PRELIMINARY

Report of the 2nd Consultation meeting on CSS/SSbD, January 31, 2024

List of Steering Committee members and co-authors of the report.

Name	Gender	Affiliation	Country	Sector	email address
Annegaaike Leopold	F	Ibacon GmbH	NL	Business	annegaaike.leopold@ibacon.com
Leo Posthuma	M	RIVM	NL	Government	leo.posthuma@rivm.nl
Hans Sanderson	M	U. Aarhus	DK	Academia	hasa@envs.au.dk
Ksenia Groh	F	EAWAG	CH	Academia	ksenia.groh@eawag.ch
Paul Thomas	M	KREATiS	FR	Business	paul.thomas@kreatis.eu
Michelle Bloor	F	U. Glasgow	UK	Academia	mbloor@yahoo.com
Bruno Campos	M	Unilever	UK	Business	bruno.campos@unilever.com
Hanna Schreiber	F	Umweltbundesamt GmbH	AU	Government	hanna.schreiber@umweltbundesamt.at
Evangelos Daskalopoulos	M	EC - RTD	BE	Government	Evangelos.Daskalopoulos@ec.europa.eu
Christoph Schür	M	EAWAG	CH	Academia	christoph.schuer@eawag.ch
Serenella Sala	F	EC - JRC	IT	Government	serenella.sala@ec.europa.eu

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Executive Summary

In an online SETAC/EC-organized Consultation meeting on 31 January 2024, experts involved and/or interested in the development and implementation of the *Safe and Sustainable by Design* (SSbD) approach joined in, for a second time. The meeting was organized the Sounding Board of SETAC-members, which supports SETAC's representation at the High-Level Roundtable for the implementation of the Chemical Strategy for Sustainability (HLRT CSS), in collaboration with the European Commission (EC) (DG RTD). This 2nd Consultation Meeting is the result of a SETAC partnership with the EC through the Sounding Board and is a direct follow-up to our highly successful 1st Consultation Meeting held on 2 October 2023, which attracted 114 participants, including representatives from the EC and its stakeholders, SETAC scientists and other associated scientists from across the planet.

This second event was targeted to provide specific scientific support the European Commission (EC) in the implementation of the SSbD framework by introducing and progressing science- and experience- based ideas from the width of SETAC's membership and beyond, to identify and create added value to the Chemicals Strategy for Sustainability (CSS). The point of departure was the crucial need and the science-based opportunities to further develop the SSbD as identified in the 1st Consultation. The objective of the 2nd Consultation meeting is the to further expand on and develop the scientific ideas for the implementation of SSbD, in a form that would feed straight into the Green Deal SSbD Workshop organised in conjunction with the SETAC Europe 34th Annual Meeting. That workshop is aimed at deriving pathways to effectively enable the SSbD vision and the CSS as a whole, with emphasis on three types of useful outputs, namely (1) science and tools are ready to use for SSbD-assessments, (2) science is- , but tools are not yet available, and (3) both science and tools are not available but key for SSbD assessments.

The Consultation meeting resulted in lively presentations, and a further expansion of the list of scientific opportunities to improve the concepts and applicability of the SSbD framework. In this preliminary report, the results of Consultation are presented in an initial form. That is: the different Chapters summarize the contents, and when applicable some questions and answers, of the plenary presentations, followed by a concise overview of outputs of breakout groups.

The present Preliminary Report, and the underlying 'raw results' (contributions and ideas formulated by the attendees) will be further edited, sorted and categorized, to form the input for the aforementioned workshop in Seville.

1. Opening (Annegaaike Leopold, Sofie Nørager and Bart Bosveld)

Annegaaike (meeting chair and SETAC-SB chair) and Sofie (meeting co-chair; Deputy Head of Unit E3 Industrial Transformation at DG Research & Innovation at the European Commission) open the meeting, highlighting the exciting journey we are on, followed by Bart (SETAC- Executive Director). Together they highlight that we all bring together a large amount of knowledge needed for optimal scientific design for- and effective implementation of the EU's Chemicals Strategy for Sustainability (CSS) and Safe and Sustainable by Design (SSbD) vision.

All three emphasise that the collated brainpower of the attendees are key for the efforts towards an optimal, valid and useful SSbD approach.

2. Motivations and setting the scene by Sofie Nørager

Sofie welcomes all participants of the 2nd SSbD Consultation by SETAC/EC, and specifically highlights the attendance of PARC representatives. PARC – Partnership for the Assessment of Risks from Chemicals – is a large European project seeking to improve on concepts, approaches and tools for chemical risk assessment. PARC-led work on a toolbox for SSbD involves several national agencies that are brought together to build an accessible toolbox for SSbD, each with different roles to play. The EU-network called IRISS – the International SSbD Network – brings all actors together with the goal of accelerating the transition to SSbD materials, products and processes and permanent networking on this (see https://iriss-ssbd.eu/). The SETAC-scientists are now added to this landscape of collaborations and networks, with the aim of tapping the broad knowledge- and experience base to propose, design and forward 'bold solutions' to the most intricate scientific (and science-practice) problems encountered under the SSbD vision.

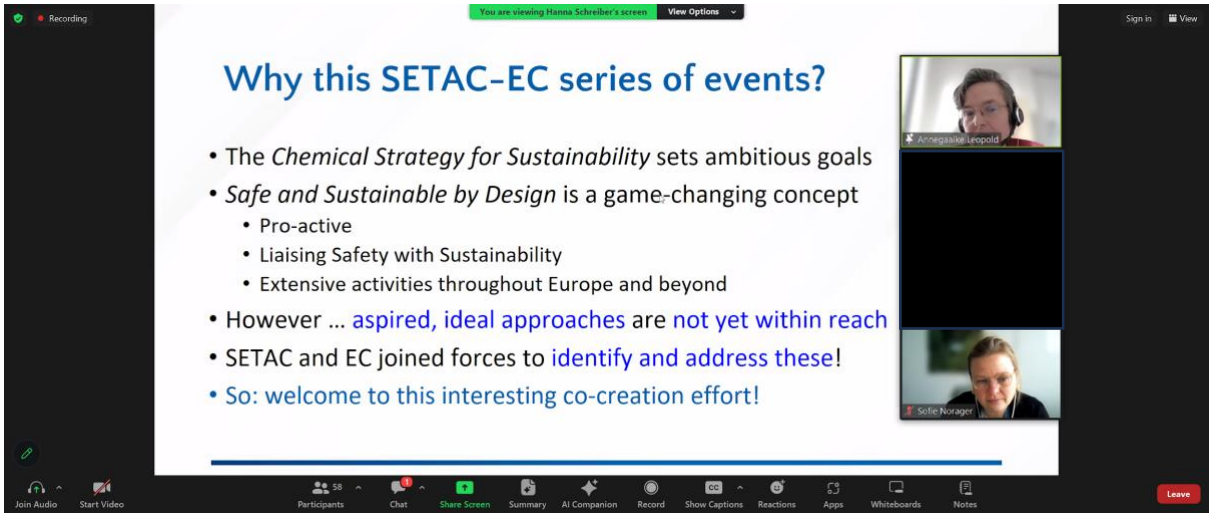
Currently, we entered a second year of EU-wide testing for the SSbD framework. Currently, SSbD development has two major tracks:

- ➔ An industry-operational track, where utility is key for bigger but especially also smaller industry partners
- ➔ A scientific track, where innovative tools and methods are key

The EC stimulates both, a forward-looking vision requires that the SSbD framework is both scientifically valid and fully operational in practical terms. The EC hopes to see that these matters are bridged together in the course of further development work.

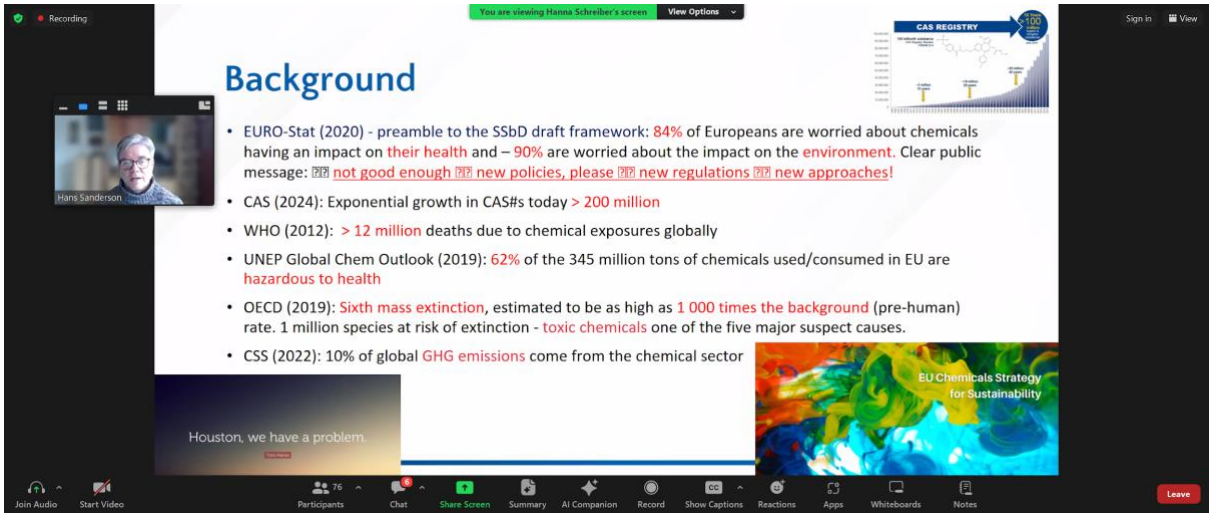
As we are working in this complex landscape, we should all aim at opening up new opportunities within the SSbD framework.

Sofie wraps up by wishing us all plenty of exciting discussions, like there were last time (i.e., during the 1st SETAC/EC SSbD Consultation held in October 2023).



3. Birds-eye view on SSbD pathways (Hans Sanderson)

Hans (SETAC-SB member) takes the floor to describe the big picture explaining the background and motivation for SSbD development. Hans stresses that (i) there are (too) many chemicals, 'and counting'; and (ii) there are public concerns regarding health and biodiversity, which gain additional importance in the context of the ongoing climate change.



Hans also stresses the relevance of the chemical sector for our society, looking at both products, revenues and labour. These matters mean an aspiration for 'make-not-break' approaches under the CSS.

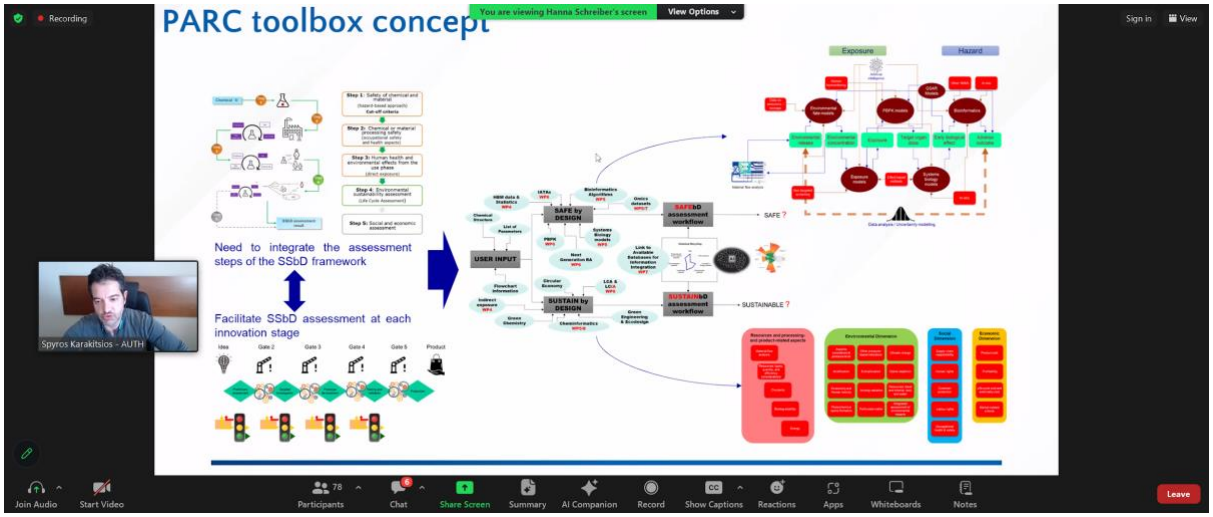
➔ So: how can science be of help for this conundrum?

