No. C 591
April 2021

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

Lisbeth Dahllöf (IVL), Tomas Rydberg (IVL), Ian A Cotgreave (RISE), Charlotte Nilsson (RISE), Hanna Holmquist (IVL) and Francesco Bignami (RISE)

In cooperation with RISE

Author: Lisbeth Dahllöf (IVL), Tomas Rydberg (IVL), Ian A Cotgreave (RISE), Charlotte Nilsson (RISE), Hanna Holmquist (IVL) and Francesco Bignami (RISE)
Funded by: The Swedish Foundation for Strategic Environmental Research (Mistra) Dnr DIA - 2015/31
Report number C 591
ISBN 978-91-7883-275-0
Edition Only available as PDF for individual printing

IVL Swedish Environmental Research Institute Ltd.
P.O Box 210 60, S-100 31 Stockholm, Sweden
Phone +46-(0)10-7886500 // www.ivl.se

This report has been reviewed and approved in accordance with IVL's audited and approved management system.

Preface

This is a summary report describing the approach for environmental and human health assessment as applied in the Mistra-founded research program TerraClean. Additional reports and outputs from the program can be found at https://mistraterraclean.com/.

Table of contents

Summary

In the Swedish research programme Mistra TerraClean a tiered approach for life cycle based environmental and human health assessment early in process development was introduced. In the project smart filters for water and air purification are under development. Innovative materials and devices are applied and evaluated with a systems perspective. In our tiered approach life cycle assessment (LCA), chemical safety assessment and applied eco and human toxicity assessments are combined, with a particular focus on the inclusion of toxicity potential impacts in LCA. To this end, the consensus model USEtox has been applied, complemented with the method ProScale, that focusses on human direct exposure. The life cycle-based approach has so far been applied to material development and a pilot scale case study. The case study focuses on water purification of per- and polyfluoroalkyl substances (PFAS) for which we have a PFAS adapted life cycle impact assessment framework at hand. This tiered approach is relevant to process developers, people within the field of water and air treatment as well as the broader LCA community.

Sammanfattning

I det svenska forskningsprogrammet Mistra TerraClean introducerades ett stegvis tillvägagångssätt för livscykelbaserad miljö- och hälso-värdering tidigt i processutvecklingen. I projektet utvecklas smarta filter för vatten- och luftrening. Innovativa material och konstruktioner tillämpas och utvärderas ur ett systemperspektiv. I vår stegvisa metodik ingår livscykelanalys (LCA) kombinerat med kemikalie-säkerhetsbedömning och tillämpad eko- och human-toxicitetsbedömning med ett särskilt fokus på införandet av toxicitetspotentialeffekter i LCA. För att göra detta tillämpas konsensusmodellen USEtox, kompletterat med metoden ProScale, som fokuserar på direkt humanexponering. Den livscykelbaserade metoden har hittills tillämpats på materialutveckling och en pilotstudie. Denna pilotstudie fokuserar på vattenrening av per- och polyfluorerade alkylsubstanser (PFAS) för vilka vi har ett PFAS-anpassat ramverk för miljöpåverkansbedömning i LCA till hands. Detta stegvisa tillvägagångssätt är relevant för processutvecklare, personer inom vatten- och luftbehandling samt den bredare LCA-intressesfären.

Introduction to the project

The Mistra TerraClean Program (MTP) was initiated in 2017 to unite academia, research institutes, commercial filtration companies and end-user industries to establish a research and development platform to bring forward "smart" material chemistry and application device innovations directed at remediation of problematic chemical exposures in society. This ambitious program was constructed to be fed by innovations largely based on materials being developed at the various academic groups involved at Stockholm University (SU), The Royal Institute of Technology (KTH) and Uppsala University (UU), which then would be combined with smart device constructions aimed at various aspects of performance optimization in the field. The platform would then direct application in a variety of case studies, largely based on existing environmental pollution issues, or industrial process needs. In Figure 1 the organizational set-up of the project is shown.

