially escape into the environment via waste-water streams. Conventional waste-water treatments usually employ one or other of the following approaches: granular acticated carbon (GAC) filtration, direct ozonation, chemical flocculation and biological degradation. Each of these approaches has its own limitations, in terms of energy requirements, carbon foot-print issues, recyclability problems and limited capacities of treatment.

This case study aims to take one of Mistra TerraClean's high TRL material/device combinations and mate it to a PoC study to examine if the technique can be utilized to remove APIs and intermediates from water streams representing those normally encountered within AstraZeneca's manufacturing facilities in Södertälje, Sweden.

Progress and achievements during 2021

The work has begun on multiple fronts. Regular meetings have been established between the various partners (AstraZeneca, RISE, KTH and SWT) and several practical needs have been identified and work initiated. Due to the pandemic situation, however, site visits have been precluded, which will need to be resolved as soon as it is allowed by national restriction regulation, and AstraZeneca's internal policies.

The active pharmaceutical ingredients (APIs) for study have been discussed and prioritized for testing. These represent various chemicals which are currently in the water streams which AstraZeneca have to deal with continuously. The initial selection has considered physico-chemical parameter variations, to give as wide a range of structures for testing as possible. Target chemicals have been ordered. Chemical structures have been communicated to RISE, to begin designing the various analytical approaches required when initial laboratory testing begins.

A plan has been developed for initial laboratory-scale tests at KTH using the CDI technique on simulated water flow mixtures of selected APIs. The concentrations which are relevant have been decided upon and the initial mixture complexity has been determined. Initial laboratory tests are planned to commence early in 2022.

Design of pilot unit to be installed at RISE's or AstraZeneca's facilities has been outlined. Size and flow will be dimensioned to match the AstraZeneca lab test rig parameters. Parts and components are ordered for pilot. Work plan and flow are agreed between KTH and SWT. KTH will initiate testing on bench scale with samples, followed by pilot installation by SWT, once operating parameters are defined via the bench scale tests. Initial contact has been made with RADMA Carbon, and a preliminary plan for application of their magnetic carbon technology has been developed, with reference to combination with the CDI technology.

CASE PACKAGE 5:
AIR AND GAS

Case package Leader: Hjalmar Granberg (RISE)

Key questions and scope

The removal of gas molecules, such as SOx, NOx, CO_2, and low-boiling point VOCs (volatile organic compounds), including formaldehyde, from indoor air are targeted. This includes material suppliers, filter manufacturers, installers and end users of air filters, forming the value chain of air-purification solutions. By combining the competences in separation methods and smart materials with the needs of users, innovative concepts for new and versatile systems for heating, ventilation, and air conditioning (HVAC) can be targeted, aiming at a combination of better economy and healthier air.

The work will focus on the following:

- New combinations of materials will be tailored and brought to TRL 4, evaluated in lab-scale. To achieve this evaluative tailoring, it will be important to study aspects such as airflows, pressure drops, adsorption/removal efficiency, and regeneration potential in HVAC systems during use.
- Based on the results, selected materials, or combinations of materials will be considered for further refinement, and techno-economical hotspots of production, operations and regeneration will be identified.
- Together with manufacturers and/or end-users, one or more material platforms may be prepared for upscaling with the necessary parts (cartridge, ducts, sensors etc.) fabricated for performance tests under realistic conditions/simulators.

Progress and achievements during 2021

We started the work with a kick-off meeting including all the involved academic and industrial partners. It was decided to set up thematic meetings during the programme's first six months to better understand the full scope of the gas adsorption and ventilation problems and how to target them.

This meeting series started with a technical discussion on flow rates through filtering media, based on results from the flow rate review of filtering media geometry from Mistra TerraClean phase I, and how these fits with the demands from industry and end use. Other seminar topics that were identified relate to adsorption and related kinetics, how graphene can be used in water and air filters, end user needs on ventilation systems and how these can be tested in realistic conditions, continuation of the development of aerogel air filters, and how to make ventilation systems smart. The topics involve both industry and academia, and may in some cases cut inter-disciplinary through the Mistra TerraClean program. Further seminars are planned to be executed in the beginning of 2022.

Work on producing different filter media in the lab has started and one can foresee lots of collaboration between CSP 5 with WP 1 and CSP 3.

