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

Ingjerd S. Krogseth,[1] Knut Breivik,[1,2] Jon Arnot,[3,4] Frank Wania[3]

[1]NILU – Norwegian Institute for Air Research, The Fram Centre, Tromsø and Kjeller, Norway; [2]University of Oslo, Oslo, Norway; [3]University of Toronto Scarborough, Toronto, Canada; [4]Arnot Research & Consulting, Toronto, Canada

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 reduce 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]

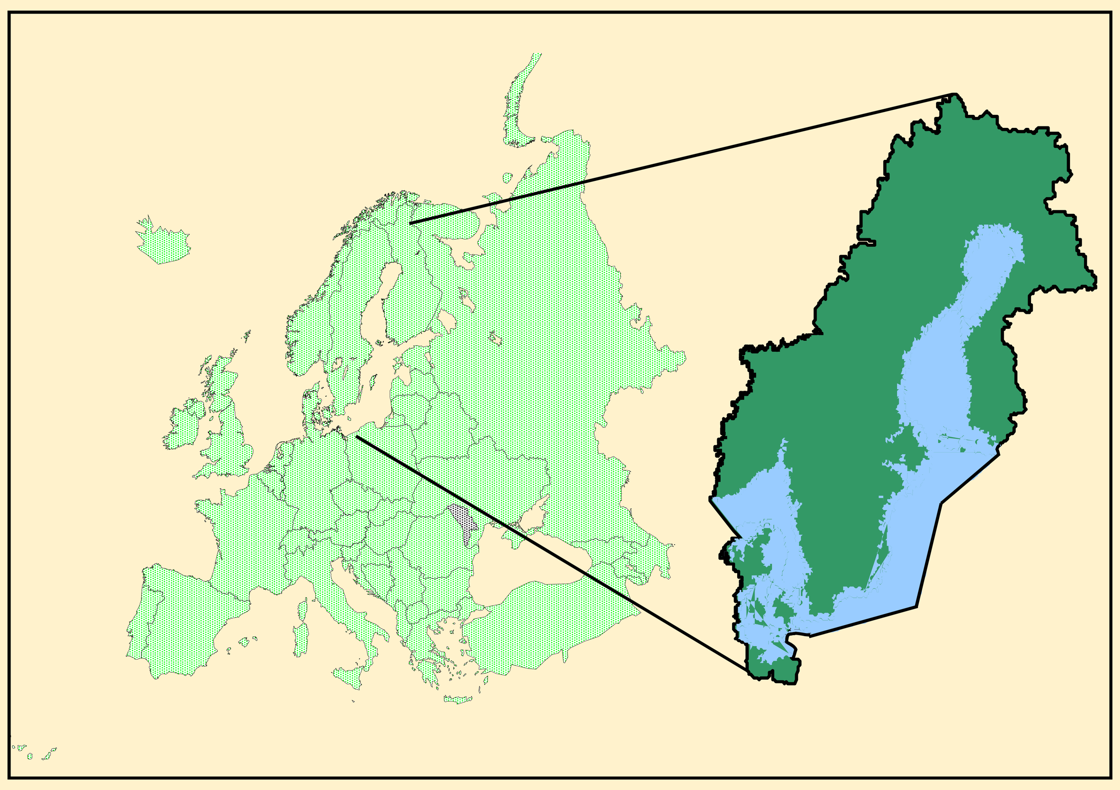

Figure 1: Map of Europe with national borders (left) and model domain of CoZMoMAN (right).[6]

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 simulation time step of 1 hour.
- Predicted chemical concentrations in humans was used as an endpoint. In CoZMoMAN the human was a 29-year old female born 41 years after emission start.

