INTEGRATING MASS BALANCE MULTI-MEDIA MODELS TO LINK NPRI DATA WITH CHEMICAL FATE AND EXPOSURE IN THE ENVIRONMENT AND THE POTENTIAL FOR ADVERSE EFFECTS

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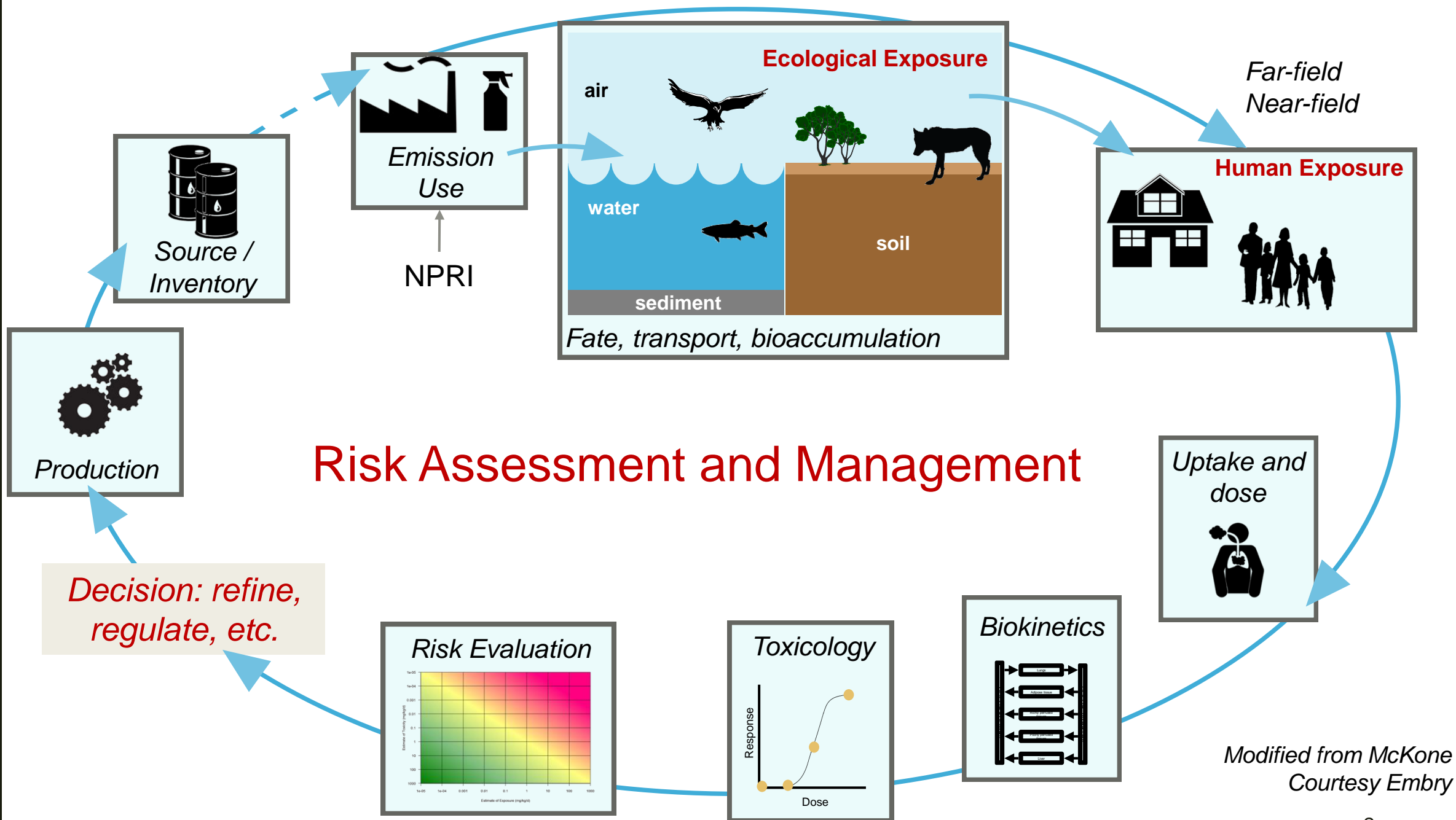NPRI Data Users Workshop

February 25, 2020

Montreal, QC, Canada

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Outline

- Background

- Objectives and rationale

- Introduction to RAIDAR

- Project tasks

- Results

- Dashboards

- Conclusions

- Future work/next steps

Risk Assessment and Management

Far-field
Near-field

Ecological Exposure

air
water
sediment
soil

Fate, transport, bioaccumulation

Human Exposure

Emission
Use

NPRI

Source /
Inventory

Production

Decision: refine, regulate, etc.

Risk Evaluation

Toxicology

Response

Dose

Biokinetics

Uptake and dose

Modified from McKone
Courtesy Embry

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CEPA 1999: Risk Assessment and Management

- Considers chemical *impacts* on human and non-human organisms, i.e., <u>risk</u>.

- Risk includes the hazard posed by a substance <u>**and exposure**</u>

$$Risk = Exposure/Hazard$$

- Exposure depends on *the amount of substance released* <u>*and its fate*</u>.

