Executive summary

Mistra TerraClean develops smart and safe engineered materials and devices for clean air and water.

Ensuring clean 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. 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 goals.

The 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 the world's 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.

Regardless of the source, current cleaning technologies must be improved to sufficiently address current and future challenges with respect to energy efficiency and sustainability (reuse, recycle, waste reduction, raw materials...). Yet a limitation with today's solutions is that they do not have the ability to adapt to variations in operating conditions. Another challenge is that traditional filters and membranes will not be able to capture all types of pollutants, especially substances that occur in minute quantities.

In essence: we need smart solutions to help industry and society address these issues!

Contaminations in effluent water and air are issues that cut across the industry and society.

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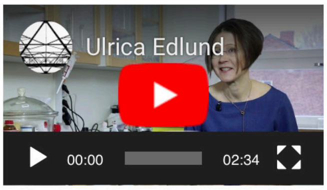
INTERVIEWS

"Most importantly, the iterative feedback processes that interlink all activities are established."



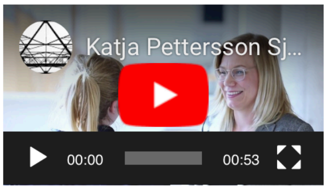
Our partners represent a variety of sectors and have complementary experiences, they also span from academia, institutes, trade organizations, start-up companies, and SMEs to multinational industries.

Heavy metals, volatile organic compounds, and nitrogen oxides are examples of substances that our programme is targeting with more effective materials and methods of separation. In addition, we are adding new “smart” functions to the materials – both at the molecular level and by embedding sensors in the material. The smart functions allow for the controlled and interactive removal of contaminants from ambient water and air in the environment and industrial effluents. Our material precursors are selected on the basis that i) they can be manufactured within Sweden, ii) Swedish researchers are in the forefront of research, and iii) they can be produced in a sustainable way.

In practical terms, it is about developing the materials from the bottom-up and validate them under both laboratory and field conditions. The latter is done within case studies where our materials are tested under realistic conditions together with partner companies to drive the research and development within this program towards real-world problems.

This report presents an overview of the Mistra TerraClean programme and the achievements and progress done during 2018. During the past year, we have moved from the start-up phase to full scale operation. With the hope of the coming year becoming as fruitful and rewarding as the past, 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 like this advance far beyond the borders of each discipline. Not in the least, we thank Mistra for their support and the confidence put in us to advance research and innovation in the field of smart materials.

“I see great potential in developing new smart materials that will also be dynamic and communicating.”



MISTRA TERRACLEAN

1. What is the main goal with Mistra TerraClean?

Mistra TerraClean develops smart and safe engineered materials and devices for clean air and water. More specifically, we aim to tailor-make membranes and filters that adsorb chemicals (such as NOx, VOCs, and heavy metal ions) from contaminated air and water.

By smart, we mean materials that interactively respond to, and perform in a controlled fashion, based on stimuli from the environment in operation and the condition of a filter.

We aim to evaluate our materials with regard to environmental and safety aspects in a safe-by-design manner.

Ultimately, we want to contribute to reach the national and global environmental and health aims in air and water quality and to establish a strong interdisciplinary research and innovation platform.

2. Any specific achievements during this past year?

It is great to see the momentum set in the entire programme. All work packages are up and running and – importantly – the iterative feedback processes interlinking all activities are established.

Materials with high and selective adsorption capacities are being produced. We demonstrated the first hybrid materials with embedded sensors, for instance, cellulose

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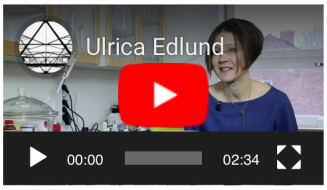


membranes with printed electronics photocatalytic activity. Our first Life cycle assessment is currently underway where we screen the chemistry of our material candidates from a sustainability and toxicology point of view. The LCA data is key in the selection of relevant materials and solutions which will proceed into the specific case studies.

3. Any challenges that you have encountered?

One of the major challenges for the program is to move from promising laboratory-scale trials to working products in larger scales. The volumes of polluted air or wastewater to be purified are considerably larger in a real industrial setting, and the controlled conditions prevailing at the lab never become the same in industry.

4. What impact do you think the research within this programme will have on our society?

Our materials may improve environmental conditions in Sweden: better air and water quality, and support the growth of Sweden's smart materials industry.

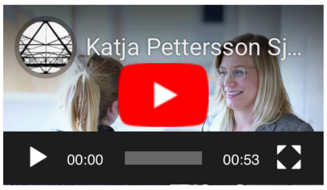
The products that are developed have the potential to significantly improve current technologies and solutions, which would have a positive effect on competitiveness.

We hope and believe that Mistra TerraClean will foster a long-term national hub capable of providing competence and expertise required to keep Sweden in the forefront with respect to research and enterprise in new materials for cleantech applications.

