Screening chemicals in commerce in the Nordic countries using multimedia fate and bioaccumulation models

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Objectives

- Emission estimates are the largest source of uncertainty in risk-based screenings of chemicals in commerce to identify potentially harmful substances.[1,2] The first objective of this study was to address this uncertainty by using more detailed information about usage of chemicals to gain better emission estimates.[3]
- The second objective was to compare two multimedia fate and bioaccumulation models; a steady-state model for an evaluative environment (RAIDAR)[4,5] and a dynamic model for the Nordic region (CoZMoMAN).[6]

Methods

- Emissions were estimated from the database for Substances in Preparations in the Nordic Countries (SPIN)[3] and a high-throughput estimation method.[1]
- Physico-chemical properties were estimated using previously published methods.[2]
- CoZMoMAN was run with constant emissions for 70 years, and a time step of 1h.
- Predicted chemical concentration in humans was used as an endpoint. In CoZMoMAN the human was a 29-year old man born 41 years after emission start.

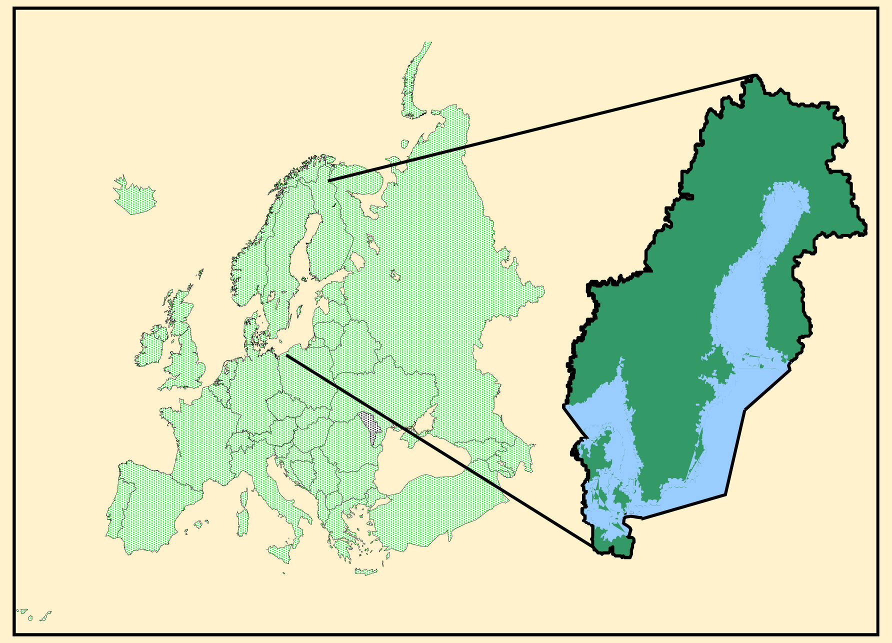

Figure 2: Map of Europe with national borders (left) and model domain of CoZMoMAN (right).[6]

