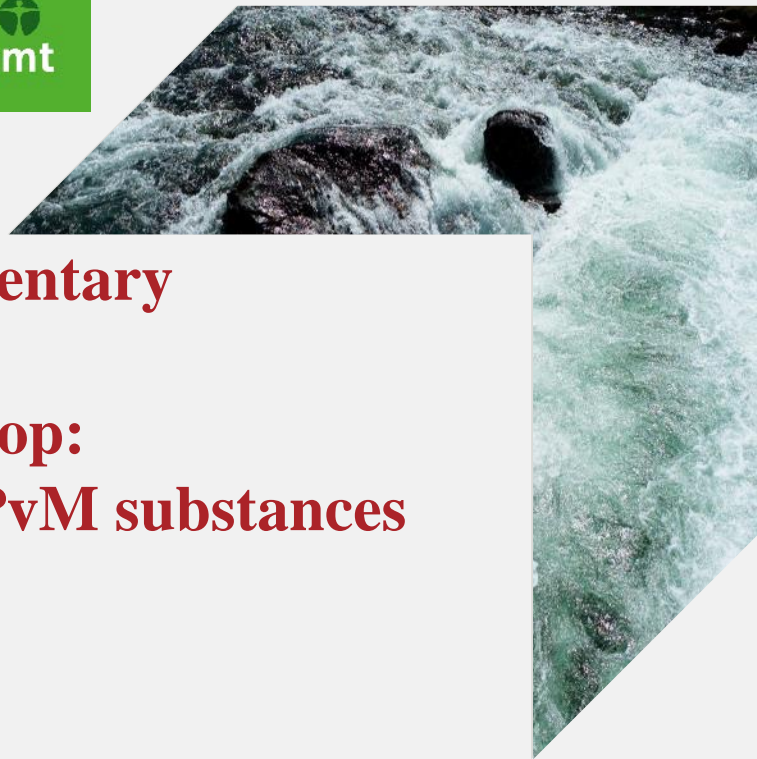# Poll results and Commentary from the Third PMT workshop: Getting Control of PMT and vPvM substances under REACH

Hans Peter H. Arp

25'th – 26'th March, 2021
Poll results and commentary

Contact: hpa@ngi.no

Poll # 1: What are the most important gaps for PMT substances ? (Please pick 3)
Timepoint: Start of workshop

Substance Assessment

- Availability of Persistency data?
- Availability of Mobility data?
- Availability for Toxicity data?
- Availability of Analytical methods?
- Availability of Monitoring data?
- Availability of transformation products and mixture composition?

Risk Governance

- Missing risk assessment tools/models?
- Missing water remediation infrastructure?
- Missing chemical legislation?
- Missing safe and sustainable substitutes?

Reemtsma et al. ES&T 2016

Results of Poll #1*

1. Availability of transformation products and mixture composition? (**48%**)
2. Availability of analytical methods? (44%)
3. Availability of monitoring data? (37%)
4. Missing safe and sustainable substitutes? (29%)
5. Missing risk assessment tools/models? (28%)
6. Missing chemical legislation? (26%)
7. Availability for toxicity data? (24%)
8. Availability of mobility data? (21%)
9. Availability of persistency data? (19%)
10. Missing water remediation infrastructure? (15%)

* ⌐ Data corrected for number of unique respondants,
  ⌐ Ignores «no response» and double responses
  ⌐ n=336 workshop participants responded
  ⌐ (ca 166 attendants with no response)

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Reemtsma et al. ES&T 2016

Commentary on poll # 1 (beginning of workshop)

- There was a wide spread in opinion, with 15% to 48% of each individual gap being selected as one of the top three gaps.
- "Availability of transformation products and mixture composition" was the biggest gap, with 48% of respondents putting this in their top three.
- This was followed by "Availability of analytical methods" (number 2) and "Availability of monitoring data" (number 3) data gaps. In some ways these are linked to each other, as you cannot monitor if no analytical methods are there, and you often analytical methods are not developed until there is a monitoring indication. Further the transformation product/mixture gap is also related, as transformation and mixtures can make a large amount of «unknowns» in monitoring campaigns, and also represent an «unknown» chemicals to look for, as often structures are missing.
- Information about P, M and T properties was ranked low (gaps 7-9)
- Risk governances gaps were in the middle (ranked 4-6) including the availability of appropriate risk assessment models, safe and sustainable substitutes, and chemical legislation. What is interesting in this regard as these gaps in risk governance require information on P, M and T substance properties, as well as information on all other gaps.
- "Missing water treatment infrastructure" was ranked as the smallest gap, could this mean at the audience felt that water treatment infrastructure is sufficient?

- As will be presented in the results of the next poll at the end of the workshop, there was a huge shift in the opinion of gaps, in part due the workshop giving a better understanding of the state-of-the art and providing a clearer definition of the gaps.

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Poll # 2: What is the SIZE of the gaps for PMT substances ? Pick «huge», «closing» or «small» Timepoint: End of workshop

Huge gap

Gap closing

Small gap
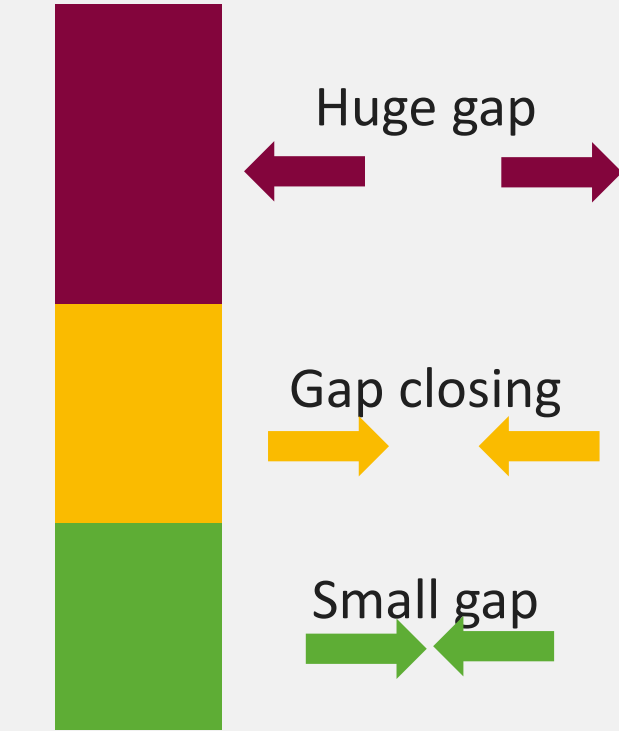
⌐ For the same gaps as the first poll, we presented the first glimpse at new project results and a summary of the workshop in relation to each "gap"

⌐ *Then at the end of the presentation, the audience was given 20 minutes if they thing each gap is huge, closing or small*

⌐ Hans Peter **made a prediction of audience response** before the polls were open. This was not necesserly Hans Peter's personal opinion, but how he anticipated the audience would respond by the end of the workshop.