5. Hopes for 2019?

When the materials are developed and their functions validated in the laboratory, it is time to level up: to test their function on a larger scale and with real effluents under more authentic conditions. I hope that the first case studies at the partner companies will start in 2019.

"I see great potential in developing new smart materials that will also be dynamic and communicating."



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WP1

WP1 deals with identifying and developing different tailored functionalized materials for use as filters. Key questions involve development of materials with functionally-enhanced natural and engineered porous materials, synthesis, refining, functionalization, characterization and structuring. A vital question is how to integrate stimuli-responsive functions through targeted chemical functionalization and/or structuring.

Involved partners: SU, KTH, UU, RISE, MoRe Research, Disruptive Materials
WP 1 Leader SU (Hedin)

Below is a summary on activities performed during 2018.

Materials for removal of heavy metal ions

This task includes investigation of materials for selective adsorption of heavy metal ions and modification of activated carbon for enhancement of capacitive device performance.

Amine modification of mesoporous magnesium carbonate (UU) has been developed as a sorbent for azo dye removal from wastewaters. This work was published recently in ACS Omega https://pubs.acs.org/doi/10.1021/acsomega.8b03493. Work is performed towards mesoporous inorganic carbonates for high temperature CO_2 capture and a paper has been drafted. Two Masters students have started in January 2019 and their theses are on the heavy metal removal using inorganic carbonates and the removal of pharmaceutics using inorganic carbonates.

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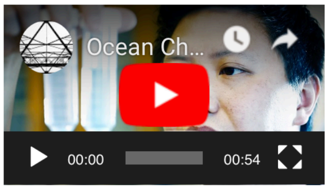
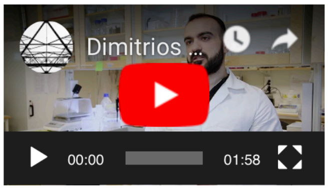
"To make a material smart enough to meet today's challenges, we often have to think about sustainability."



"I have the chance to work with people, institutes and companies that have many years of experience in the field!"

Modifications of the capacitance of carbon electrodes of a typical capacitive de-ionisation device is performed (KTH). Hexagonal boron nitride (h-BN) is well-known high band-gap material (5.9 eV), that has high resistant to dielectric breakdown. Preliminary characterization of the h-BN nanoflakes and the electrode modification was performed with scanning electron microscopy (SEM) and Raman spectroscopy, Figure 1.



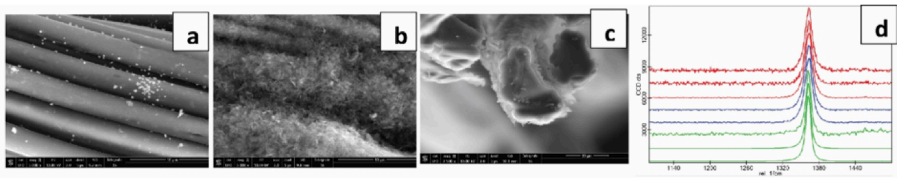


Figure 1. a) SEM image of unmodified activated carbon cloth fibres; b) SEM image of carbon cloth fiber after coating with h-BN nanoflakes; c) cross section view of the carbon cloth fiber with the h-BN flakes visible at its outer surface; d) Raman spectra of h-BN flakes-red and blue traces are from h-BN nanoflakes and the green traces are from bulk h-BN. (not to be published elsewhere).

The coating process is being optimised, to obtain a more homogeneous coating, especially in the corners between the weaves of the carbon fibres. Preliminary electrochemical C-V measurements carried out at KTH did not show any increase in specific capacitance possibly due to inhomogeneous coating as well as detachment of the h-BN flakes from the carbon cloth. At RISE, efforts will now focus on the development of an aerosol-based method to coat the carbon cloth to obtain an integral coating in order to achieve the target of increasing specific capacitance of the devices.

Surface modification of cellulose versions and hybrids with hemicellulose

The research work in this task has involved the preparation and characterization of lignocellulose nanoparticles, and their functionalization with zwitterionic polymers. Nanoparticles were extracted with high-pressure homogenization from the residue of a bioethanol pilot plant, which has been reported to consist of crystalline cellulose and lignin. Prior to the mechanical treatment, the material was partially bleached to be able to remove part of the lignin. Residual lignin is expected to improve on the adsorption performance of the material and provide chemical groups useful for functionalization. The nanoparticles were functionalized by grafting of zwitterionic sulfobetaine polymers providing high adsorptivity towards heavy metal ions and metalloids. Bi-layered membranes were prepared with cellulose microfibers as support layer and the zwitterionic lignocellulose as the functional layer.

The work in this task started in January 2018 and planned to last 30 months. One PhD student is involved.

Self-organized wet-stable nanocellulose functionalized aerogels

Studies on how different preparation processes affect the properties of porous, light-weight cellulosic materials have been done, to select special material structures for given end-use applications. Further, suitable candidate contaminants will be selected for additional studies. By including electrically conducting materials, such as nanocarbons or conducting polymers, further material smartness will be demonstrated.