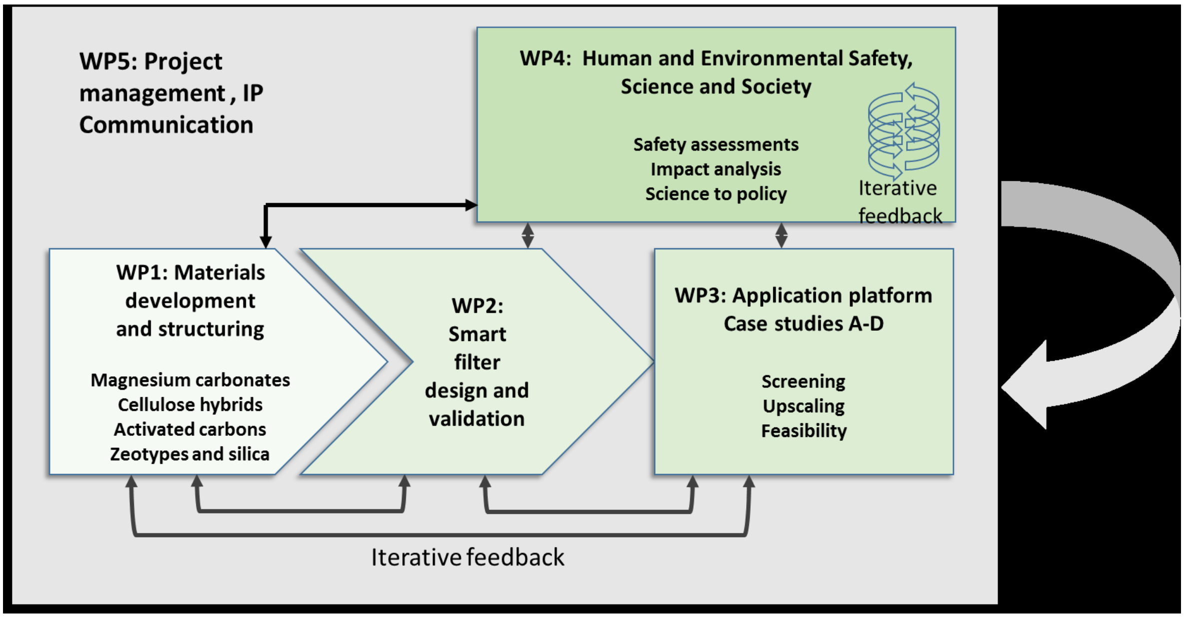

Figure 1. Material development set-up and flow in the Mistra TerraClean Program.

The MTP decided to use the concept of "safe by design" which has been traditionally employed by only a few areas of chemical design and production. This is particularly evident in various areas of the life science industry, such as pharmaceuticals, food additives and medical devices. In contrast, the concept is only now being introduced in other areas of industrial chemical design, manufacture and use. In the pursuit of smart chemical design, prospectively unifying desired functionality with optimal safety characteristics, the MTP has "front-loaded" this paradigm at the very heart of the chemical design and synthesis performed at the various academic laboratories partaking in the program.

Thus, the MTP has introduced LCA approaches covering the entire life cycle of the materials and devices from the very onset of the innovation process to the upscaled applications (work package WP4, Figure 1). A 2-tier LCA approach was established and screening LCA studies were performed at a very early stage of the development of materials and devices and full LCAs were planned, and one is being done now for the most promising solutions which had passed the tollgate, see figure 2. There the integral parts of the development and testing strategies in the MTP tollgate (TG) process towards full assessment in individual case studies are illustrated. Thus, a 2-tiered approach has been defined and systematically applied throughout all projects.