- Strategies are developed to determine how best to manage "toxic" substances, i.e., potential actions required to mitigate risk of adverse effects.

- Social, economic and other factors are integral to risk management.

Project Objectives

- Apply a tool to bridge the gap between NPRI emission estimates and exposures and potential risk to various ecological species and humans

- Improve understanding of exposure and exposure pathways of NPRI chemicals (can inform possible mitigation steps, if necessary)

- Similar efforts of using mass balance models to link with NPRI data have recently been explored
  - *USETox 2.0*

RESEARCH ARTICLE

A toxicity-based analysis of Canada's National Pollutant Release Inventory (NPRI): a case study in Nova Scotia

Stephanie Taylor[1] · Stuart Johnston Edwards[1] · Tony R. Walker[1]

Risk Assessment IDentification And Ranking (RAIDAR)

A continued evolution of fugacity-based, mass balance multi-media models for **discrete neutral and ionogenic organic chemicals** pioneered by Don Mackay and colleagues

- *RAIDAR combines environmental fate and food web bioaccumulation models in an evaluative regional-scale environment*

- *Exposure and risk simulations require chemical-specific information:*
  - Partitioning, e.g., Kow, Kaw
  - Medium-specific degradation half-lives, e.g., reaction half-life in air
  - Emission rates, e.g., how much chemical is released to air, water or soil
  - Toxicity thresholds, e.g., LC50s, NOAELs

- *Some primary model output of regulatory interest:*
  - Fate, Overall Persistence, Long-Range Transport Potential, Bioaccumulation metrics
  - Concentrations in physical environment and biological receptors
  - Exposure potential, and exposure and risk estimates

- *Currently coded in Visual Basic for Applications in Microsoft Excel*

- *Current User Interface is Excel spreadsheets*

RAIDAR model concepts

Steady state; regional scale; diffuse emissions
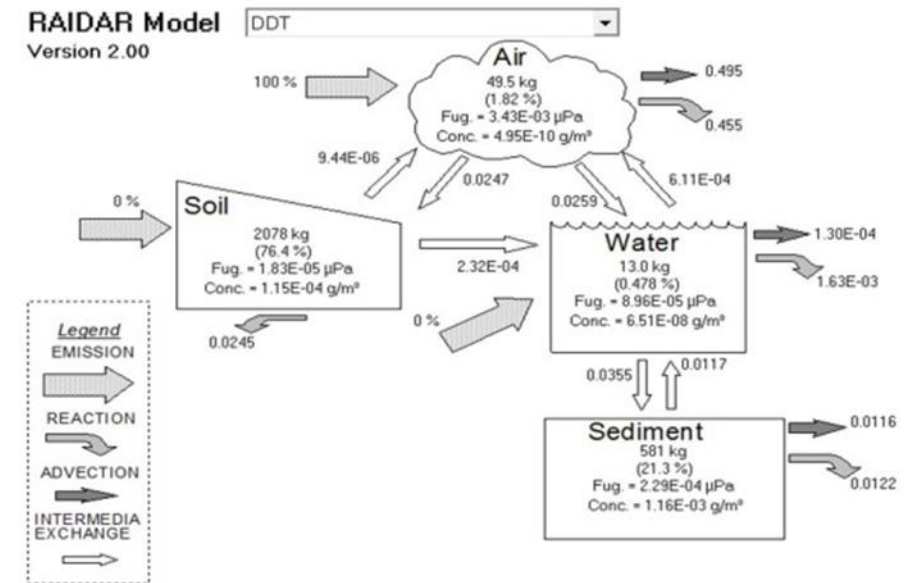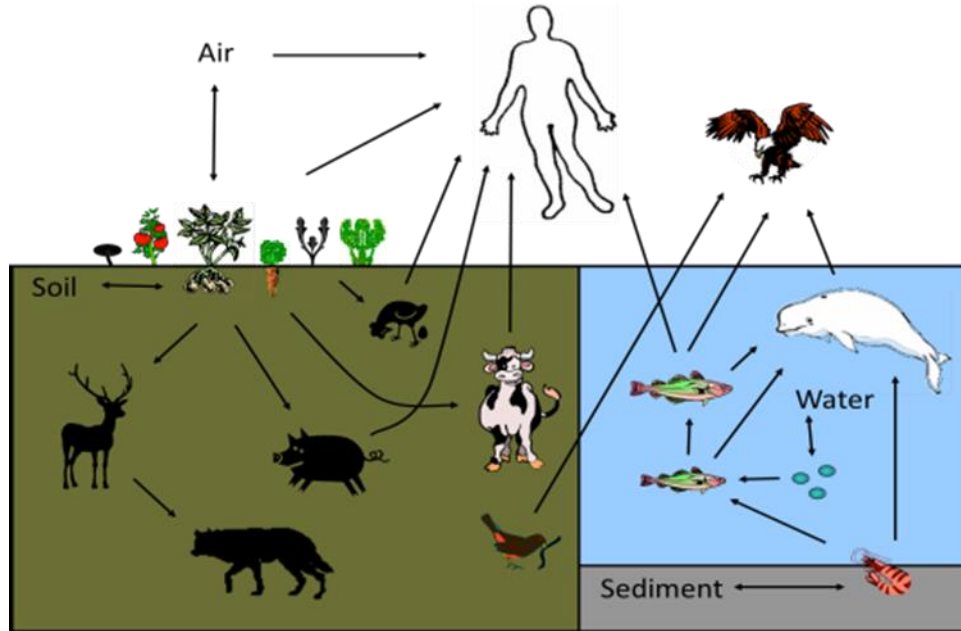
Water-ventilating organisms
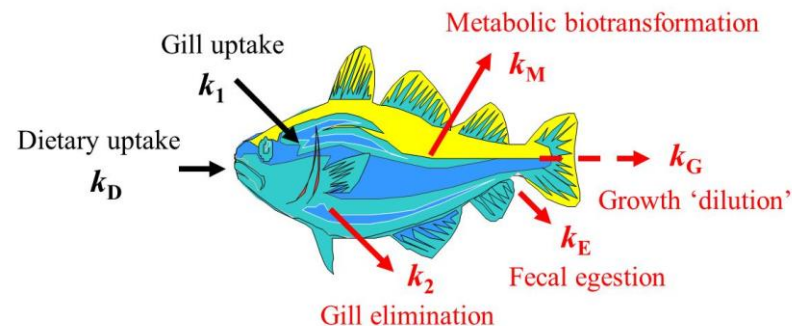
Air-respiring organisms
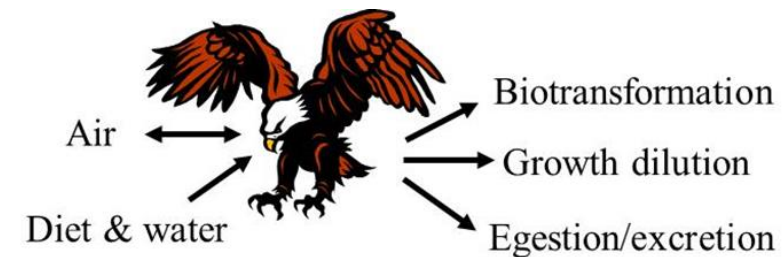
RAIDAR hazard and risk-based metrics for ranking chemicals