Different methods to control the pore size in nanocellulose aerogel particles have been in focus for the work at RISE.

Activated carbons and porous polymers derived from relevant biomass and waste

Refined hydrochars have been prepared, starting with the preparation of activated carbons and from glucose and amines/polyamines. One manuscript on the valorization of waste milk by hydrothermal carbonization has been prepared and is to be submitted.

Unexpected result

During the preparation of iron impregnated activated carbons for the preparation of magnetically activated carbon for water purification applications, an unexpected result occurred.

As shown in Figure 2., one of the hydrochars had a golden-like luster. A thin film had been deposited on the assembly of hydrochar particles. The size of those particles was gradually increasing when going down in the particles' assembly. Those at the bottom had diameters of about 5 micrometer while those at the top were about 1 micrometer in top. Further studies are undertaken to rationalize the golden luster and the ordered carbon spheres.

Apart from the unexpected results, which may have applications in water purification and gas separation processes, our objective is to prepare magnetically activated carbon which can be manipulated by a magnetic field.

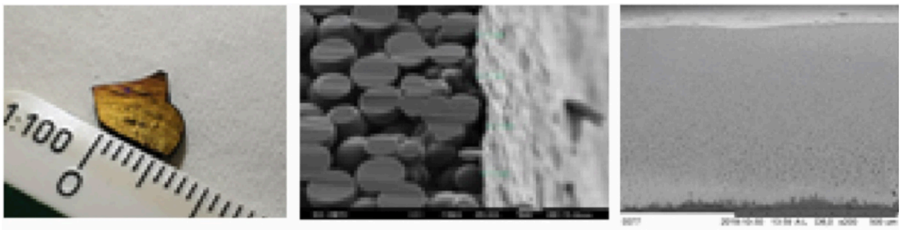


Figure 2 (left) Golden-like luster of the hydrochar, (middle) cross sectional SEM image zoom in, (right) cross sectional SEW image. (do not use elsewhere, high quality images can be provided later).

So far, glucose had been used as the carbon precursor. The prepared samples did not show any response to a magnetic field which means iron is not impregnated (EDS shows less than 0.08w %) in the prepared samples. Other sources or changes in the work up procedure will be tested.

Publications

Amine-Modified Mesoporous Magnesium Carbonate as an Effective Adsorbetn for Azo Dyes, https://pubs.acs.org/doi/10.1021/acsomega.8b03493

Students

Master Thesis by Stivan Sabir "Minimizing pore size of nanocellulose aerogel particles".

2019

Two Masters students have started in January 2019 and their theses will cover heavy metal removal using inorganic carbonates and the removal of pharmaceutics using inorganic carbonates. Presentable results from the thesis students are expected later in 2019. Together with MORE, UU is testing different protocols for producing papers with inorganic carbonates embedded. The results are so far very preliminary now but we are in continuous discussion. Discussions with Camfil, and UU is to be sending samples for testing soon.

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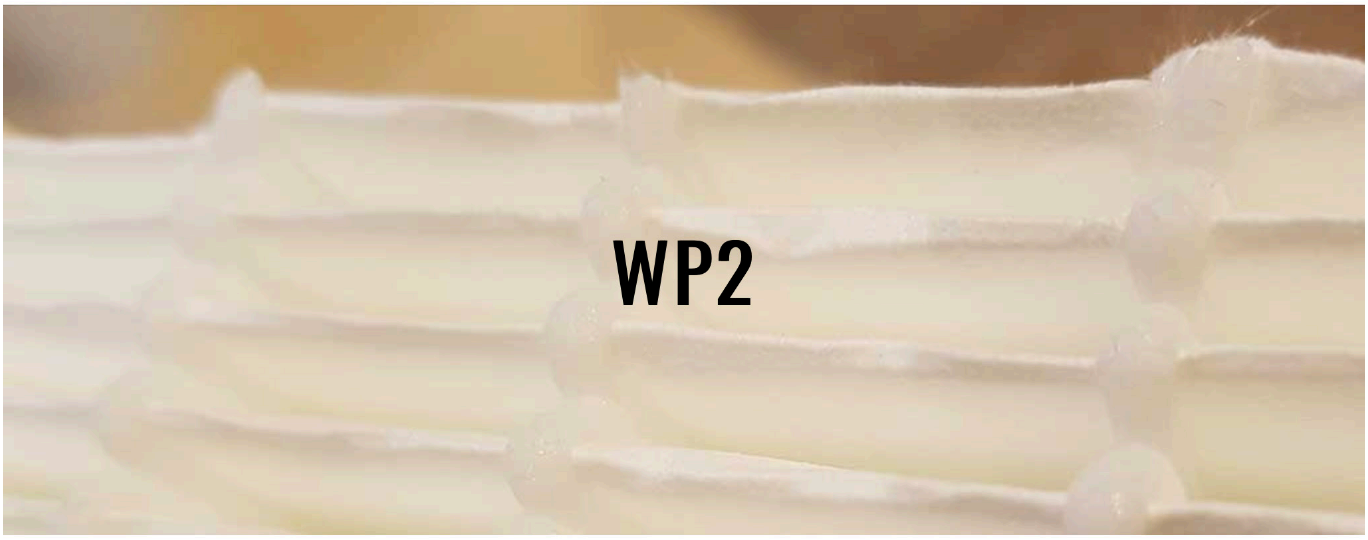

WP2

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 against existing solutions.