⌐ **The slides below compare Hans Peter's prediction of audience poll with the audience polling, and also of the first poll**

Approx. n= 120 audience members responded to poll #2 ;
Approx. n =240 did not respond, depending on question

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Gap 1: Availability of **Persistency** data? Prediction

HPA's prediction

40% ⌐ Little/no information for low volume/intermediate REACH substances

40% ⌐ Mandatory PBT assessment for substances > 10 tpa contributes to more testing: Effect of PBT/vPvB regulation

20% ⌐ Screening tests for ready/inherent biodegradability useful for demonstrating «Not P»

Persistency Conclusions all REACH

No. REACH registered substances

not P: 4026, Potential P/vP: 4829, Potential P/vP++: 843, P: 141, vP: 237, no or conflicting data: 5884

Persistency Conclusions REACH > 10 tpa

No. REACH registered substances

not P: 2603, Potential P/vP: 1276, Potential P/vP++: 372, P: 98, vP: 148, no or conflicting data: 889

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Gap 1: Availability of **Persistency** data? Results
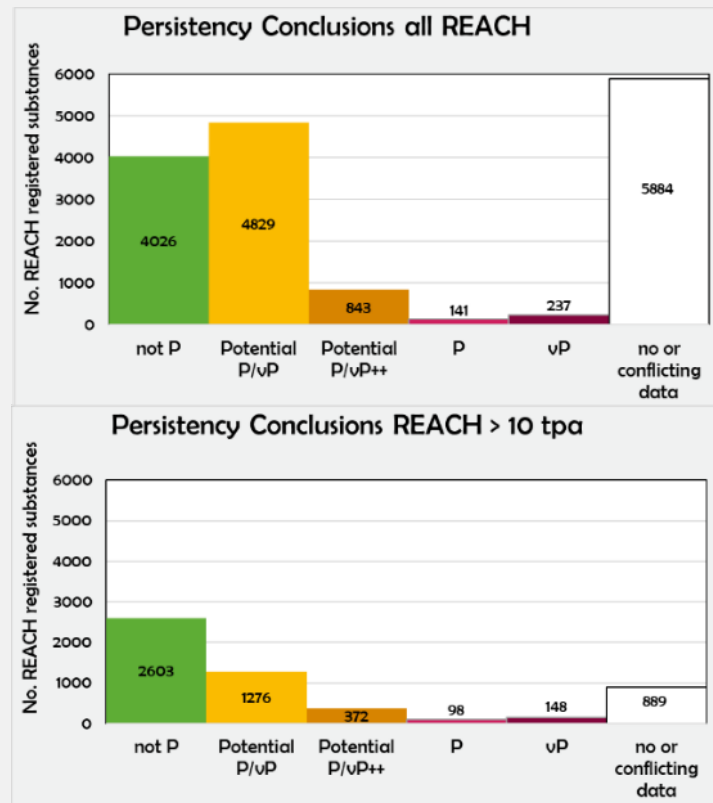
HPA's prediction

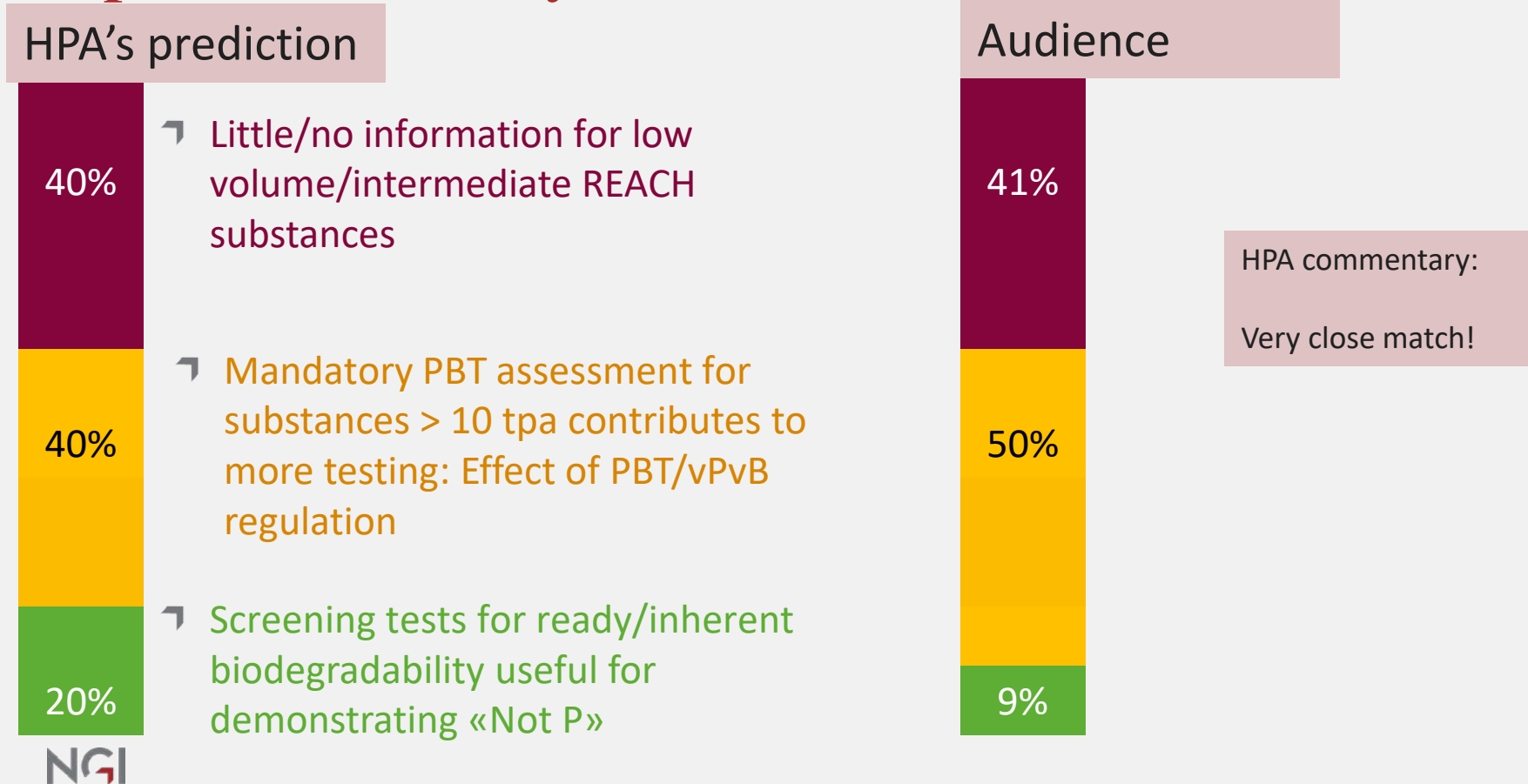|	
40%	⌐ Little/no information for low volume/intermediate REACH substances
40%	⌐ Mandatory PBT assessment for substances > 10 tpa contributes to more testing: Effect of PBT/vPvB regulation
20%	⌐ Screening tests for ready/inherent biodegradability useful for demonstrating «Not P»