Screened Chemicals

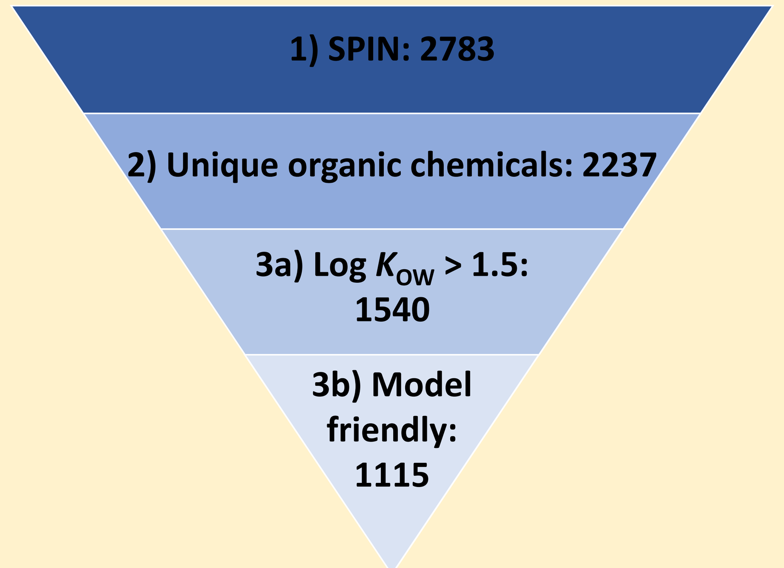

Figure 3: Schematic illustration of the number of chemicals that were included in the study.

The chemicals were filtered in the following way:

1) There were 2783 chemicals registered in SPIN as used in Norway, Sweden, Finland and/or Denmark in the years 2000-2007.[3]
2) Duplicate, inorganic, and organometallic substances were removed, leaving 2237 chemicals.
3) The CoZMoMAN model is unstable for chemicals that react quickly or that are very volatile or hydrophilic. All chemicals with log K_{OW} > 1.5 were included (n=1540), and 1115 of these chemicals could be simulated.

RAIDAR & CoZMoMAN

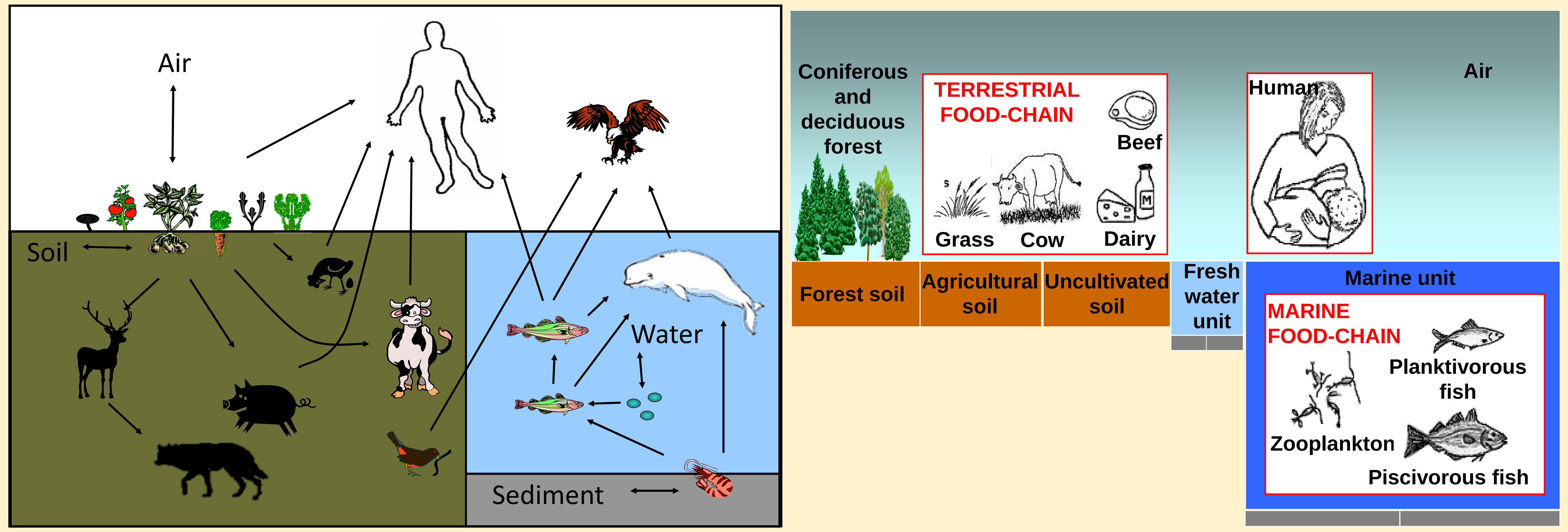

Figure 1: Schematic illustrations of compartments in RAIDAR[4,5] (left) and CoZMoMAN[6] (right).