Involved partners: RISE Acreo, Stockholm University (SU), Borregaard, MoRe Research, Swedish Aerogel, KTH, RISE Bioekonomi, NeoZeo, IVL, RISE Biovetenskap och material samt Boliden.

WP2 leader: RISE Acreo (Sandberg); WP2 Co-leader: SU (Matthew)

Below follows a summary in text and in illustrations on activities performed during the year combining all Tasks, with contributions from all parties.

Filter materials

Research work will be done to manufacture filter materials and how to integrate different cellulose grades into multilayered membranes has been focused on (SU, MoRe). The ambition for the coming year is to have in hand functionalized cellulose membranes manufactured from WP1, integrate the membranes with electrochemical sensors and study the permeability, mechanical properties, adsorption performance and scalability of the obtained smart filtering systems. In collaboration (SU, MoRe, Acreo), support layers of the membranes will be developed, and electrochemical tests of the prepared material will be conducted. The observations from these studies are expected to result to at least one publication by the end of 2019.

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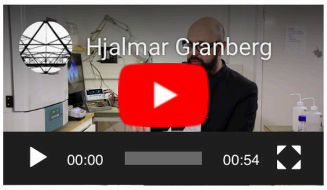
"These hydrogels are transformed into aerogels that are porous filters."



Electronic sensors in filter paper

Lab work on the integration of optical light guides and electronic sensors into filter paper has been performed. The results so far indicate that the challenges are non-trivial, and the plan is to develop improved ideas and concepts during 2019. Fig 1 illustrates illuminated optical fibers in paper.

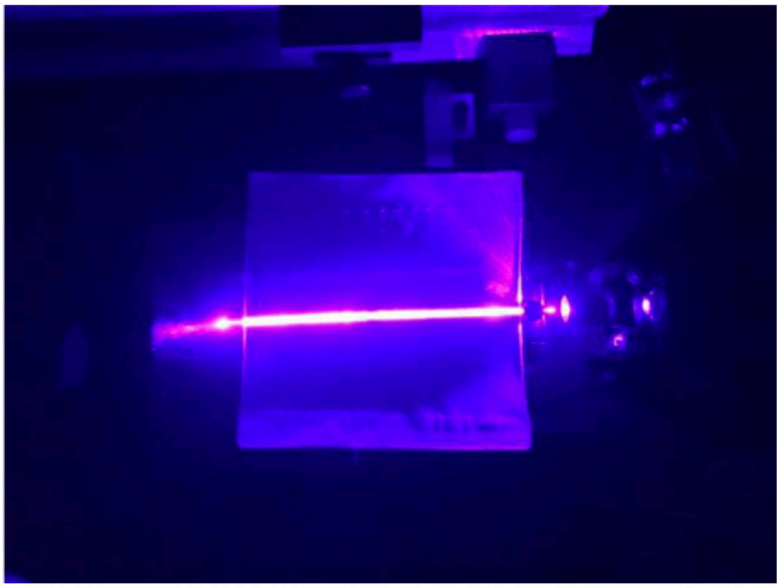


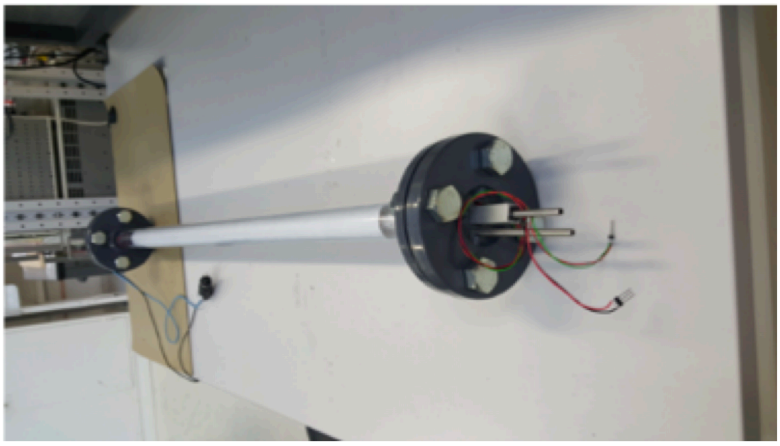
Fig 1. Illuminated optical fiber in paper.

Photocatalytic activity in zink oxide paper

The photocatalytic activity in ZnO-paper based on photocatalytic activity indicator inks has been studied. The results are promising, and the plan is to submit a scientific article based on the finding during 2019.