The Chemicals

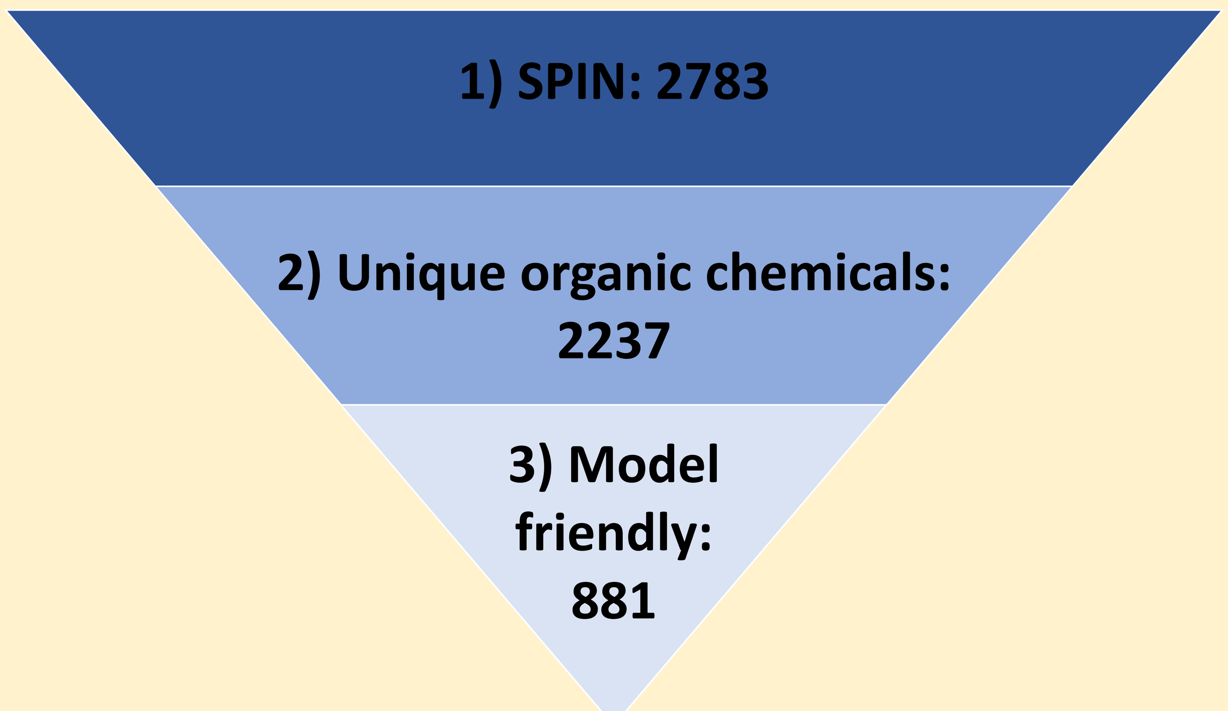

Figure 2: Schematic illustration of the number of chemicals that were included in the study.

The chemicals were filtered in the following way (Fig. 2):

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 can become unstable for chemicals that react quickly or that are very volatile or hydrophilic. Hence, initially 881 model-friendly chemicals were included, i.e. where there were no numerical instabilities. More chemicals could possibly be added later.

