DISCUSSION SESSION

Group 1: Policy need

Chair: Solvår Hardeng

Possible themes

1. How should screening exercises address needs for data in international conventions?
2. Should national policy needs, e.g. national priority lists, be addressed with screening exercises?
3. Are some conventions more important than others when it comes to need for and reporting of screening data?
4. What type of screening data is most useful in convention work (matrix, geography etc)?
5. How can policy makers use networking (e.g. Norman) in their work?
6. Are results for certain matrices more valuable than others? If yes, which ones?

Group 2: Substance selection

Chair: Eva Brorstrøm-Lundén

Possible themes

1. What data-sources are available for information on screening candidates?
2. Could there be instances where uncertainties introduces during any one or more of the steps in the chain of events in going from sample selection to analytical analyses could lead to the deselection of a candidate substance?
3. What substance would you select for screening if you were to choose?

Group 3: Networking

Chair : Bernd Gawlik

1. How can policy makers use networking (e.g. Norman) in their work?

Group 4: Modelling/selection

Chair: Michael McLachlan

1. What are the requirements for optimizing the prioritization of candidates for screening based on modelling?
2. Which compounds would be prioritized for screening if the selection is based on modelling?
3. What is the difference between the list prioritized for screening in the work of McLachlan compared to others, like Muir and Howard, 2006 and Brown and Wania, 2008?
4. Discuss the suggestion by Zhang et al. 2010.

Derek C. G. Muir*‡ and Philip H. Howard§ Are There Other Persistent Organic Pollutants? A Challenge for Environmental Chemists[1] *Environ. Sci. Technol.*, **2006**, *40* (23), pp 7157-7166

TABLE 2. Top 30 Bioaccumulative and Persistent Substances Based on Data Assembled for the Environment Canada DSL Categorization[a]

no.	chemical name	CAS no.	log K_{ow}	Log BCF[b]	log BCF[c]	degradation[d] $t_{1/2}$ (d)	media[e]	production volume[f]
1	[1,1'-biphenyl]-4,4'-diamine, *N,N'*-bis(2,4-dinitrophenyl)-3,3'-dimethoxy-	29398967	6.94	4.74	4.65	182	W	LPVC
2	benzenamine, 4,4 -[(1-methyl-ethylidene)bis(4,1-phenyleneoxy)]bis-	13080869	6.88	4.76	4.60	182	S	TSCA
3	1-naphthalenemethanol, α,α-bis[4-(dimethylamino)phenyl]-4-(phenylamino)-	6786830	7.21	4.63	4.52	182	W	LPVC
4	1-octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-	24448097	7.29	4.59	4.42	182	A	HPV
5	spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(diethylamino)-	509342	6.63	4.82	4.41	182	S	LPVC
6	spiro[isobenzofuran-1(3H),9 -[9H]xanthen]-3-one, 6 -(diethylamino)-3 -methyl-2 -(phenylamino)-	29512490	7.32	4.57	4.38	182	S	HPV
7	peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)	25155253	7.34	4.56	4.35	182	S	HPV
8	peroxide, (1,1,4,4-tetramethyl-1,4-butanediyl)bis[(1,1-dimethylethyl)	78637	6.55	4.82	4.35	182	AS	HPV
9	anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone, 2,9-bis(3,5-dimethylphenyl)-	4948156	7.36	4.54	4.31	182	W	LPVC
10	anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone, 2,9-bis(4-chlorophenyl)-	2379773	6.46	4.83	4.28	182	W	LPVC
11	spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2',4',5',7'-tetrabromo-3',6'-dihydroxy-	15086949	6.91	4.75	4.22	182	S	LPVC
12	1,4-benzenediamine, *N,N* -di-2-naphthalenyl-	93469	6.39	4.83	4.22	60	W	LPVC
13	cyclohexasiloxane, dodecamethyl- (D6)	540976	6.33	4.83	4.17	60	A	LPVC
14	perylo[3,4-cd:9,10-c'd']dipyran-1,3,8,10-tetrone	128698	6.26	4.82	4.12	182	S	LPVC
15	1-naphthalenepropanol, α-ethenyldecahydro-2-hydroxy-	515037	6.00	4.78	3.92	182	S	

TABLE 3. Top 30 Persistent and Bioaccumulative Substances with long Range Atmospheric Transport Potential Based on Data Assembled for the Environment Canada DSL Categorization