As scientists, we are well-equipped and trained to contribute to SSbD-like activities. But can we also re-think, improve and arrange with the different ways that we are familiar with on the one hand, to chart a passable road toward effective and valid SSbD on the other? Can we link to the innovation cycle, being a reality in society and industry?

The idea of the Consultations of the SETAC experts is to address the problems that came forward in the design and testing of SSbD. For this, we need to look outside the light-circle of the things we already know ….

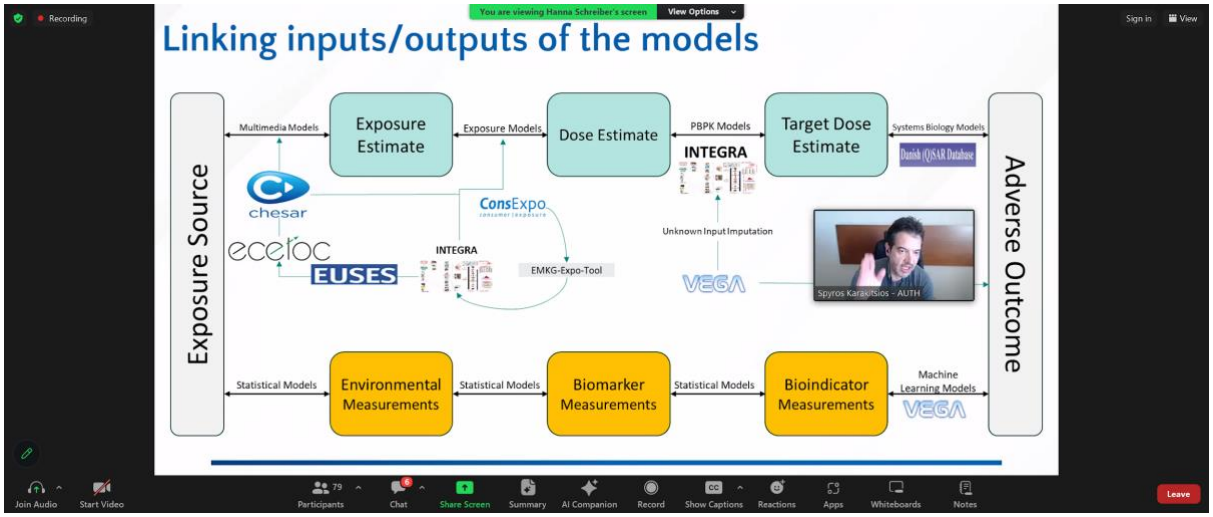
4. Complementarity of the current effort to PARC activities on SSbD (Spyros Karakitsios)

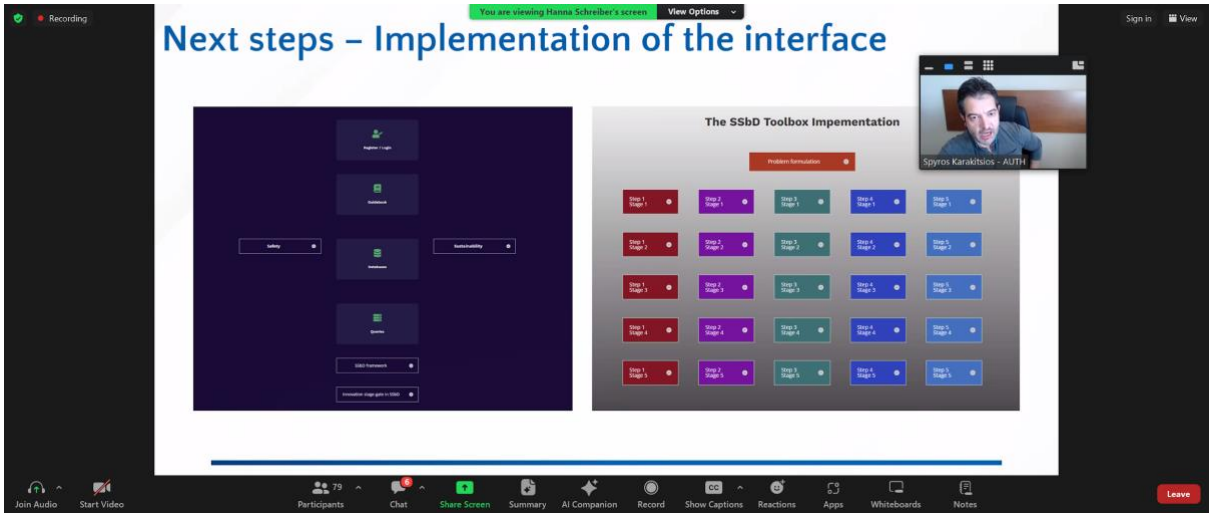
Spyros (the leader of PARC's SSbD-toolbox project) introduces PARC as a Europe-wide project that – amongst its many other activities – brings together the existing science-based tools and approaches to make them useful for SSbD. PARC has been running for 2 years now, and will continue for another 5 years.



The PARC's SSbD-toolbox concept builds on principles that are both scientifically strong and operationally effective. PARC then addresses specific aspects of all principles, models, databases – and so on and so forth – aiming to establish the required interconnections (science part) as well as the user-oriented "pipelines" and tools for end-users (practical operation part). The latter aspires to be "easy-to-use" and also implements several wizards to help the end users. Clever approaches, such as blockchain-techniques, can help in management of proprietary data, because they can allow using data that at the same time would remain proprietary.

The complexity of current tasks at hand is high, but it can be arranged in logical steps, to build the proper linkages between the different models and implement the necessary interface (see top and bottom slides below):

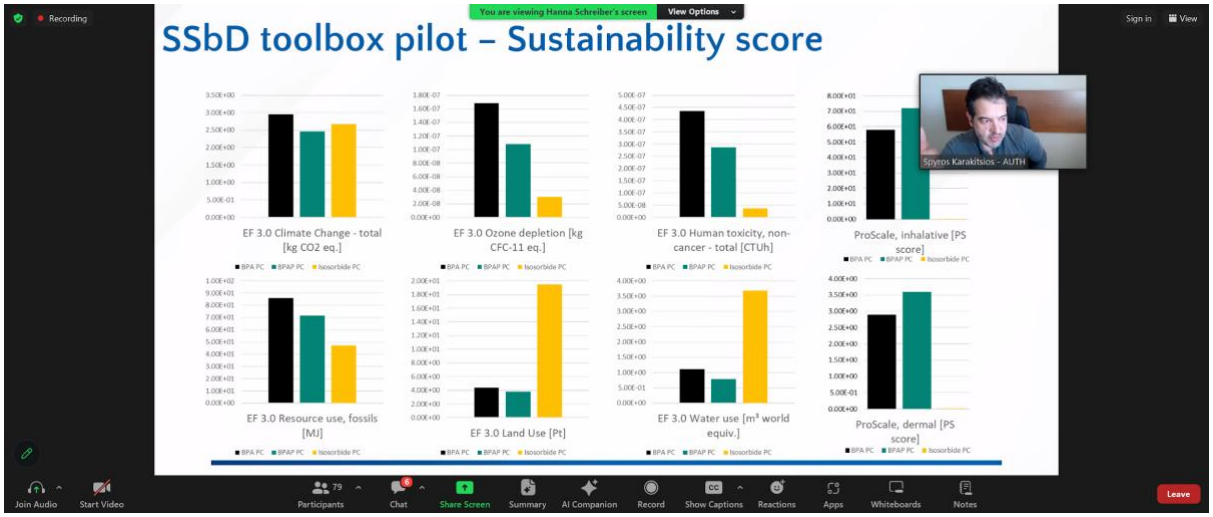




A “wizard”-approach will assist the end-users to make all connections that are needed. The toolbox is being trialled and will be improved based on experiences gained in several case studies.

Amongst the most complex matters to be addressed, Spyros highlights the early-development stages of innovation processes, where the toolbox needs to be able to generate safety and sustainability scores under data-poor conditions.

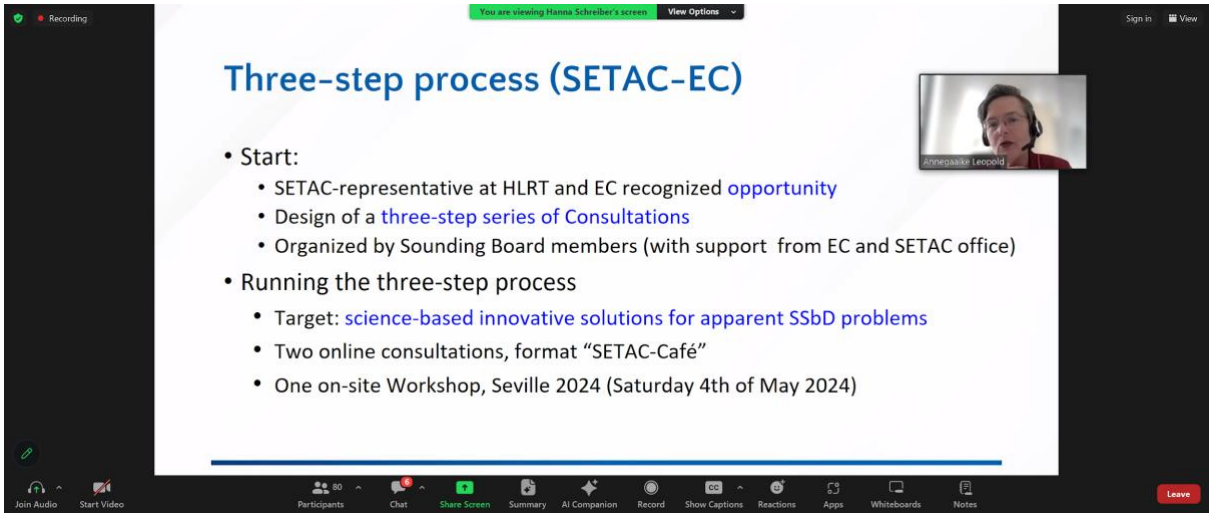
The outcomes – for now – include multi-dimensional measures, which will then be evaluated via Multi Criteria Decision Analysis:



Spyros concludes by explaining that there are still multiple steps ahead of the PARC’s SSbD toolbox project, which will be based on an open and inclusive IT-design.

5. The SETAC/EC SSbD Consultation Process (Annegaaike Leopold)

Expanding on Sofie's introduction (above) Annegaaike explains that we are following a three-step process which was initiated based on meetings and discussions with Peter Dröll (Director for Prosperity, Directorate-General for Research and Innovation at the European Commission), suggesting that SETAC scientists represent a wide array of scientific knowledge and could thus provide valuable ideas that could be of help in solving the complex (remaining) problems on the path toward successful implementation of SSbD.

