New approach methods for high throughput risk-based screening and prioritization for ecosystem health

Jon A. Arnot[1,2], Liisa Toose[1], James M. Armitage[1,3], Alessandro Sangion[1,2], Li Li[4], Mark Bonnell[5]

[1]ARC Arnot Research and Consulting Inc, Canada; [2]University of Toronto Scarborough, Canada
[3]AES Armitage Environmental Sciences Inc, Canada; [4]University of Nevada Reno, USA; [5]Environment and Climate Change Canada, Canada

INTRODUCTION

- Under US law (TSCA / LCSA [1]) thousands of commercial chemicals are subject to risk evaluations.
- TSCA ***requires*** that EPA use best available science and base decisions on the weight of scientific evidence.
- An EPA white paper [2] outlines their current plan to use a rather complex ***multiple category approach*** in which chemicals are scored and binned (a "PBT approach") for prioritization (**Fig. 1**); "high-priority" chemicals proceed to risk evaluation while "low priority" chemicals are left behind.
- Models are routinely used to estimate chemical fate & persistence (P), bioaccumulation (B) and exposures which can then be combined with toxicity (T) data for risk estimates in a ***holistic (& transparent) approach*** for prioritization [3]. For example, the Risk Assessment IDentification And Ranking (RAIDAR) model (**Fig. 2;** [3]) combines environmental fate and bioaccumulation models to simulate aggregate exposure to various ecological receptors (water-respiring and air-breathing) and can include toxicity data for risk estimates to ***prioritize a large number of chemicals quickly and efficiently based on risk allowing limited resources to on data gaps.***
- A previous case study for 400 chemicals ***demonstrated and explained why*** a multiple category (PBT) approach is generally ineffective at prioritizing chemicals for ecological risk [3].

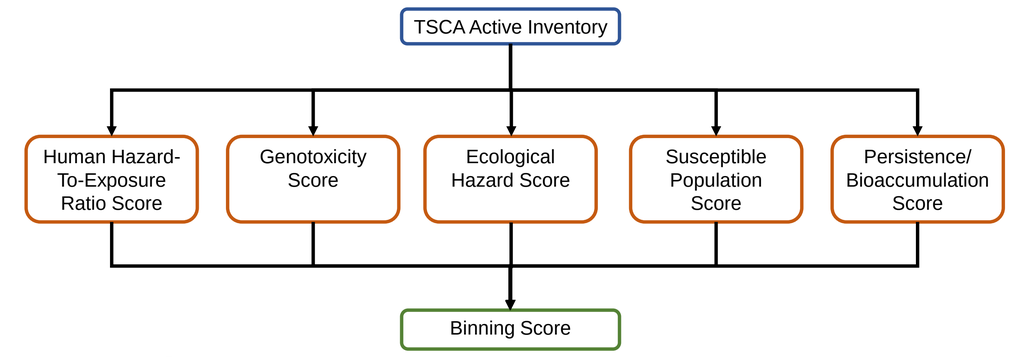
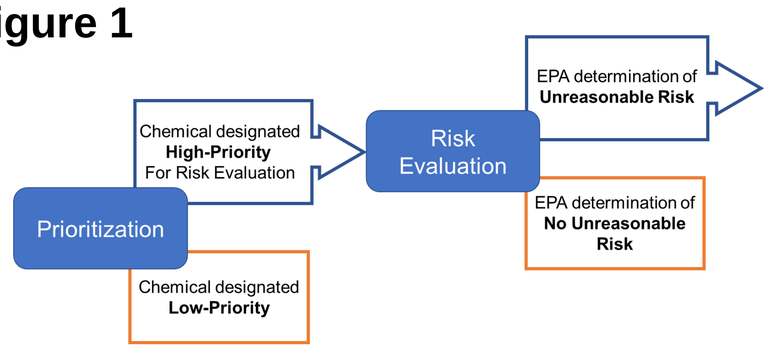