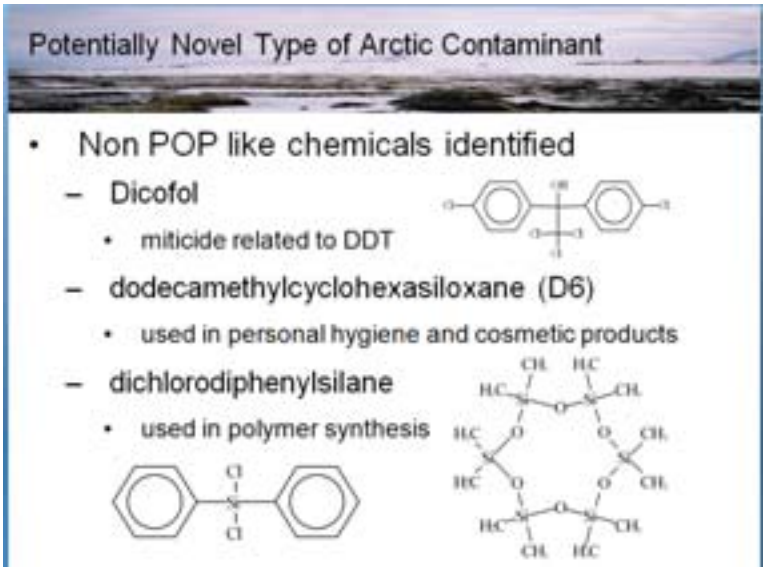
no.	chemical name	CAS no.	degradation[a] $t_{1/2}$ (d)	AO[b] $t_{1/2}$ (d)	Log BCF[c]	log K_{ow}[d]	production volume[e]
1	1,3-isobenzofurandione, 4,5,6,7-tetrachloro-	117088	182	338.4	3.9	−4.1	HPV
2	benzenethiol, pentachloro-	133493	182	76.7	4.7	−2.3	HPV
3	benzene, 1,1 -oxybis-, hexabromo deriv. (hexaBDE)	36483600	182	30.4	3.6	−4.7	TSCA
4	1,3-cyclopentadiene, 1,2,3,4,5,5-hexachloro- (HCCP)	77474	182	27.2	3.9	−1.1	HPV
5	benzene, 1,3,5-tribromo-	626391	60	22.0	3.9	−1.9	LPVC
6	benzene, 1,1 -oxybis-, pentabromo deriv. (pentaBDE)	32534819	182	19.4	4.4	−4.3	HPV
7	cyclohexane, tribromotrichloro-	30554735	60	16.9	3.8	−3.4	
8	cyclohexane, tetrabromodichloro-	30554724	60	16.4	3.9	−3.9	
9	cyclohexane, 1,2,3,4,5-pentabromo-6-chloro-	87843	60	15.7	4.0	−4.4	TSCA
10	benzene, 1,3-diiodo-	626006	37.5	12.6	3.6	−1.9	
11	sulfonium, triphenyl-, chloride	4270706	37.5	8.6	4.6	−4.2	
12	benzene, 1-(1,1-dimethylethyl)-3,4,5-trimethyl-2,6-dinitro-	145391	60	7.3	4.4	−4.9	
13	benzene, 1,3,5-tribromo-2-methoxy-4-methyl-	41424366	60	7.2	4.4	−3.0	
14	benzene, 1,1-oxybis-, tetrabromo deriv.	40088479	182	7.1	4.8	−3.9	
15	peroxide, bis(2,4-dichlorobenzoyl)	133142	182	6.1	4.8	−4.4	TSCA
16	benzene, 1,2,3,4-tetrachloro-5,6-dimethoxy-	944616	182	4.4	4.1	−3.6	
17	peroxide, bis(4-chlorobenzoyl)	94177	60	4.3	4.0	−4.1	
18	butanoic acid, 3,3-bis[(1,1-dimethylethyl)dioxy]-, ethyl ester	55794202	60	3.4	4.2	−4.1	TSCA
19	1,1-biphenyl, 4-bromo-	92660	37.5	3.1	3.9	−2.2	
20	silane, dichlorodiphenyl-	80104	37.5	2.7	4.3	−2.5	HPV
21	benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethyl]-	53190	182	2.5	4.7	−2.8	
22	naphthalene, dichloro-	28699889	37.5	2.4	3.8	−1.9	
23	cyclotetrasiloxane, 2,2,4,6,6,8-hexamethyl-4,8-diphenyl-, cis-	33204761	37.5	2.2	4.4	−1.9	
24	cyclohexane, 1,2-dibromo-4-(1,2-dibromoethyl)-	3322938	37.5	2.2	4.4	−2.8	TSCA
25	cyclododecane, 1,2,5,6,9,10-hexabromo- (HBCD)	3194556	60	2.1	4.3	−4.2	HPV
26	benzenemethanol,α-(trichloromethyl)-, propanoate	31643148	60	2.0	3.66	−4.4	