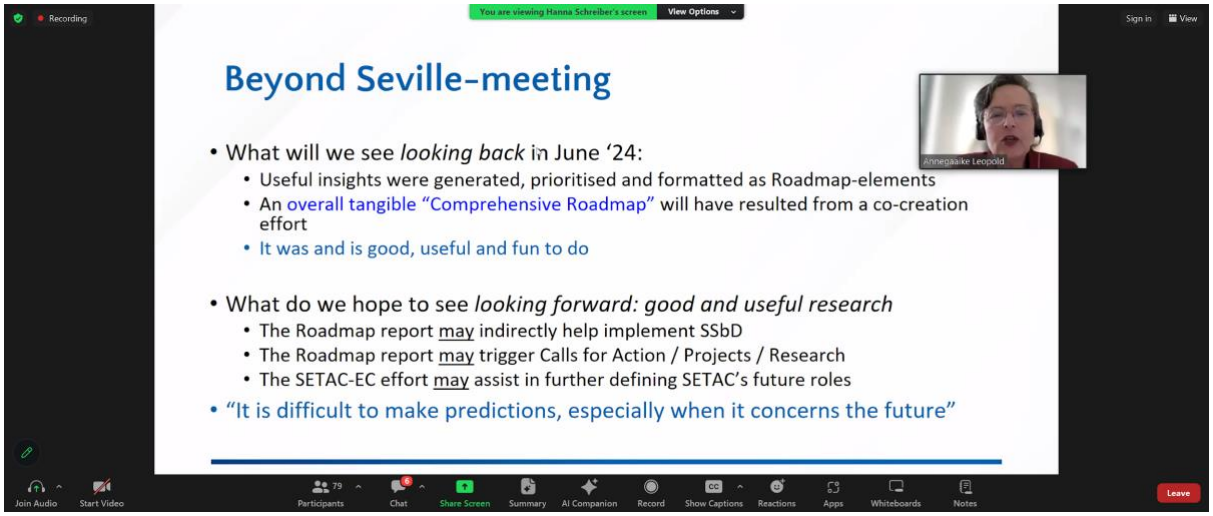


Following the 1st (October 2023) and 2nd (taking place now, January 2024) online Consultations, the process will end with an on-site workshop in Seville (May 2024, adjacent to the annual meeting of SETAC Europe). The outcome of the Seville workshop will be a *Comprehensive Roadmap for the pressing scientific problems that could be solved to forward the scientific basis and utility of SSbD*.

Annegaaike invites volunteers to get involved in the preparations for the workshop in Seville and contribute to the co-creation of its foreseen end-product.

Annegaaike also addresses our aspirations for the time beyond the Seville: what are we aiming for, when are we happy? We are happy, if we have tangible results, in the form of a comprehensive Roadmap that supports optimization (science, utility) of SSbD, and that can serve as the basis for strategic planning of scientific and practical innovation. We are aware that this tangible product is seen as important by the EC, but that a follow-up action has not been formulated.

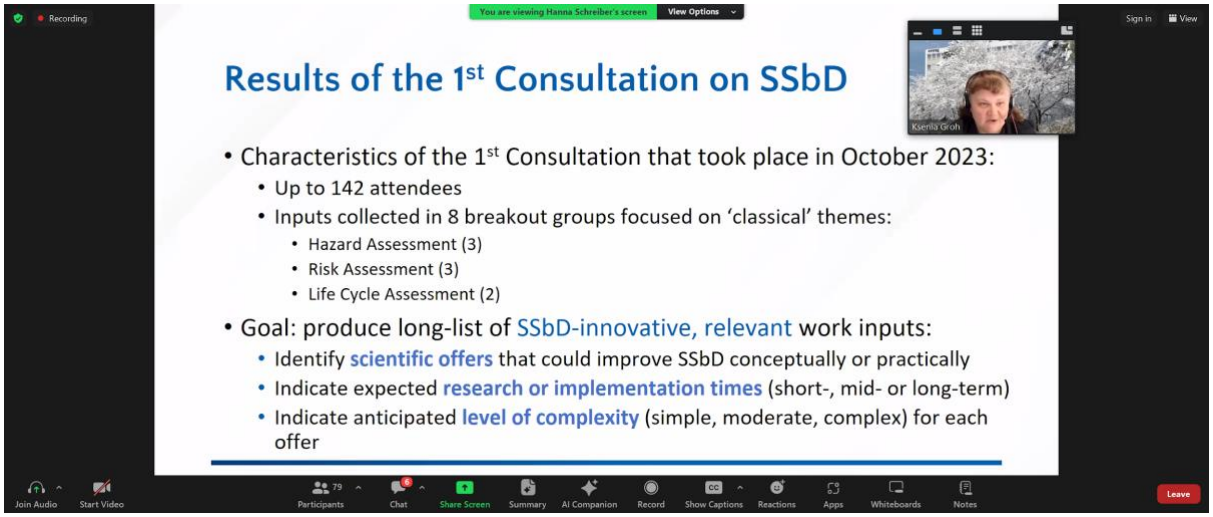
Note that the report of the 1st Consultation meeting can be found on the SETAC-website: file:///N:/Documents/Downloads/20231208Preliminary-report-of-the-1st-SSbD-Consultation-meetingreported-to-EC-final-005.pdf.



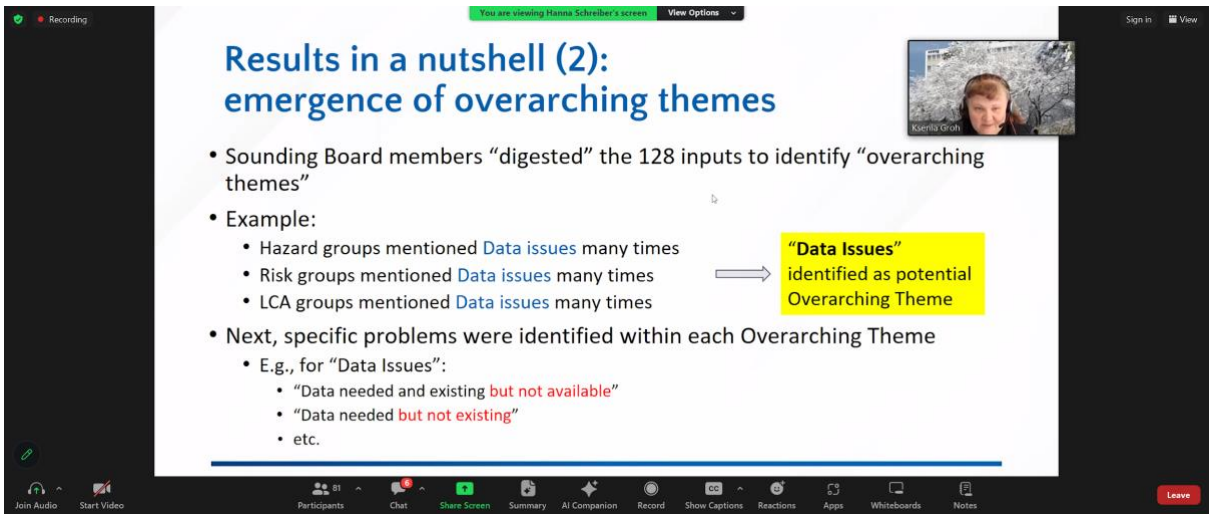
Annegaaike ends with presenting the program of today. The first part of today's program is planned as a plenary, introducing the current status reached after the 1st Consultation, whilst the second part is aimed at *work!*

6. Results of the 1st Consultation meeting (Ksenia Groh)

Ksenia Groh (SETAC-SB member) introduces what happened so far. With close to 150 international attendees taking part in the 1st Consultation, there is evidence for ample attention of both SETAC-EC-affiliated scientists and other stakeholders. Those attendees contributed with many ideas, to yield an initial long-list of innovative and relevant ideas.



As shown in the example slide below, the analysis of inputs collected during the 1st Consultation identified three major "overarching themes", such as one on "Data": early in the innovation process, lack of data is common - so that this subject was frequently mentioned in different ways. Various other themes were also found more frequently. For each of these themes we then described "problems" and "aspired solutions", following specific Roadmapping techniques (following the so-called Cambridge-approach, described in Phaal et al., 2011). The first question of this technique is not "*What can we do tomorrow as the next step we can easily foresee in our planned workflow*", but the question "***Where do we want to go?***" as starter-question. In the terms of this effort: ***"Can we set some Aspirational Goals to solve scientific or practical SSbD problem items, encountered in the test phase of SSbD, or even problems that we expect in future applications of SSbD and not apparent from tests so far?"***



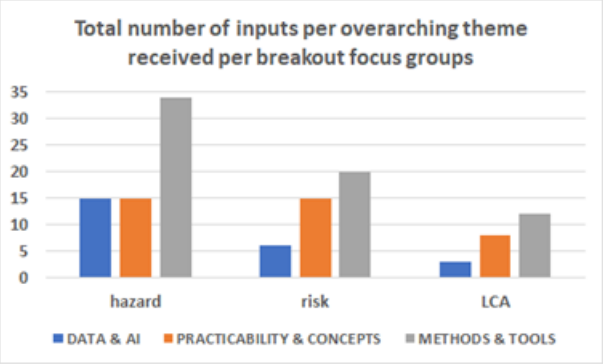
The three “overarching themes” on SSbD include:

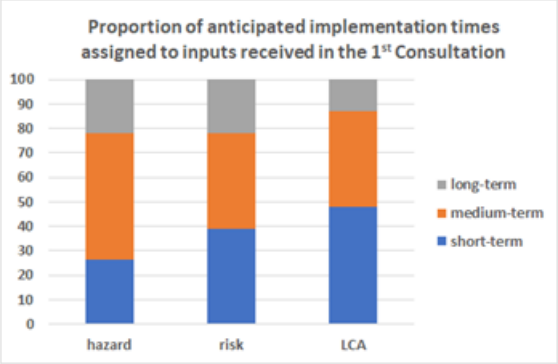
(1) Data & Data methods,

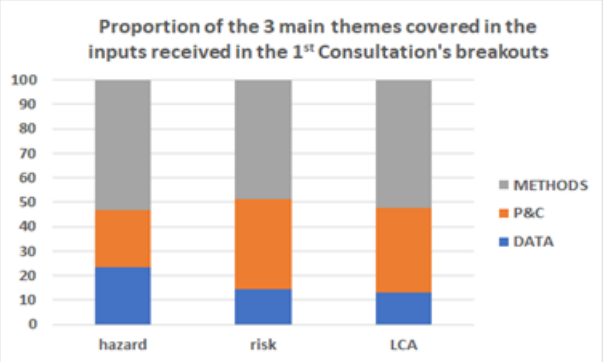
(2) Practicability & Concepts, and

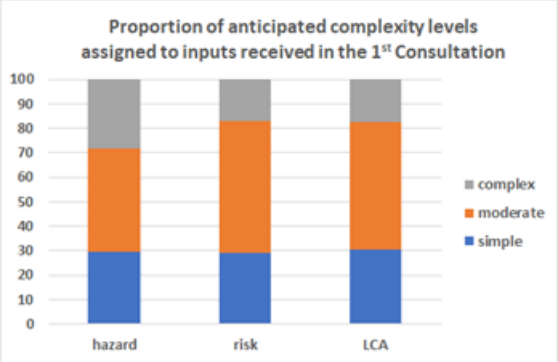
(3) Methods & Tools.