1. Exposure Assessment Factor (EAF) $\approx f$ (P + B)

2. Hazard Assessment Factor (HAF) $\approx f$ (P + B + T)

3. Risk Assessment Factor (RAF) $\approx f$ (**E** + P + B + T)

E = Emission rates (NPRI data)

RAIDAR Application: NPRI chemicals

Obtained required chemical input parameters from databases and QSARs
Two Sets of Simulations:

2015-2017 NPRI reporting years - 342 NPRI substances

1. 252 chemicals (RAIDAR input data obtained)
   a. *Full chemical emission (release) data unavailable*
   b. *Therefore only RAIDAR **EAF** and **HAF** output provided*
2. 137 chemicals (2017 NPRI reporting year, release data only)
   a. *NPRI emission estimates used to obtain RAIDAR **RAF***

Results-1

Exposure *potential* (**EAFs**) spans 14 orders of magnitude
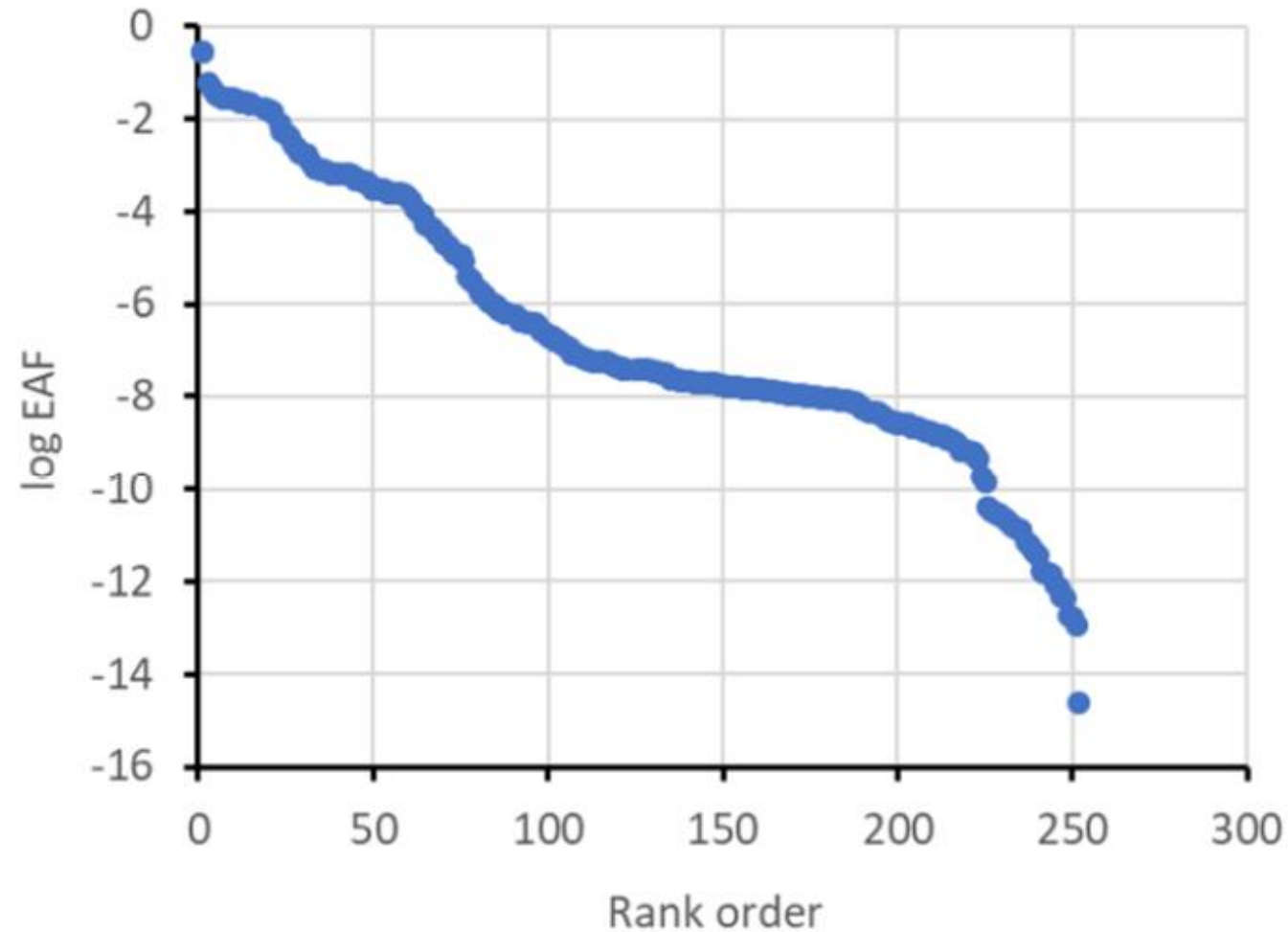
Results-2