CASE PACKAGE 6: MICROPLASTICS

Case package Leader: Sven Norgren (RISE)

Key questions and scope

Anthropogenic generation of microplastics is a pertinent and global problem that is escalating steadily. Two of the major sources of microplastics in Sweden are particles generated by traffic and washing machine effluents. Early capture, and water-phase capture will lower the risk of particles becoming airborne and the risk of particle down-sizing (Fig. 16).

Traffic-generated particles end up in run-off waters and are not captured, while household-generated microplastics are removed in water-treatment plants. This case package will look for potential synergies with studies within the programme Mistra Nanosafety and the possibility of joint activities.

Progress and achievements during 2021

The case package work is started, as some literature study and learning in the area has been done. As a fist proof-of-concept study, we will develop filters for the outlet of domestic washing machines. Filters will be prepared by structuring (e.g. 3D-printing, air-laid technology, papermaking-like process).

FIGURE 16. Filtering of washing wastewater may capture released microfibers and mitigate microparticle pollution.

OUTREACH AND SCIENTIFIC OUTPUT

SCIENTIFIC OUTPUT AND OUTREACH ACTIVITIES – PUBLICATIONS

Georgouvelas, D., Nasser Abdelhamid, H., Li, J., Edlund, U., Mathew, A.P. (2021) All-cellulose functional membranes for water treatment: Adsorption of metal ions and catalytic decolorization of dyes. Carbohydrate Polymers, 264, 118044. https://doi.org/10.1016/j.carbpol.2021.118044

Åhlén, M.; Jaworski, A.; Strømme, M.; Cheung, O. (2021) Selective adsorption of CO_2 and SF6 on mixed-linker ZIF-7–8s: The effect of linker substitution on uptake capacity and kinetics. Chemical Engineering Journal, 422, 130117. https://doi.org/10.1016/j.cej.2021.130117

Åhlén, M.; Kapaca, E.; Hedbom, D.; Willhammar, T.; Strømme, M.; Cheung, O. (2021) Gas sorption properties and kinetics of porous bismuth-based metal-organic frameworks and the selective CO_2 and SF6 sorption on a new bismuth trimesate-based structure UU-200. Microporous and Mesoporous Materials, 329, 111548. https://doi.org/10.1016/j.micromeso.2021.111548

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SUBMITTED

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Nasser Abdelhamid, H., Georgouvelas, D., Edlund, U., Mathew, A.P. (2021) CelloZIFPaper: Cellulose-ZIF Hybrid Paper for Heavy Metal Removal and Electrochemical Sensing. Submitted manuscript

Zhou, X., Shen, B., Lyubartsev, A., Zhai, J., Hedin, N. (2021) Semiconducting Piezoelectric Heterostructures for Piezo- and Piezophotocatalysis. Submitted manuscript

Hao, W., Yang, J., Wang, X., Hedin, N. (2021) Activated fibers for CO_2 capture derived from electrospun fibers based on polyvinylpyrrolidone and colloidal hydrochar. Submitted manuscript

Saadattalab, V., Jansson, K., Hedin, N. (2021) Blue hydrochars formed on hydrothermal carbonization of glucose using an iron catalyst. Submitted manuscript

Hsini, N., Saadattalab, V., Wang, X., Dhaouadi, H., Dridi-Dhaouadi, S., Hedin, N. (2021) Activated carbons from hydrothermally carbonized prickly pear seed waste. In manuscript for rework and resubmission

CONFERENCES

Georgouvelas, D., Edlund, U., Mathew, A.P. (2020, June) Cellulose nanocrystals with zwitterionic polymer grafts – a material with enhanced antifouling and antibacterial properties [Oral presentation] Conference on Nanotechnology for renewable materials (TAPPI), Helsinki, Finland.

Granberg, H., Gimåker, M., Fall, A., Håkansson, K., (2021, Oct) Opportunities for production of non-woven bio-based electronics [keynote presentation], INDEX™20, Geneva/Online.

Hedin, N. (2021, March) Biomass-derived carbons for adsorption in gas phase [Keynote presentation] International Symposium on Functional Biomass-derived Carbon Materials, Spain/Online.

Saadattalab, V. (2021, March) Hydrothermal carbonization of glucose in the presence of iron ions [Oral presentation] Sweden International Symposium on Functional Biomass-derived Carbon Materials, Spain/Online.

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