Audience

41%
50%
9%

HPA commentary:

Very close match!

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Gap 2: Availability of **Mobility** data? Prediction
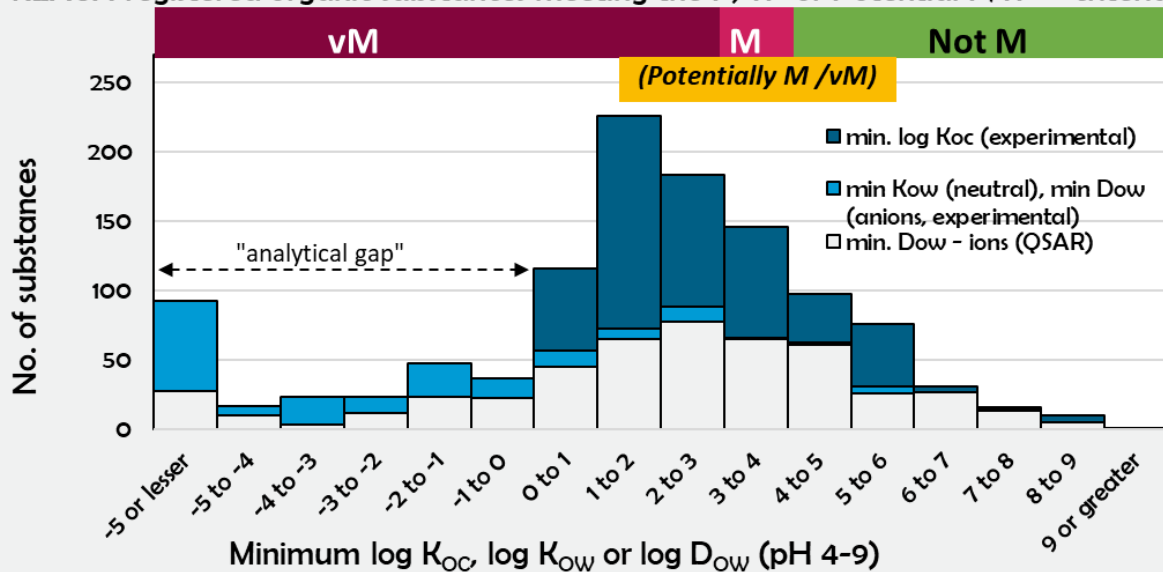
HPA's prediction

20%

20%

60%

- K_{oc} data for ionic substances rare and scattered, D_{ow} does not account for ion-exchange

- Neutral substances – lots of data and good models. Many ionic substances have K_{oc} values orders of magnitude from threshold

REACH registered organic substances meeting the P, vP or Potential P/vP++ criteria

vM   M   Not M

(Potentially M /vM)

No. of substances

250

200

150

100

50

0

- min. log Koc (experimental)
- min Kow (neutral), min Dow (anions, experimental)
- min. Dow - ions (QSAR)

"analytical gap"

Minimum log K_{OC}, log K_{OW} or log D_{OW} (pH 4-9)

-5 or lesser, -5 to -4, -4 to -3, -3 to -2, -2 to -1, -1 to 0, 0 to 1, 1 to 2, 2 to 3, 3 to 4, 4 to 5, 5 to 6, 6 to 7, 7 to 8, 8 to 9, 9 or greater

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Gap 2: Availability of **Mobility** data? Results