Including NPRI emissions – each point is a facility reported value
Risk **(RAF)** estimates for these chemicals span 17 orders of magnitude, easy to prioritize chemicals and facilities based on RISK!
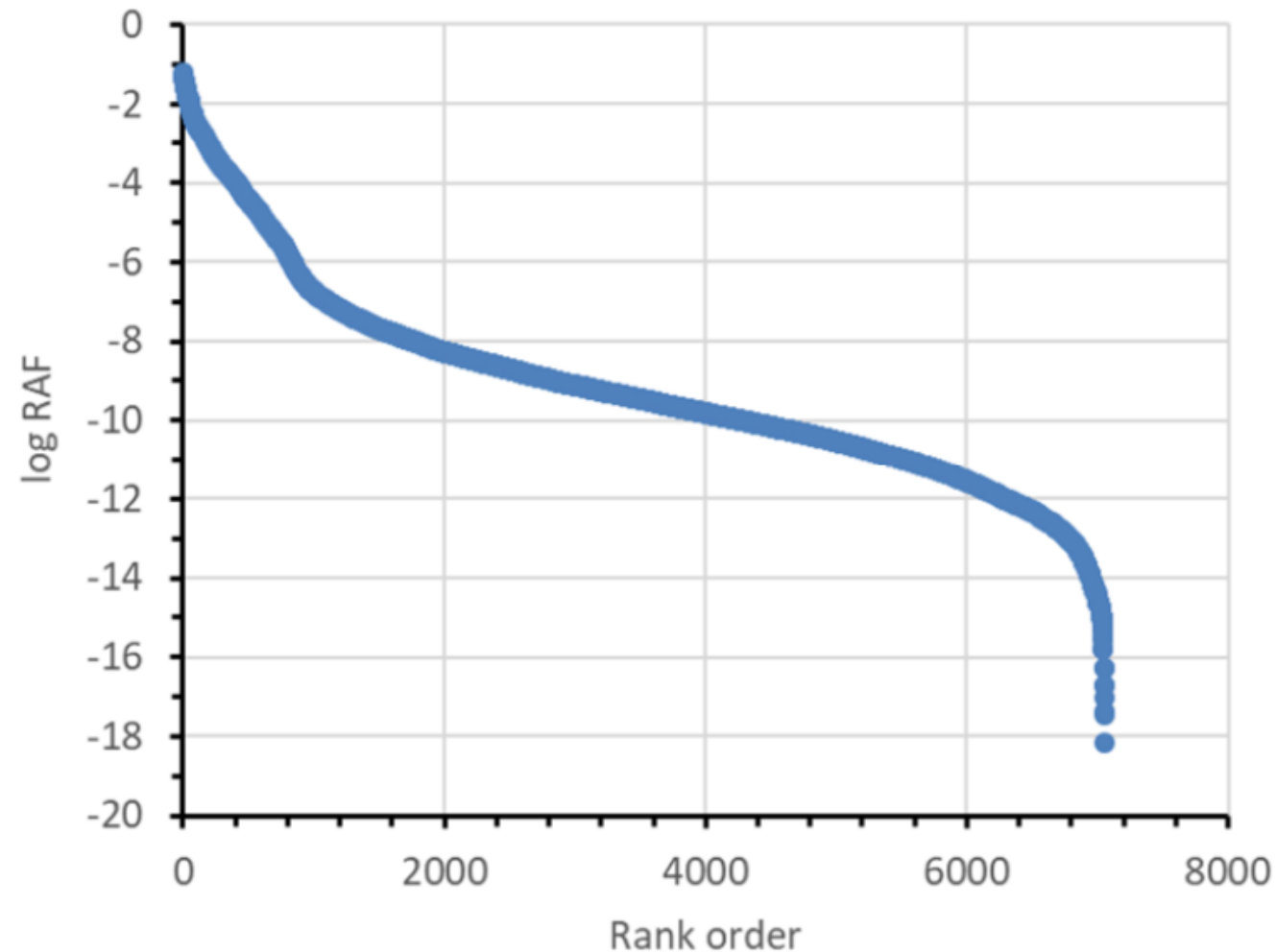
Results-2