Test reactor

A test reactor for sheet-formed photocatalysts for air purification in a plug-flow configuration has designed and built (Sandberg et al.). Compared to other evaluation tools for photocatalytic air purification, the MTC validation tool for photocatalysis has several distinguishing features. It is a reactor of plug-flow type with a high aspect ratio, and the photocatalytic sheets are illuminated directly by the light source without any barrier in between, such as quartz glass. The light source is a water-cooled UV-LED aggregate of own construct. Compact sensors are integrated into the reactor. Function of photocatalytic papers and the validation tool has been confirmed.



Design, manufacturing and testing of electrochemical in and at filter membranes

Sensor electrodes has been integrated into filter materials in one approach to realize smart and connected filter materials, to provide a new tool set for the development of “sensor-absorbent filter materials”.

Validation tool for sheet-formed photocatalysts for air purification

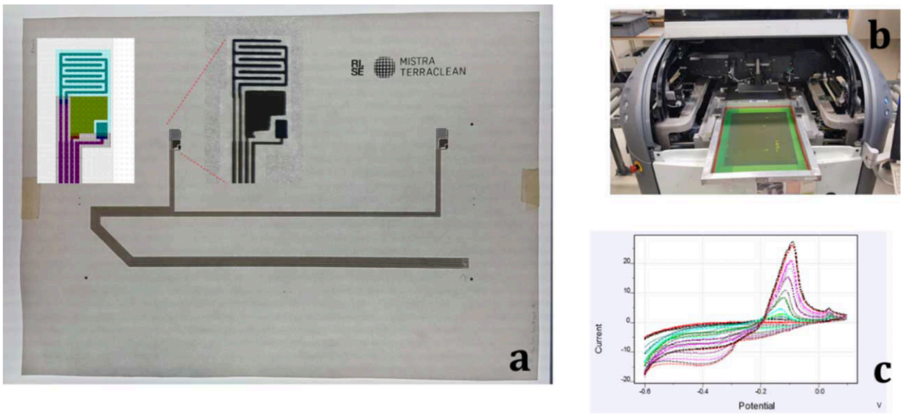


Fig 2. Two sets of electrochemical sensors printed directly on filtration media Insets show details of the electrode structure, a. Each set of sensors have one interdigit electrode structure for impedance measurements and one two electrode structure with a working electrode and a large reference counter electrode. Printing of materials for electrochemical sensors, b. Electrochemical response to metal ion absorption in the filter medium, c. The sensors can be facing into the filter medium or into the bulk liquid and can be applied on both sides of a membrane.

Unexpected results

The role of CO_2 on irradiated ZnO surfaces is under debate and is of great importance for evaluation and operation of photocatalytic reactors. With the sensors mounted inside the reactor it become clear that the dynamics of CO_2 release from an irradiated photocatalyst is slow, significant and must be considered.

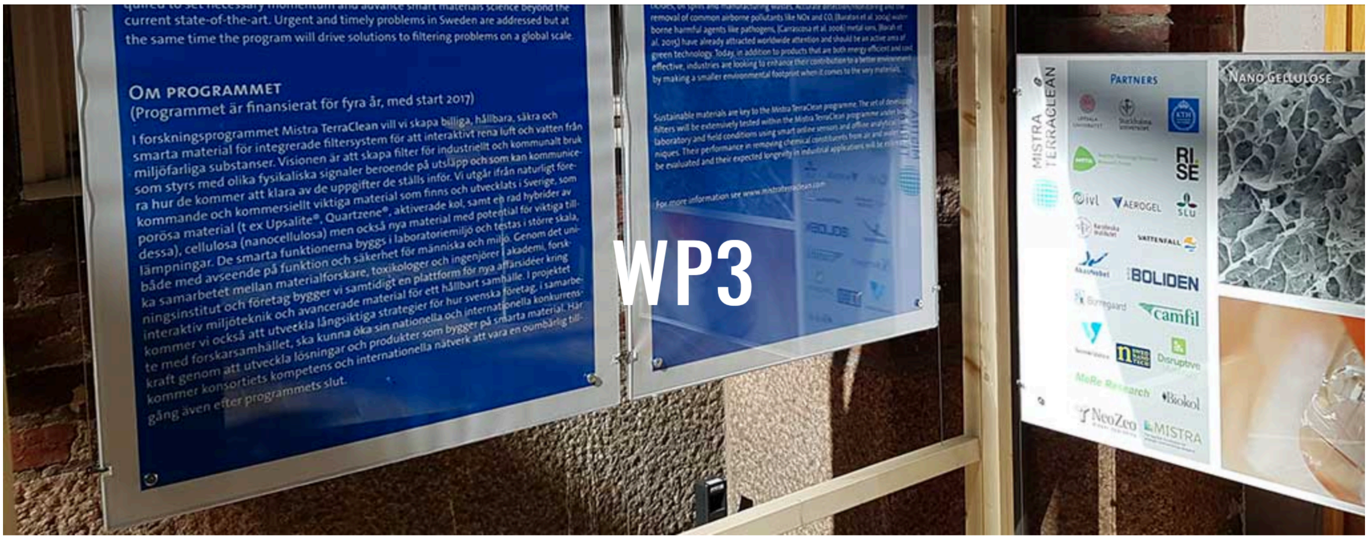
Experiments have indicated that printing electrodes on membranes can be useful tool for understanding, development and economic operation of filter membranes. The conducting traces, i e the printed electrochemical sensors on filtration membranes, are well insulated by the printed dielectric. Metal ions in the membrane can be distinguished from metal ions in the bulk.

