A high-throughput method to screen organic chemicals in commerce for emissions

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Introduction

Only chemicals which combine harmful properties with emissions in significant quantities are expected to represent a real risk to the environment and humans. A high throughput method to screen chemicals in commerce for emissions has therefore been developed, applied and preliminary evaluated.

Methods

The method builds upon the approach outlined in the EU Technical Guidance Document [1] and requires information on quantity, chemical function (industrial and use categories) and physical-chemical properties (vapour pressure, water solubility). It is applied to organic substances on various high production volume (HPV) lists within Europe, Japan, USA, Canada and OECD [2]. The uncertainty in the resulting emission scenarios are additionally estimated as vital input data remain fragmented or inaccessible.

Results

Overall results are presented for 12,616 discrete organic substances, ranked from high to low in Figure 1.

• **Fig 1A** presents the estimated overall quantity across all HPV lists. The uncertainty reflects quantities being presented as bins on the original HPV lists, often spanning orders of magnitude.

• **Fig 1B** presents the estimated total environmental emissions to air, water and soil across key stages of the life-cycle. Larger uncertainties in emission scenarios typically reflect lack of data on chemical function, which is more frequently occurring for substances produced in lesser quantities.

A number of Risk Assessment Reports (RARs) have been prepared by EU member states on individual substances of possible concern. Figure 2 shows a comparison between quantities and emission data from these RARs and our estimates for Europe alone.

• **Fig 2A** shows that estimated quantities from this study are typically higher, which partially reflect our conservative approach at an initial tier. Recent RARs may also have captured recent reductions in quantities not captured on the EU HPV list. Still, 80% and 96% of the data are within 1 and 2 orders of magnitude, respectively.

• **Fig 2B and C** illustrates the additional uncertainties that are introduced when emissions are estimated. Although these are often significant, about 60% and 80% of the data falls within 2 and 3 orders of magnitude for both air and water, respectively. In comparison, estimated emissions across all substances vary over ~10 orders of magnitude (Fig 1B).

Discussion

Following refinement, the emission screening tool will be integrated into a large effort to screen for exposure that also seeks to account for the uncertainty in other input parameters (see WE051 by Arnot et al.). The latter results are, in turn, expected to identify a subset of substances for which more accurate emission estimates are needed at consecutive tiers, facilitating a rational way forward.

Acknowledgements

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Figure 1 Estimated overall quantity (A) and environmental emissions to all media (B).