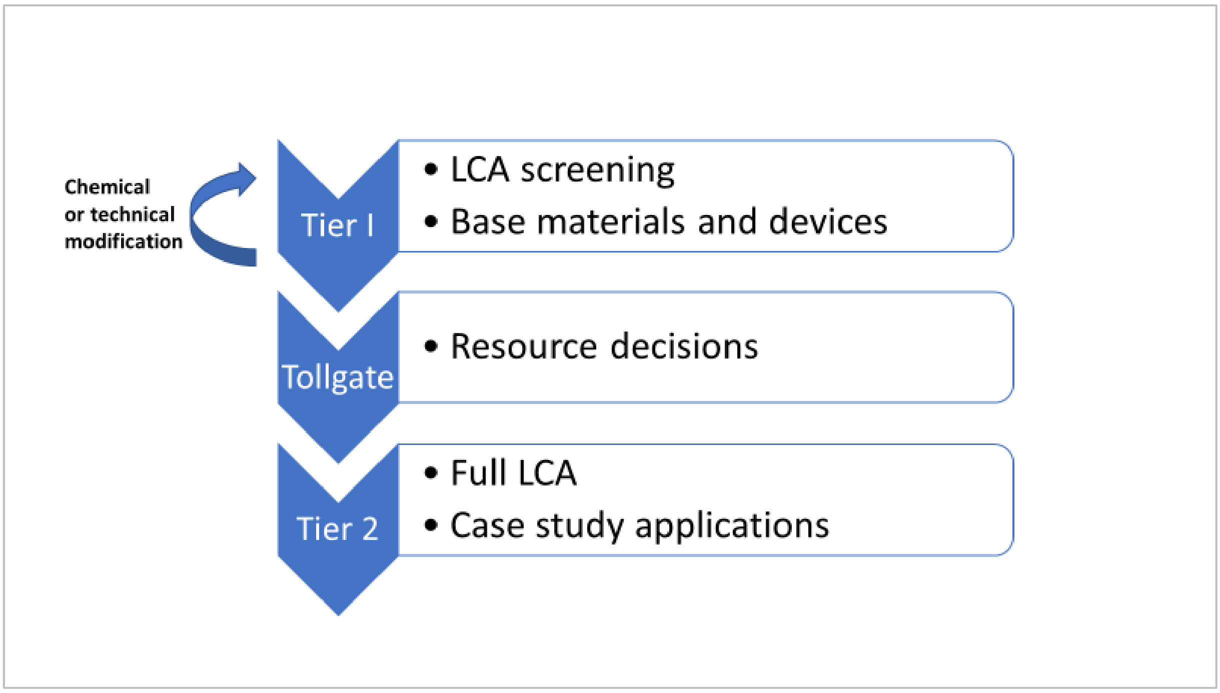

Figure 2. The Mistra TerraClean 2-tier LCA approach

Description of environmental LCA

Environmental LCA is the calculation and evaluation of the environmentally relevant inputs and outputs and the potential environmental impacts of the life cycle of a product, material or service (ISO 14040:2006 and 14044:2006) and involves various phases of scoping, information collection, impact assessment, interpretation and iterative feedback (figure 3 and 4).

