Mistra TerraClean
Annual Report 2020

MISTRA
TERRACLEAN

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FÖRORD

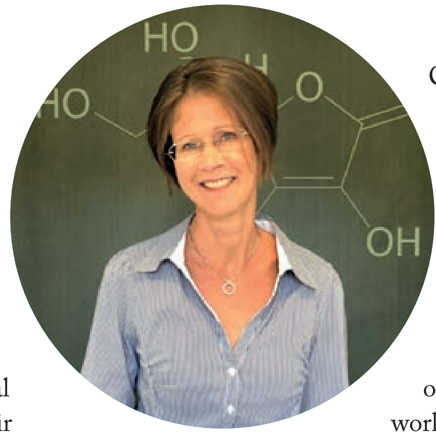
Det har varit en ovanlig utmaning att aktivt utveckla och koordinera detta omfattande projekt med alla människor och skilda aktiviteter under detta pandemiår.

Jag anser att jag har bred erfarenhet av att bedöma projekt från mitt långa arbetsliv i ledande ställning och jag är uppriktigt imponerad av den projektledning och det fokus på resultat som karakteriserar denna verksamhet.

Projekten och dess olika s.k. work packages har rullat på bra och koordinerats väl under det gångna året och det har gått lätt att följa olika aspekter av framdriften trots begränsningen i fysiska möten. Vi är nu inne i en fas där vi får möjlighet att pröva forskningsresultat direkt på marknaden och det är mycket spännande.

Bo Olsson, 18 mars 2021
Member of the programme board

A MISTRA TERRACLEAN PERSPECTIVE ON 2020



Mistra TerraClean develops smart and safe engineered materials and devices for clean air and water. Our vision is to establish a strong research and innovation environment enabling the development and use of smart materials engineered from indigenous raw materials, to provide substantial contributions to the national environmental and health aims in air and water quality. The programme addresses two of the main global challenges for the future – clean air and clean water – and how smart materials can be part of the solution to these challenges. This report presents an overview of the Mistra TerraClean programme, our achievements, challenges, and progress during 2020.

It was an eventful year. Materials with high and selective adsorption capacities were produced and the capacitive deionization technology proved highly effective for the capture of pollutants in water. The screening life cycle analysis was completed and provided important feedback to the material and device developing partners, allowing adjustment of process parameters, when applicable, to improve the safety and sustainability of the technical solutions iteratively. The Mistra Fellow programme enabled Mistra TerraClean to send a partner for an internship at World Health Organization (WHO) in Geneva to work strategically with water policy issues. We prepared for the first pilot study and made photocatalytic devices, membranes and materials with integrated sensors for water treatment and gas separations.

Clearly, the Covid-19 pandemic has affected Mistra TerraClean activities, the consortium, and the way we interact in many ways. Being a research programme devoted to chemistry and technology innovation, many of our partners work in laboratories, with instruments, testbeds, and/or production on a daily basis. Restricted access to work premises and lockdowns took a toll on progression and our ability to produce materials and validate them under both laboratory and field conditions. There are many lessons learned from the pandemic, aside from medical and social aspects. The pandemic has shed light on the importance of addressing the water crisis and air circulation infrastructures with innovation. Lack of access to clean water has during the pandemic been highlighted in developed countries in ways not previously noticed.

We look forward with confidence to the coming year. I thank all 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. We thank the programme board for their continuous support and valuable advice. We thank Mistra for their support and their trust in us to advance research and innovation in the field of smart materials.

Ulrica Edlund, March 2021

ABOUT MISTRA TERRACLEAN

Mistra TerraClean develops smart and safe engineered materials and devices for clean air and water. To ensure clean and safe air and water for all is an integral challenge for a sustainable future and directly addressed by the United Nations 2030 Agenda for Sustainable Development. The global and domestic need to more effectively capture pollutants released into the air, water, and industrial effluents is continuously increasing. Climate change, exponential population growth, and man-generated emissions threaten our supply of water resources with severe implications for the economy, environment, and human health. Also, emissions to air and insufficient cleaning technologies pose threats to social, economic, and environmental sustainability. Innovation and technologies that support the improvement of water and air quality, resource and waste management are urgently needed. Knowledge is the key to progress and to reach the 2030 goals. Contaminations in effluent water and air are issues that cut across the industry and society. Our partners represent a variety of sectors and have complimentary experiences; they span from academia, institutes, trade organizations, start-up companies, SMEs to multinational industries.

PROGRESS AND RESULTS 2020

WORK PACKAGE 1
MATERIALS DEVELOPMENT AND STRUCTURING

WP 1 Leader: Stockholm University (Niklas Hedin)

WP1 deals with identifying and developing functionalized materials that are differently 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 various fields or adaptive chemistries. The major challenge of WP1 is to develop, combine, and integrate materials with such stimuli-responsive functions that simultaneously fulfill the general and specific goals of the Mistra TerraClean programme — 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 and to securing 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 the Mistra TerraClean programme.

1.1 Materials for removal of heavy metal ions

We explored a possible sorbent based on a metal-organic framework, mixed-linker ZIF-7/8 as a possible sorbent. To understand further its possibilities to remove heavy metal ions, we studied the CO_2 and SF_6

sorption and separation in detail. Mixed-linker ZIF-7/8 can be fine-tuned for physisorbption of CO_2 or SF_6 over N_2 with high selectivity. The high selectivity of this sorbent is directly linked to the effective pore size, which can be tuned by varying the linker rations. A manuscript has been submitted for publication.

A typical capacitive deionization (CDI) device consists of two conductive electrodes, separated by a spacer to provide electrical isolation of the electrodes. A modified electrode configuration by placing two electrodes with different points for zero charge was used in an asymmetric electrode configuration. The electrosorption capacity was found to be improved on an asymmetric electrode configuration, and an activated carbon cloth doped with fluorine was used to redistribute the electric potential. The energy use during the desalination of a sodium chloride solution of 1000 ppm was 0.71kWh/m^3 for a symmetric electrode configuration and reduced by 36% with the asymmetric configuration. This study showed some of the benefits of asymmetric configuration to achieve an optimal operation of CDI device, and improvements of the related energy use.

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

Activities were mainly devoted to the development of multifunctional porous sorbents. These multifunctional porous sorbents are based on mesoporous magnesium carbonate (MMC) and new functionalities are introduced by possibly using MMC as a support for other porous materials.

1.3 Surface modification of cellulose versions and hybrids with hemicellulose

Cellulose nanoparticles offer a high versatility towards chemical functionalization because of the abundance of hydroxyl groups on their surfaces. These groups can be modified to enhance the properties of the materials as adsorbents, such as selectivity, adsorption capacity, antibacterial and antifouling properties. To that aim, we have developed methods of grafting zwitterionic polymer chains from cellulose nanocrystals which shown to prevent protein adhesion and reduce bacterial viability on the surface of the material. A lignocellulosic material has been developed and tested similarly, however despite having good antibacterial activity it did not prevent proteins from adhering to its surface.