RAIDAR vs. CoZMoMAN

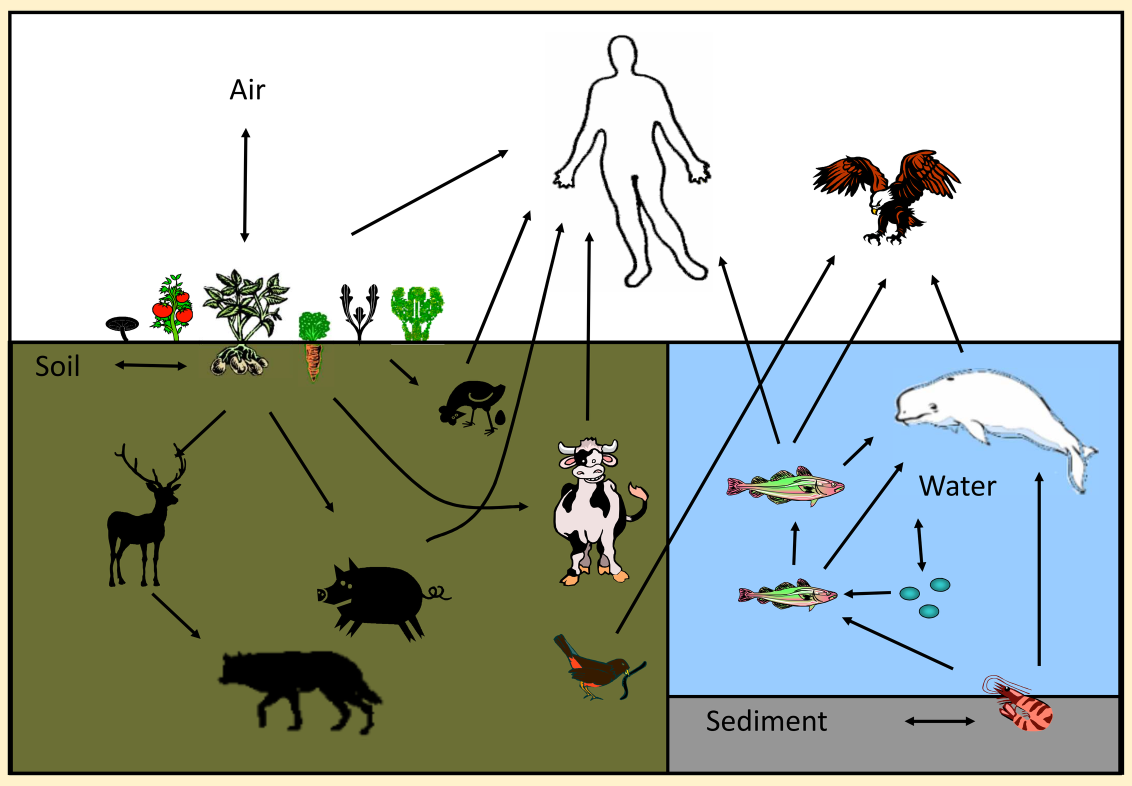

Figure 3: Schematic illustration of compartments in RAIDAR.[4,5]