Abstract

The past 5 years have seen some major successes in terms of global measurement and regulation of persistent, bioaccumulative, and toxic (PB&T) chemicals and persistent organic pollutants

(POPs). The Stockholm Convention, a global agreement on POPs, came into force in 2004. There has been a major expansion of measurements and risk assessments of new chemical contaminants in the global environment, particularly brominated diphenyl ethers and perfluorinated alkyl acids. However, the list of chemicals measured represents only a small fraction of the approximately 30,000 chemicals widely used in commerce (>1 t/y). The vast majority of existing and new chemical substances in commerce are not monitored in environmental media. Assessment and screening of thousands of existing chemicals in commerce in the United States, Europe, and Canada have yielded lists of potentially persistent and bioaccumulative chemicals. Here we review recent screening and categorization studies of chemicals in commerce and address the question of whether there is now sufficient information to permit a broader array of chemicals to be determined in environmental matrices. For example, Environment Canada's recent categorization of the Domestic (existing) Substances list, using a wide array of quantitative structure activity relationships for PB&T characteristics, has identified about 5.5% of 11,317 substances as meeting P & B criteria. Using data from the Environment Canada categorization, we have listed, for discussion purposes, 30 chemicals with high predicted bioconcentration and low rate of biodegradation and 28 with long range atmospheric transport potential based on predicted atmospheric oxidation half-lives >2 days and log air−water partition coefficients ≥5 and ≤1. These chemicals are a diverse group including halogenated organics, cyclic siloxanes, and substituted aromatics. Some of these chemicals and their transformation products may be candidates for future environmental monitoring. However, to improve these predictions data on emissions from end use are needed to refine environmental fate predictions, and analytical methods may need to be developed.

Brown and Wania SETAC 2008;



www.utsc.utoronto.ca/~**wania**/.../**Brown**%20and%20**Wania**%20SETAC%20Platform%20Presentation

Xianming Zhang[a, b], **Trevor N. Brown**[a, b], **Frank Wania**[a, b], , **Eldbjørg S. Heimstad**[c] **and Kai-Uwe Goss**[d]:
Assessment of chemical screening outcomes based on different partitioning property estimation methods
(Available online 6 May 2010). Env. Int. 23

Abstract

Screening is widely used to prioritize chemicals according to their potential environmental hazard, as expressed in the attributes of persistence, bioaccumulation (B), toxicity and long range transport potential (LRTP). Many screening approaches for B and LRTP rely on the categorization of chemicals based on a comparison of their equilibrium partition coefficients between octanol and water (K_{OW}), air and water (K_{AW}) and octanol and air (K_{OA}) with a threshold value. As experimental values of the properties are mostly unavailable for the large number of chemicals being screened, the use of quantitative structure–property relationships (QSPRs) and other computational chemistry methods becomes indispensable. Predictions by different methods often deviate considerably, and flawed predictions may lead to false positive/negative categorizations. We predicted the partitioning properties of 529 chemicals, culled from previous prioritization efforts, using the four prediction methods EPI Suite, SPARC, COSMOtherm, and ABSOLV. The four sets of predictions were used to screen the chemicals against various LRTP and B criteria. Screening results based on the four methods were consistent for only ~ 70% of the chemicals. To further assess whether the means of estimating environmental phase partitioning has an impact, a subset of 110 chemicals was screened for elevated arctic contamination potential based on single-parameter and poly-parameter linear free energy relationships respectively. Different categorizations were observed for 5 out of 110 chemicals. Screening and categorization methods that rely on a decision whether a chemical's predicted property falls on either side of a threshold are likely to lead to a significant number of false positive/negative outcomes. **We therefore suggest that screening should rather be based on numerical hazard or risk estimates that acknowledge and explicitly take into account the uncertainties of predicted properties.**

Notes from the group discussions

POLICY NEED AND NETWORKING GROUP

Chair: Solvår Hardeng

Rapporteur. Bernd Gawlik

How should screening exercise address needs for data in international conventions?