Across the three breakouts held during the 1st Consultation (i.e., breakouts on hazard, risk, and life cycle assessment (LCA)), these themes were represented in various proportions, the largest of them being taken by Methods & Tools. The participants were also asked to provide their estimates of the implementation time (short term, medium term or long term) and complexity (simple, moderate or complex) of the solutions and paths forward, which they were proposing. While the largest number of submitted inputs were tagged as “medium term” and “moderate” in terms of time and complexity, there were also short-term and simple solutions which were judged as being ripe for immediate implementation. As well, several highly complex development needs and visions were identified, which could be pursued for implementation in the long-term horizon. Respective graphs are shown below as an impression.









7. Plenary warp up: questions and answers

Questions for the presenters were addressed mostly orally, in line with the presentation and clarifying aspects of the presentations.

Questions and answers posed during the session were further captured in the Chat-function. They pertained to practical questions, such as:

- "Will the results be reported"? - answer: Yes

and to in-depth questions on matters such as:

- on the SSbD-framework: e.g., "[it was observed that] Life Cycle Assessment plays a key role, but would there be more options for the Sustainability Assessment parts of SSbD?"

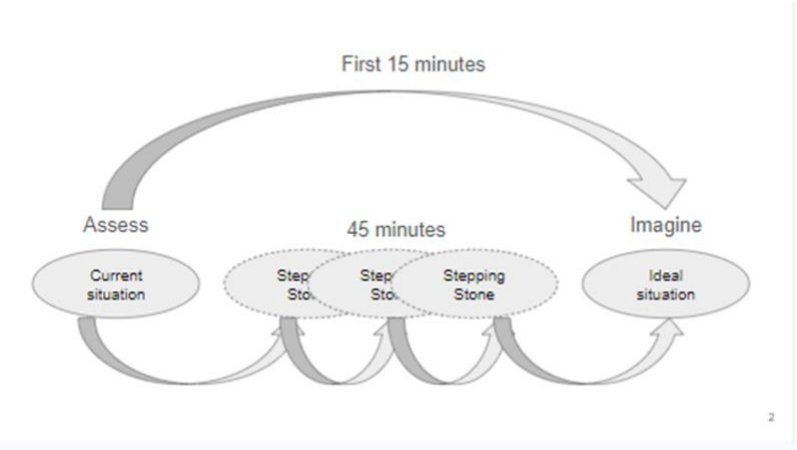
The Q&A was further handled during and after the Breakout sessions.

8. Breakout sessions (Leo Posthuma and Hanna Schreiber)

Moving towards the ***work*** of the participants in the Breakout sessions, Hanna Schreiber (SETAC Council member) and Leo Posthuma (SETAC-SB member) make a dual presentation of the subjects and approaches of the Breakout groups foreseen for the 2nd Consultation.

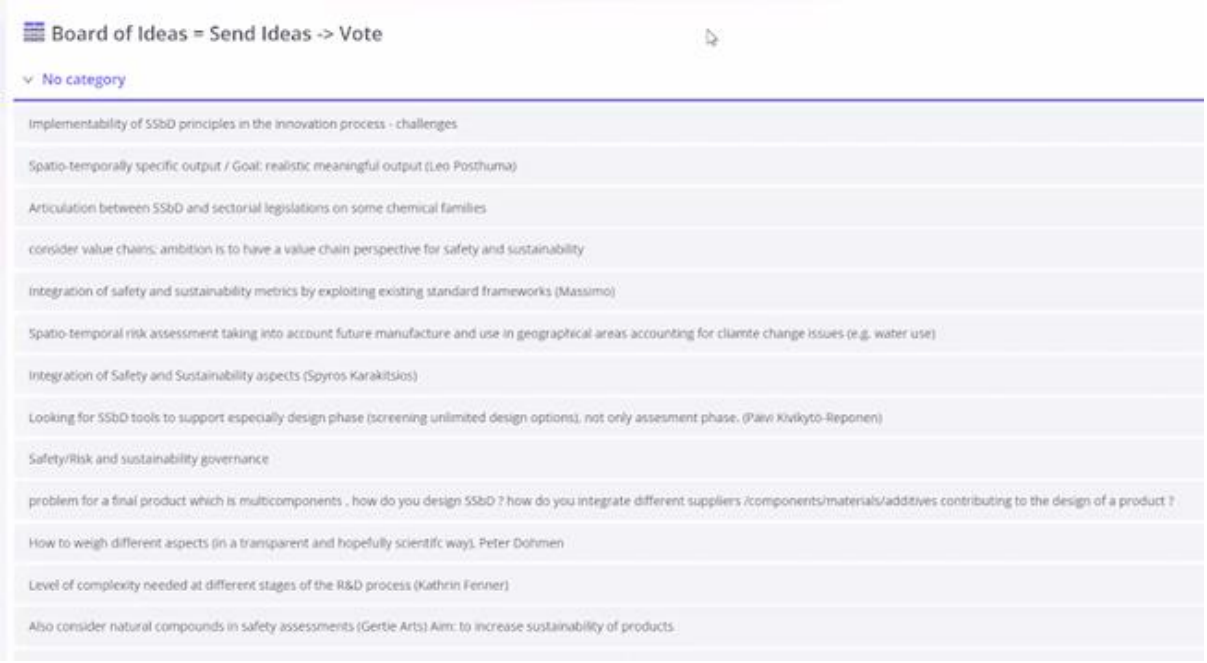
The primary aim of these breakouts was presented as "... to collect ideas on scientific solutions for apparent SSbD-problems and start outlining the detailed development paths - with stepping stones as explicit intermediate steps - to solve those….".

The approach that was selected to run the breakout groups, originating from the Cambridge Roadmapping concept, is summarized in the figure below:

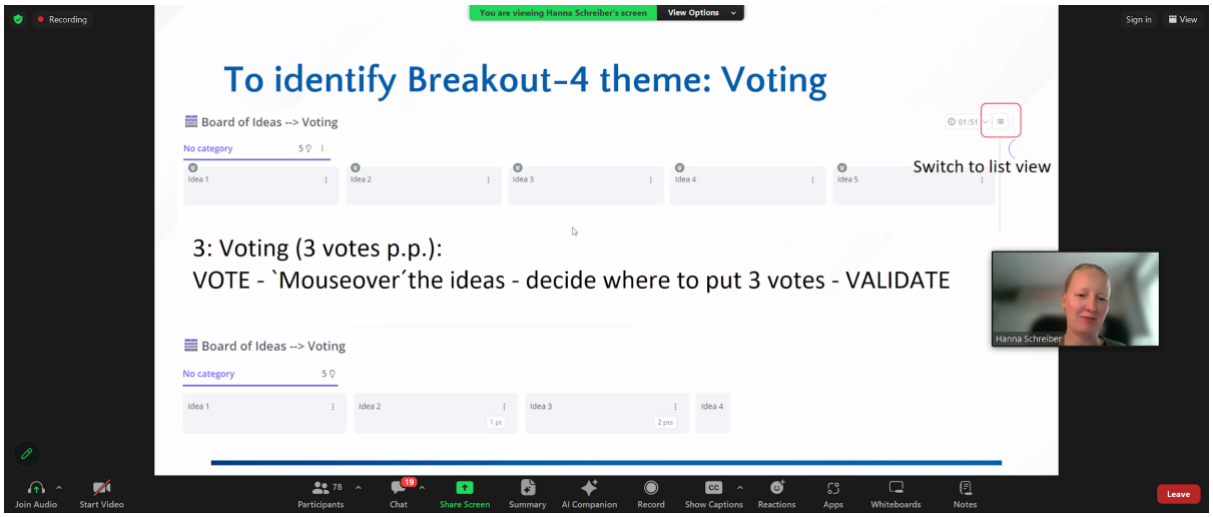


While three of the planned breakouts had been pre-defined to correspond to each of the three "overarching themes" identified on the basis of the results of the 1st Consultation, attendees are now uniquely given the opportunity to contribute further ideas and identify additional topics/themes that have not been covered so far. That is, there were three "identified themes" but also an option for an as yet undefined "freecard"-session on topics that were deemed important by today's attendees.

The "freecard"-session was identified by asking the attendees whether they had an idea that would substantially improve the output of the Consultation, by focusing on a particular SSbD-related subject of high interest. This process was supported by the Beekast online tool for workshop feedback. Upon a short period in which all attendees could describe their high-interest proposed subjects, those results were shown and voted on, again by the full audience. A suite of potential "freecard"-Breakout group Themes were proposed. Details of proposed items (yet without voting) are in the illustration below.



After sufficient time to enter Theme-proposals, attendees voted as in the picture below, allowing them to give three points to the Themes they identified as key to potentially improve (one attendee could give all three points to one Theme, or spread them over maximum of three different Themes).



The chairs of Breakout session 4 considered which topics received most votes and as absolute top-2, the following Themes were considered of highest relevance for (future) SSbD consideration/development, by the chairs of Breakout Group no. 4. :

1. The final evaluation and weighting (including interpretation and communication) of outcomes of SSbD studies
2. Considering spatially-differentiated outcomes of SSbD assessments

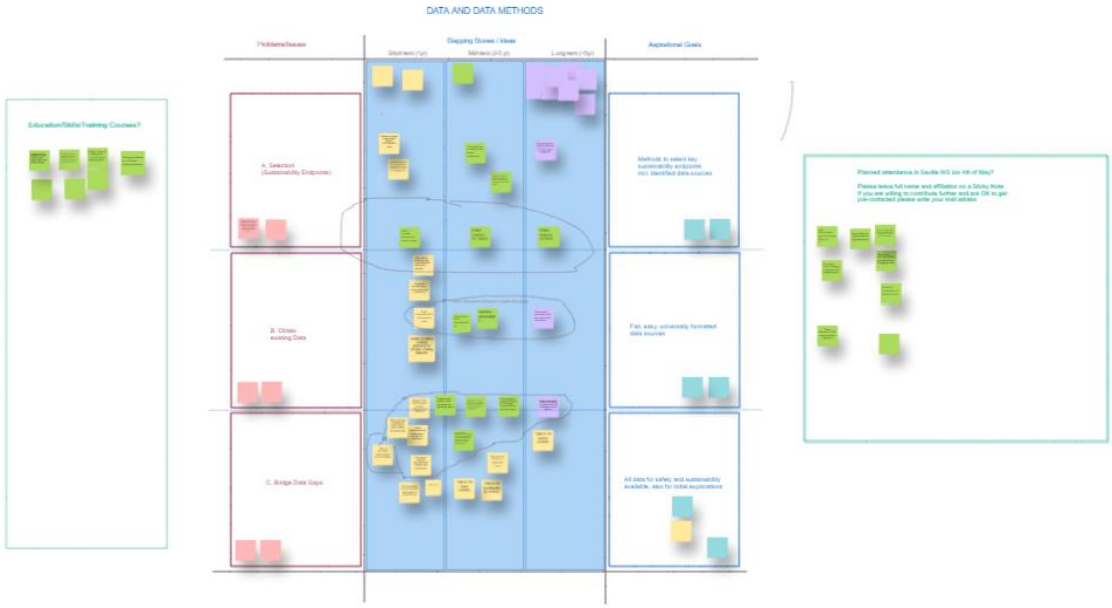
The assigned Chairs of the breakout for this novel Theme thereupon prepared for their session, whilst attendees could have a short break. All attendees could thereupon select the Theme group of their interest, and move to the selected Breakout room.