Figure 1

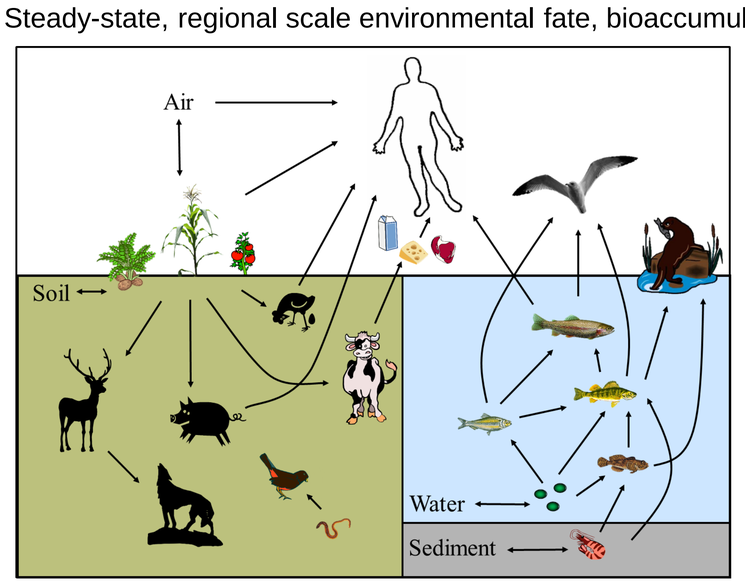


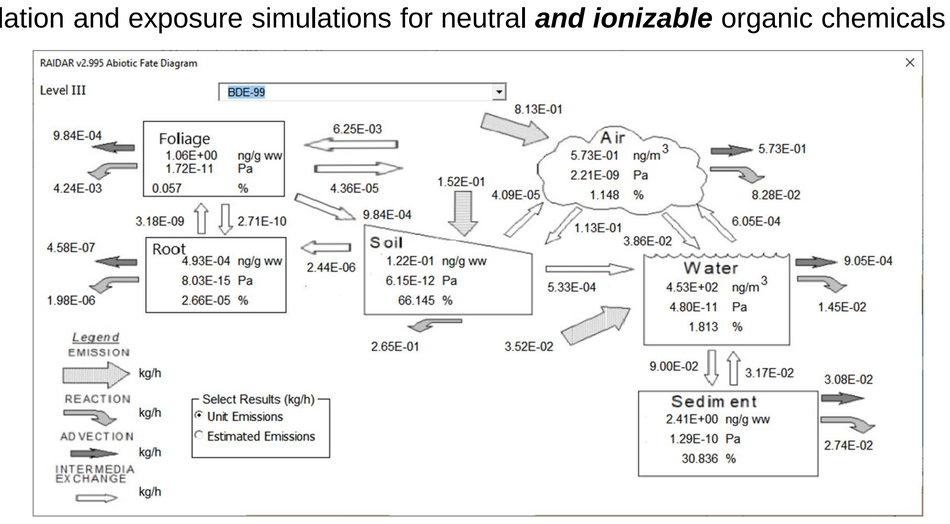
OBJECTIVE

- Compare a **holistic risk-based priority setting method** (RAIDAR) against PBT classification method results for 12,000 organic chemicals (**Fig. 3**). RAIDAR also provides overall persistence calculations and bioaccumulation metrics, e.g., BAFs, BMFs.

Figure 2

Steady-state, regional scale environmental fate, bioaccumulation and exposure simulations for neutral ***and ionizable*** organic chemicals





Physiologically-based toxicokinetic models for a range of ecological receptors *including biomagnification and biotransformation processes*