The developed zwitterionic material, together with pristine cellulose nanocrystals and TEMPO mediated oxidized cellulose nanofibers were incorporated into functional layered membranes. The membranes were tested as adsorbents for the removal of metal ions (Au, Co, and Fe) and cationic organic dyes (methylene blue and rhodamine B), and metal-free catalysts in the decolorization of the aforementioned dyes via hydrolysis. The results highlighted the high adsorptivity and the high catalytic activity of the membranes.

FIGURE 1. Water purification membrane prepared from cellulose, microfibrillated cellulose and functionalized nanocellulose with high adsorption capacity.

Recently, we have been working on the development of systems for the removal of negatively-charged contaminants from water streams such as fluorides, nitrates, phosphates, and sulphates. For this purpose, cellulose pulp was functionalized with positively charged chemical groups and then brought down to the nano-scale via mechanical treatment.

1.4 Interactive filters based on wet-stable aerogels and foams to selectively remove metal ions and bacteria from water, and bacteria and other air-borne particles, such as pollen and viruses, from air

Industrial organic pollutants and oily wastewater are becoming a serious environmental problem leading to a demand for more efficient and less expensive approaches for water clean-up. To target this issue, wet stable and shapeable aerogels based on cellulose nanofibrils (CNF) were prepared and modified through a molecular layer by layer (m-LBL) technique for oil/water separation.

The contamination of water with heavy metals and organic contaminants is a major global risk factor for the illness and death of humans, animals, and different microorganisms. Thus, the design and fabrication of sustainable functional materials from renewable resources for water purification has been and is an emerging research area. β-lactoglobulin is a low-cost milk protein and is the major component of whey. By denaturation of β-lactoglobulin under appropriate pH and temperature conditions, amyloid fibrils are formed which have a high affinity for different metal ions and organic compounds. We have prepared wet-stable aerogels by combing dialdehyde CNFs and amyloid fibrils followed by conventional freezing and solvent exchange, the related amyloid/CNF composite aerogels were prepared, characterized, and optimized for dye adsorption.

High flux bio-hybrid wet stable membranes based on cellulose fibers/polydopamine have been developed. The wet stability of the structure originates from the polymerization of dopamine molecules in between cellulose fibers, which leads to a wet stable, and semi-interpenetrating network. Catechol groups in polydopamine have a high affinity toward metal ions. To further improve the adsorption properties and to create a dual affinity network, the so-created structure was decorated with amyloid fibrils.

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

In the progress of preparation of the hydrochars, we have noted that some display white light interference effects relating to thin films formed at the interface of the liner of the hydrothermal bombs. Hydrochars are derived by hydrothermal carbonization of biomass or simple sugars. We have used various characterization techniques such as Raman, IR, NMR, XPS, and UV-vis to characterize the colorful hydrochars. A manuscript has been submitted. Activated carbons have also been prepared from the activation of chars derived from electrospun fibers. The fiber comprised a polymer and hydrochars. These activated carbons have very CO_2 adsorption capacities. A manuscript is being drafted.

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

We have used grass cuttings for preparing hydrochars during the year and are exploring the activation of these hydrochars by selective chemical activation procedures combined with integrating iron compounds. The activated carbon will be later used for water purification applications.

1.7 Synthesis of zeotype materials suitable for biogas upgrading

We have synthesized and ion-exchanged a range of zeolite sorbents and studied the CO_2-over-N_2 selectivity that maps with the CO_2-over-CH_4 selectivity. The details of the task concern how the synthetic parameters of the ion exchange affected the ability of the sorbent to select CO_2 in gas mixtures. The latter is of importance for biogas upgrading of raw biogas. A manuscript is being drafted.

WORK PACKAGE 2 SMART FILTER DESIGN AND VALIDATION

WP2 Leader: RISE (Mats Sandberg)

WP2 deals with the design and manufacturing of filters based on smart materials and the development of methods to benchmark and validate the performance of smart materials filters (SMF) against existing solutions.

Connectivity is a key design parameter for SMFs. Smart materials in filters can influence the absorption properties of a pollutant by external stimuli by channeling the stimuli into the material by various connections. By changing the electrochemical potential, electromagnetic fields, pH, ion strength, or photochemical effects, the material can be functional if smart materials connections are allowing the stimuli to enter the responsive material.

The key question of WP2 is to combine connectivity with mechanical and fluidic properties in a filter design that allows scaling of manufacturing to large volume filters. For photocatalytic purification devices, providing illumination inside 3D structures it will also be important to optimize fluid flow in 2D structures and find scalable designs and materials for photocatalytic fuel cells.

Iterative feedback to WP1 to refine the materials development and functionalization for fine-tuning performance will be crucial for this WP.

As for the materials development part, efforts during 2020 were focused on hybrids of cellulose and metal-organic frameworks (MOFs), evaluation of water and/or air purification performance or anti-microbial activity, and scalability evaluation. Another focus of the activities 2020 was the investigation of the efficiency of capacitive deionization for removal of per- and polyfluoroalkyl substances (PFAS) and PFOS (perfluorooctanesulfonic acid). The positive results of these investigations were the main achievement during 2020. In the construction of filters built to enable direct measurements of filter material state-of-health, the efforts were redirected towards optics from electrochemistry.

The confirmed finding that capacitive deionization is an efficient method for the removal of ionic PFAS species was unexpected and very positive.

In Mistra TerraClean WP2, building devices utilizing the smartness of materials is a key activity with the following tasks.

2.1 Sensory filter material and actuators development

Nanocellulose and zwitterionic-grafted cellulose membranes were evaluated for adsorption of metal ions and anti-microbial effects. Figure 2 shows membranes before and after absorption of different metal ions. The effect of absorption on the optical properties can be used to monitor absorption optically.

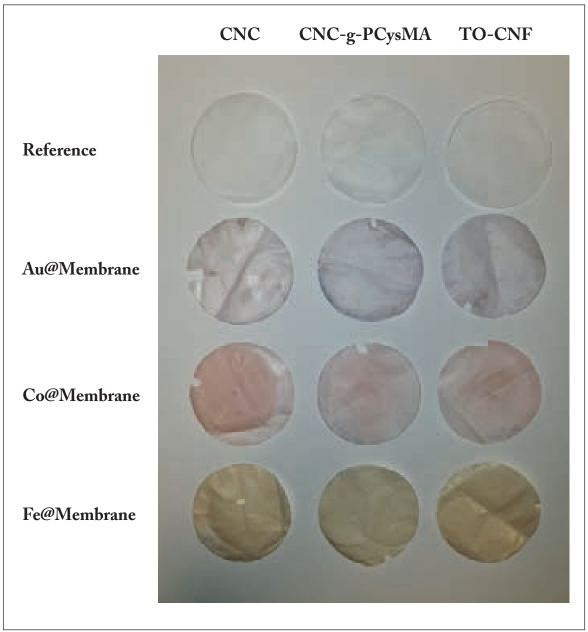


FIGURE 2. Photographs of functional cellulose-based membranes before and after the adsorption of metal ions.