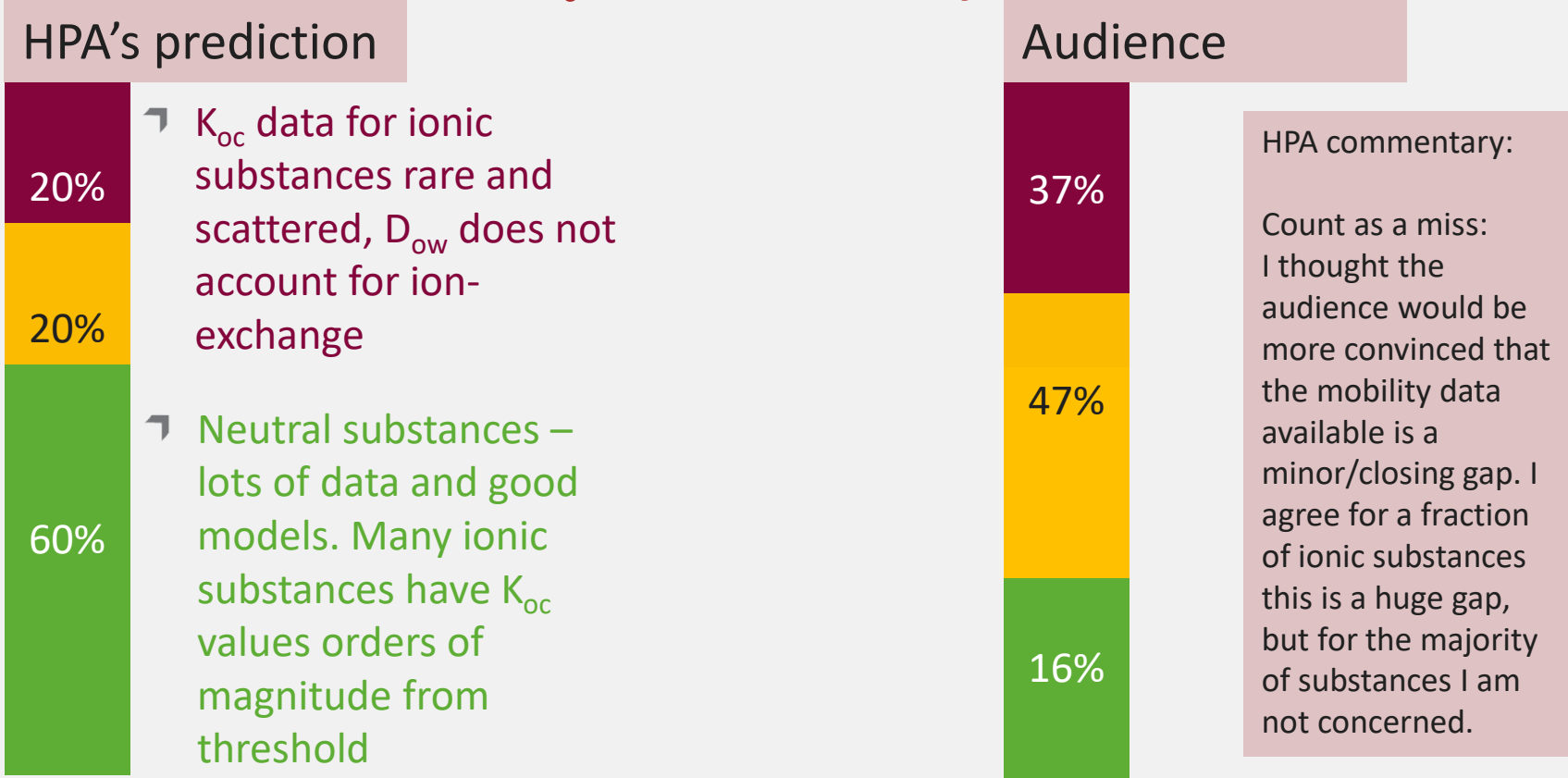## HPA's prediction

- 20%
- 20%
- 60%

↱ K_{oc} data for ionic substances rare and scattered, D_{ow} does not account for ion-exchange

↱ Neutral substances – lots of data and good models. Many ionic substances have K_{oc} values orders of magnitude from threshold

Audience

- 37%
- 47%
- 16%

HPA commentary:

Count as a miss: I thought the audience would be more convinced that the mobility data available is a minor/closing gap. I agree for a fraction of ionic substances this is a huge gap, but for the majority of substances I am not concerned.

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Gap 3: Availability of **Toxicity** data? Prediction

HPA's prediction

40% — Lack of data on PM/vPvM chemicals, despite chronic exposure. Few long-term physiologically based pharmokinetic (PBPK) models.
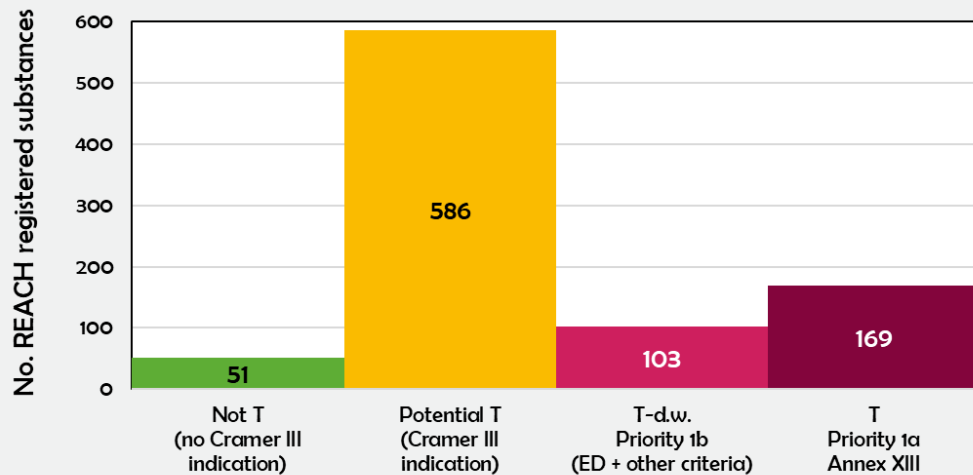
20% — Attention on PFAS is inspiring increasing research on effects from chronic water exposure

40% — Lots of required testing due to CLP

Toxicity Conc. for PM/vPvM substances registered under REACH

No. REACH registered substances

Not T (no Cramer III indication)	Potential T (Cramer III indication)	T-d.w. Priority 1b (ED + other criteria)	T Priority 1a Annex XIII
51	586	103	169

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Gap 3: Availability of **Toxicity** data? Results

HPA's prediction

40%	Lack of data on PM/vPvM chemicals, despite chronic exposure. Few long-term physiologically based pharmokinetic (PBPK) models.
20%	Attention on PFAS is inspiring increasing research on effects from chronic water exposure
40%	Lots of required testing due to CLP

Audience

60%
30%
10%

HPA commentary:

Partial hit/miss

I thought a larger fraction of the audience would think there is enough toxcity testing and conclude «minor gap». I personally agree this is a major gap, but was surpriesed the audience did too