Upon identifying the priority-subject of the fourth Breakout group, and as introduced by the organisers, the Breakout groups were asked by Hanna and Leo to deliberate on the various Aspects of

SSbD (Scientific, or Utility, but also Training & Skills), in an effective way for the future step of Roadmapping. That is, the Breakout groups were offered a specific “whiteboard”, pre-formatted in the Beekast software, according to the scheme depicted in the Figure below.

The Figure below gives **one short and visual impression of the results of the Breakout groups.** The detailed results are in the Appendix.

In this example, the pink Post-Its to the left represent three **types of Problems** handled by this Breakout group, and the blue Post-Its to the right show that the group defined (as first step) some **Aspirational Goals**. The yellow and green Post-its in the middle reflect the science- and experience based ideas that were offered by the Attendees to solve either of the Problems in the three types of Problems. Those can be characterised as intermediate Stepping Stones. **From left to right, in the blue area, there is an indication of time- and sequence needed to solve a problem, via one or more Stepping Stones**.



Further results of the Breakout groups are summarised in the **Appendix**, and the present report proceeds with **summarising observations** collated from the Breakouts.

9. Key findings – Presented in the 2nd Plenary

Upon return from the Breakout sessions, Annegaaike Leopold re-opened the 2nd Plenary session, which is committed to reporting on the most important observations that were made during the Breakouts. That is, all detailed results were promised to be "digested further, and surely kept" as preparatory information for the Seville-workshop, but for now, given time limits, we focus on highlights and potential breakthrough ideas.

Annegaaike invited the four presenters to show their Highlights, of which the picture below is one example impression. The impression makes clear, that the Attendees have really made an "organized brain dump" of their ideas. They indeed:

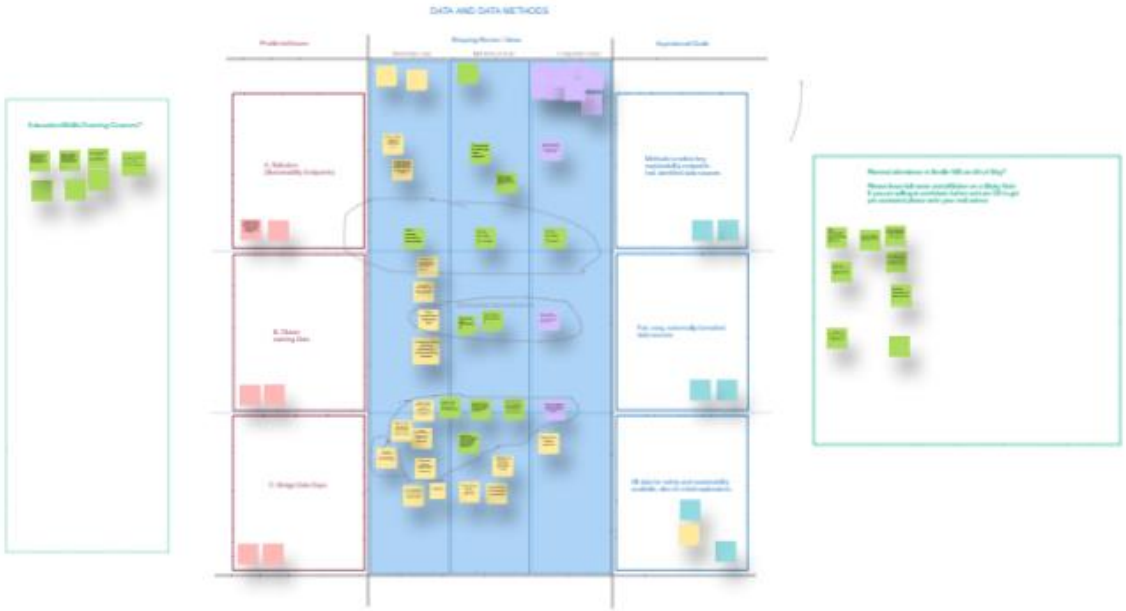
- amended the Aspirational Goals (amended or added right-hand side Post-its)
- amended and refined currently-experienced Problems (amended or added left-side Post-its)
- but especially created preliminary roadmap by formulating their "sorted" ideas, positioning those as Post-it in the form of sequential Stepping Stones between a problem and a goal.

The picture shows that - despite the very time-compact format of a SETAC Cafe / Consultation - a suite of ideas was brought forward, whilst those were even sorted in **Preliminary Roadmap shapes/sequences.**

With details provided in the Appendix, the sections below sketch summary outputs of the Breakout groups, for the selected themes. Note that the Pictures are not meant to be readable, as the details are shown in the Appendix.

Data-related issues

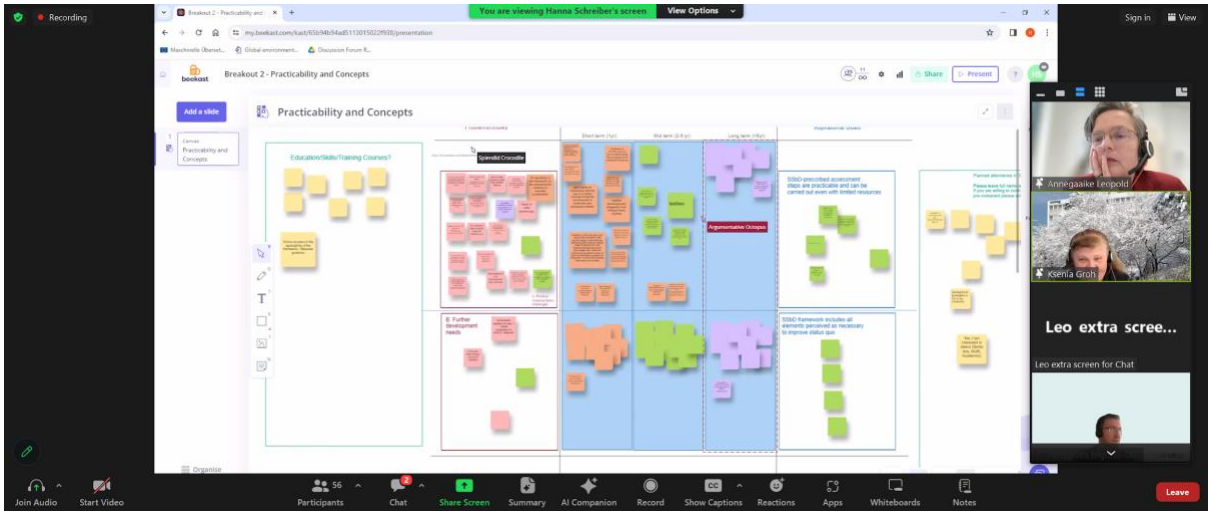
The group working on **Data-related issues** considered three pre-recognized categories of Data-related problems to be solved, that is: (a) identifying which sustainability impact categories are key for a specific SSbD case, (b) identifying problems with and solutions for existing data that are as yet not easily obtained and collated for SSbD practices, and (c) identifying problems with and solutions for bridging data gaps in safety and sustainability assessment steps.



The group activity resulted in various ideas for Education and skills (green Post Its, left), little amendments of the defined problems and aspirational goals (left and right red/blue boxes), but some clear incentives and draft-sequential stepping stones (liaised by the lines) to solve some of the problems. The groups clearly identified the need for central and accessible data sets, so that SSbD-practices are facilitated. The group identified three main comprehensive 'pathways', which would relate to (1) a systematic design of course material (teaching, skills, top encircled Post Its), (2) prescribed data formats and alike, to support easy access and use, and (3) an extensive pathway to address data gaps for safety as well as sustainability assessment, for example for Artificial Intelligence methods (especially for early-stage SSbD applications, for data-poor conditions).

Practicability & Concepts issues

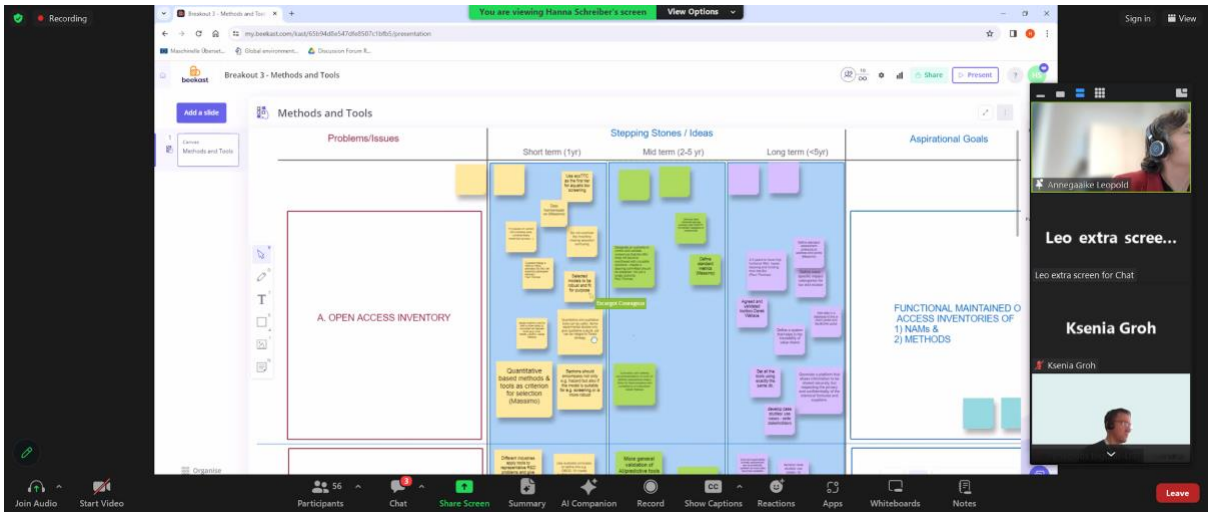
Here we see, as illustration from the breakout group on Practicability & Concepts, that participants provided their thoughts on Problems existing in the two predefined areas, along with of the Aspirational Goals and Stepping Stones.



Note: the figure is not meant to be legible. Ksenia informed that some of the issues discussed in her Breakout group seem to correspond to those discussed in other Breakouts, e.g. data handling, development of specific methods, and challenges with integration and weighing of multiple data streams and assessment outcomes. This again highlights that interdisciplinarity is key and paves the way for putting together the respective preparatory teams and discussion groups for Sevilla workshop, based on the interests indicated by the participants.

Methods & Tools

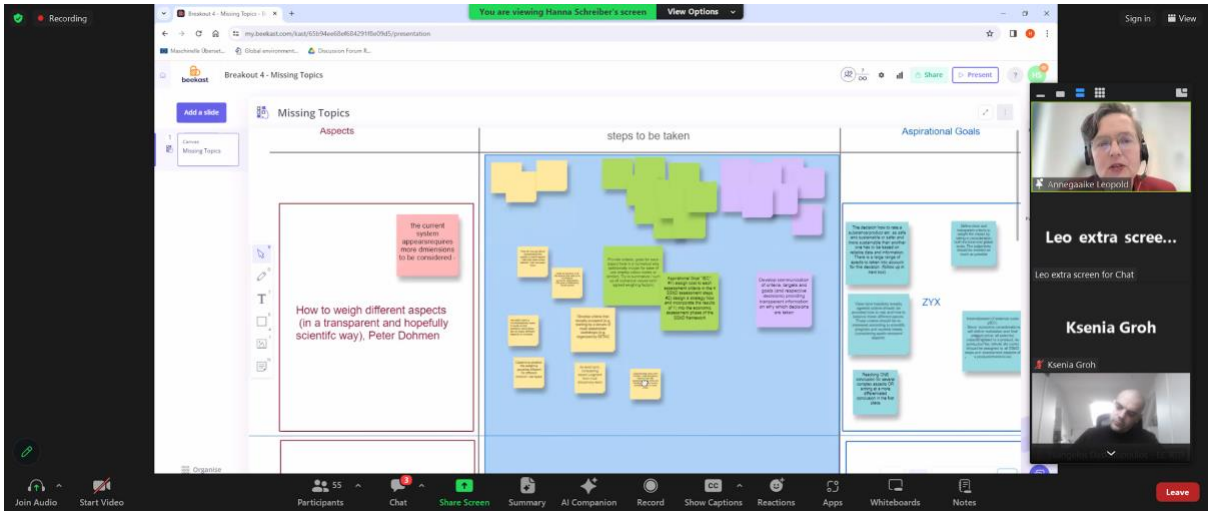
Likewise, the "Methods and Tools" group also showed an extensively loaded collection of Stepping Stones, as shown in the overview below (note: not intended to be legible).