2.2 Smart material filter design and manufacturing

Oxidized cellulose was used as a substrate and host for the crystal growth of cellulose-metal-organic-framework hybrids, MOFs. More specifically, MOF crystallites of the type zeolitic imidazolate framework (ZIF) were grown on cellulose to provide CelloZIF's of two types: CelloZIF-8 and CelloZIF-L, see figure 3. The CelloZIF's are effective adsorbents of anionic dye molecules, metal ions, and carbon dioxide, and catalyzes hydrogenation and degradation of organic dyes. The materials can be synthesized in water at ambient temperature without alkali and can be regenerated in several recycling cycles. Sheets of CelloZIF's were manufactured with a Rapid Köthen method, and crystal growth of MOF's can be done in the pulp or after paper formation. Future work includes tests in filter devices for water or air purification, the latter in cooperation with Camfil, and scaling manufacturing at MoRe.

2.3 Photocatalyst materials. Photocatalytic fuel cells

Tests of NO_2 abatement planned for 2020 were delayed as the access to the test facility is restricted during the Covid-19 pandemic.

2.4 Identification of applications and scalability issues

Performance evaluation of sorbent media based on cellulose aerogel hybrids for gas separation studies is ongoing in collaboration with Camfil. To potentially increase the molecular adsorption of acidic gases such as SO_2 from air, the cellulose aerogel hybrids are modified to get basic surface functional groups. The surface modification techniques tested so far, layer-by-layer assembly and plasma technology, both introduced basic surface functional groups as was characterized by methods such as X-ray photoelectron spectroscopy (XPS, figure 4).

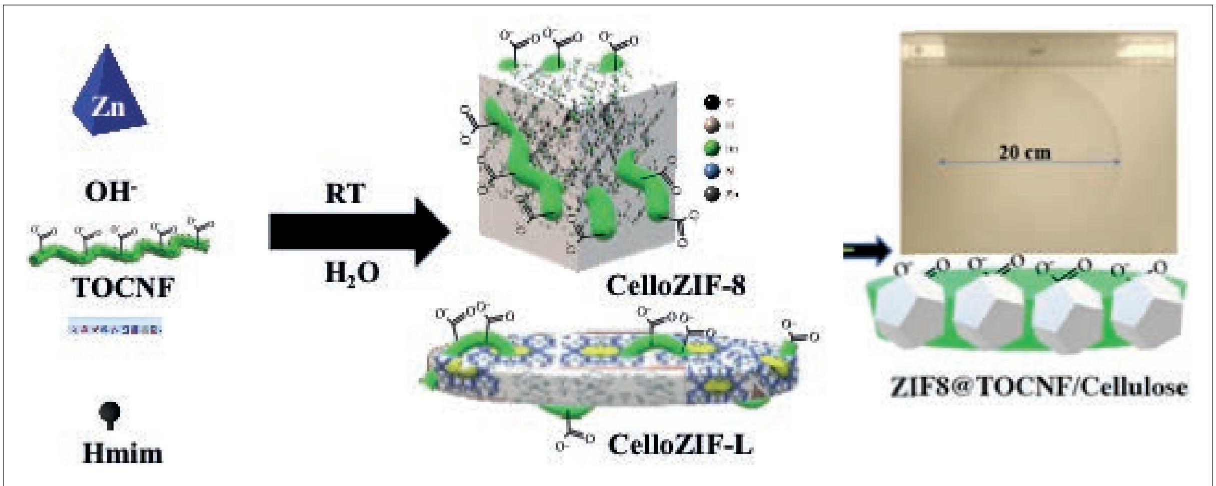


FIGURE 3. Schematic representation of the synthesis of CelloZIFs and membranes with cellulose substrates.

FIGURE 4. The XPS instrument at RISE was used to analyze the surface chemical composition of Mistra TerraClean materials.

2.5 Benchmarking of filter material smartness

Spectroscopy and measurements using optical fiber technology open interesting possibilities of monitoring and analyzing absorbent materials under operation. To this end, we have constructed with the use of additive manufacturing and fittings for optical fiber bundles, a cartridge for membranes enabling spectroscopy or measurements of absorbed light reflected at the filter medium, figure 5. This type of device provides a useful tool for the development of new absorbent media and for testing media against different water matrices and serves as a prototype for a smart filter where the filter operation is controlled with the aid of direct monitoring of absorbent state-of-health.

2.6 Active capacitive deionization device

Electrically driven adsorption, electroadsorption, is at the core of technologies for capacitive deionization wherein modeling can be crucial for understanding and optimizing these devices, and hence different approaches have been taken to develop multiple models, which have been applied to explain capacitive deionization (CDI) device performances for water desalination.

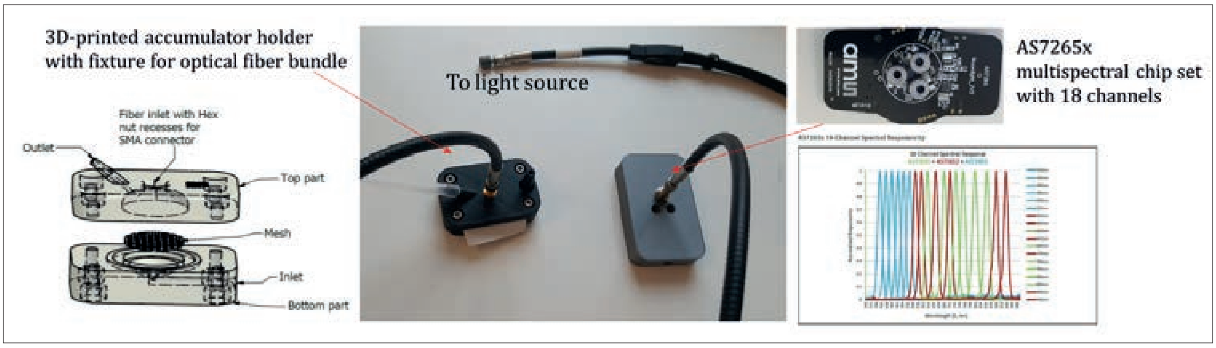


FIGURE 5. An optical fibre filter cartridge for monitoring of accumulation during filter operation.

Three CDI models, namely, the more widely used modified Donnan (mD) model, the Randles circuit model, and the recently proposed dynamic Langmuir (DL) model were developed. Crucially, the common physical foundation of the models allows them to be improved by incorporating elements and simulation tools from the other models. Ideally, electroadsorption should be the only process occurring in the pores but Faradaic reactions can lead to a transfer of charge from the electrode through the solution. Also, it was generally found that micropores can carry a net charge, which is balanced by ions from the solution even before an external potential is applied, altering the point of zero charge (PZC).