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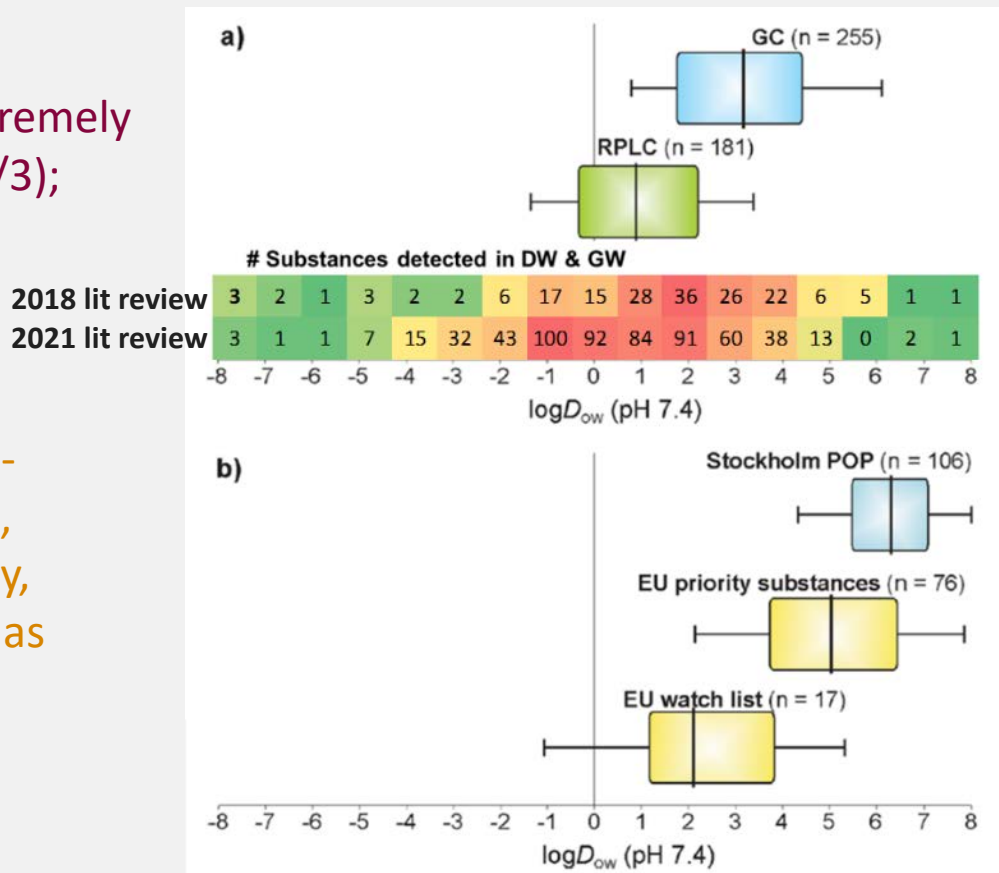## HPA's prediction

30%

⌐ Target analysis still needed for extremely mobile substances (e.g. log D < -2/3); standards HARD to come by

40%

30%

⌐ VAST improvements in the past 5 years in relation to target and non-target analysis (e.g. HILIC columns, Super critical fluid chromatography, suspect screening databases such as the Norman Network SLE)

a)

GC (n = 255)

RPLC (n = 181)

Substances detected in DW & GW

2018 lit review	3	2	1	3	2	2	6	17	15	28	36	26	22	6	5	1	1
2021 lit review	3	1	1	7	15	32	43	100	92	84	91	60	38	13	0	2	1
	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8

$\log D_{ow}$ (pH 7.4)

b)

Stockholm POP (n = 106)

EU priority substances (n = 76)

EU watch list (n = 17)

-8 -7 -6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6 7 8

$\log D_{ow}$ (pH 7.4)

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Figure adapted from Reemtsma et al. ES&T 2016
2018 review: Arp and Hale, UBA Texte, 126/2019, 2021 review: Arp et al. in prep.

Gap 4: Availability of **Analytical methods**? results

HPA's prediction

30%	⌐ Target analysis still needed for extremely mobile substances (e.g. log D < -2/3); standards HARD to come by
40% / **30%**	⌐ VAST improvements in the past 5 years in relation to target and non-target analysis (e.g. HILIC columns, Super critical fluid chromatography, suspect screening databases such as the Norman Network SLE)

Audience

33%

57%

11%

HPA commentary:

Very close prediction!

Though I thought a somewhat larger portion of the audience would say there was «no analytical gap» as we have so many great methods out ther.

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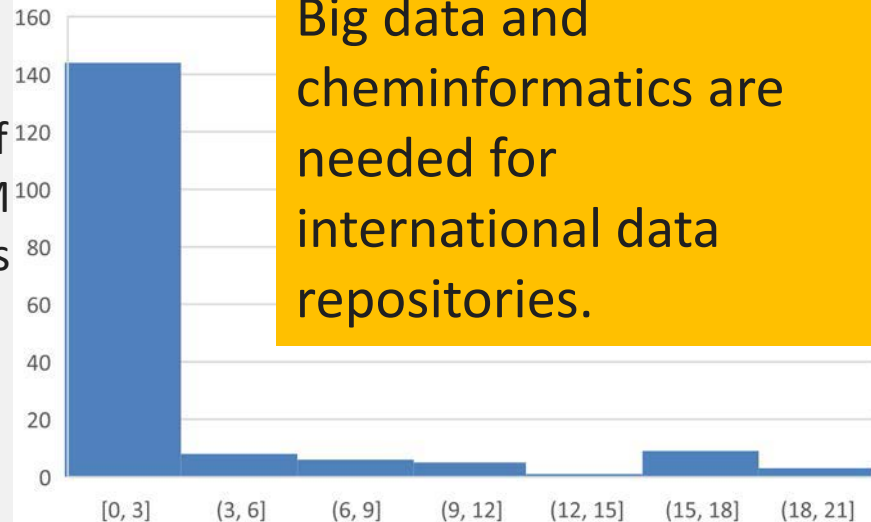# Gap 5: Availability of Monitoring Data? Prediction

70%

↰ An **incentive** gap: why monitor unless requested/share data unless requested. Only seeing tip of the «chemical iceberg» via research community

20%

↰ State-of-the-art research labs paving the way!

10%

Number of PMT/vPvM substances

Big data and cheminformatics are needed for international data repositories.

Number of water analysis labs in Germany that routinely analyze for them

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Gap 5: Availability of Monitoring Data? Results

70%

An **incentive** gap: why monitor unless requested/share data unless requested. Only seeing tip of the «chemical iceberg» via research community

20%

State-of-the-art research labs paving the way!