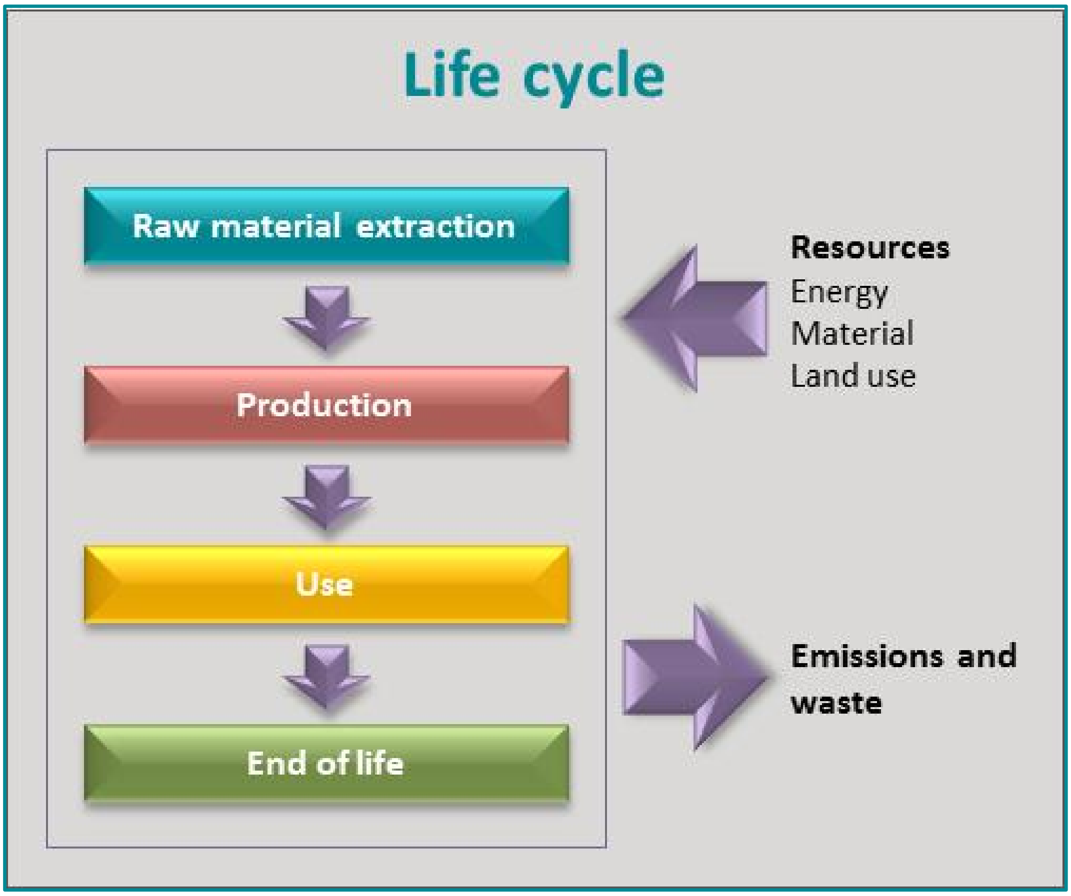

Figure 3. Illustration of the LCA system of the life cycle of a product, material or service.

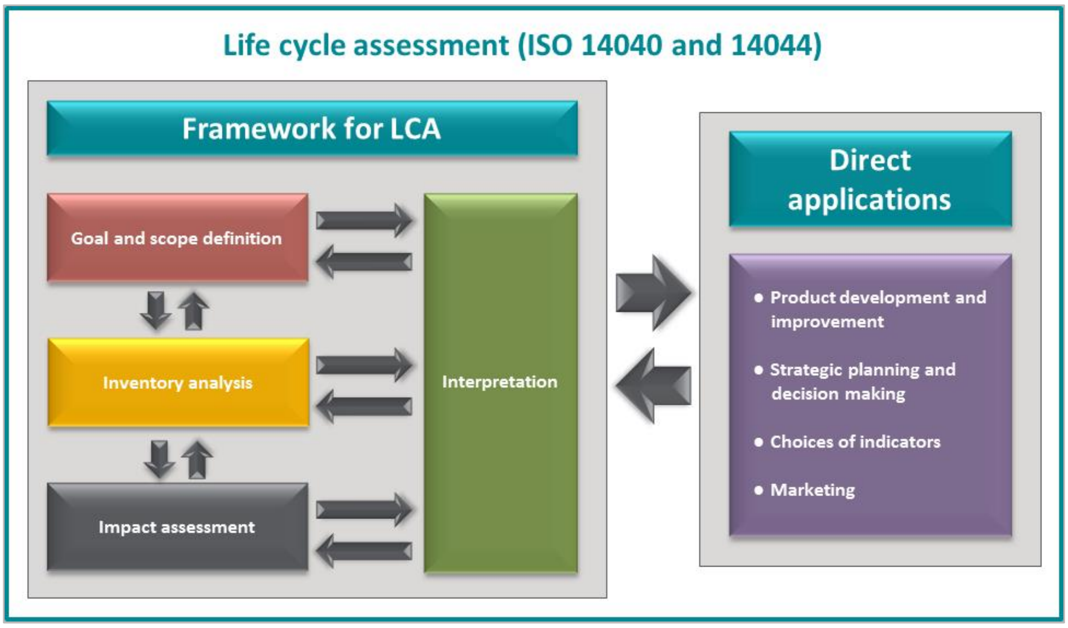

Figure 4. Illustration of the LCA process.

Description of screening LCA in MTP

During the pre-TG initial phase, tier 1, an "LCA light" or screening LCA process, coupled with toxicological evaluations, was applied to all base materials and chemistries in the project, in order to guide initial efforts at the laboratory bench towards producing a pool of potentially interesting materials and devices assessed both to be safe and to have acceptable environmental performance characteristics in terms of energy use, water consumption, raw materials, regeneration possibilities, resulting wastes and by-products.