Some of these balancing ions present in the micropores (well-known Langmuir adsorption) are expelled upon the application of an electric field. This means not all charges induced on the electrodes will have corresponding counterions adsorbed from the solution. In a typical model, the micropores, macropores, and channels were considered for building up the mathematics as water naturally passes through open spaces, making the macropores the primary pathways for water flow, while the micropores intuitively hold most of the surface area because of their high area-to-volume ratio, rendering them suitable as the primary location for ion adsorption, figure 6.

The models were then validated using data from reports in the literature and also from our own experiments showing significant prospects in combining modeling elements and tools to properly describe the results obtained in these experiments. Developing efficient and cost-effective water deionization technology design principles for scaling from small CDI cells to larger units and modules is becoming increasingly important. We investigated the flow distribution in single flow-through CDI cells and interconnected modules to determine architectural principles that can feasibly reduce the pressure drop with good throughput, thus increasing energy efficiency. Massive parallelism, open regions to symmetrically distribute flow and tailoring the permeability of the electrodes and spacers were found to influence the efficiency of treatment processes. Implementing the design principles leads to a significant reduction in pressure drop and energy consumption of a CDI system, which is essential for upscaling to larger modular systems for practical use.

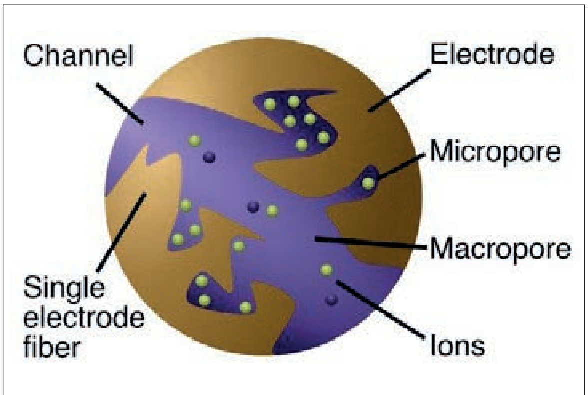


FIGURE 6. A CDI model for Langmuir adsorption

PFAS/PFOS Degradation studies

There are water and ground sites around Sweden with a significantly higher content of PFAS/PFOS compounds than the allowed limit of 90 ng/L. For example, for providing drinking water, Uppsala Vatten employs an additional final polishing step in their five pumping stations but still, there are problems to capture the shortest chain PFAS as they are less prone to be blocked by the filters.

To understand the mechanism(s) for sorption and transformation a more thorough study of the effect of the CDI process on different PFAS molecules needs to be conducted. However, plans to use CDI device operating in "Catch and Destroy" mode, capturing short chains (as they are electrically charged) was tested and if successful at a larger scale would be a breakthrough. Initial tests with the CDI device on a spiked solution of deionized water (500 ng/L) demonstrated >97% removal of C_4-C_{10} perfluoroalkyl carboxylic acids (PFCAs), C_4, C_6, and C_8 perfluorosulfonic acids (PFSAs) (Table1).

PFSAs appeared to be more rapidly removed compared to PFCAs indicating that the sulfonic acid head group results in more favorable electrostatic interactions. The recovery tests demonstrated that 39-87% of the PFAS present in the spiked water solution were permanently removed from the water solution. Although a small fraction of the removed PFAS (<12%) could be attributed to non-specific sorption these results provide indicative evidence for chemical transformation of PFAS in the CDI device. Overall, the lowest recoveries (i.e. more efficient transformation) were observed for longer-chained PFCAs and PFSAs which is consistent with the literature.

TABLE 1. Results from lab-scale tets of PFCAs and PFSAs removal with the Mistra TerraClean CDI device.

	PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFBS	PFHxS	PFOS
Non-specific sorption	6.6%	2.4%	11.1%	0.4%	11.8%	2.7%	9.2%	3.0%	10.6%	9.6%
LOW VOLTAGE										
Removed 30 min	58%	59%	59%	60%	57%	59%	70%	71%	72%	76%
Removed 120 min	96%	97%	98%	98%	98%	97%	94%	99%	99%	97%
Recovered	40%	46%	44%	41%	34%	35%	29%	42%	45%	50%
HIGH VOLTAGE										
Removed 30 min	97%	98%	98%	98%	98%	97%	95%	98%	98%	98%
Removed 120 min	97%	98%	99%	100%	99%	99%	99%	99%	99%	99%
Recovered	55%	61%	46%	44%	33%	20%	10%	39%	29%	13%

WORK PACKAGE 3
APPLICATION PLATFORM

WP 3 Leader: IVL Svenska Miljöinstitutet (Henrik Kloo)

Case studies address our core aims of managing air quality, water quality, and chemicals. WP3 will manage the testing and evaluation of the novel filter materials and online sensors developed in WP1 and WP2 under realistic conditions. A key for driving innovation and implementation is to have efficient communication between the needs and competence provided by the problem owners (industry representatives), and the possibilities provided by the solution providers (research organizations and suppliers).

The aim is to use four specific cases within water purification/ air purification to drive the research and development within this program towards real-world problems. This approach can bridge the multidisciplinary task of water and air purification by focusing the interest of all the involved organizations towards those four chosen and concrete case studies.

The major task of WP3 is to up-scale the production of the most promising materials and system solutions, evaluate the performance and design a technical product that can be used on an industrial scale. In this work package industrial environmental problems are identified at industrial partners and the intention is that the project will provide promising solutions with the potential to show improved functionality and economy compared to existing methods.

During 2020 two industrial case studies have been in focus, flue gas cleaning and condensate water in waste incineration at Vattenfall and PFAS removal from water. Apart from this a method to reduce nitrogen oxides in gas has also been studied.

In the case of flue gas and water condensate from waste incineration, it was decided not to proceed as the identified case study was not addressing the latest technology. Initially, the sorption properties of available materials were tested in lab-scale with a sample of condensate water from the Vattenfall incineration plant in Uppsala. However, later Vattenfall declared less interest in the Uppsala plant, as this plant was not designed according to the future standard for waste incineration plants. Instead, they proposed to make tests at the plant in Jordbro. This plant has a closed-loop water system, meaning that the properties of the water are quite different and with much less content of heavy metals.

In WP 2 tests on PFAS removal were performed with a CDI – device and showed promising results. Based on this a separate project with funding from the “Blue Sky fund” on PFAS removal with a CDI pilot plant designed by Stockholm Water has been initiated. The project comprises lab-scale tests at KTH and the pilot trials at IVL including chemical analysis. An environmental evaluation is also performed as a subtask in the project. Initially, the plan was to apply this on ground water from Bromma Airport, but due to practical difficulties with access to this site treated wastewater from Uppsala water was selected. However, due to site restrictions caused by the Covid-19 pandemic the tests were redirected to the joint KTH/IVL facilities at Hammarby Sjöstadsverk.

The applicability and scalability as well as the prospect for cost level on the various adsorption and absorption materials from WP1 have been reviewed. The result of this will be used for future case studies and are implemented in case descriptions in the application for Mistra Terra Clean phase II.