Paul highlighted that – for example – in the third Problem Aspirations pathway discussed in this Breakout, there is a need to look at meaningful results, whereby Artificial Intelligence along with other NAMs would be combined, so that this also develops into cost-effective and useful combinations of approaches. Such AI-matters were also discussed in the Data-oriented Breakout group.

"Missing theme"= weighing in SSbD

The "Missing Theme" breakout group had different starting points, whereby the question "How to weigh the different aspects of Safety and Sustainability" introduced by an attendee received among the largest number of votes as a point of major interest. The general feeling was that indeed the subject is a highly-relevant aspect to explore in greater detail. Thereupon, the group formulated the Aspirational Goals and started identifying Stepping Stones to get there. Criteria should be formulated in advance, but there should also be readiness for improvement-adjustment when experiences come in for real-life cases.



An important Aspirational Goal would be to get a 'clear answer' for a true case, so that the net outcome of an SSbD assessment is very clear for decision making. This group did not attempt to align their thoughts along the short-medium-long term continuum but preferred to rather focus their discussion on the bigger picture: all aspects are important, and timing of efforts in research can be done later. Regarding Education & Skills, this group suggested to make sure that SSbD becomes part of educational programs at e.g. universities, so that it becomes a 'natural approach' to be followed by the next generation of environmental science professionals. Peter Dohmen, who introduced the subject finally suggested that SETAC would be a good organisation to organise the way-forward, given its tripartite structure (because interdisciplinarity "is in SETAC's genes").

Turning to the cross-cutting relevance of Education & Skills, all Breakout groups defined this as a subject for specific attention, as it is Science + Utility + Skills that eventually make SSbD operational. Various remarks were made during the breakouts, generally supporting the idea that indeed Education & Skills are key for the successful application of SSbD and all its aspects. Specifically, the plenary highlighted the need for / ideas on:

1. A need for a Definitions / Glossary across the disciplines
2. Interdisciplinarity defines a need for having people who can "bridge``, who have roots in both Safety and Sustainability assessment, due to the high degree of interdisciplinarity required in the process. These people should be identified, and asked for their help to substantiate the bridge between long-term independently-evolved scientific tracks.
3. The points above expand beyond the experts, in fact also to the more general public and decision makers.

As an overview, the set of results presented by the four co-chairs - Annegaaike concluded - showed to be a rich resource to prepare for the Seville on-site workshop. Moreover, a relevant collection of volunteers put their names on the Beekast screens, in reply to the invitation to contribute to preparing for the Seville-workshop as Volunteer.

1. All four groups were highly productive, for all aspects of the Whiteboard space
2. The raw results surely require some further 'digestion and sorting', so as to derive some clear "preliminary roadmaps" for specific Aspects of SSbD.
3. The raw results also showed to be multi-relevant, that is: some solutions were earmarked by the plenary attendees as having multiple forms of use to improve SSbD, for example, a solution for a Data Problem surely also helps the Modeling development and implementation.

There is clear latitude to study the Aspect roadmaps not per item, but also via cross-cutting linkages.

4. All attendees were informed on, and their feedbacks showed, the view that Education & Skills are indeed cross-cutting issues for SSbD.

The observation was made that the Breakout group proposed a set of wonderful ideas, marking the involvement of the attendees - in fact there were group members still working together during the 2nd plenary (and upon request they will also do so after the 2nd Cafe!)!

Further details of the Breakout group products are in the Appendix.

For sure, some work has to be done by the organisers and the volunteers, who so clearly offered their willingness to support the Seville preparations (as shown by explicit sets of names of volunteers with each Breakout group).

10. Closure and next steps

In the closing session, Annegaaike first asks feedback from Sofie Nørager. Sofie mentions that she is rather overwhelmed to see a lot of movement and ideas, and that Education & Skills was indeed mentioned multiple times. Sofie will look forward to the more detailed "digestion" of the breakout results with great interest. Annegaaike remarks from her own point of view, that today's meeting was rich, and getting results to "a next level", where >75 participants actively and innovatively contributed.

Annegaaike and Sofie thereupon expressed their sincere thanks to all attendees, for their open-minded contribution to the breakout "pressure cookers". They were impressed by the wide array of potentially important ideas, and by the group-effect of making preliminary roadmaps. Explaining on the way forward, Annegaaike once more thanks the volunteers for putting their names forward, and states that the Organising Committee and the volunteers will act to "digest" all detailed results prior to the Seville workshop.

Annegaaike thanked all attendees profusely for their creativity, SETAC for their hard work behind the screens, and the Organising Committee for all scientific and organisational matters.

The 1st and 2nd SETAC-Cafe-style Consultation Meetings on SSbD have proven to be a step-up for a potentially very effective workshop at Seville, where the results obtained so far, and novel ideas, will likely be ***shaped into the ambitious goal of the Comprehensive Roadmap for addressing current SSbD problems***.

Once more, Annegaaike and Sofie thank the Attendees for their contributions, and they point at the SETAC-office and website, as well as specific mailings, to keep each of us informed on progress to the next step.

Upon stating that, Annegaaike closes the meeting.

11. Appendix A: Results breakout "Data and Data methods"

This breakout group was co-chaired by Leo Posthuma (RIVM; SETAC-SB member) and Christoph Schür (Eawag).

Introduction

SSbD is a concept that asks for assessments to be made under data-poor conditions, given the fact that novel chemicals and products are to be evaluated at an early Technological Readiness Level (TRL). This has practical consequences for the issue of obtaining and using data. On the basis of the results of the 1st Consultation meeting, and reported findings of SSbD-case studies and development processes, this Breakout focused on three Problems with their corresponding Aspirational Solutions, that were pre-defined as input for the 2nd Consultation:

1. **Problem 1** concerns clarity on what data are necessary to perform an assessment. This is less of a challenge for safety, but varies widely depending on the object of a sustainability assessment. Here, a clear framework to prioritise aspects of a sustainability assessment, and thus the needed data, for a specific object group is needed. As a solution, effective SSbD asks for easily-obtainable data sets that can – moreover – be combined smoothly, fruitfully and validly, for both safety and sustainability assessments.
2. **Problem 2** concerns process aspects of obtaining and re-using *existing data*, whereby formalities (rather than scientific problems) imply limitations to get, use, re-use or extract data from format-wise "unfriendly" sources. Evidently, a relevant aspect is proprietary information that was financed by one company which consequently wants to prevent its use by another. As a solution, we seek for any process that removes barriers for the re-use of existing data without violating economic laws. Another way to look at this is to work towards all necessary data to be aligned with the FAIR principle (Findable, Accessible, Interoperable, Reusable).
3. **Problem 3** concerns *missing data and how to bridge* data gaps, especially for data-poor, lower TRL-situations, for both safety and sustainability assessments. The aspirational solution would be here to have reliable and validated methods that are easily usable and indeed bridge existing data gaps.

Approach

The breakout group started with an introduction, followed by transferral to a Beekast Canvas with empty post-its. The canvas was prepared following the principles of Phaal et al. (2011) and featured on the vertical axis the major Problems identified (left) and associated Aspirational Goals (right). In the beginning of the Beekast work session, attendees were asked to make a "brain dump" to identify potential Stepping Stones that could allow bridging from identified Problems to their respective Aspirational Goals, i.e., what will be reached when these problems are solved. Stepping Stones are defined as science-based innovations, through which (if needed in a stepwise manner) the current Problem's status can be moved toward the aspired Solution, or, Aspirational Goal. The attendees positioned their ideas, thus, as stepping stones for all of the identified Problems/Goals. They were also allowed to refine the Problem and Aspirational Goal definitions, and were, moreover, asked to provide their thoughts on SSbD education and training needs, as well as indicated their interest and availability to attend the workshop in Seville as well as assist in its preparation.

Results - overview

The Breakout group generated 42 stepping stones. An impression of the results positioned on the Canvas is shown in Figure 1.

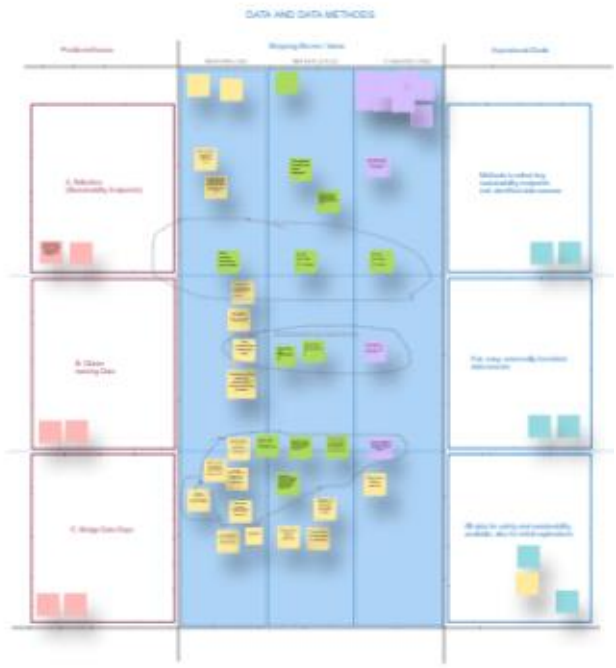


Figure 1. Overview of the Canvas-results of the Breakout group on Data and Data Methods, showing that there were numerous stepping stones generated for all three problem-goal pathways. The figure is not meant to be readable. Top to bottom: the three Problem/Aspirational Goal aspects. Left to right: (White) Problems (Blue) short/middle/long-term stepping stones for scientific development (white) Aspirational goals.

Results - detailed

The set of results concerns various aspects of Problem 1: Existing data that need to be obtained and combined in order to execute scientifically sound SSbD analyses, based on available/existing/combined data.

This problem was further subdivided into some more detailed categories, with two slightly different aspects of the problem definition and suggestions for improvements/stepping stones (see results shown in the next table).