The results of the initial screening have been provided as important feedback to the bench chemists, allowing adjustment of various aspects of their work, such as route of synthesis and use of solvents and other potentially toxic materials, all in an iterative fashion. Standardisation of the screening procedure across all materials and devices provides support to decision making process at the TG for defining which materials pose the best opportunities for application in specific case studies. It is fully recognized that the parameters derived and utilized at this early (laboratory/pilot) stage of material and device development may change at a later stage, when scale up to test batch production occurs. The intention is that the outcome of tier 1 can guide such changes, to avoid foreseeable issues which may lead to increased hazards.

Description of full LCA in MTP

The second tier of more in-depth LCAs is then applied to prioritized material/device combinations for pilot scale applications and encompasses a full appraisal of all relevant parameters for assessment of the further development, scale-up and performance of the approach, which would support relevant advancement of TRL levels from industrial and regulatory perspectives.

In this review we present our initial findings and experiences from the application of this tiered LCA approach in chemical innovation at the interface between academia, research institutes and industry in the MTP, and illustrate how the approach may be useful to other efforts where the development of "safe and sustainable by design" is important, which should always be the case.

Tier 1: screening LCA

The screening LCAs were applied "cradle to gate", thus only the production phase was quantified. The materials or devices encompassed were at different stages of maturity, with some being at lab scale and others at pilot scale and one at production scale. Data for chemical substance use, water use, and energy consumption were collected for the production steps and potential environmental impact was calculated. Global warming potential (CML, 2001 with the most recent IPCC data), environmental damage costs (EPS 2015dx excluding impact form secondary particles) and human and ecotoxicity potential (USEtox 2.1) were all calculated. Datasets and factors that were published in the database of the LCA software GaBi[1] were used for the screening LCAs. As a consequence, there were some data gaps regarding toxicity assessment. For data gaps in the inventory analysis, "proxies" were used instead. Additionally, toxicological assessments of the precursors and produced materials were also performed outside the LCA.

Qualitative assessment of the performance and handling of the various materials after use, for example involving possible regeneration, was also performed as a complement and outside the LCA calculations. The overall process was iterative and made in close communication with the research teams for each material and device type.

Below is a description of how this tier 1 approach has been applied to the MTP and the usefulness for the researchers in the project. Table 1 shows the different materials covered by screening LCA in the MTP.

Table 1. Materials covered by the screening-LCA approach

Scale	Materials	Company/academia
Production	Micro-fibrillated cellulose	Exilva from Borregaard
Pilot	Magnesium carbonate	Upsalite from Uppsala University and Disruptive Materials AB
Pilot	Amorphous hydrophilic silicon dioxide,	Quartzene from Swedish Aerogel
Lab	Wet-stable nanocellulose aerogels	RISE
Lab	Iron-impregnated activated carbon	Stockholm University
Lab	Nano-lignocellulose	KTH

Two devices from the MTP were considered. ZnO immersed in paper and in glass cylinders illuminated on the inside with UV light and a capacitor covered with a cloth of activated carbon (capacitive deionisation; CDI).

Although there were uncertainties in the data, environmental hot spots could be found in the production of each of the materials. Environmental hotspots are activities or substances with relatively large contribution to the environmental impact in the studied system. For the pilot and lab scale products, these findings were discussed directly with the material researchers, together with suggestions about possible regeneration and release of toxic chemical substances, which

[1] https://sphera.com/life-cycle-assessment-lca-software/ (professional version 4b, was the preferred one and ecoinvent 3.51 was used as a complement)

should be avoided whilst filtrating out the targeted pollutants. For example, for the lab synthesis of the nano-lignocellulose, the probable high energy use in the homogenization step was identified as a hot-spot worth attention. Additionally, in this particular case, the toxicity properties of one chemical substance led to a recommendation of either substitution with a less toxic reagent or implementation of occupational measures to avoid exposure.

For further improvements of the filter materials, chemical modifications/functionalisation have been proposed by the research teams for future developments and, to this end, the iron impregnated activated carbon, which is a chemically modified type of active carbon, is the only physical example. If other modifications are presented in the future, these should also be analysed with our tiered life cycle approach.

In terms of the zinc oxide device, the screening LCA was complemented using the relatively new Proscale™ method for assessing human toxicity (Lexén *et al.* 2017). An index for ZnO was calculated, including all its production steps, which is a common chemical substance and therefore the index is useful for the LCA community.