Water-ventilating AND air-breathing organisms

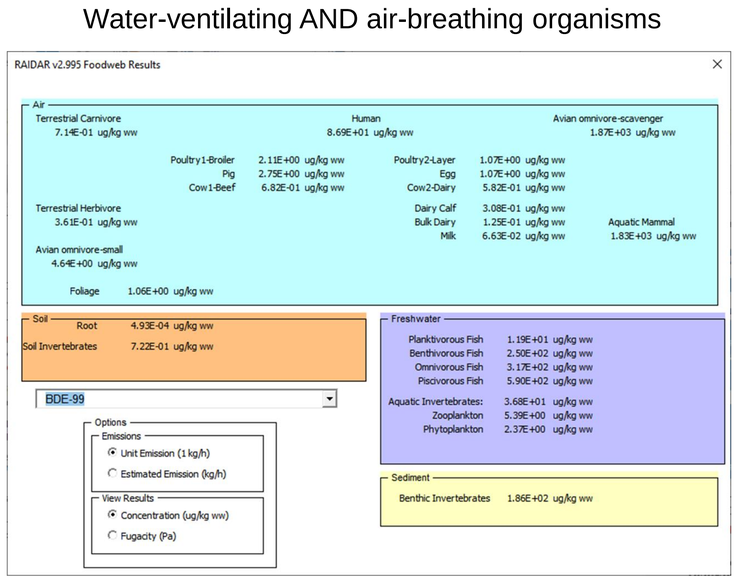
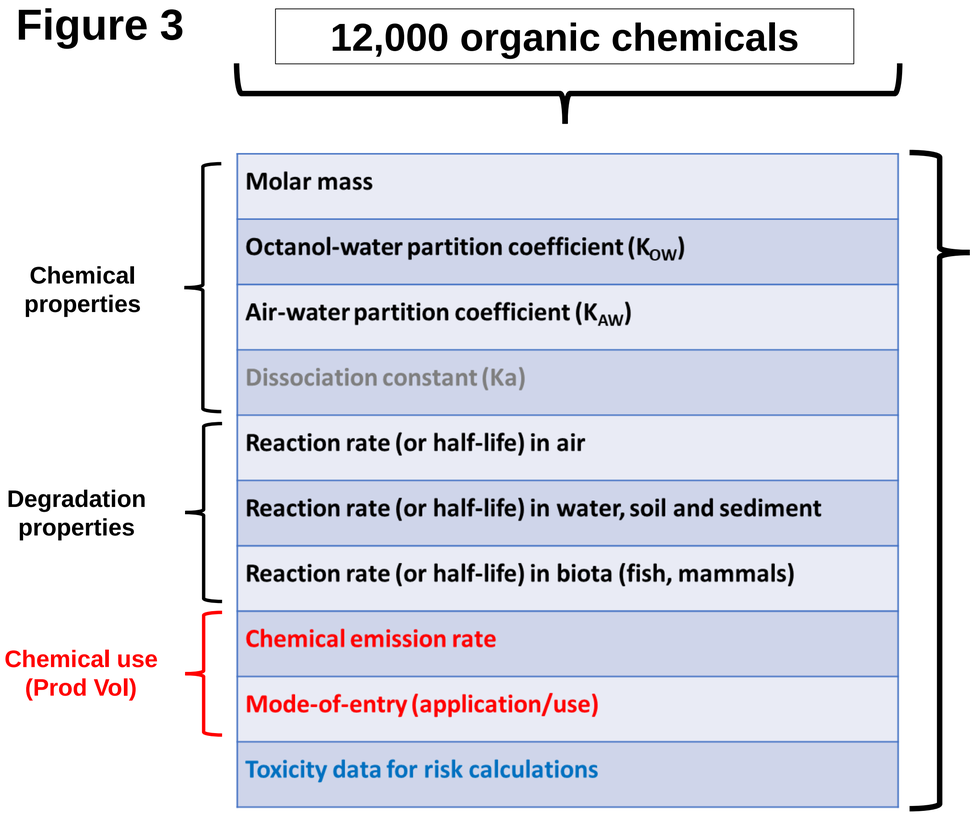