RAFs as a function of actual emission rates (E_A) for 7000 instances of NPRI data for 135 organic substances based on 2017 reporting data

$y = 0.6245x - 7.6754$
$R^2 = 0.2499$
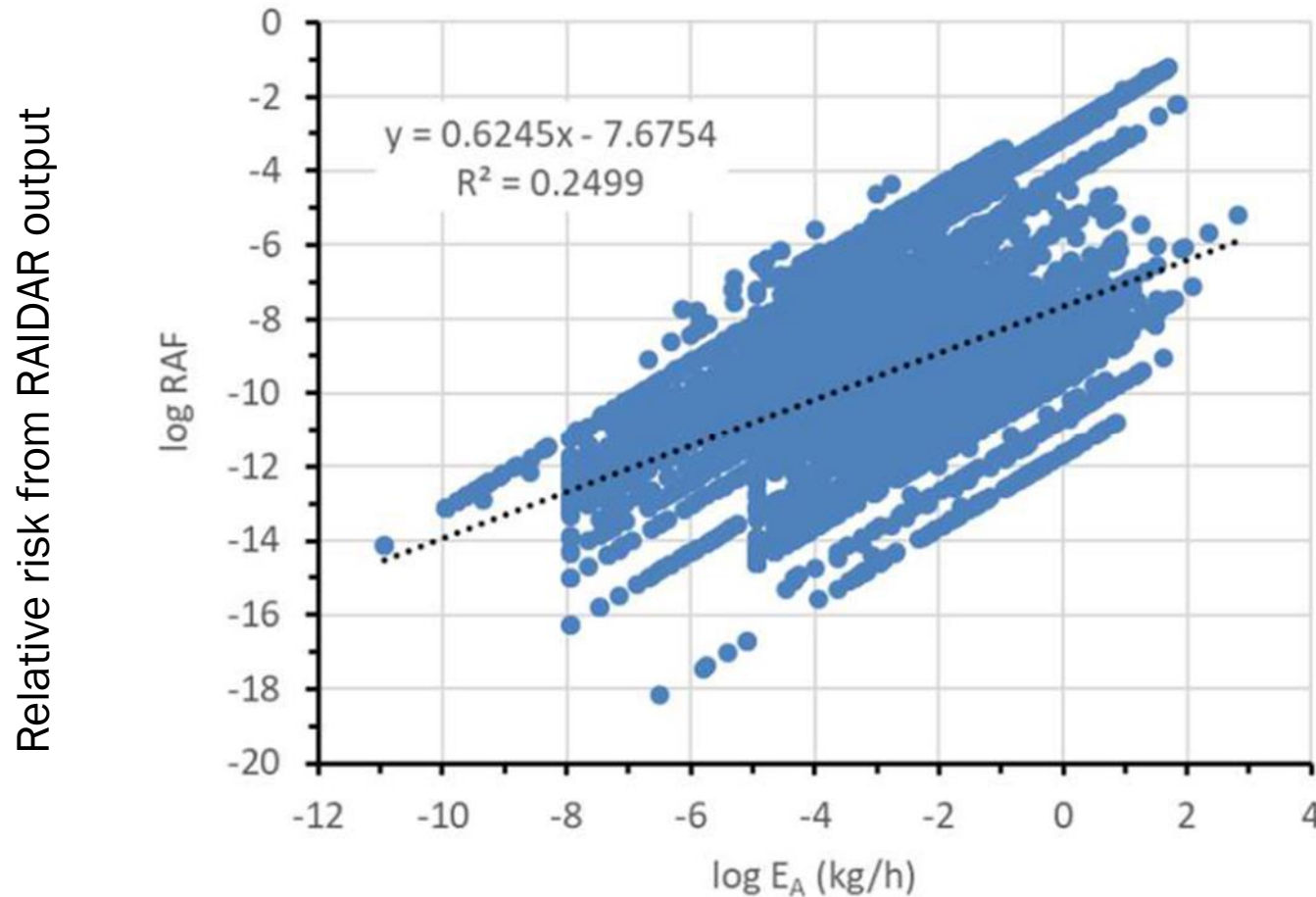
Only a weak relationship between chemical release and risk to the environment