- What types of substance are included in the conventions?
- Screening helps to enlarge the list of substances to look at. This is not a purely static process.
- Should the screening be more targeted from the beginning?
- Need for a methodology to decide on substances to be screened?
- Do you want to change something as it is done now?
- Screening are producing arguments necessary to introduce it into continuous monitoring, e.g. Stockholm Convention.
- Scope of data by screening is to identify new topics, which eventually are confirmed/not confirmed by others → importance of networking.
- Early-alert system to produce candidate substances.
- Other application is in the EU-Policy Context: WFD/REACH
    - In WFD a safety net function by screening.
    - Need for measured concentration in order to confirm/adjust PEC in the REACH process.
    - Screening as a decisional tool to refine the risk assessment.

CONCLUSION: Screening helps to enlarge the list of substances to look at. This is not a purely static process. Screening are producing arguments necessary to introduce it into continuous monitoring, e.g. Stockholm Convention. It forms an early-alert system to produce candidate substances. Other application is in the EU-Policy Context: WFD/REACH: In the WFD screenig offers a safety net function In the REACH Process there is a need for measured concentration in order to confirm/adjust PEC in the REACH process.Screening as a decisional tool to refine the risk assessment.

Should national policy needs be addressed with screening (context of candidate priority lists for various purposes).

CONCLUSION: Yes, this is important to draft candidate priority lists (Example of river basin specific pollutants). This is important also for in inter – national e.g. bilateral context. There is an issue of trust vs. mistrust, which can be addressed by screening information. There are different use patterns between countries. National data are useful here for the understanding.

Are some conventions more important than others when it comes to reporting screening

CONCLUSION

Again, some conventions e.g. Stockholm Convention, favour the reporting of screening data.Timing is a bigger issue than actually the convrntion, e.g. screening in the drafting/revision phase of a Convention/Directive is more important than in the implementation phase.

What type of screening data is most useful in Convention work

CONCLUSION

Some conventions are more specifically addressing the needs of monitoring data.Screening data are valuable. If available, use them as much as possible.(→ Networking!). Screening is not done for a specific convention. It the knowledge, which can find its way to various conventions.*A priori* this is not known.

<u>WFD requirements</u>: Screening data are useful to evaluate effectiveness measures or to prioritise them →Key words: Intelligent sampling, point sources by WWTP, industrial sites.

Screening is providing additional data which otherwise is not obtained.

How can policy makers use networking in their work

- Cross borders comparison.
- Example of NORMAN: It is used, but no structure for funding? Everybody wants it: → Institutionalisation of such a network ?
- Comment: Policy has to learn how to use it.→ Need to create ownership.
- NORMAN is seen as being a useful example.
- LR-Transport does not stop at EU. Look outside?
- BREACH REACH – REACH ECHA?

CONCLUSION

NORMAN is a successful example of a platform for screening and monitoring data, yet in its beginning. More network activity of this type of activities is needed, in particular targeted to Member States. A more (pro)<u>active approach may be necessary to bring this to the attention to the policy maker</u>. (Need for a "FACEBOOK" for screening). Number of databases is an issue.

Results for certain matrices more valuable than others? Which:

CONCLUSION

Encourage the use of time-capsuled samples. Time-trends (time-integration) is an issue for the assessment of long-term effects of policies→ Network on European Specimen Banks.Choice of matrix

depends on the scope of the screening: Samples/Matrix for long-term storage must fulfil different requirements than those for exploratory investigations.