10%

Audience

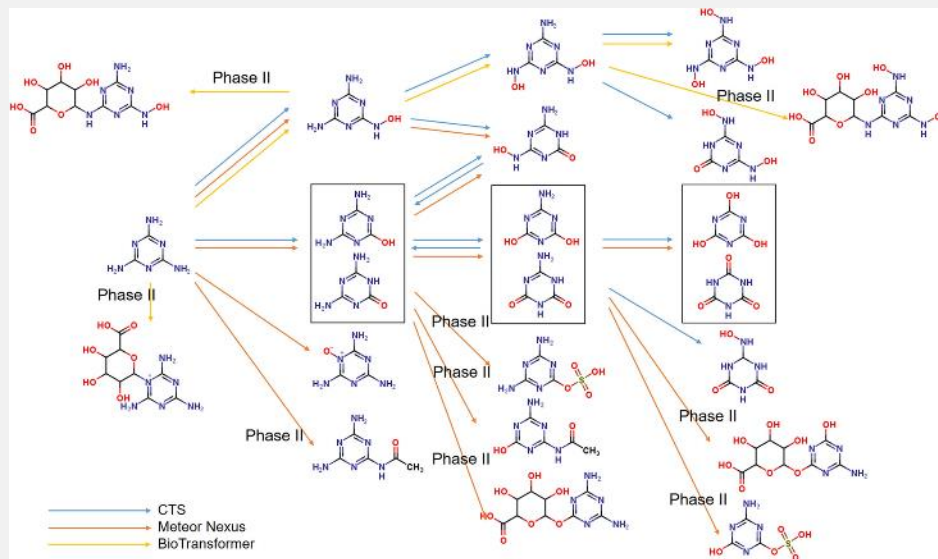64%

32%

4%

HPA commentary:

A very close prediction!

NGI

HPA's prediction

80%

For all REACH:

- ONLY 451 transformation products identified through **experimental** databases (EAWAG BBD, Norman SLE)
- QSARs give multiple predictions (see Zheng et al.)
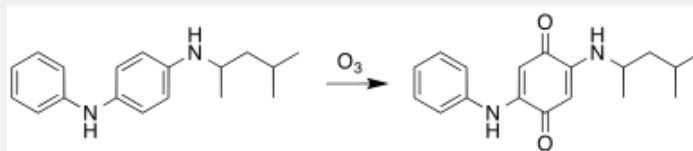- Ca 30% of organic substances in REACH are complex mixtures (UVCBs)

10%

10%

Melamine transforming to even more vPvM chemicals (Zheng et al. ES&T 2020, 10.1021/acs.est.0c02593)

6PPD (REACH vPvM & PMT) -> killer of Coho Salmon (Tian et al. Science 2020 https://science.sciencemag.org/content/371/6525/185)

Gap 6: Transformation products and mixture composition? (Results)

HPA's prediction

80%

10%

10%

- ⌐ For all REACH:
  - ⌐ ONLY 451 transformation products identified through **experimental** databases (EAWAG BBD, Norman SLE)
  - ⌐ QSARs give multiple predictions (see Zheng et al.)
  - ⌐ Ca 30% of organic substances in REACH are complex mixtures (UVCBs)

Audience

91%

7%

2%

HPA commentary:

Another very close prediction, and maybe the least surprising one.

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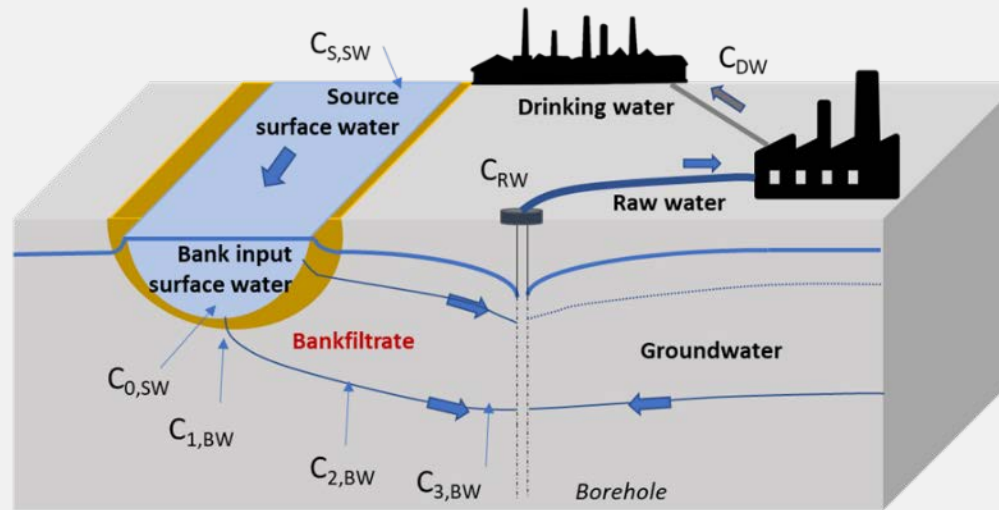# Gap 7: Missing risk assessment tools/models? Prediction

60%

- Mobility gap – ionic substances have complex behaviour
- Toxicity gap – unknown long term exposure effects
- Diffuse emissions, bank filtrate/ground water are inherently complex and not covered by generic models

10%

30%

- Well established agriculture plant protection product (PPP) and waste water treatment plant (WWTP models for specific scenarios (EUSES, SimpleTreat)

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Gap 7: Missing risk assessment tools/models? Results

HPA's prediction

60%

- Mobility gap – ionic substances have complex behaviour
- Toxicity gap – unknown long term exposure effects
- Diffuse emissions, bank filtrate/ground water are inherently complex and not covered by generic models

10%

30%

- Well established agriculture plant protection product (PPP) and waste water treatment plant (WWTP) models for specific scenarios (EUSES, SimpleTreat)

Audience

34%

53%

10%

HPA commentary:

I will call this a miss prediction, as clearly more of the audience though risk assessment tools were adapting to PMT/vPvM substances than I did. Personally I still think the gap is quite large, as it represents the sum of many gaps (e.g. emissions, M, T)

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Gap 8: Missing water remediation infrastructure? (rank 10)

HPA's prediction

A gap that cannot be fully closed. Many "pristine", or developing countries have limited drinking water production infrastructure – rely on chemical regulation to ensure protection.

Regrettable remediation: Most PMT/vPvM only removable with RO / super expensive, resource intensive treatment: Economic, Efficiency and Sustainability concerns.

Advance treatment methods work best at emission source

70%

20%

10%

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Screening of 158 PMT/vPvM substances Arp and Hale 2019. Suitable water treatments:

Technique	%
Neither O_3 nor AC	52,5
Only O_3	15,8
Only AC	20,9
Both	10,8

K.Nödler, preliminary results

Setting the agenda in research

Comment

One of five water-reuse plants in Singapore, which together supply about 40% of the nation's water for drinking and other uses.