Data presentation using dashboards

- Dashboards help to convey the data and analysis to broader audiences

- Tableau software (www.tableau.com)

- Data analytics

- Distill and compare large datasets of results

- Tabular, graphical, spatial data types

Ranking based on assessment factor

Comparison of different approaches to rank priorities among NPRI release data 2008-2017

Match to RAIDAR?	Reporting Year	Release type	Most Sensitive Orga..
☐ False	All	All	All
☑ True			

Release type by Quantity

Colour legend - Release..
- Total Air
- Total Land
- Total Water

Most Sensitive Organism

Colour legend - Most Sensitive Organism
- Foliage vegetation
- Root vegetation
- Plankton

	Rank by Quantity released (NPRI data)			Rank by Exposure Assessment Factor (EAF)				Rank by Hazard Assessment Factor (HAF)				Rank by Risk Assessment Factor (RAF) (in most sensitive organism)	
1	Methanol		1	Dioxins and furans - total	0.04825		1	1-Nitropyrene	1.08e-01		1	Methanol	17.641662
2	Ethylene glycol		2	Hexachlorobenzene	0.00880		2	Dioxins and furans - total	5.05e-02		2	Isopropyl alcohol	1.040837
3	n-Hexane		3	Decabromodiphenyl oxide	0.00081		3	Indeno(1,2,3-c,d)pyrene	1.29e-02		3	Formaldehyde	0.097218
4	Xylene (all isomers)		4	Dibenzo(a,e)pyrene	0.00067		4	Hexachlorobenzene	1.04e-02		4	Nitrilotriacetic acid (and its salts)	0.042227
5	Toluene		5	Dibenzo(a,l)pyrene	0.00067		5	Benzo(j)fluoranthene	6.75e-03		5	N-Methyl-2-pyrrolidone	0.003548
6	Styrene		6	Dibenzo(a,h)pyrene	0.00067		6	Benzo(g,h,i)perylene	3.97e-03		6	Nonylphenol and its ethoxylates	0.003058
7	Ethylene		7	Dibenzo(a,i)pyrene	0.00067		7	Isopropyl alcohol	3.72e-03		7	Indeno(1,2,3-c,d)pyrene	0.001800
8	Formaldehyde		8	Benzo(g,h,i)perylene	0.00063		8	Benzo(a)anthracene	2.60e-03		8	Anthracene	0.001616
9	Methyl ethyl ketone		9	Dibenzo(a,h)anthracene	0.00063		9	Benzo(a)pyrene	1.92e-03		9	2-Mercaptobenzothiazole	0.001385
10	Isopropyl alcohol		10	Dibenzo(a,e)fluoranthene	0.00061		10	Benzo(e)pyrene	1.87e-03		10	Phenol (and its salts)	0.001073
11	Acetaldehyde		11	Polymeric diphenylmethane..	0.00049		11	Chloroacetic acid (and its salts)	1.73e-03		11	Acrolein	0.000759
12	Cyclohexane		12	7H-Dibenzo(c,g)carbazole	0.00044		12	Anthracene	9.93e-04		12	Peracetic acid (and its salts)	0.000753
13	Benzene		13	Dibenzo(a,h)acridine	0.00042		13	Benzoyl peroxide	8.70e-04		13	Benzo(g,h,i)perylene	0.000692
14	1,2,4-Trimethylbenzene		14	Dibenzo(a,j)acridine	0.00042		14	Pyrene	8.19e-04		14	Benzo(e)pyrene	0.000691