Current problem	Aspirational Goal	Timeline	Redacted content
1_Data flows unclear or badly organised	1_SSbD AND DATA & SCIENCE	(0) NA	Proposal to improce the understanding of limitations for both Prediction and Measurement tools and techniques
		(1) short	Proposal to combine data of different souces (repositiries, monitoring)
			Proposal to define criteria for data quality (safety and sustainability)
			Proposal to make data FAIR and make data flow processes (Data provenance, also known as data lineage, is a form of metadata that captures the history of data, detailing its origins, transformations, and journey through various processes.)
			Proposal to mimic EUCLID for safety and sustainability data
		(3) long	Porposal to create scientific data quality evaluation of documentation standards
2_Existing data not traceable or useful	2_SSbD AND DATA PROCESSES	(1) short	Proposal to develop approach(es) to compile relevant data sets
			Proposal to make clear rules to collect existing data
			Proposal to make data FAIR (Data provenance, also known as data lineage, is a form of metadata that captures the history of data, detailing its origins, transformations, and journey through various processes.)
			Proposal to organize consortium for data sharing
			Proposal to standardize FAIR data reporting for chemical data submissions (safety and sustainability)
		(2) medium	Proposal to harmonize data documentation

Next, a specific set of suggestions was provided for scientific methods to bridge data gaps, via the application of Artificial Intelligence methods. The associated results are in the Table below. The attendees hinted clearly at the opportunities to develop, and make user-friendly, methods that employ Machine Learning techniques for bridging data gaps. Regarding the scientific underpinning of urgently needed solutions, the table below might be amongst the most important set of suggestions, which have not been handled in full depth so far (due to the limited time during the 2nd Consultation meeting).

Current problem	Aspirational Goal	Timeline	Redacted content
3_Need to bridge data gaps	3_SSbD, DATA AND ARTIFICIAL INTELLIGENCE	(1) short	Proposal to design principles for the use of Artificial Intelligence for Safet and Sustainability
			Proposal to identify database resources for Artificial Intelligence in Safety and Sustainability
		(2) medium	Proposal to execute trial studies for the application of Artificial Intelligence to bridge Chemical Safety data gaps
			Proposal to execute trial studies for the application of Artificial Intelligence to bridge Sustainability metrics data gaps
			Proposal to execute validation studies of data generated by Artificial Intelligence methods
			Proposal to improve scientific data sources for Artificial Intelligence modeling
Grand Total			

If one proceeds through an SSbD assessment process, this yields a diverse set of outcomes (including data) that need to be interpreted. This forward-looking aspect was covered by various attendees, with results as shown below:

Current problem	Aspirational Goal	Timeline	Redacted content
4_Need to focus sustainability assessment	4_SUSTAINABILITY-KEY IMPACT Categories	(1) short	Proposal to develop methods to identify priority Impact Categories for Sustainability Assessment step
		(2) medium	Proposal to trial methods to identify priorityl Impact categories for Sustainability Assessment step
		(3) long	Proposal to make an operational guidence to help identifying priority Impact Categories in Sustainability Assessment step
5_Need to integrate SSbD output	5_SSbD_FINAL INTEGRATION	(2) medium	Proposal to develop weights or another methods to deal with trade-offs among environmental issues
Grand Total			

Thinking ‘outside the box’ also generated some interesting outputs, whereby attendees reminded each other that it may be very helpful to generate showcase-data and SSbD-outputs, to serve as example for future SSbD designs, thereby including standards for often-to-be-evaluated base chemicals.

Current problem	Aspirational Goal	Timeline	Redacted content
6_SSbD utility can improve generally	6_DATA-MISCELLANEOUS IDEAS	(1) short	Proposal to define documents that resemble Product Category Rules for basic chemicals and materials
		(2) medium	Proposal to develop and publish SSbD steps and outcomes for "model substances" as basis for other SSbD analyses
			Proposal to encourage Open Access publishing on SSbD analyses of novel compounds
			Proposal to publish open and free LCA-profiles for basic chemicals to be reused in SSbD assessments
Grand Total			

One of the subjects of every breakout was also: Education and Skills for SSbD. This triggered some input, with key indications that (a) there is a need for a systematic design of training steps, based especially on (b) a bridging of the historical divergence between safety and sustainability assessments. This repeatedly was pointed out to, for example, manifest in differing use of specific vocabulary. Suggestions were made as follows:

Current problem	Aspirational Goal	Timeline	Redacted content
7_Insufficient combined Safety and Sustainability expertise and skills	7_EDUCATION AND SKILLS: IMPROVING SSbD BY PROPER TRAINING	(0) NA	Proposal for SSbD courses (1): introductory and pinciples
			Proposal for SSbD courses (4) Statistical analysis and interpretation of results and errors (Confidence intervals, error proppigation)
			Training/ guidance on LCA data sharing standards
		(1) short	Proposal for SSbD courses (1): introductory and pinciples
		(2) medium	Proposal for SSbD courses (2): cases
		(3) long	Proposal for SSbD courses (3) tools
		(blank)	Proposal for SSbD courses (4) integration and interpretation

The breakout finally yielded also some further suggestions in the form of miscellaneous problems identified, that could be taken up (if applicable and feasible) in the Seville workshop in any of the pertinent groups there:

Current problem	Aspirational Goal	Timeline	Redacted content
8_Miscellaneous problems	8_DATA-MISCELLANEOUS REMARKS	(0) NA	Proposal to better define safety endpoints and their assessment
			Proposal to evaluate published SSbD cases to verify logical interpretations, and avoid under- or over-interpretation and wrong decisions (leanr by doing)

A further take-away was that data problems cannot be addressed independently of the methods and models which these data are to be used for. These two topical groups are closely intertwined and need to be addressed in an integrative way.

12. Appendix B: Results breakout “Practicability and Concepts”

This breakout group was co-chaired by Ksenia Groh (Eawag; SETAC-SB member), Serenella Sala (EC, JRC - Joint Research Centre) and Evangelos Daskalopoulos (EC, DG RTD - Research & Innovation).

Introduction

During the 1st Consultation, attendees identified several challenges related to the practical implementation of the SSbD framework. These referred to, for example, the overall complexity of the SSbD assessment schemes, resulting in extensive demands for different types of expertise and high degree of interdisciplinarity; lack of agreement on some operational aspects, such as criteria, thresholds or sequence of assessment steps, etc.; as well as limitations related to the lack of necessary tools, experience, training or resources. In addition, several conceptual needs for further developing or amending the SSbD framework were highlighted, e.g., developing approaches for handling the mixture toxicity issue, for assessing multi-component substances or for dealing with trade-offs, etc. While these issues are quite diverse and many require availability of subject experts to move forward with solutions, the aim of this breakout was to first identify the specific Problem(s) that this particular group of people wants to work on, and only then move to discussing the respective Aspirational Goals and Stepping Stones, if time allows. In addition, participants were asked to suggest SSbD education/training needs, as well as to identify their interest to participate in the Sevilla workshop and assist in its preparation.

Approach

The breakout group started with an introduction, followed by transferral to a Beekast Canvas with empty post-its. The canvas was prepared following the principles of Phaal et al. (2011) and featured on the vertical axis the two focus areas for this group, namely “A. Practical implementation challenges” and “B. Further development needs”. Participants were invited to add post-its describing the Problems they see in the respective focus areas, followed by identification of respective Aspirational Goals as well as short-, mid- and long-term Stepping Stones on the way toward solutions. Simultaneously, a discussion on the already-added input was started, leading to further clarification of the arguments as well as identification and addition of further Stepping Stones. Due to the limited time, the process of arranging individual paths from Problem to Goals through specific Stepping Stones could not be finalised during the breakout running time. The collected ideas were later evaluated, categorised and sorted into groups, in order to identify useful material that could be channelled toward further work in Seville. Main results are presented below.

Results - overview

This breakout group received in total 53 inputs. An impression of the results positioned on the Beekast Canvas is shown below.

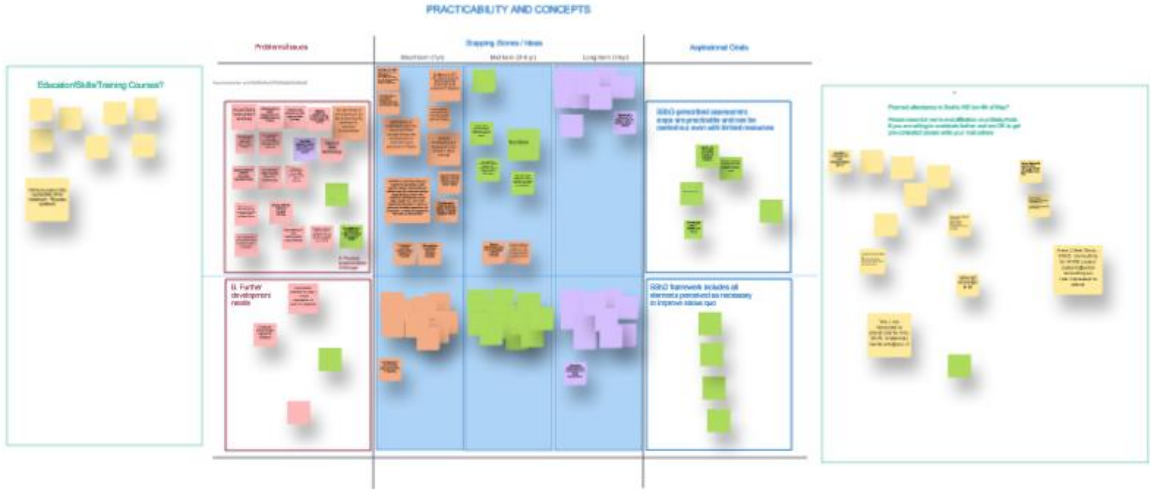


Figure. Overview of the Canvas results of the breakout group on Practicability and Concepts, showing that most inputs were generated in the upper problem-goal area, while much less notes were placed in the lower problem-goal area. The figure is not meant to be readable. Top to bottom: the two Problem/Goal aspects. Left to right: (White) Education/Skills ⇒ (White) Problems space (Blue) space to record short/middle/long-term stepping stones for scientific development (White) Aspirational goals space ⇒ (White) Volunteers capturing space

Results - detailed

To evaluate the received content, individual inputs were reviewed and assigned to different categories, which enabled their grouping and allowed building some provisional pathways linking specific Problems with associated Goals and Stepping Stones, where available. This evaluation revealed that many discussions held in this group were closely related to the topics handled in other groups, e.g., data, methods, or integration approaches. This is understandable, given the close interconnection of concepts with the subjects they are handling, such as e.g. collection and interpretation of data. Several more specific topics were also proposed by some participants, such as the need for developing SSbD guidelines / criteria in support of SSbD application in molecular design.

The excerpts presented below provide insights into received inputs. These inputs are grouped according to overarching categories identified, and placed in a sequence moving from Problem to Stepping Stones to Aspirational Goal(s) for specific subtopics, where available and whenever it was possible to assume association based on the input originally provided by the participants. (Note that it is possible that the proposed grouping does not fully correspond to the original idea that a specific participant had in mind when providing that input.)