Meetings

The WP2 team participate regularly in the monthly WP2 Skype meetings.
A filter workshop was held at Camfil for the entire Consortium, with focus on air filters in Feb 2018.

Workshop on membranes (processing and testing) took place at SU, hosted by Aji Mathew at her lab. This full day event was very successful, with about 20 participants from the MISTRA TerraClean program seeing some of the lab work we conduct in the WP2 tasks.

At the Consortium meeting in Uppsala in October, 2018, the partners could benefit from a lecture on LCA, held by IVL.



WP3

The overarching aim in WP3 – application platform, 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.

Involved partners: IVL, Boliden , Vattenfall, Svenskt Vatten, MoRe
WP Leader: IVL (Nordström) WP Co-leader: RISE (Granberg)

In the first year of the programme, focus has been on four areas:
Case A – Flue Gas Liquids and Heavy Metals
Case B – NOx SOx VOC Dioxins
Case C – Mining Effluents
Case D – PFAS and Drinking Water

In **Case A**, real flue gas condensate from the acid stage, wastewater tank and condensate stage have been run through WP1 concept apparatuses and analyses for heavy metals are in progress presently. Once all samples are characterized, we can calculate the energy input to give estimates on volumetric capacity and energy requirements for the process with a potentiality to remove hazardous heavy metals. Similar tests have been done for **Case D**. The challenge we are focusing on is if PFAS can be reduced from levels 700 ng/l to acceptable levels (less than 90 ng/l). New tests are to be performed and further details will evolve during next year.

Clearing gases from harmful levels of contaminants is one topic in **WP3**. The NOx case has been studied in **Case B**, simulating car tunnels with levels of 2 ppm that have been neutralized in initial trials using concepts created in **WP2**. Additional promising results of higher levels have been tested (up to toxic 30 ppm levels). The harmful levels have been beneficially diminished to acceptable levels. Long-run verification trials are to be made to further verify the good results.

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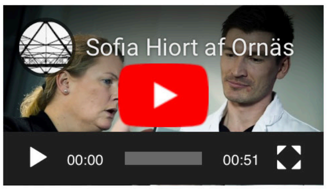
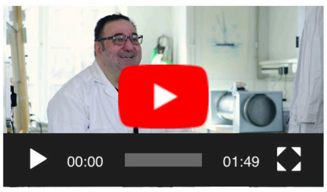
“The program has already given us access to a great network with good people and great expertise.”



“The performance requirement must be fulfilled. Another parameter is the cost-performance value.”



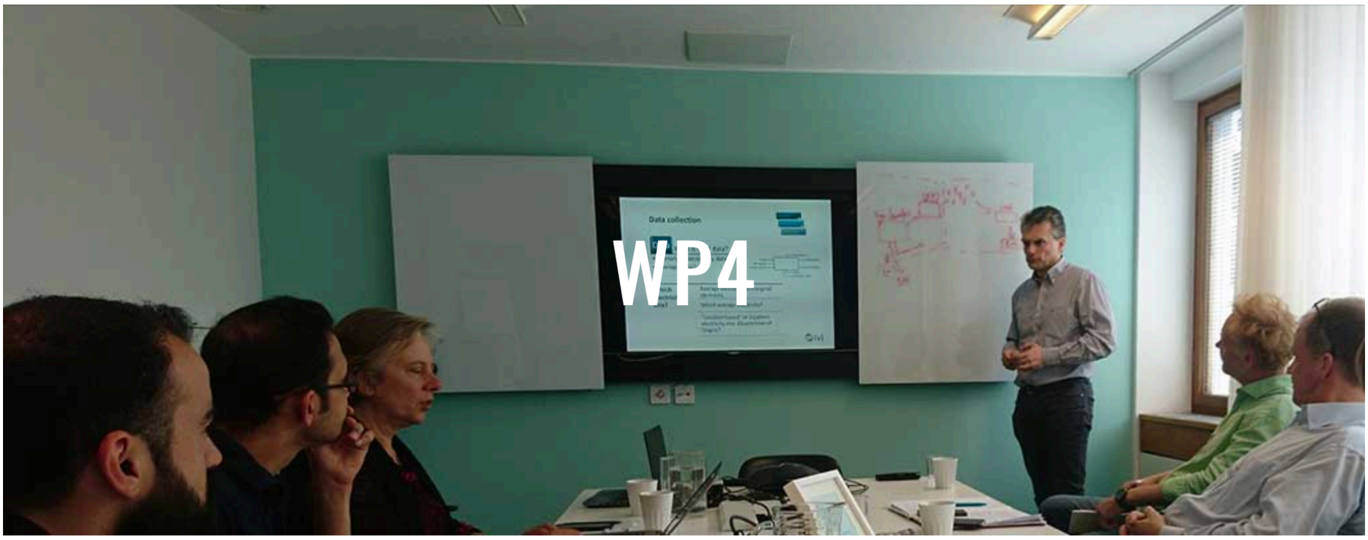
The consortium partner representing the mining industry has provided us with samples of mining effluents. We have succeeded to screen the samples for all involved organic and nonorganic ingredients. In addition to characterizing mining waters thoroughly, it has turned out some filter materials evaluated initially can really catch some materials that (e.g. determining REE – Rare Earth Elements) in the mining waters that are not detected in conventional methods.