Ranking based on release pattern

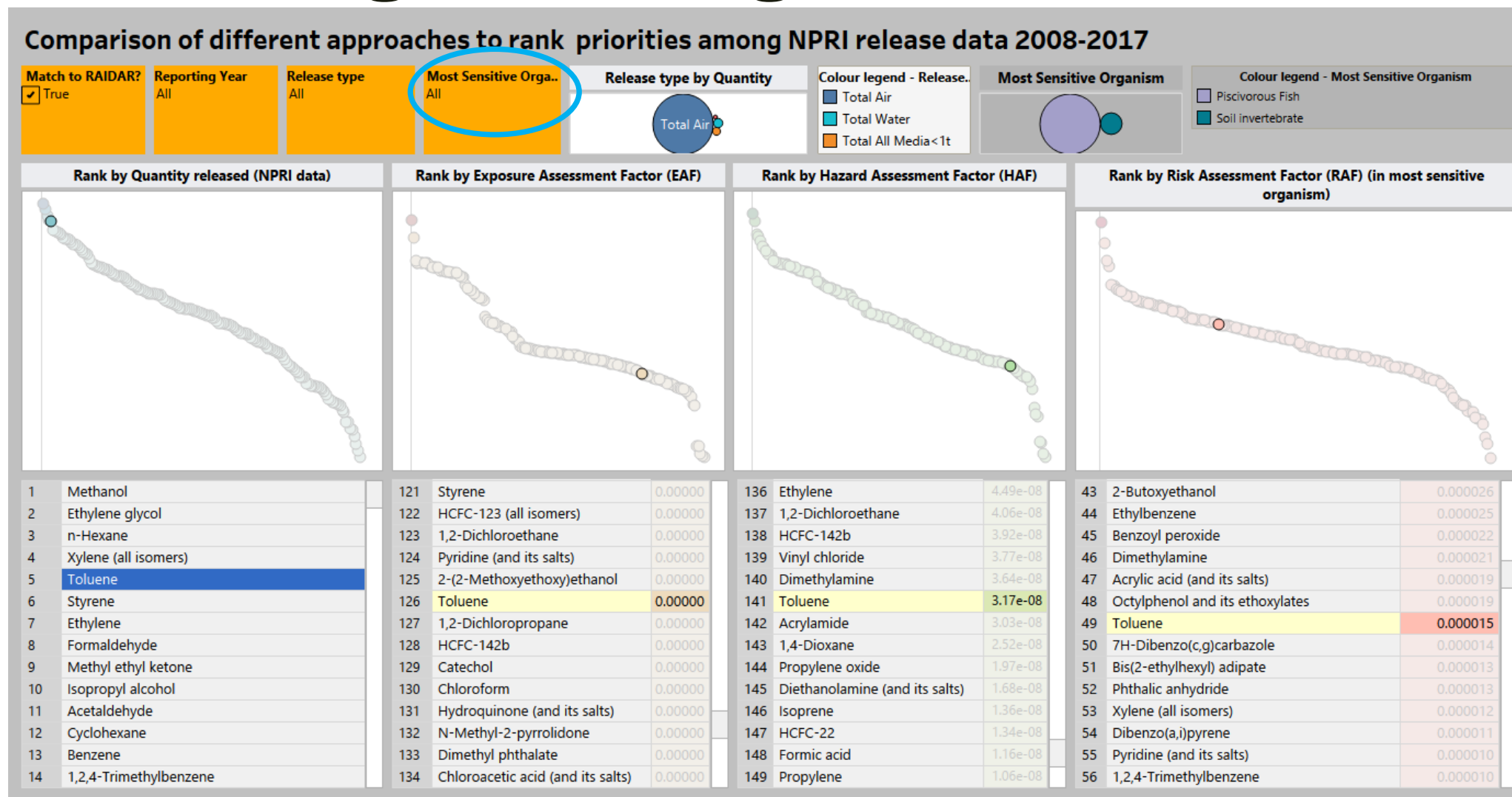## Comparison of different approaches to rank priorities among NPRI release data 2008-2017

Match to RAIDAR? ☑ True | **Reporting Year** All | **Release type** All | **Most Sensitive Orga..** All

Release type by Quantity — Total Air

Colour legend - Release..
- 🟦 Total Air
- 🟦 Total Water
- 🟧 Total All Media<1t

Most Sensitive Organism

Colour legend - Most Sensitive Organism
- 🟪 Piscivorous Fish
- 🟦 Soil invertebrate

#	Rank by Quantity released (NPRI data)	#	Rank by Exposure Assessment Factor (EAF)	#	Rank by Hazard Assessment Factor (HAF)	#	Rank by Risk Assessment Factor (RAF) (in most sensitive organism)	
1	Methanol	121	Styrene	136	Ethylene	44	Ethylbenzene	0.000025
2	Ethylene glycol	122	HCFC-123 (all isomers)	137	1,2-Dichloroethane	45	Benzoyl peroxide	0.000022
3	n-Hexane	123	1,2-Dichloroethane	138	HCFC-142b	46	Dimethylamine	0.000021
4	Xylene (all isomers)	124	Pyridine (and its salts)	139	Vinyl chloride	47	Acrylic acid (and its salts)	0.000019
5	Toluene	125	2-(2-Methoxyethoxy)ethanol	140	Dimethylamine	48	Octylphenol and its ethoxylates	0.000019
6	Styrene	126	Toluene	141	Toluene	49	Toluene	0.000015
7	Ethylene	127	1,2-Dichloropropane	142	Acrylamide	50	7H-Dibenzo(c,g)carbazole	0.000014
8	Formaldehyde	128	HCFC-142b	143	1,4-Dioxane	51	Bis(2-ethylhexyl) adipate	0.000013
9	Methyl ethyl ketone	129	Catechol	144	Propylene oxide	52	Phthalic anhydride	0.000013
10	Isopropyl alcohol	130	Chloroform	145	Diethanolamine (and its salts)	53	Xylene (all isomers)	0.000012
11	Acetaldehyde	131	Hydroquinone (and its salts)	146	Isoprene	54	Dibenzo(a,i)pyrene	0.000011
12	Cyclohexane	132	N-Methyl-2-pyrrolidone	147	HCFC-22	55	Pyridine (and its salts)	0.000010
13	Benzene	133	Dimethyl phthalate	148	Formic acid	56	1,2,4-Trimethylbenzene	0.000010
14	1,2,4-Trimethylbenzene	134	Chloroacetic acid (and its salts)	149	Propylene	57	Dibutyl phthalate	0.000009

Ranking based organism of interest

Comparison of different approaches to rank priorities among NPRI release data 2008-2017