Topic: Data and digitalization

Redacted Content	Roadmap element
differentiation of SSbD assessment info available data set	Problem
no common data sharing base	Problem
Automation needed for step 1 - Avoid duplication of work	Problem
Centralised dashboard-portal to upload results of SSbD assessments	Stepping Stone
Computer aided design approach validated	Problem
The digitalization is there as an enabler for making the evaluation simpler	Problem
Conceptual re-use of results and assessment	Stepping Stone
Development of automated streamlined tools for different steps	Stepping Stone

Topic: Handling many disciplines

Redacted Content	Roadmap element
large number off different disciplines require	Problem
Several different expertise required	Problem
Map the required expertise info the different steps of SSD	Stepping Stone
To overcome the multidisciplinary aspect develop the concept of a SSbD integrator	Stepping Stone
Multidisciplinary collaboration and this cafe is a really good way to start discussions	Stepping Stone

Topic: Methods/Tools – Implementation and Integration

Redacted Content	Roadmap element
Find appropriate best practices that fit for different sectors and industries	Problem
how to implement safety and sustainability assessment together from the phase 1	Problem
Weighting of different steps (hazardous substance used in a controlled way leading to more sustainable result)	Problem
No specificity of the framework on assessing the methods to evaluate 'sustainability'	Problem
step by step process on the case studies	Problem
Best practices from different fields are described	Stepping Stone
Training: Practitioners can derive from best practices how their process/product/service can be more sustainable	Stepping Stone
Need for overarching methods covering several regulations	Problem
method development and integration from different fields	Stepping Stone
No consensus on boundaries for each assessment; possible subjective options	Problem
Guidance on EC/JRC level on how to define/divide the processes to be assessed	Stepping Stone
Aspirational Goal: One flexible tool for all	Asp. Goal
SSbD is implemented	Asp. Goal

Topic: Methods/Tools – Specifics

Redacted Content	Roadmap element
Effect data needed at a very early stage in the process: lack of validated methods	Problem
The SSbD evaluation should be possible on a multi component product	Problem
Boundaries of LCA (downstream use)	Problem
Improve the in silica tools for hazard, exposure, process design, etc.	Stepping Stone
Develop a fit-for-purpose approach related to the TRL level of the development	Stepping Stone
Develop SSbD assessment capacity building on available capacity for tools used in SSbD	Stepping Stone
Develop SSbD toolbox	Problem

Topic: Molecular design in SSbD

Redacted Content	Roadmap element
How to use SSbD criteria for molecular design (early innovation of chemicals, in academia chemistry and material sciences)	Problem
gain hands on experience with the use of SSbD concept during the development of molecules and processes	Stepping Stone
explore the potential to add specific design criteria addressing the molecular design stage (more bridging more with early-stage chemical development); the criteria are should clarify which chemical properties are desirable and which need to be avoided	Stepping Stone
SSbD is an actionable concept for academic chemists	Aspir. Goal
SSbD is an actionable concept for industrial chemists involved in product/process design	Aspir. Goal

Topic: Terminology issue and education needs

Redacted Content	Roadmap element
Need of clear terminology	Problem
Roundtables/interactive workshops can help to have a comprehension of terminologies differently used by different expertise (e.g., use, function, endpoint, intermediate)	Stepping Stone
No common understanding of sustainability (environmental, social, economical)	Problem
A consensus common understanding is agreed upon	Stepping Stone
Training: Stakeholders know how sustainability is defined	Stepping Stone
Mainstream SSbD thinking/skills in chemistry/material sciences, integration in curricula	Stepping Stone
Online courses on the applicability of the SSbD framework - Stepwise guidance	Stepping Stone

13. Appendix C: Results breakout "Methods and Tools"

This breakout group was co-chaired by Hans Sanderson (Aarhus University; SETAC-SB member) and Paul Thomas (KREATiS, SETAC-SB member).

Introduction

In the first Consultation meeting 65 remarks were made on Tools and Models. New regulatory needs yield new data needs which yields new methods and tools needs. We identified challenges regarding lacking data due to lacking methods. In preparing for the 2nd Consultation meeting, several problems that are experienced were identified. In this breakout group several themes were addressed relating to methods and tools required to effectively develop SSbD materials.

Approach

An approach similar to that described above was used.

Results - overview.

A: Open Access Inventory

Three main steps are envisaged chronologically but also as a tired approach to allow the process to be handled in a methodological way.

Step 1. Short term, precursor methodology: Develop case studies/ use cases - wide stakeholders. One can use ecoTTC as a very first tier for aquatic tox screening with minimum data. Add data in a database to the e-chem portal and the ECHA portal.

Step 2. Medium term: Develop a single location (can be link to other sites) to document all relevant tools (e.g. LCA, NAMs, QSAR) to support quantitative based methods & tools as criterion for selection. Fix expected issues of current DB (missing data, confidentiality, restricted access...). Define the standard metrics that are needed. Develop data consortia among industry see REACH for similar categories of compounds. The data base should also include evaluation and ranking (recommendation) of tools for defined assessment steps to drive for harmonisation and consistency in evaluation. The database platform should allow information to be shared securely, but respecting the privacy and confidentiality of the chemical formulas and suppliers.

Step 3. Longer term, more complex: Define the standard metrics needed. Within 2-3 years establish a fully functional Wiki: needs backing and funding from the EU. Designate an authority to control and validate content (so that the Wiki does not become overflowed with unusable solutions - maybe a steering committee should be assigned, not just a single authority. The system should help in the traceability of value chains.

B: DEFINE APPLICABILITY DOMAIN/RELIABILITY OF TOOLS

Three main steps are envisaged chronologically but also as a tired approach to allow the process to be handled in a methodological way. The first initial stepping stones to set up a stronger base to increase the use of NAMs in SSbD would be:

Step 1. Short term, precursor methodology: Inventorise what is already available and what isn't. Reassess the fitness of purpose of the tools to deliver SSbd requirements.

Identify specific gaps/endpoints in tools with a broad range of stakeholders. Verify they answer the questions posed under SSbD. Develop/fund development of tools that can deliver the outcome we want based on the data currently available. Don't reinvent the wheel. Consider targeted research to fill data gaps to complete limitations in existing tools.

Consider using combinations of NAMs to strengthen confidence and predictive outcomes and to confirm their reliability. Create case studies to challenge and help develop confidence in the tools.

Step 2. Medium term: Create stronger alignment between authorities e.g. EFSA, ECHA, US EPA should be developed for NAMS, QSAR and prospective LCA without compromising the contributions proposed by private enterprise. For example for QSARs, Good Modelling Practice could be set up (along the lines of GLP) with accredited producers thus harmonising regulatory requirements between experimental and in silico laboratories.

Broaden defined approaches to make them appropriate based on a knowledge of current tools and their likely short term future development.

Step 3. Longer term, more complex: Widen scope of QAF to make it a better tool for estimation of hazards and open up weight of evidence approaches. Use available principles to define this e.g. OECD. Or create guiding principles when absent.

We will need to develop AI tools - and to ensure their integrity and accuracy avoiding error. These can be integrated into a new, more complex assessment framework.

C: Higher Throughput Methodologies

Step 1. Short term, precursor methodology: Need data harmonization as well as global collaboration – not only EU based tools. We need to use NAMs in a WoE approach and demonstrate in general in case studies. These should be based on tiered approaches. Ideally we can develop more powerful algorithms that may address multiple KPIs in the use of AI in ascertaining the suitability of AI tools for optimizing chemical and material design from safety and sustainability perspective, validation of new methods using AI and data science to manage input data into models. Tiered strategies IATAs should be assessed. Quick screening tools for e.g. raw material selection in substitution cases for design phase. Substitution phase: also technical performance and functionality models outputs may be integrated. Downscaled experimental hazard assessment methods could be developed such that they are consistent with simulation study outcomes.

14. Appendix D: Results breakout “Weighing”

This breakout group was co-chaired by Annegaaike Leopold (AFFILIATION; SETAC-SB member) and Michelle Bloor (AFFILIATION, SETAC-SB member).

Overview: relevancy of the prioritized theme

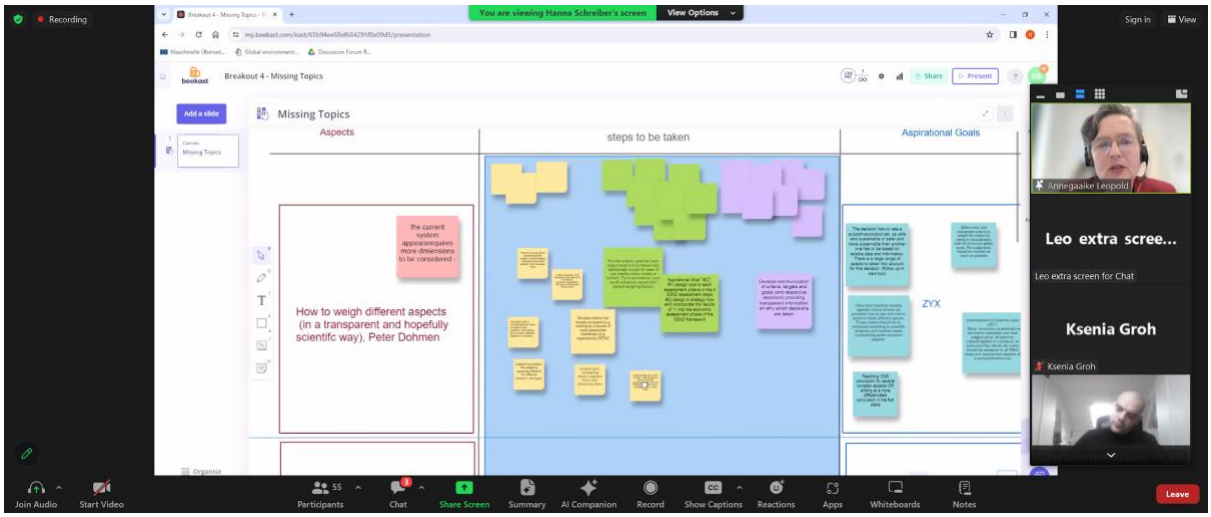
As stated earlier, the Organising Committee wanted to keep ample room for suggestions by the Attendees to pay attention to a specific Aspect of high interest. As working title, this was the “Missing theme”. But they had a different starting point for their group, whereby the question “*How to weigh the different aspects of Safety and Sustainability*” introduced by an attendee of the 1st Plenary was the highest-voted Aspect of SSbD that would ask for attention in one of today’s Breakout groups. The general feeling was that indeed the subject is a highly relevant aspect to explore in greater detail.

On goals

As starter, the group formulated the Aspirational Goals and started identifying key problems and their potential science-based solutions.

On solution pathways

This yielded a set of well-formulated, and thus inviting “Stepping Stones” to get to the aspired results, which were also defined in a highly-specific way. In fact, whereas the Data-group had three pre-identified major Aspects (problem types), the present group was able to identify multiple layers, of increasing proximity to the final communication of “the” SSbD outcome for a case. That is, the group identified Aspects such as (a) What constitutes a good SSbD approach, (b) the added subject of the Economics of an SSbD assessment, (c) the identification of the key drivers of non-sustainability as key SSbD metrics, (d) criteria for each of the separate impact categories of the SSbD, and the (e) weighting and (f) summary communication of the final outputs of an assessment. Criteria should be formulated in advance, but there should also be also readiness for improvement-adjustment when experiences come in for real-life true cases.



An important very high Aspirational Goal (reflecting the last point) would be to get a ‘clear answer’ for a true case, so that the net outcome of an SSbD assessment is very clear for decision making.

This group did not attempt to align their thoughts along the axis of short-medium-long terms of research and implementation, as they focused their discussion on the bigger picture: all aspects are important, and timing can be done later.

On Education and skills

Regarding Education & Skills, this group suggested that the idea is to make sure that SSbD becomes a core part of educational programs at e.g. universities, but also of current professionals, so that it becomes a 'natural approach' to be followed by the next generation of environmental science professionals. The attendee who introduced the subject of this Breakout group finally suggested that SETAC would be a good organisation to organise the way-forward on the matters of the whole collaborative action of SETAC and EC, given its the tripartite organisation structure (because interdisciplinarity "is in SETAC's genes").

15. References

Phaal, R., E. O'Sullivan, M. Routley, S. Ford and D. Probert (2011). "A framework for mapping industrial emergence." Technological Forecasting and Social Change **78**(2): 217-230

SETAC/EC: Preliminary report of the 1st Consultation meeting: file:///N:/Documents/Downloads/20231208Preliminary-report-of-the-1st-SSbD-Consultation-meetingreported-to-EC-final-005.pdf