No screening LCA was performed for the CDI approach since the environmental impact was expected to be very low for the production of the device. This is because it consists of a long-lasting metal-based equipment (steel) and an activated carbon cloth. This cloth is regenerated every time the electrical charge used for collection of charged impurities is discharged in the regeneration step. Originally the device was intended for desalinisation, but in the MTP we will test its application in removal and destruction of per- and polyfluoroalkyl substances (PFAS) in various urban water sources. However, an in-depth analysis is currently performed on this in a second tier (below).

Tier 2: in depth LCA of the CDI device

The laboratory CDI device for cleaning ionic, microbial and other charged (and some uncharged) contaminants from water, was designed, manufactured and tested by the Functional & Nano Materials (FNM)[2] group at KTH (see Mistra TerraClean annual report 2019 for more information). One of the CDI prototypes was applied to removal of PFAS, more specifically 10 perfluoroalkyl acids (PFAA), in a lab-scale test. When water spiked with these PFAA was treated in the CDI, more than 95% removal was achieved. In addition, laboratory measurements could confirm that, at voltage between 2.5 – 4.0 volt DC application, the PFAA were also disintegrated, i.e. this technology has the potential not only to remove but also to degrade PFAS. The optimum voltage is still being determined in pilot trials, but it will be below 4.0 volt DC.

The CDI recently passed the MTP TG as it progressed from TRL5 towards TRL6 and pilot scale testing was initiated with modules designed, manufactured, installed and tested by Stockholm Water Technology. In this pilot the CDI will be applied for PFAS removal from drinking water in a testbed facility in Stockholm, Hammarby Sjöstadsverk.

[2] https://www.kth.se/start/2.8955/groups/mnp/research-groups/functional-materials?l=e

A full-scale LCA on the CDI, as applied in this pilot, is now planned (Figure 5). The aim is to compare different environmental aspects between the CDI and conventional PFAS treatment, without claiming any environmental superiority.

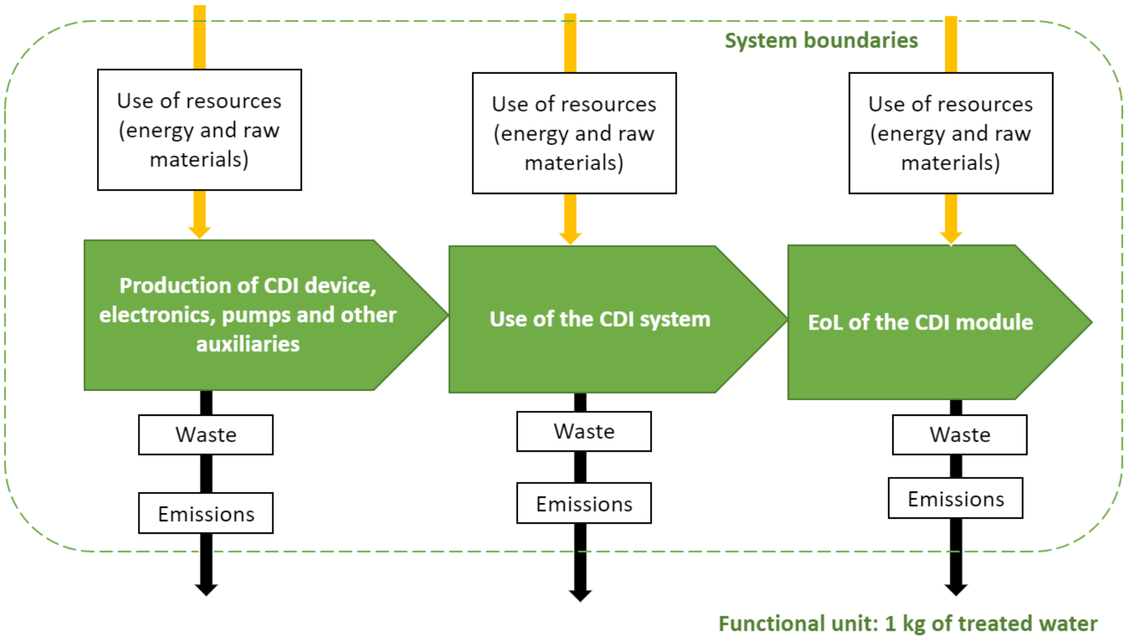

Figure 5. Schematic picture over the life cycle of the CDI device with various parameters highlighted for incorporation in the in-depth LCA