Conclusions

- Successful "proof of concept" linking NPRI data with mass balance models for fate and exposures and potential risk of **discrete neutral and ionogenic organic chemicals** to biological receptors in Canada

Possible future work

- Improved spatial simulation of release, exposure and risk
  - *Determine "hotspots" for not only emissions, but for risk*
  - *Parameterize RAIDAR for regional-specific environments in Canada*

- Evaluate model predicted environmental concentrations with monitoring data in these regions (partnerships with other government agencies)

- Consider using NPRI disposal data (not currently modelled in RAIDAR) using EASE Suite which includes a chemical life cycle emissions module (CiP-CAFÉ)

Acknowledgments

■ Environment and Climate Change Canada, National Pollutant Release Inventory Program for funding and collaboration.

■ The RAIDAR model and other tools can be found at www.arnotresearch.com

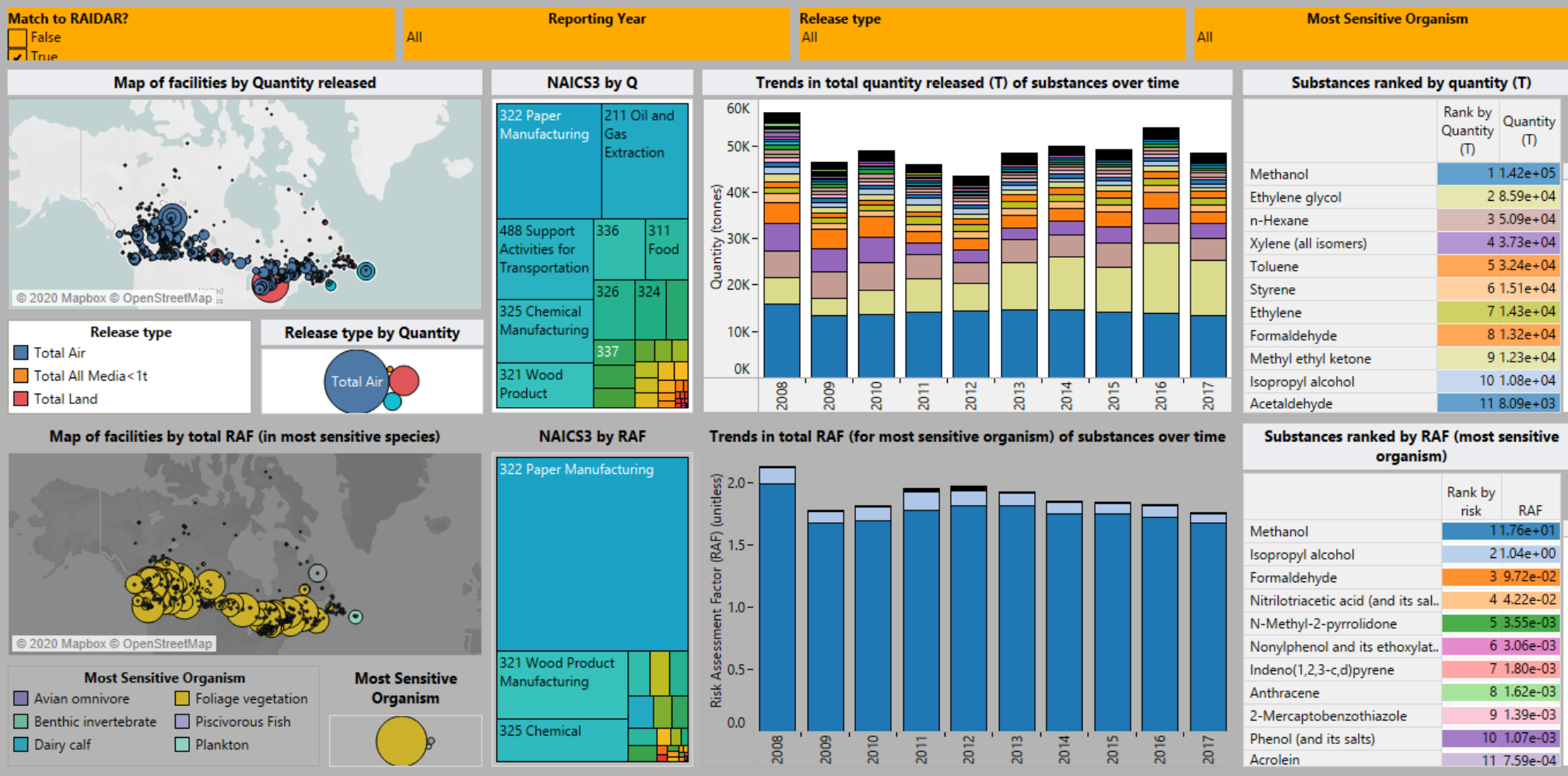ARC Arnot Research & Consulting   About   Research   Models   Databases   Contact

■ Please contact liisa.toose@gmail.com, jon@arnotresearch.com or Alicia.Berthiaume@canada.ca for more information

Impact of industry type

Trends and hotspots by 2 different approaches (by quantity and by risk)

Trends in emissions and risk