Ranking of Chemicals

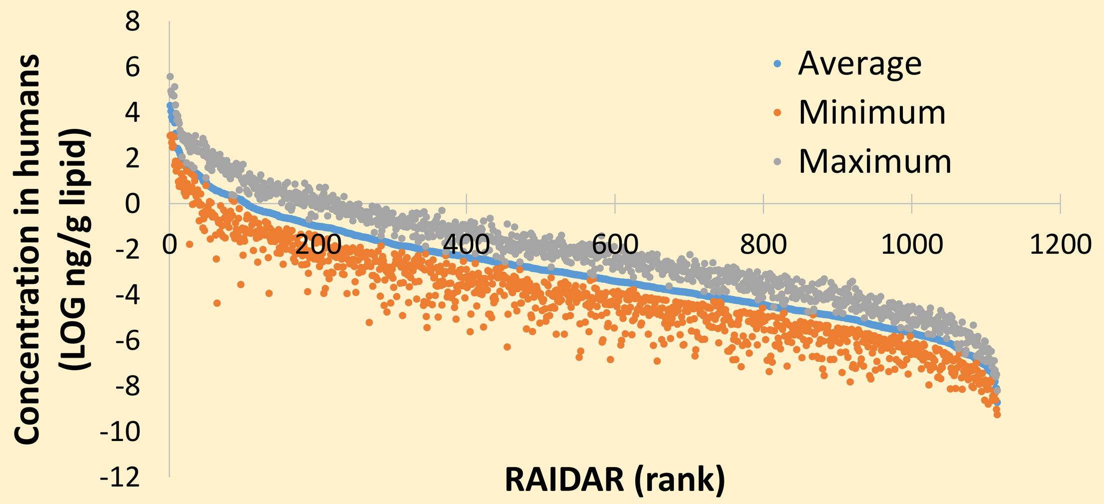

Figure 4: Predicted concentrations in human from RAIDAR for the 1115 chemicals, based on minimum, average, and maximum emission scenarios.

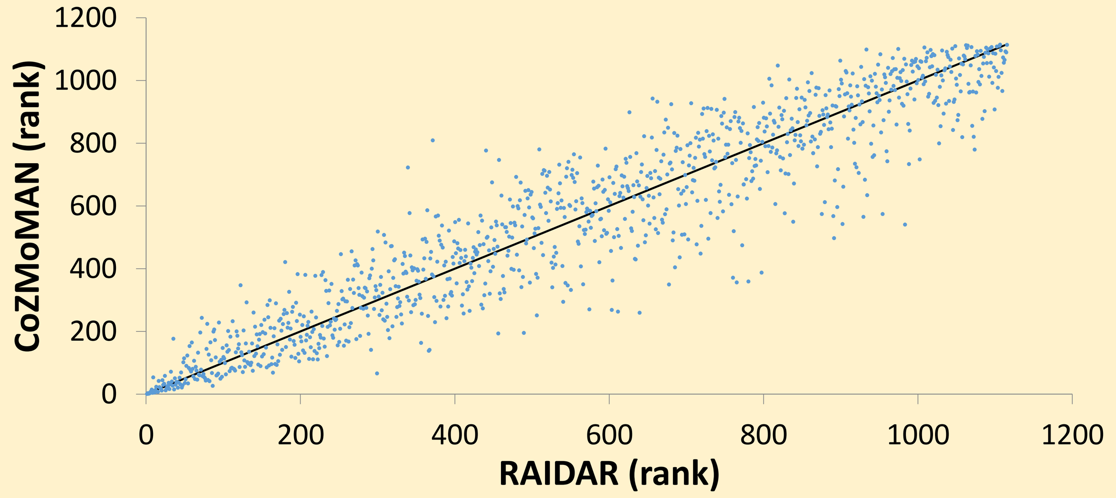

Figure 5: Predicted relative rank of the 1115 chemicals from CoZMoMAN and RAIDAR based on predicted concentration in humans.