Environmental performance (including human health aspects) is to be compared to the more conventional techniques already in place, e.g. granular activated carbon (GAC) filters. With a functional unit set to a treated volume of water to a specific standard, e.g. an updated drinking water standard or based on the recent EFSA risk assessments (EFSA Panel on Contaminants in the Food Chain *et al.* 2018, EFSA Panel on Contaminants in the Food Chain *et al.* 2020), comparisons will be made across the two systems of potential impacts for the whole life cycles as well as hot spot patterns. As mentioned earlier, hot spot in an LCA is an activity with a large contribution to the environmental impact of the product. In scenario analyses, varying characters in the incoming waters, both with regards to PFAS profile, and other properties (e.g. content of dissolved organic carbon (DOC), particulates etc.), will be considered. These comparisons will hopefully generate valuable insights into under what circumstances the CDI has the potential to be a favourable technique and what aspects of the CDI life cycle that can be improved in order to enhance its environmental performance.

In addition to an ecotoxicological appraisal of the treated effluent, eco and human toxicological ((eco)toxicological) potential impacts are to be included in the LCA. This will, by use of a recently developed framework for life cycle impact assessment (LCIA) for PFAS (Holmquist *et al.* 2020), potentially allow us to compare (eco)toxicological impacts within the life cycles; e.g. the treated effluents potential impacts with direct and indirect chemical emissions from the manufacturing.

Conclusions

The concept "safe by design" which was achieved by using a 2-tier LCA approach with (eco)toxicity analysis was fruitful because:

- unlike many commercial producers, university chemistry groups are generally not used to performing LCA in their research, but with this concept they got acquainted with the usefulness,
- introduction of LCA in these environments requires close, iterative communication with the researchers at the chemistry bench which creates a fruitful dialogue,
- application of screening LCA has clearly guided the scientific thinking behind improvements in material design where applied,
- the academic researchers involved in the MTP have demonstrated the value of early application of LCA in material development.

The application of the 2-tier LCA approach to ensure full "smartness" in material and device design will continue throughout the lifetime of the program and beyond, helping to steer wave upon wave of novel synthesis towards functional and safe materials for minimising potentially harmful chemical exposures via water and air.

References

EFSA Panel on Contaminants in the Food Chain, H. K. Knutsen, J. Alexander, L. Barregård, M. Bignami, B. Brüschweiler, S. Ceccatelli, B. Cottrill, M. Dinovi, L. Edler, B. Grasl-Kraupp, C. Hogstrand, L. Hoogenboom, C. S. Nebbia, I. P. Oswald, A. Petersen, M. Rose, A.-C. Roudot, C. Vleminckx, G. Vollmer, H. Wallace, L. Bodin, J.-P. Cravedi, T. I. Halldorsson, L. S. Haug, N. Johansson, H. van Loveren, P. Gergelova, K. Mackay, S. Levorato, M. van Manen and T. Schwerdtle (2018). "Scientific Opinion on the risk to human health related to the presence of perfluorooctane sulfonic acid and perfluorooctanoic acid in food." EFSA Journal **16**(12): e05194.

EFSA Panel on Contaminants in the Food Chain, D. Schrenk, M. Bignami, L. Bodin, J. K. Chipman, J. del Mazo, B. Grasl-Kraupp, C. Hogstrand, L. Hoogenboom, J.-C. Leblanc, C. S. Nebbia, E. Nielsen, E. Ntzani, A. Petersen, S. Sand, C. Vleminckx, H. Wallace, L. Barregård, S. Ceccatelli, J.-P. Cravedi, T. I. Halldorsson, L. S. Haug, N. Johansson, H. K. Knutsen, M. Rose, A.-C. Roudot, H. Van Loveren, G. Vollmer, K. Mackay, F. Riolo and T. Schwerdtle (2020). "Scientific Opinion on the risk to human health related to the presence of perfluoroalkyl substances in food." EFSA Journal **18**(9): e06223.

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

Lexén, J., 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 and 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/.

IVL Swedish Environmental Research Institute Ltd.
P.O. Box 210 60 // S-100 31 Stockholm // Sweden
Phone +46-(0)10-7886500 // www.ivl.se