A lot of new ideas have emerged during this productive year. The case studies will continue in the iteration processes with **WP1** and **WP2**, where we anticipate testing the functionalized materials for further implementation into industrial applications.

LCA and LCC

LCA and LCC are important tools in evaluating new materials. Both methods have already been taken into consideration in this stage. and will be deepened when we find a potential full-scale application to be run the next coming years in the program. Co-operation with WP4 has been very fruitful and deep discussions are already now prevailing in where the aim should be put to gain a sustainable future.

MISTRA TERRACLEAN



WP4

The work package will provide 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. 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 public.

During 2018 WP4 has focused on building interactions with key groups and individuals within WP1 and WP2, who are driving the development of novel chemistries and devices for application in the various case studies.

Involved partners: RISE, IVL, SwedNanoTech
WP Leader: RISE (Cotgreave), WP Co-leader: SwedNanoTech (Hartmanis)

LCA in early research

Regular work package leadership meetings have been conducted, primarily focusing on discussions around how to introduce Life Cycle Assessment (LCA) earlier than originally projected into the project.

In order to avoid a situation where new materials for water and air cleaning present less benefit for the environmental and human health than conventional solutions, it was considered that the project would benefit greatly from early introduction for LCA "light" thinking into the workstreams involved in novel chemical synthesis within WP1. Similarly, WP 2 devise design processes were also identified as beneficiaries of early LCA analyses.

A Life Cycle Assessment describes environmental aspects and impacts throughout the whole life cycle of a product, i.e. raw material extraction, production, use and end-of-life management. The function of the product is central for the calculations because only then

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"I hope that that this project will contribute to a better environment."

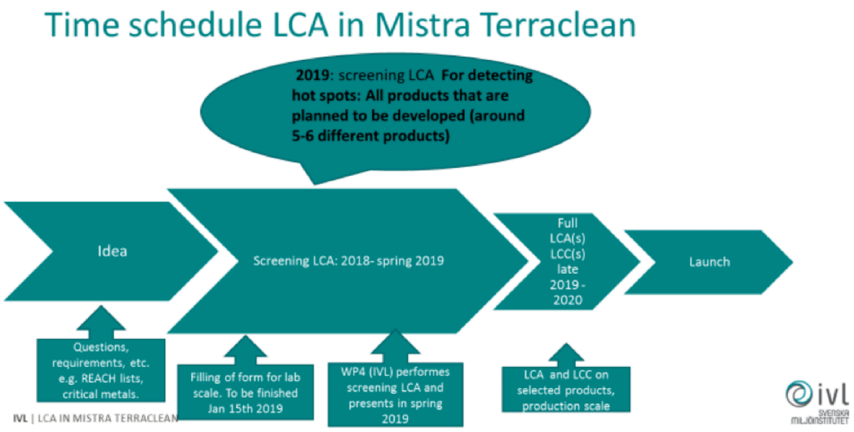
comparisons are possible. This is also extendable to potential aspects on human health, during scale-up production of materials and utilization in device construction.

To have good collaboration in the study, it was important to educate the material researchers in the project and to discuss the advantages with the assessment with them. We therefore started with an LCA course open to all consortium researchers in May. Around that time, it was also decided to perform screening LCA studies on six currently existing new materials and/or sensors early in the project. This will be supplemented later with other materials/devices as they appear within the workflow of the project. This will not detract from the plan to introduce a full LCA/Life Cycle Cost (LCC) analysis on 1-2 of the material(s)/device(s) deemed closest to commercialization.

The overall LCA plan was presented in the autumn 2019, together with a repetition of the LCA methodology, first at a meeting with WP1 on September 12th and thereafter in a meeting for all project participants on October 4th. Toxicity and metal scarcity aspects were also addressed as important to keep track on when choosing synthesis route.

Data collection from each WP1 and WP2 project involved was initiated late in 2018 and is ongoing presently. Data appraisal will be carried out in q1 of 2019 and active feedback driven with each of the chemistry/device development groups. It is the ambition of this initial LCA-screening interaction to provide confidence to the the groups with a "heads-up" on environmental and/or human risk issues and problems with the individual chemistries/syntheses/processes already employed at the bench. This will either reveal a lack of foreseeable issues, or where applicable, help to suggest alternatives to circumnavigate potential issues.