Case PFAS removal from water

In cooperation between KTH and the start-up enterprise Stockholm Water Technology AB, a pilot-scale system based on the CDI-technology was designed. Due to the Covid-19 pandemic, it was not possible to get access to the premises at Uppsala Water. As a back-up solution the pilot tests will proceed on spiked tap water at the research facility owned by KTH and IVL in Stockholm (Hammarby Sjöstadsverk).

Initial lab-scale tests with the CDI device were performed by KTH in spring 2020. PFAS removal was investigated with promising results. These preliminary results were followed by more lab-scale tests which started in autumn 2020. The removal/degradation of PFAS was studied by treating spike solutions of specific PFAS in deionized water (one PFAS per experiment, not in a mixture). These experiments aimed to investigate if the PFAS are mineralized completely or not. In case of incomplete degradation other, potentially toxic, PFAS can be created. The results obtained so far confirmed the previous results on the high removal efficiency of PFOS and PFOA. Some degradation products were detected in the treated water, but the extent of degradation is yet to be investigated.

A CDI pilot test plant was commissioned and trials have started in February 2021.

Case NOx removal in gas phase

A pilot study has been prepared for testing removal of NOx, SOx and VOC in the gas phase. Building on the achievements in WP 2, the focus has been to reduce nitrogen oxides. Tests for NO_2 adsorption and photocatalysis are performed at Camfil. Adsorption on papers with different amounts of carbonate is tested at IVL. The method, based on a pilot-scale produced tetrapodal ZnO-filled paper in a photocatalytic reactor and visible light, has passed the first toll gate in the gate model we developed in 2019.

There is evidence that NO_2 can be trapped and converted to nitrate in a reactor with pilot scale produced tetrapodal ZnO filled paper. It is possible that the retention time in the equipment can be prolonged if nitrate can be buffered by an alkaline compound such as carbonate and at lower concentrations of NO_2. Adsorption test shows increased uptake when carbonate is added to the paper material.

Further testing is proposed on the reduction of N_2O with a paper filled with different amounts of ZnO and with different amounts of carbonate. The aim is to investigate the adsorption and possible conversion to NO for these different paper materials and to test the same paper in the catalytic cell.

Results show that pilot-scale produced low cost ZnO-filled paper and visible light can reduce NO_2. However residential time is long and the effect is decreasing after a few days but on the other hand, papers can be produced at low cost and the catalytic paper might be incorporated in existing room surfaces such as curtains and wallpaper, or as titanium dioxide in paints for reducing NO_2 in a concrete wall.

WORK PACKAGE 4
HUMAN AND ENVIRONMENTAL SAFETY, LIFE CYCLE ASSESSMENT, SCIENCE AND SOCIETY

WP4 Leader: RISE (Ian Cotgreave)

WP4 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. Life cycle assessment of potential environmental impacts and a risk assessment of hazards to humans and the ambient environment will be performed and documented for relevant regulatory body interaction and approval. 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 work will also cover 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 will 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.

4.1 Toxicological appraisal of material production, application, post-consumer fate and management

Much progress was made during the initial half of the year on "cradle to gate" analysis of the raw materials being used/developed in WP 1. This resulted in a report to the governing body of Mistra TerraClean in June 2020.

Individual LCA assessments were delivered to and discussed with the individual chemistry groups involved, focussed on magnesium carbonate (Upsalite), microfibrillated cellulose (Exilva), wet-stable nanocellulose aerogels, ZnO-filled cellulose structures, iron-impregnated activated carbon, quartzene and nano-lignocellulose.

One interesting and unusual finding from the activities was the ready uptake of the information by the academic scientists. This indicates that there is a large interest in the application of LCA-based analyses to projecting consequences of novel chemical synthesis at the bench, into potential application zones, with respect to the concept "safe by design". This lays a solid foundation within this consortium to continue education of academic and industrial chemists in their efforts to introduce novel and smart modifications of these materials towards application in real world cases.

4.2 Toxicological appraisal of material performance in individual case studies in WP3

During the year, laboratory scale experiments utilizing the CDI equipment provided by Stockholm Water Technology (SWT) on water contaminated with per- and polyfluoroalkyl substances (PFAS) have been performed at KTH. Analyses were performed by IVL (see report from WP 3). Due to problems with sighting the scale up work first at Swedavia's site at Bromma Airport, and then at Uppsala Water, a case study involving scale up of the CDI/PFAS application at Hammarby Sjöstadsverket was undertaken during 2020 (See WP3 report). Work of WP4 has been centered on identifying critical LCA parameters for application to a full scale LCA including ecotoxicity and toxicity potential impacts. In addition to LCA, plans were made for ecotoxicity testing of the polluted water, before and after treatment, an activity that will be executed by SLU.

A case-study structure has been generated, figure 7, covering the CDI at pilot scale, and a comparison with standard Granular Activated Carbon (GAC) treatment as a benchmark technology. Scenario design was initiated where the CDI is to be modelled in at least two scenarios, high and low voltage, to identify hot spots in the system (i. e. activities causing high potential impact). To ensure a fair comparison between the CDI and the benchmark, close interaction and information exchange with water treatment experts in the larger case study team was foreseen to be needed and working groups were established. A "Goal and Scope" document for the LCA has been drafted, describing the goal of the LCA:

"The goal of the LCA is to compare the environmental performance of two different water treatment technologies: the novel capacitive deionization (CDI) with conventional granulated active carbon (GAC). The goal is furthermore to identify hot spots within the life cycle of the CDI device as such information can guide improvement of environmental performance. In particular, it is of interest to investigate the relationship between human and ecosystems toxicological risk exposure with environmental impacts in other impact categories."

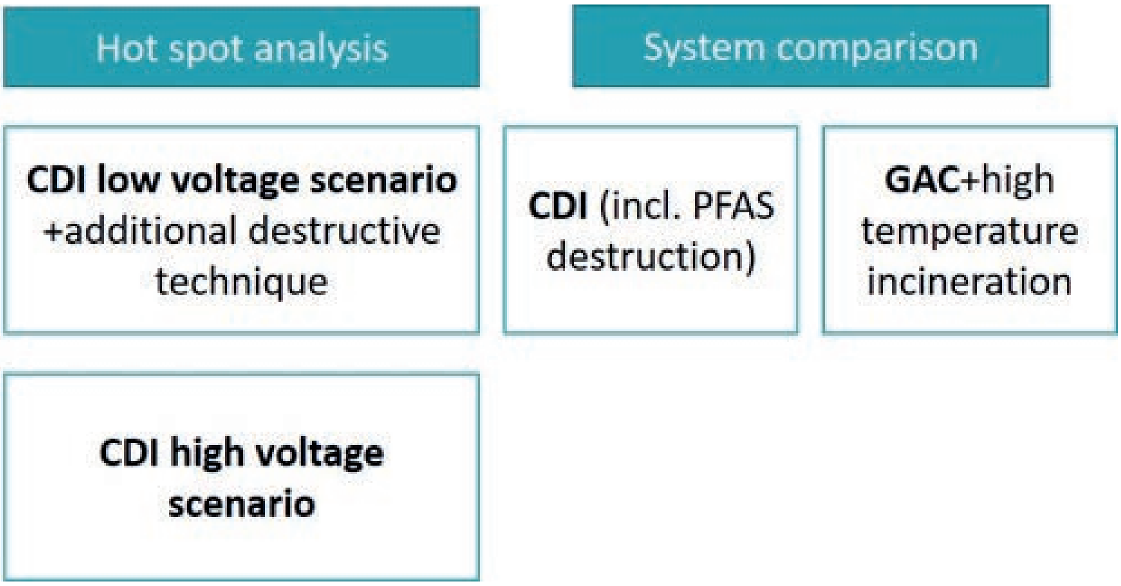


FIGURE 7. Overview of the case study structure in Mistra TerraClean.