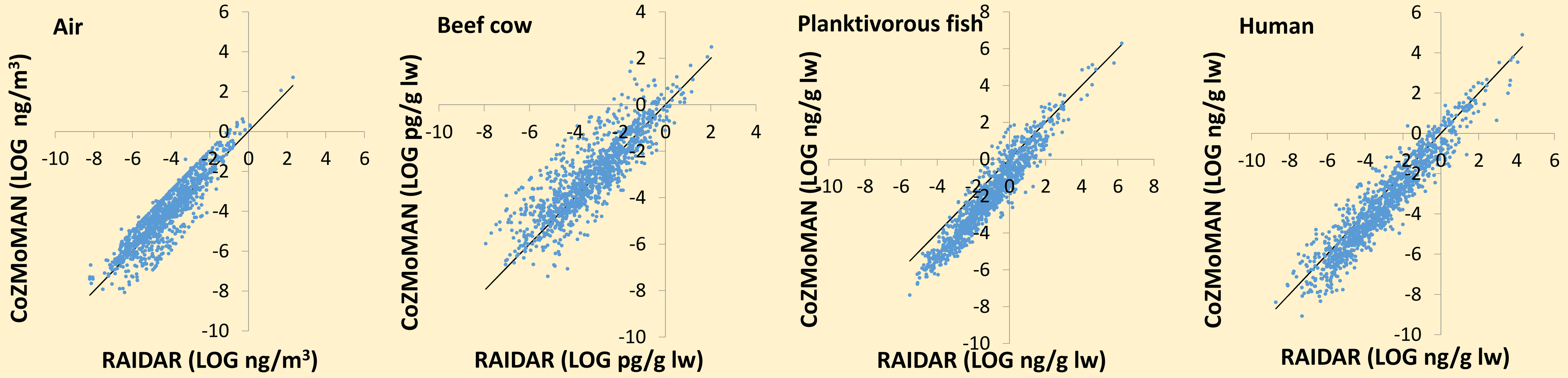

Figure 6: Predicted concentrations in air, beef cow, piscivorous fish, and human (male) from RAIDAR and CoZMoMAN for the 1115 chemicals, based on average emission scenarios. The diagonal line is the 1-to-1 line, lw = lipid weight.

References: [1]Breivik, K. et al. *J. Environ. Monit.* 2012, 14, 2028-2037. [2]Arnot, J. et al. *Environ. Health Persp.* 2012, 120, 1565-1570. [3]SPIN-substances in preparations in Nordic countries, www.spin2000.net. [4]Arnot, J. et al. *Environ. Sci. Technol.* 2006, 40, 2316-2323. [5]Arnot, J. and Mackay, D. et al. *Environ. Sci. Technol.* 2008, 42, 4648-4654. [6]Breivik, K. et al. *Environ. Int.* 2010, 36, 85-91. **Acknowledgements:** We thank the Norwegian Research Council (196191/S30) for financing the study, and Trevor Brown for assistance.