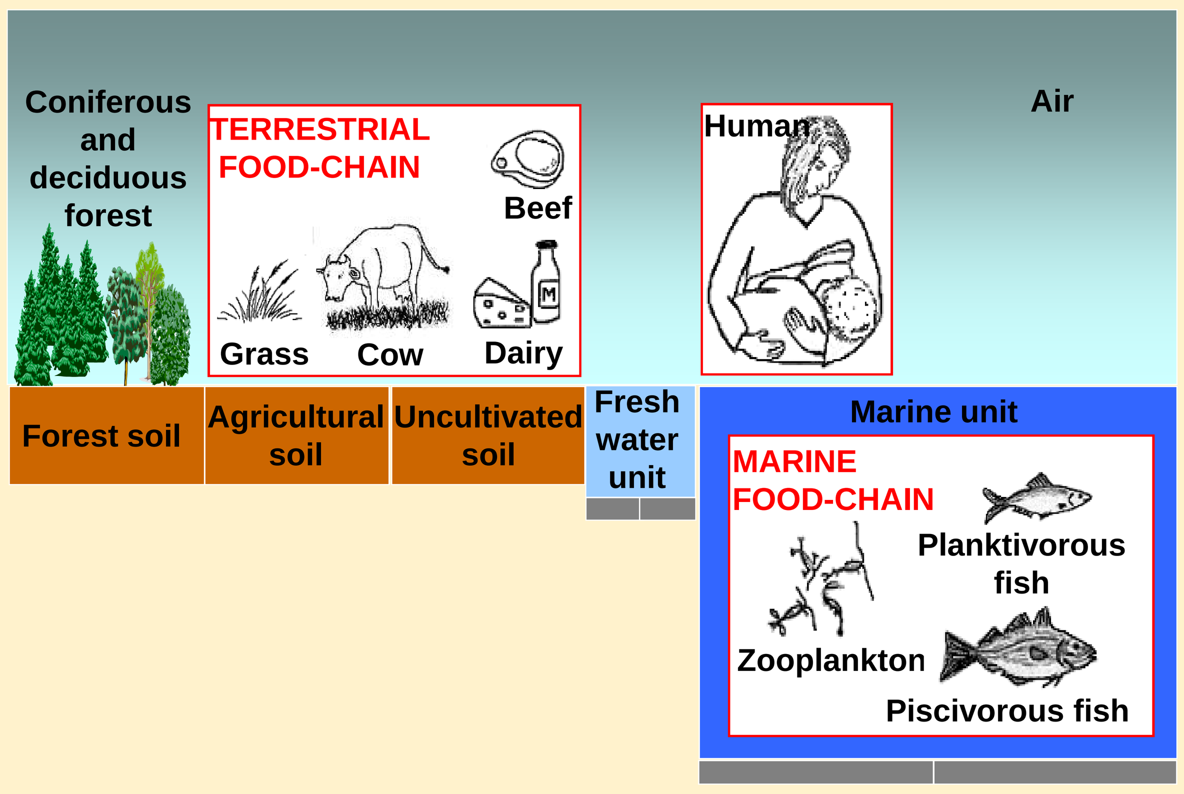

Figure 4: Schematic illustration of compartments in CoZMOMAN.[6]

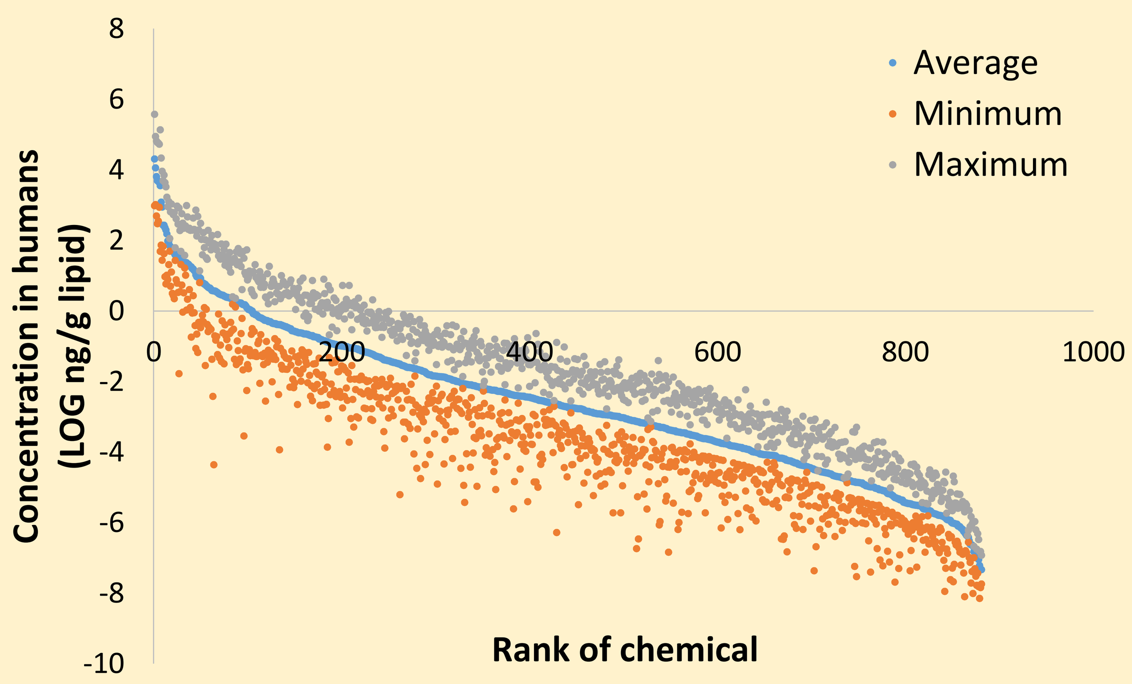

Figure 5: Predicted concentrations in human from RAIDAR for the 881 chemicals, based on minimum, average, and maximum emission scenarios.