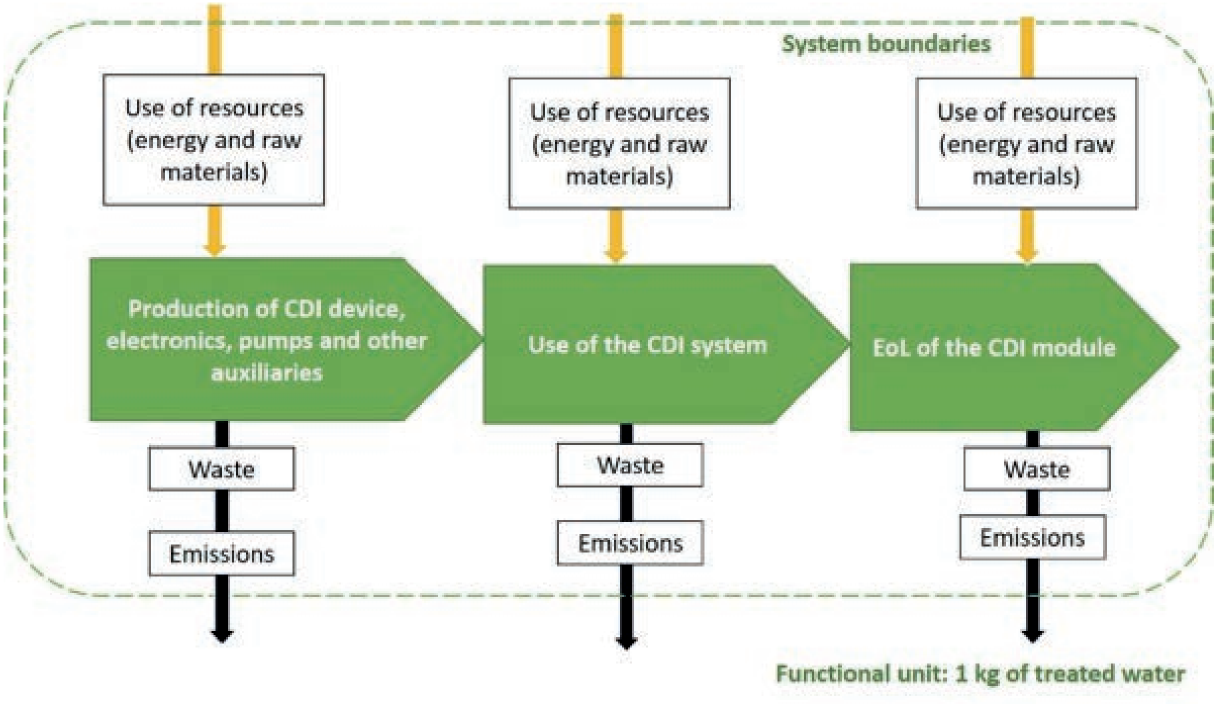


FIGURE 8. Schematic flowchart of the life cycle of the CDI device. This is not a complete picture of the LCA model, for example, transports and material re-use are not shown.

As part of the scoping, in dialogue with KTH and SWT, the CDI system was described, and system borders defined, figure 8.

Life cycle inventory (LCI), i.e. data collection, on the CDI and GAC process and its materials/consumables has been initiated. This included a visit to the site for the laboratory scale work and SWT and contact with a supplier of one of the key components, for better understanding of the process/device.

Plans were made for life cycle impact assessment (LCIA) in the LCA. The ProScale method (Lexén et al. 2017)[1] was decided to be used for assessment of direct human toxicity. Further, plans were made to apply a recent framework by Holmquist et al. (2020)[2] for PFAS characterization to differentiate the treated effluents based on PFAS composition.

Work will continue in 2021 on both the data collection and impact assessment to define the overall suitability of the remediation process for scale-up and utilization in the remediation of PFAS and, indeed, other applications. Focus is on environmental LCA, but plans have also been made for a limited life cycle cost (LCC) assessment. This will be important when weighing up the impact and costs of using the CDI approach against the hazards and societal costs of inaction in the case of PFAS remediation, as well as with respect to the burden remaining on recycling the GAC material and subsequent destruction of PFAS by high temperature incineration.

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1 J. Lexén, E. Belleza, C. L. Lindholm, T. Rydberg, N. Amann, P. Ashford, A. Bednarz, P. Coërs, P. Dornan, R. Downes, M. Enrici, M. Glöckner, E. Gura, Q. d. Hults, C. Karafilidis, E. v. Miert, P. Saling, T. Tiemersma, A. Wathelet, X. Weinbeck (2017). ProScale – A life cycle oriented method to assess toxicological potentials of product systems, Guidance document, version 1.5 October 2017, UetlibergPartners on behalf of the ProScale consortium, Oetlikon, Switzerland. Retrieved 2021-01-25, from https://www.proscale.org/.

2 H. Holmquist, P. Fantke, I. T. Cousins, M. Owsianiak, I. Liagkouridis, G. M. Peters (2020). "An (Eco)Toxicity Life Cycle Impact Assessment Framework for Per- And Polyfluoroalkyl Substances." Environmental Science & Technology 54(10): 6224-6234.

4.3 Societal stakeholder interactions with the program

PROGRESS IN 2020

Conferences and meetings were planned and discussed with TechConnect Malmö, EIT Raw Materials, NanoForum and Almedalen, however, they all were postponed due to the Covid-19 pandemic. The activities are planned to occur before the end of 2021 but remain insecure. Collaborations with these organizations are continuing.

During 2020 the Industrial Emissions Directive and EU Chemical Strategy has been identified as important policy instrument for the program to get contact with. Collaborations with Mistra Safe Chem have begun during 2020 on the "Safe-By-Design" concept as overarching between the two sister programs.