Figure 3

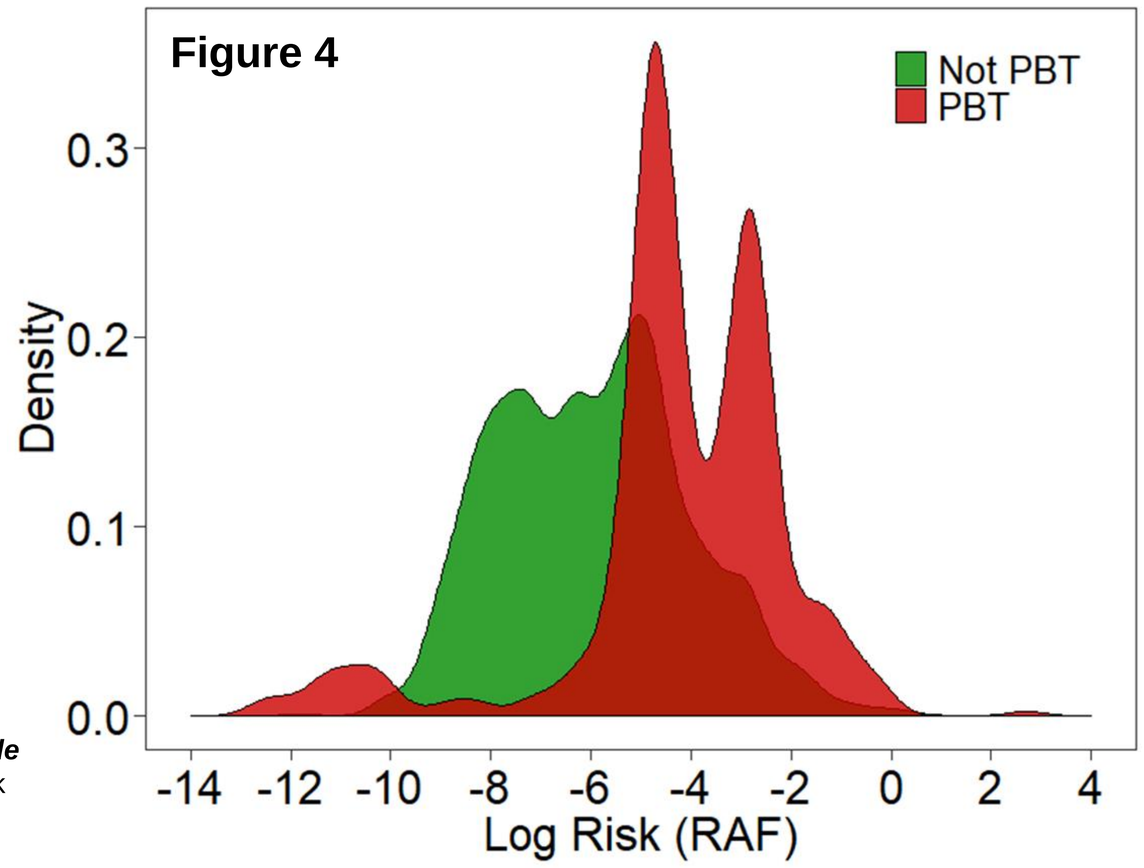


Same basic data used in both holistic and category approaches!

RESULTS

1. Category method output – PBT (vPvB) classifications
2. Holistic risk-based method output – Risk Estimate (RAIDAR Risk Assessment Factor, RAF)
3. Compare the results of the two different prioritization methods…

Figure 4



KEY FINDINGS

- RAIDAR RAFs span approximately ***18 orders of magnitude*** providing a simple means for risk-based prioritization to a wide range of ecological receptors (**Fig. 4**).
- Chemicals classified as "PBT" and "not PBT" show an ***overlap of approximately 14 orders of magnitude*** when compared based on RAFs. Many chemicals classified as "low priority" using PBT methods have risk estimates comparable to or greater than chemicals classified as "PBTs" and vice versa (**Fig. 4**).
- Significant effort and resources can be spent assessing chemicals that present negligible risk in the environment (i.e., not of concern under current use patterns), primarily due to a wide margin of exposure, while other chemicals with relatively higher potential risk are overlooked from further evaluation.

REGULATORY AGENCIES ARE ENCOURAGED TO USE READILY AVAILABLE HOLISTIC METHODS TO COMPLEMENT OTHER METHODS FOR CHEMICAL PRIORITIZATION TO MINIMIZE TYPE I AND TYPE II ERRORS

References

1. Congress, U. S., Frank R. Lautenberg Chemical Safety for The 21st Century Act. In *Public Law 114–182*, Washington D.C. **2016**.
2. US EPA. A Working Approach for Identifying Potential Candidate Chemicals for Prioritization, Washington D.C. September **2018**.
3. Arnot, J. A.; Mackay, D. Policies for chemical hazard and risk priority setting: can persistence, bioaccumulation, toxicity and quantity information be combined? *Environ. Sci. Technol.* **2008,** *42*, (13), 4648-4654.

Acknowledgements

American Chemistry Council Long-Range Research Initiative (ACC-LRI)