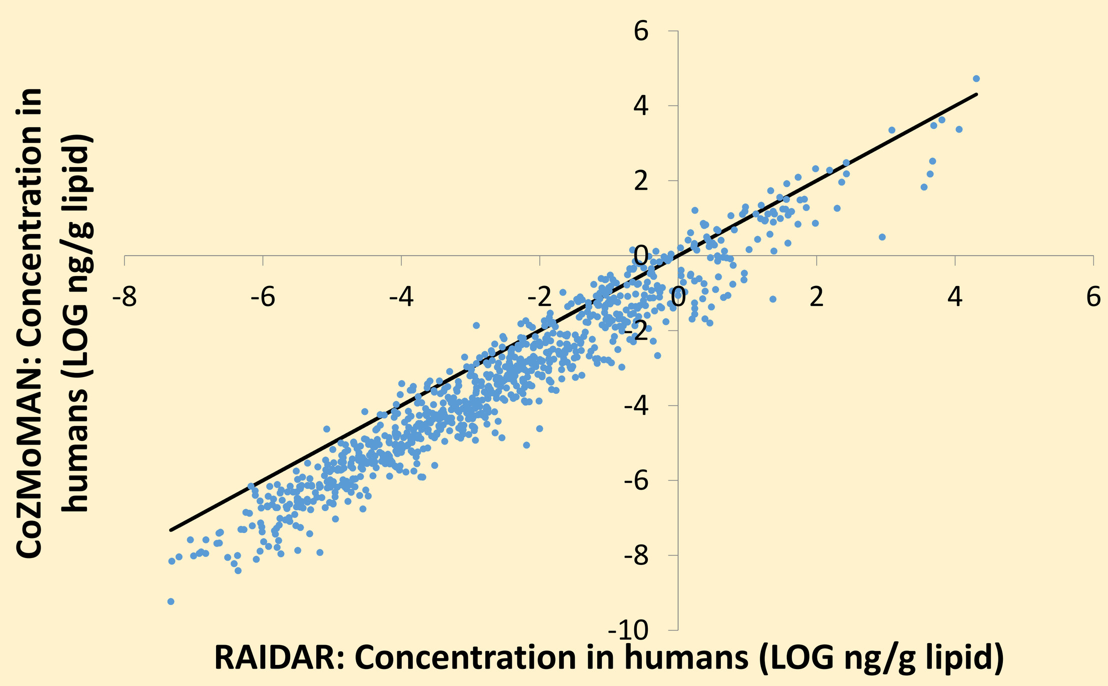

Figure 6: Predicted concentrations in human from RAIDAR and CoZMoMAN for the 881 chemicals, based on average emission scenarios. The diagonal line is the 1-to-1 line.