Below is the time schedule showed and agreed at the consortium meeting in Uppsala in October, 2018.



On the communication side of WP4, plans were laid to initiate external communications on project specific matters related to human and environmental safety when enough data is obtained from the LCA screening procedure. Initially it was agreed that this should be in the form of a publication on the application of LCA methods in screening chemistries in large consortium projects such as Mistra Terraclean.

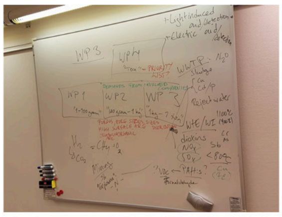
MISTRA TERRACLEAN

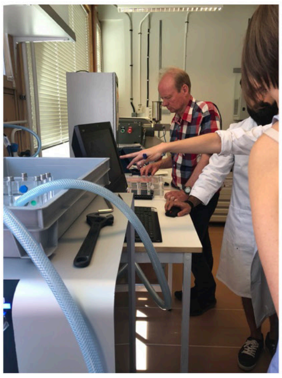
Knowledge Dissemination

Mistra TerraClean Academy

Mistra Terraclean Academy is an initiative to give added value in terms of competence and insights in issues related to the program's overarching aim, to the team members. The goal is to organize a site visit in connection with the annual consortium meeting. Every work package is also invited to arrange a special workshop, for other team members to attend. With this initiative, the program will foster an open and learning environment.





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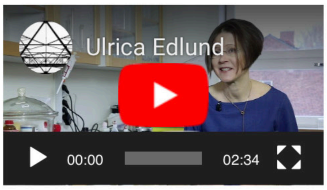
INTERVIEWS

”Most importantly, the iterative feedback processes that interlink all activities are established.”



During 2018, the following workshops and site visits have been arranged:

Oct 1, 2017
Site visit to Käppala water treatment plant, Lidingö
Kick-off Consortium meeting

Jan 29, 2018
Site visit Camfil, Trosa
Filter Workshop

May 8, 2018
WP 4 Workshop, How to Assess the Environmental Impact of the Mistra Terraclean Project Solutions, Stockholm

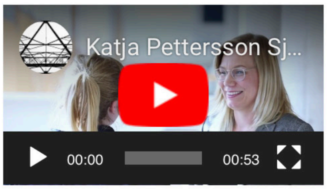
May 29, 2018
Workshop, Sensors, technical session, KTH Kista

May 30, 2018
WP2 Membranes workshop, Stockholm University

Sept 12, 2018
Workshop, Uppsala university

Oct 4, 2018
Site visit to Vattenfall fjärrvärme, Uppsala
Consortium Meeting

"I see great potential in developing new smart materials that will also be dynamic and communicating."



Publications

Activated Carbons from Hydrothermal Carbons Prepared in Milk
*Salwa Haj Yahia, Kian Keat Lee,‡ Niklas Hedin, Tamara L. Church**
Materials and Environmental Chemistry, Stockholm University. Submitted for publication.

Inorganic carbonate composites as high temperature CO2 sorbent with enhanced cycle stability
Maria Vall, Jonas Hultberg, Maria Strømme and Ocean Cheung**
Nanotechnology and Functional Materials Division, Department of Engineering Sciences, The Ångström Laboratory, Uppsala University. Submitted for publication.

Amine modified mesoporous magnesium carbonate (aMMC) as an effective adsorbent for azo dyes
Maria Vall, Maria Strømme and Ocean Cheung**
Nanotechnology and Functional Materials Division, Department of Engineering Sciences, The Ångström Laboratory, Uppsala UniversitySubmitted for publication.

A universal model for describing the dynamics of capacitive deionization
Johan Nordstrand, Karthik Laxman, and Joydeep Dutta
Functional Materials, Applied Physics Department, SCI School, KTH Royal Institute of Technology. Published

The Team

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Zoheb Karim, MoRe Reserach AB
Åsa Claesson, RISE Acreo
Åsalie Hartmanis, SwedNanoTech

MISTRA TERRACLEAN

Financial report

INCOME	
Contribution from Mistra	6793900
TOTAL INCOME	6793900
EXPENSES	
Personnel	6976866
Travels	96997
Consumables	609386
Depreciations	25589
Other costs	221751
Services	8375
DIRECT COSTS	7344506
Indirect costs incl facilities	2729364
TOTAL COSTS	10668328
BALANCE	1198035
PROGRAM INKIND CONTRIBUTION	1379258
inkind part of total cost	13%

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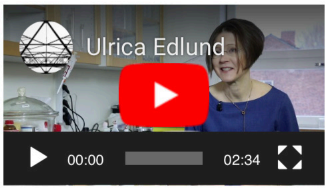
INTERVIEWS

"Most importantly, the iterative feedback processes that interlink all activities are established."



"I see great potential in developing new smart materials that will also be dynamic and communicating."