4.4 Long-term/post-program viability

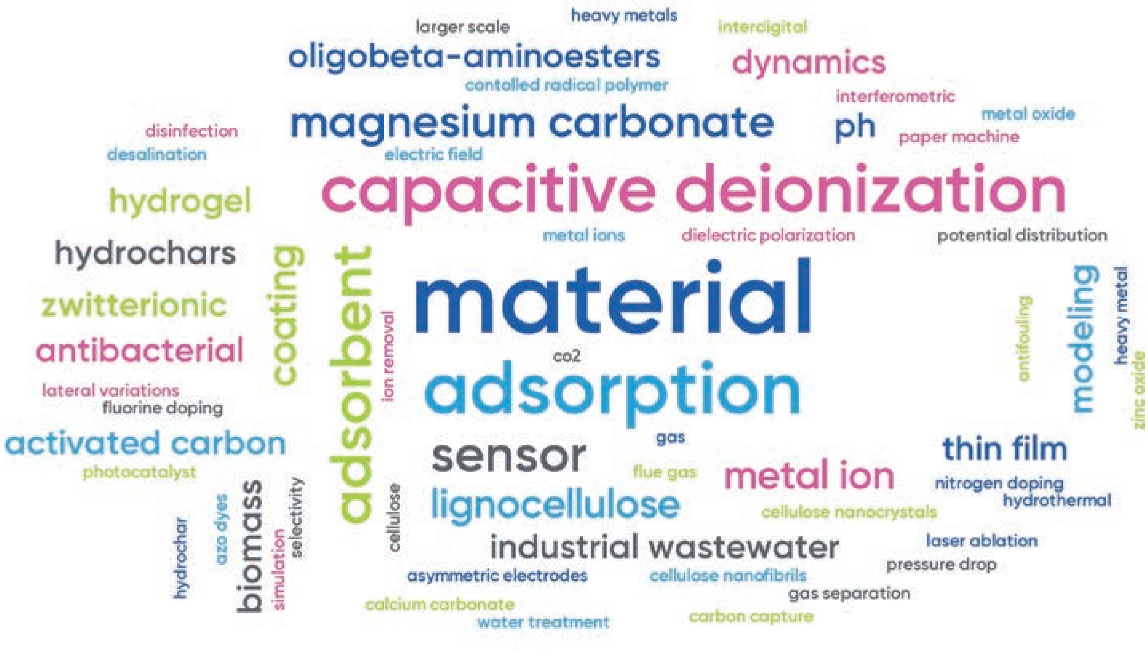
During the remaining period of phase I, we are committed to create an action plan for enhancing Swedish companies' competitive advantage, through sustainable innovations based on advanced materials. The action plan will be based on an analysis of the companies in Sweden that work with advanced materials related to Mistra TerraClean areas of research. The analysis will be used to predict other companies that can benefit from our work, thus providing a stronger network to collaborate in phase II. The action plan has been defined and will be implemented in 2021.

WORK PACKAGE 5
MANAGEMENT, IP HANDLING AND COMMUNICATION

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

WP5 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 RTD 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. And to facilitate an effective cooperation and communication between the different WPs.



OUTREACH

The Mistra TerraClean team has made extensive efforts in communicating smart, advanced materials as being part of the solution to the global challenges in general, and specifically as solutions to the challenges regarding clean water and clean air. Below are some selected initiatives.

Mistra Fellow – a WHO internship

Within the Mistra Fellows Programme, the research council enabled a one-year internship at World Health Organization (WHO) in Geneva. The objectives with the Mistra Fellowship were knowledge transfer to the programme, a strategic outlook, deeper insight in global water management policies and processes that govern the same, and a valuable network. Dr. Johan Strandberg started the fellowship in July 2020. The original plan was to do a full-time fellowship on-site. However, the pandemic clearly limited the networking possibilities and on-site work. Dr. Strandberg has visited the office in Switzerland twice in 2020 and is currently working remotely. To increase the outcome, the fellowship duration was extended for several months as to facilitate networking and allow for site visits later in the spring. In the meantime, Dr. Strandberg works part time as a fellow, and part time in other Mistra TerraClean activities. As a fellow, Dr. Strandberg is working strategically with water policy issues regarding revising amendments to the drinking water quality standards. His primary tasks include the contaminant Mn, asbestos, and PFAS. He is also involved in a project concerning Pb in water, where some countries are facing problems. Updating data sheets on microorganisms in water is another area of interest.

IVA's "100 List"

Both the programme Mistra TerraClean and the consortium partner Stockholm Water Technology AB, where the CDI technology for remediation of PFAS in WP 2 was developed, were selected to IVA´s "100 List" for 2020. IVA is the Royal Academy of Engineering Sciences. The list aims to highlight researchers and research teams with high scientific quality and with interest in increased contacts with the business sector and surrounding society. The selection is not only based on scientific excellence but primarily on the research´s potential for business development, innovation and benefit for users, companies and society.

IVA reports the following impact of the "100 List":

- The "100 List" website was the most visited page on iva.se for large parts of 2020.
- Great attention and frequent sharing on social media - the posts about the list have the best spread of all IVA's posts in all channels.
- Many journalists showed interest in covering the Summit with researchers from the list, which unfortunately became completely digital and thus less interesting for the press as a result of the Corona pandemic.

- Communication has not stopped: the lit is receiving continuous attention in IVA's communication during the year, and universities and others continue to publish and disseminate.

Popular science talks

Many of the partners have in various fora given popular science briefs about the programme's vision and activities. One of them is prof. Strømme at Uppsala University, who has during 2020 delivered several presentations on themes like ”nanomaterials for a sustainable future”,” nanotechnology induces disruptive changes in industry and society”, and ”technology development and the grand challenges”. The popular scientific presentations have been held mostly in Sweden and Norway at events arranged by financial institutions, business parks, and by stakeholders in public and private sector. Prof. Strømme has furthermore been interviewed in several TV shows, and pod casts, advocating for the future of advanced materials in a sustainable society.

Meetings

Prof. Mathew and Prof. Edlund organized in collaboration with colleagues in Finland and Austria, a symposium on ”Cellulose and Renewable Materials for Gas, Air & Water/Liquid Purification”. The symposium was arranged as part of the American Chemical Society (ACS) National Meeting and a number of contributions from Mistra TerraClean partners was planned as dissemination of programme results. Due to the outbreak of Covid-19 pandemic, the conference was unfortunately cancelled.

A digital consortium meeting with Statens Geologiska Undersökning (SGU) was held in March 2020 when current and future challenges in water, sludge, and sediments remediation and the needs for smart materials in this context were discussed.

The annual consortium meeting went from what in non-pandemic times would be a full-day's event with site visits to a digital workshop. Constructive discussions set momentum to the work on how to prepare the programme for phase II and beyond. The consortium meeting was the start of many meetings within the consortium to work out our strategies for how to proceed in the coming years.

The board members represent different actors in society, most importantly governmental, trade, and expert organizations, that build bridges between research, politics, society and business. The board makes the final decisions, assisted in the decision-making by the steering group. The board met four times in 2020.

The Steering group supports the programme board in final decision making and is also responsible for the administrative management of the programme. The steering group consists of 1) the programme director, 2) the communication leader, and 3) the leader for each WP. Since the start of Mistra TerraClean in 2017, the steering group has met monthly, lately only digitally.

Sustainable water supply project

The Royal Academy of Engineering Sciences, IVA, launched an ambitious 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 serves as a working group member at IVA throughout this project and facilitate knowledge transfer to the consortium.