Drink more recycled wastewater

Cecilia Tortajada and Pierre van Rensburg

Tortajada and van Rensburg, Nature, 2019

Gap 8: Missing water remediation infrastructure? Prediction

HPA's prediction

A gap that cannot be fully closed. Many "pristine", or developing countries have limited drinking water production infrastructure – rely on chemical regulation to ensure protection.

Regrettable remediation: Most PMT/vPvM only removable with RO / super expensive, resource intensive treatment: Economic, Efficiency and Sustainability concerns.

Advance treatment methods work best at emission source

70%

20%

10%

Audience

56%

20%

13%

HPA commentary:

I will call this a good prediction, especially considering in the first poll the audience did not see water remediation as a major gap, but I think day 1 (especially) convinced them that it was.

NGI

Gap 9: Missing chemical legislation? Prediction

HPA's prediction

30% — Harmonization to be explored across risk and hazard based legislation and regulation (CLP, REACH, PPPR, WHO GV, DWD,E-PRTR)

50% — The Chemicals Strategy for Sustainability and Zero Pollution Ambition
- Inclusion of PMT/vPvM in for REACH / CLP
- PFAS restriction
- Safe and Sustainable by Design

20% — Existing tools
- Article 57f
- PPPR

Jin et al. https://pubs.acs.org/doi/10.1021/acs.est.0c04281

Safe and Sustainable Chemicals

Minimize and Control

Eliminate and remediate

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Gap 9: Missing chemical legislation? Results

HPA's prediction

30% Harmonization to be explored across risk and hazard based legislation and regulation (CLP, REACH, PPPR, WHO GV, DWD,E-PRTR)

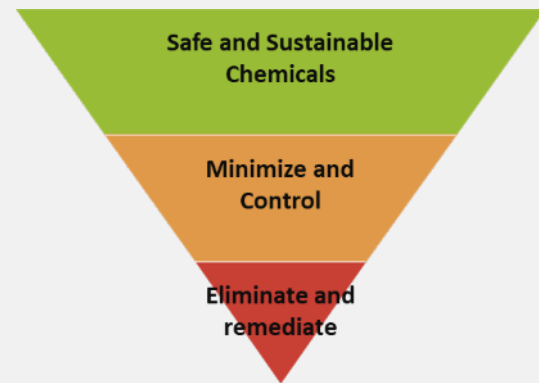**50%** The Chemicals Strategy for Sustainability and Zero Pollution Ambition
- Inclusion of PMT/vPvM in for REACH / CLP
- PFAS restriction
- Safe and Sustainable by Design
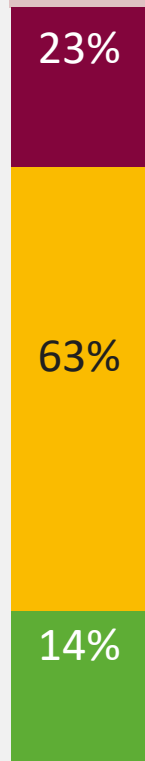
20% Existing tools
- Article 57f
- PPPR

Audience

23%

63%

14%

HPA commentary:

A fairly good prediction. The audience is generally convinced that the CSS and EU Green Deal will do a lot to close the gaps!

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Gap 10: Missing safe and sustainable substitutes (rank 4)

40%
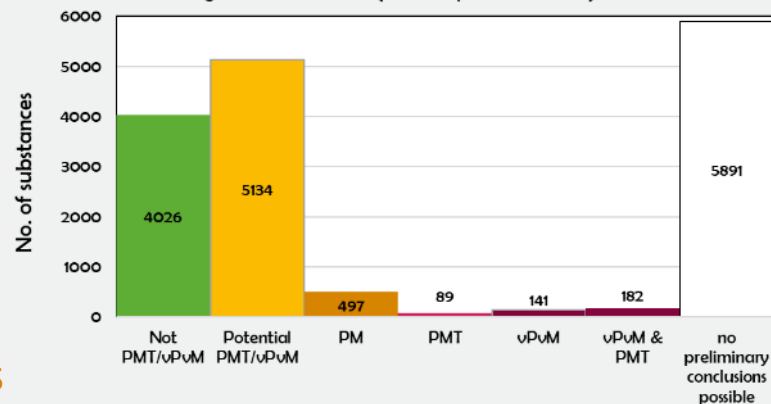- Technical / economic challenges
- Definition of «essential use»

30%
- Safe and sustainable by design / green chemistry techniques concept and techniques rapidly developing
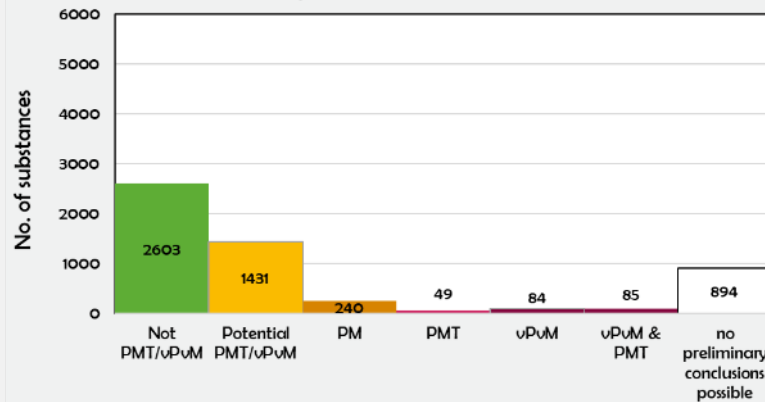- Sustainable material and process engineering

30%
- Majority of high production chemicals are NOT PMT/vPvM
- Strong societal/industry support
- Humans are innovators

A) PMT/vPvM Conclusions for all REACH Registered Substances with idenfied organic constituent (as of September 2019)

No. of substances: Not PMT/vPvM 4026, Potential PMT/vPvM 5134, PM 497, PMT 89, vPvM 141, vPvM & PMT 182, no preliminary conclusions possible 5891

B) For REACH Registered Substances with Organic Constituent > 10 tonnes per annum

No. of substances: Not PMT/vPvM 2603, Potential PMT/vPvM 1431, PM 240, PMT 49, vPvM 84, vPvM & PMT 85, no preliminary conclusions possible 894

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Gap 10: Missing safe and sustainable substitutes (Prediction)

HPA's prediction

40% — Technical / economic challenges
Definition of «essential use»