NEW: Usefulness of time trends

- See above

SELECTION OF SUBSTANCES

Discussion leader: Eva Brorström-Lunde'n, SE

Secretary: Elisabeth Nyberg, SE

Group participants:

Peter Haglund, SE, Bård Nordbø, NO, Anita Evenset, NO, Martin Schlabach, NO, Elisabeth Lie, NO, Matti Verta, FI, Susanne Boutrup, DE, Hrönn Ólina Jörundsdóttir, IS, Kristin MacBeath, NO, Heli Routti, NO, Anna Rotander, SE, Bert van Bavel, SE, Roger Lille-Langøy, NO, Kristin Olafsdottir, IS, Katrin Hoydal, FO, Anuschka Polder, NO

Substance selection

1. What data sources are available for information on screening candidates?

Summary of sources used by the Nordic countries:

- Product registers (KEMI)
- Suggestions from researchers
- Priority substances from different directives and conventions (WFD (also the waiting list), OSPAR etc)
- Pre-screening - comprehensive studies on different matrices (humans, storm water, wastewater etc)
- Literature studies
- Substances covered by media (public concern)
- Substances that appear in political discussions
- Screening studies in other countries
- Substances covered by NORMAN

New data that could be used as a source for screening candidates:

Since goods and humans are moving constantly we should use information available globally like for example:

- Data registers like NHANES
- Emission inventories
- Product registers
- Emission modelling efforts world wide
- Screening done by for example Canada and Japan
- Review papers

It was also suggested that meta-analysis should be conducted on the global research.

2. Are there any substances that are so complicated to analyse that we should leave them out?

When choosing which substances to screen for an evaluation of which level the analytical method could detect is crucial. The effect level should also be evaluated and compared to the LOQ (level of quantification) for the analytical method. If the effect level is lower then the LOQ it might be better to leave the substance out until the analytical method has improved.

A screening project should not finance method development, but it is very important that **the problem is communicated to the relevant laboratories** otherwise we might never be able to analyse the substance. It is also important that the Nordic countries discuss the analytical problems with other countries to find a solution.

Sampling strategies:

When conducting a larger geographical screening it is of utmost important to have a relevant sampling strategy from the beginning to be able to compare the results spatially. Important parameters are for example:

- Geographical location of the samples
- Matrix selection
- If biota: same size, sex and age, outside spawning season
- Sampling season: could be important if you look at for example pesticides which are very seasonal dependent or substances connected to aquaculture

A suggestion was also do the screening in three steps:

1. Literature study etc
2. Pre screening – to establish that the substance is there by for example looking at hot spots
3. Screening study on a larger scale

3. Substances?

- We should conduct broad comprehensive screening of samples, for example indoor air and then identify and semi quantify substances
- Look at substances on waiting lists of different directives (for example the 13 new compounds proposed for the priority list of the WFD) – information of occurrence of these substances is very important for the policy makers to be able to make decisions
- Lists of LRT substances
- NORMAN – database and network – suggest an expert group within NORMAN that could select chemicals for screening
- Important to not forget the unintentionally formed chemicals
- When choosing substances for screening it is important that the selection is risk based, look at toxicity information available
- Look for unknown unknowns – it is difficult but not impossible – biological methods could be used for identification another way is to take an easy matrix and see what could be found (like for example Bert van Bavels work)

MODELLING/SELECTION

Participants: Michael McLachlan (chair); Knur Breivik, Alberto Pistocchi; Kevin Thomas; Emma Undeman; Ingjerd Sunde Krogseth; Maria Dam (rapporteur).

The role the modelling could be a tool for synthesizing existing knowledge.

Models can not predict toxicity, they can predict to a certain degree lipid solubility and Bioconcentration factor. Need to run a battery of test , there are QSARs models that can model estrogen and androgen effects. You would need to model toxicity in addition to exposure in addition to get an idea of risk.

In most cases, the knowledge about quantities released into the environment is the one thing that makes the largest uncertainty in exposure modelling. The emmission data are the ones that are most needed.

Muir and Howards (2006) modelling is based on LRT potentials, and this fits with the criteria for being regulated under the Stockholm convention. Brown and Wania´s model (SETAC 2008) is based on structural similarities to exicting POPs. These models will thus not pick up for instance PFCs. The model of Muir and Brown have predicted that some compound will turn up in the Arctic and this has later been confirmed.

According to McLachlan partitioning proteries are not large sources of uncertainties in predicting exposure to POP like chemicals.

Positive aspect of models in selecting substances for screening:

- objective selection

- potentially transparent but dependent on expert judgement, which may not be reproducable

Negative aspect

- uncertainties in how the models are set up will give uncertainty in modelling outcomes, this adds to the uncertainties in the data that goes into the model.