Mentoring startups for collaboration

Prof. Edlund was one out of 13 climate champions, representing sustainable materials, in Startup Climate Action, a challenge driven initiative by the incubators Sting and Norrsken in Stockholm, aiming to create more fast-growing startups that contribute innovative and scalable solutions to combat climate change in 2020. She acted as coach to the collaboration teams.

SCIENTIFIC OUTPUT

SCIENTIFIC PUBLICATIONS 2020

D. Georgouvelas, B. Jalvo, L. Valencia, W. Papawassiliou, A. Pell, U. Edlund, A.P. Mathew. "Residual lignin and zwitterionic polymer grafts on cellulose nanocrystals for antifouling and antibacterial applications". ACS Applied Polymer Materials 2020, 2, 8 (cover page). DOI: https://doi.org/10.1021/acsapm.0c00212

K. Laxman, P. Sathe, M. Al Abri, S. Dobretsov, J. Dutta. "Disinfection of bacteria in water by capacitive deionization". Frontiers in Chemistry 2020. DOI: https://doi.org/10.3389/fchem.2020.00774

J. Nordstrand, J. Dutta. "Simplified prediction of ion removal in capacitive deionization of multi-Ion solutions." ACS Langmuir 2020, 36, 5. DOI: https://doi.org/10.1021/acs. langmuir.9b03571

J. Nordstrand, J. Dutta. "Predicting and enhancing the ion selectivity in multi-ion capacitive deionization". ACS Langmuir 2020, 36. DOI: https://dx.doi.org/10.1021/acs.langmuir.0c00982

V. Saadattalab, X. Wang, A. E. Szego, N. Hedin. "Effects of metal ions, metal, and metal oxide particles on the synthesis of hydrochars". ACS Omega 2020, 5. DOI: https://dx.doi.org/10.1021/acsomega.9b03926

M. Sandberg, K. Håkansson, H. Granberg. "Paper machine manufactured photocatalysts - Lateral variations". Journal of Environmental Chemical Engineering 2020, 104075. DOI: https://doi.org/10.1016/j.jece.2020.104075

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J. Yan, A. Karlsson, Z. Zou, D. Dai, U. Edlund. "Contamination of heavy metals and metalloids in biomass and waste fuels: Comparative characterisation and trend estimation". Science of the Total Environment 2020, 700, 134382. DOI: https://doi.org/10.1016/j.scitotenv.2019.134382

C. Xu, G. Yu, J. Yuan, M. Strømme, N. Hedin, "Microporous organic polymers as CO_2 adsorbents – advances and challenges", Materials Today Advances 2020, 6100052. DOI: https://doi.org/10.1016/j.mtadv.2019.100052

L. Dahllöf, C. Nilsson, F. Bignami, S. Örn, I. A. Cotgreave. "Life cycle assessments (LCA) and toxicological evaluations of filter materials and devices in MISTRA TerraClean". Internal report to Mistra 2020.

MANUSCRIPTS

D. Georgouvelas, H. Abdelhamid, J. Li, U. Edlund, A. P. Mathew. "All-cellulose functional membranes for water treatment: 1 Adsorption of metal ions and catalytic decolorization of dyes". Carbohydrate Polymers. Submitted.

V. Saadattalab, K. Jansson, N. Hedin. "Thin colorful films formed on hydrothermal carbonization of glucose using an iron catalyst". ACS Langmuir. Submitted.

Z. Atoufi, M. S. Reid, P. A Larsson, L..Wågberg. "Cellulose-based oil adsorbents made hydrophobic through deposition of ultrathin molecular layer-by-layer coatings".

L. Dahllöf, T. Rydberg, I. A. Cotgreave, C. Nilsson, H. Holmquist, F. Bignami. "The application of a tiered life cycle assessment (LCA) approach to safe and sustainable chemistry in the development of smart solutions for water and air purification: The Mistra TerraClean case". In preparation for publication in the IVL Scientific Publication Series.

CONFERENCE CONTRIBUTIONS

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

D. Georgouvelas, U. Edlund, A. Mathew, "Bio-based zwitterionic membranes for the removal of metalloids from industrial effluents", International Conference on Nanotechnology for Renewable Materials 2020, abstract for oral presentation.

V. Saadattalab, N. Hedin, "Hydrothermal carbonization of glucose in the presence of iron ions", 5th Green & Sustainable Chemistry Conference, Dresden, Germany,2020, poster.

U. Edlund, "Toward smart and safe engineered materials and devices for clean air and water", Abstracts of Papers, 259th ACS National Meeting, Philadelphia, PA, Unites States, 2020, CELL.

D. Georgouvelas, B. Jalvo, U. Edlund, A.P. Mathew, "Zwitterionic functionalized nanolignocellulose for removal of metalloids from industrial effluents", Abstracts of Papers, 259th ACS National Meeting, Philadelphia, PA, Unites States, 2020, CELL.

Z. Karim, D. Georgouvelas, A. Svedberg, A. Mathew, "Nanoscopically engineered microfibrillated cellulose composite membranes for removal of charged impurities", Abstracts of Papers, 259th ACS National Meeting, Philadelphia, PA, Unites States, 2020, CELL.

J. Yan, A. Karlsson, C. Nordenskjöld, U. Edlund, "Fuel Contamination in Renewable Energy Production – Demands of Materials Development for Sustainably Reducing of Emissions to Air, Water and Soils", Abstracts of Papers, 259th ACS National Meeting, Philadelphia, PA, Unites States, 2020, CELL.

U. Edlund, "Mistra TerraClean", Water at the Centre, Session C: New Horizons for Water, KTH Royal Institute of Technology, 2020, oral presentation.

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Boliden AB
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FINANCIAL REPORT

Contribution from Mistra		
	Incoming Balance	**2 224 567**
	INCOME	**7 243 600**
EXPENSES		
Personnel		7 110 961
Travel		24 306
Consumables		654 140
Depreciations		186 833
Other costs		683 068
Services		457 617
	DIRECT COSTS	
Indirect costs incl. facilities		3 267 859
	TOTAL COSTS	**12 384 784**
	BALANCE	**-2 916 617**
	PROGRAMME IN-KIND CONTRIBUTION	**3 637 245**
	TOTAL IN-KIND CONTRIBUTIONS since programme start	**7 651 652**
In-kind part of total cost 2020		29%

MISTRA TERRACLEAN

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UPPSALA UNIVERSITET

Stockholms universitet

KTH VETENSKAP OCH KONST

SLU

swt

RISE

ivl SVENSKA MILJÖINSTITUTET

Nouryon

IKEM Innovations- och kemiindustrierna i Sverige

Karolinska Institutet

VATTENFALL

AkzoNobel

NEW BOLIDEN

Borregaard

Disruptive Materials

Svenskt Vatten

camfil

MoRe Research

AEROGEL

Biokol

NeoZeo Biogas upgrading

MISTRA The Swedish Foundation for Strategic Environmental Research