The «Top100» chemicals

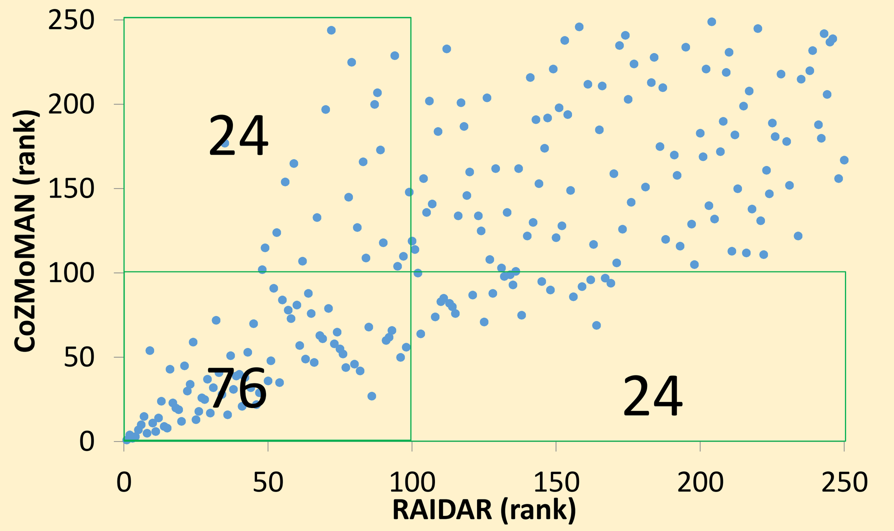

Figure 7: The predicted rank of the chemicals in CoZMoMAN and RAIDAR (detail from Fig. 5). The green squares indicate the Top 100 chemicals, with 76 chemicals ranked among Top 100 in both models.

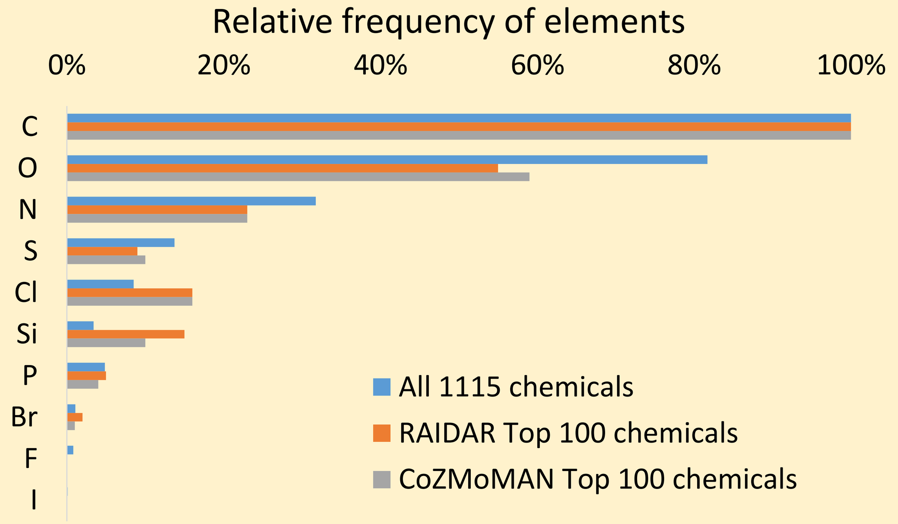

Figure 8: The relative frequency of chemicals containing selected elements.

Summary of Preliminary Results

- The predicted concentrations in humans for the 1115 chemicals ranged over 13 orders of magnitude with RAIDAR (Fig. 4) and 14 with CoZMoMAN, respectively. The average range between minimum and maximum emissions (and hence also predicted concentration in humans) was 2 orders of magnitude (Fig. 4).
- Overall, there was a good correlation in the relative ranking of the chemicals between the two models based on the predicted concentration in humans (Fig. 5). The absolute concentrations also agreed well, with a tendency for higher predicted concentrations in humans from RAIDAR than from CoZMoMAN (Fig.6). RAIDAR predicted somewhat higher concentrations in the aquatic food-chain, and somewhat lower concentrations in the agricultural food-chain than CoZMoMAN (Fig. 6)
- 76 chemicals were ranked among the Top 100 by both models (Fig. 7), and many of these were either organosilicone or chlorinated compounds (Fig. 8). The Top 100 chemicals also included already known contaminants such as PCBs (included as reference), volatile methyl siloxanes, hexabromocyclododecane, chlorpyrifos, and medium-chained chlorinated paraffins.

Future Research

- Detailed evaluation of results, with exploration of key differences between models.
- Sensitivity- and uncertainty analysis, in particular to identify the contribution of uncertainty in the emissions to the uncertainty in the predicted ranking.
- Detailed investigation of the chemicals that are ranked to be of highest concern in the Nordic environment.