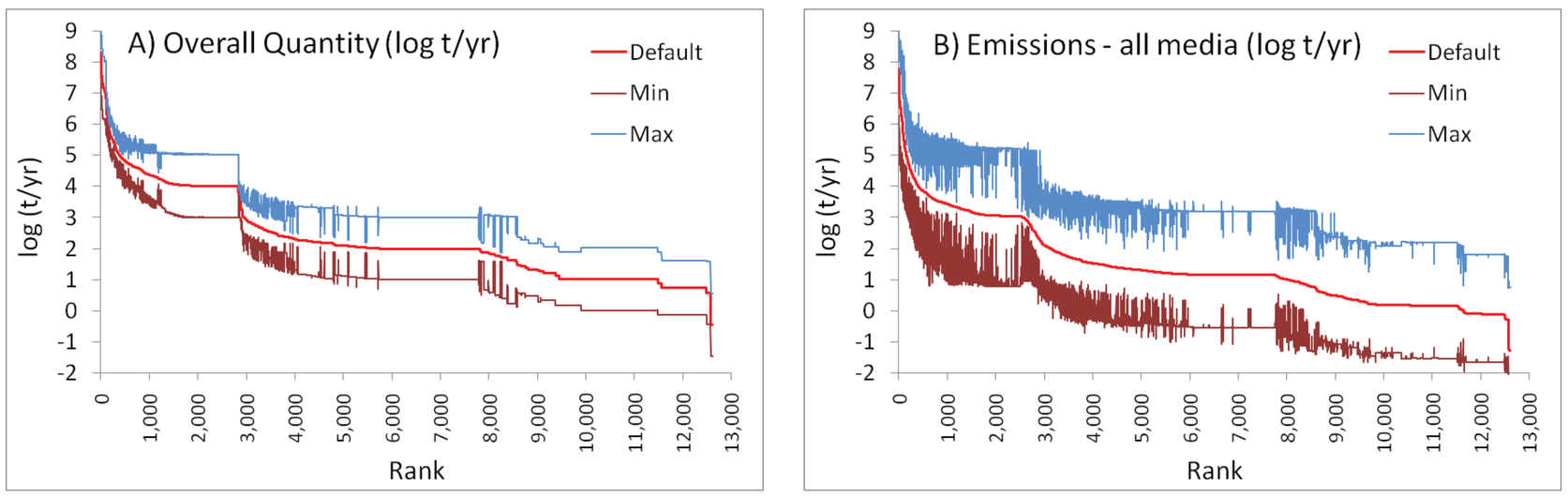
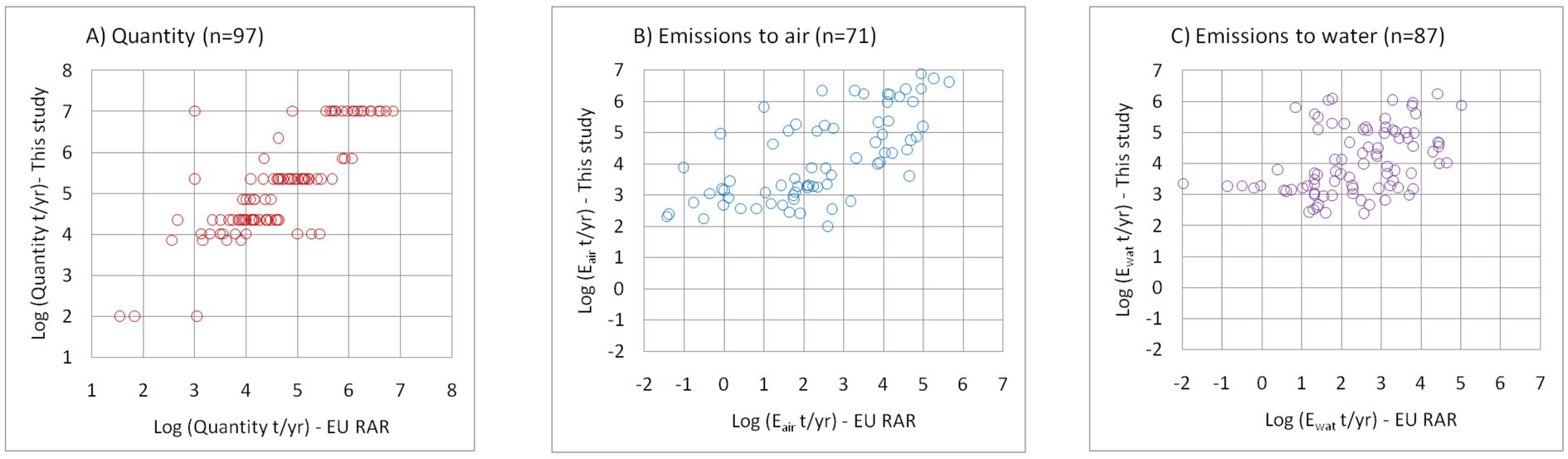


Figure 2 Comparison with estimates from various EU risk assessment reports (RARs).



References

1. ECB Technical Guidance Document on Risk Assessment; European Chemicals Bureau: 2003.
2. Brown, T. N.; Wania, F., Screening chemicals for the potential to he persistent organic pollutants: A case study of Arctic contaminants. Environ. Sci. Technol. 2008, 42, (14), 5202-5209.