30% — Safe and sustainable by design / green chemistry techniques concept and techniques rapidly developing
Sustainable material and process engineering

30% — Majority of high production chemicals are NOT PMT/vPvM
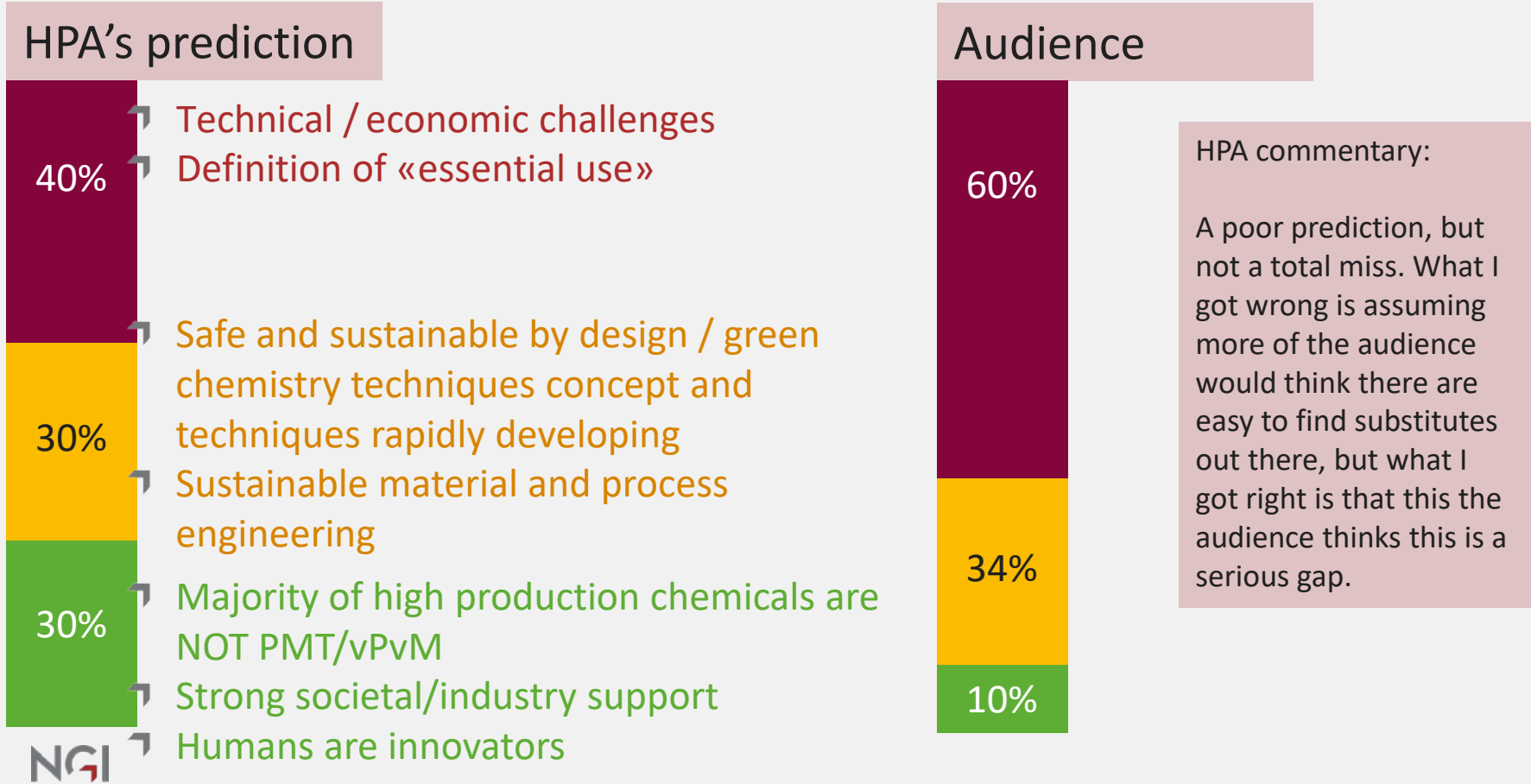Strong societal/industry support
Humans are innovators

NGI

Audience

60%

34%

10%

HPA commentary:

A poor prediction, but not a total miss. What I got wrong is assuming more of the audience would think there are easy to find substitutes out there, but what I got right is that this the audience thinks this is a serious gap.

Comparing Poll #1 and Poll #2: Changes in opinions about the biggest gaps over the workshop?

Substance Assessment

- Availability of Persistency data?
- Availability of Mobility data?
- Availability for Toxicity data?
- Availability of Analytical methods?
- Availability of Monitoring data?
- Availability of transformation products and mixture composition?

Risk Governance

- Missing risk assessment tools/models?
- Missing water remediation infrastructure?
- Missing chemical legislation?
- Missing safe and sustainable substitutes?

	Poll #1	Poll #2
When	Start of workshop	End of workshop
Time	1 hour	20 min
Structure	Top three gaps	Status of each gap: huge, closing, minor
Ranking	Frequency selected in top three	Frequency «huge gap» was selected
N value	Ca 366 of 502 participants	Ca 120 of 340 particpants
Notes	- Definition of «gaps» more clearly defined before Poll #2 - Did not control for same participants in both polls.	

Reemtsma et al. ES&T 2016

Comparison of poll ranking of «biggest gaps»

	Beginng of workshop	End of workshop	HPA's End predictions
Availability of trans. prod. and mixture comp	1	1	1
Availability of analytical methods	2	9	9
Availability of monitoring data	3	2	2
Missing safe and sustainable substitutes	4	3	6
Missing risk assessment tools/models	5	8	4
Missing chemical legislation	6	10	8
Availability for toxicity data	7	4	7
Availability of mobility data	8	7	10
Availability of persistency data	9	6	5
Missing water remediation infrastructure	10	5	3

We have the tools, let us close the gaps to get control!

Stewardship + Risk Governance + Science

Non-toxic heirarchy of the Chemical Strategy for Sustainability

Status quo

- PMT/υPυM In CLP & REACH

- Harmonization of PMT/υPυM definitions within risk assessment models and regulations

- Big data monitoring data and suspect list harmonization (e.g. non-target in E-PRTR)

- Remediation at emission sources rather than downstream

- Safe and sustainable chemistry

Safe and Sustainable Chemicals

Minimize and Control

Eliminate and remediate

Zero pollution of PM substances

#påsikkergrunn

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