The Top 100 Chemicals

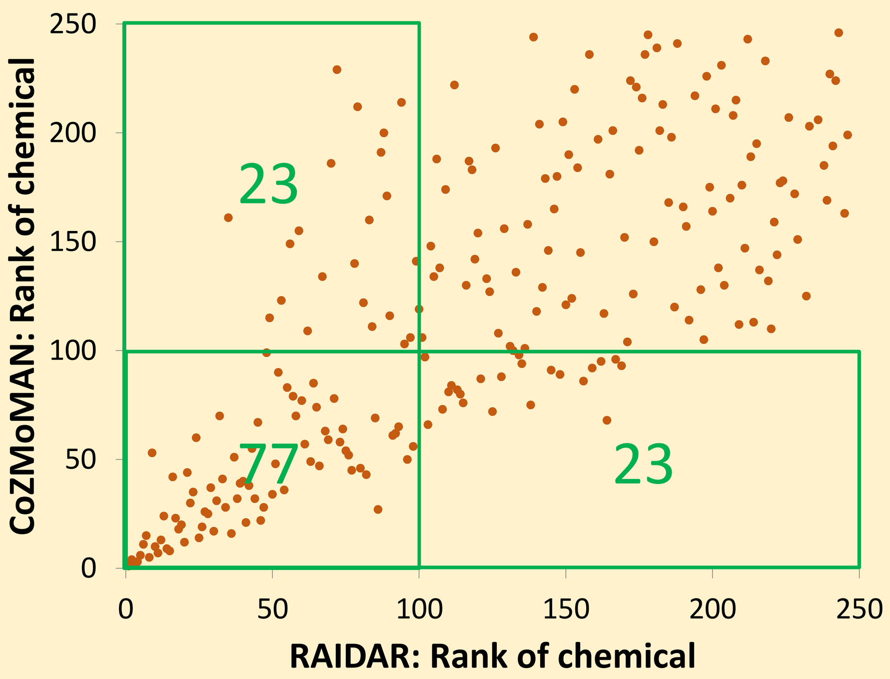

Figure 7: The predicted rank of the chemicals in CoZMoMAN and RAIDAR. The green squares indicate the Top 100 chemicals, with 77 chemicals ranked among Top 100 in both models.

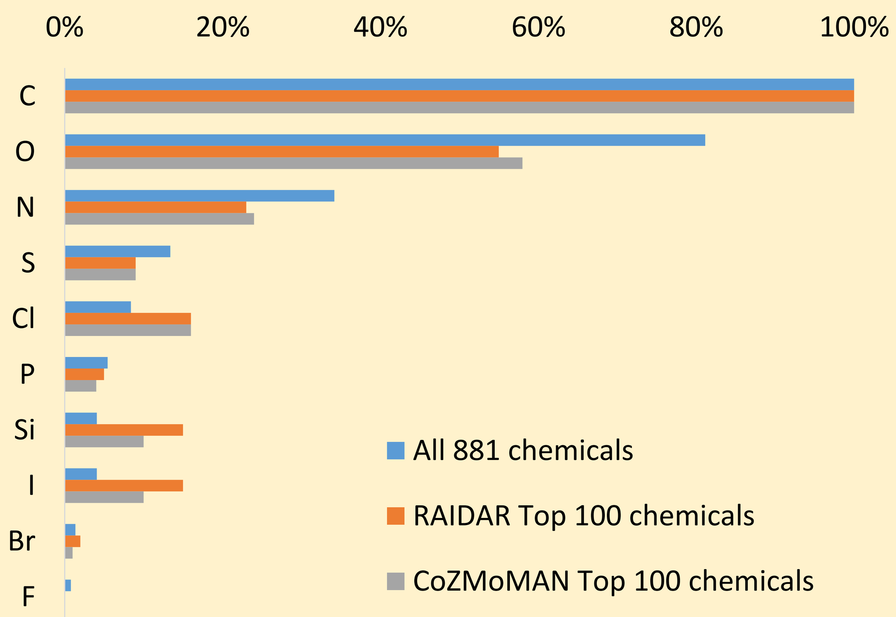

Figure 8: The relative frequency of chemicals containing selected elements.

Summary of Preliminary Results

- The average range between minimum and maximum emissions (and hence also predicted concentration in humans) was 2 orders of magnitude (Fig. 5).
- The predicted concentrations in humans for the 881 chemicals ranged over 12 orders of magnitude with RAIDAR (Fig. 5) and 14 with CoZMoMAN, respectively.
- Overall, there was a good correlation in the ranking between the two models (Fig. 6). 77 chemicals were ranked among the Top 100 by both models (Fig. 7).
- The elements Chlorine, Silicon, and Iodine were more frequent among the Top 100 chemicals than among all 881 chemicals (Fig. 8).

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.
- Investigation of different endpoints for ranking of the chemicals, such as concentration in various physical matrices and biota.
- Detailed investigation of the chemicals that are ranked to be of highest concern in the Nordic environment.

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.