Probabilistic Risk Characterisation for Chemical Mixtures:

Hierarchical Integration of Models for Similar and Different Mode of Action

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HIGHLIGHTS

- Nature-based Solutions (NbS) for urban waste-water treatment (UWWT) have been tested with six technical pilots
- We developed a multi-level probabilistic model for mixture risk calculation
- The model integrates traditional CA and IA concepts in a seamless and traceable way

BACKGROUND

- EU project MULTISOURCE: Modular tools for integrating enhanced natural treatment solutions in urban water cycles [1]
- Technical pilots in six countries: BE, DE, FR, IT, NO, US
- Example: Pilot "FR" (Lyon, France) (Fig. 1)
- Challenge: assess reduction in environmental risk for both single substances and mixtures
- Aim of Task 2.2: explore alternative approaches to mixture risk characterisation with probabilistic modelling methodology

Figure 1. Technical pilot "FR": treatment of raw wastewater and sludge in wetlands. Source: [1].

DATA PROCESSING

- Measured concentrations: in influent and effluent waters
- Data compliation and harmonisation: NIVA Risk Assessment database [2]
- Extrapolation to environmental conc.: country-specific dilution factors
- **Risk Quotient (RQ)** = concentration / [predicted no-effect concentration]
- Prioritisation: 12 substances selected by highest RQ
- Substances allocated to groups, preferably by Mode of Action
- Modelling methodology: Object-oriented **Bayesian network (BN)** [3]

PROBABILISTIC CHARACTERISATION OF MIXTURE RISK

- Definition of **Risk**: **probability (P)** of **RQ > Threshold$_{RQ}$** (Fig. 2B)

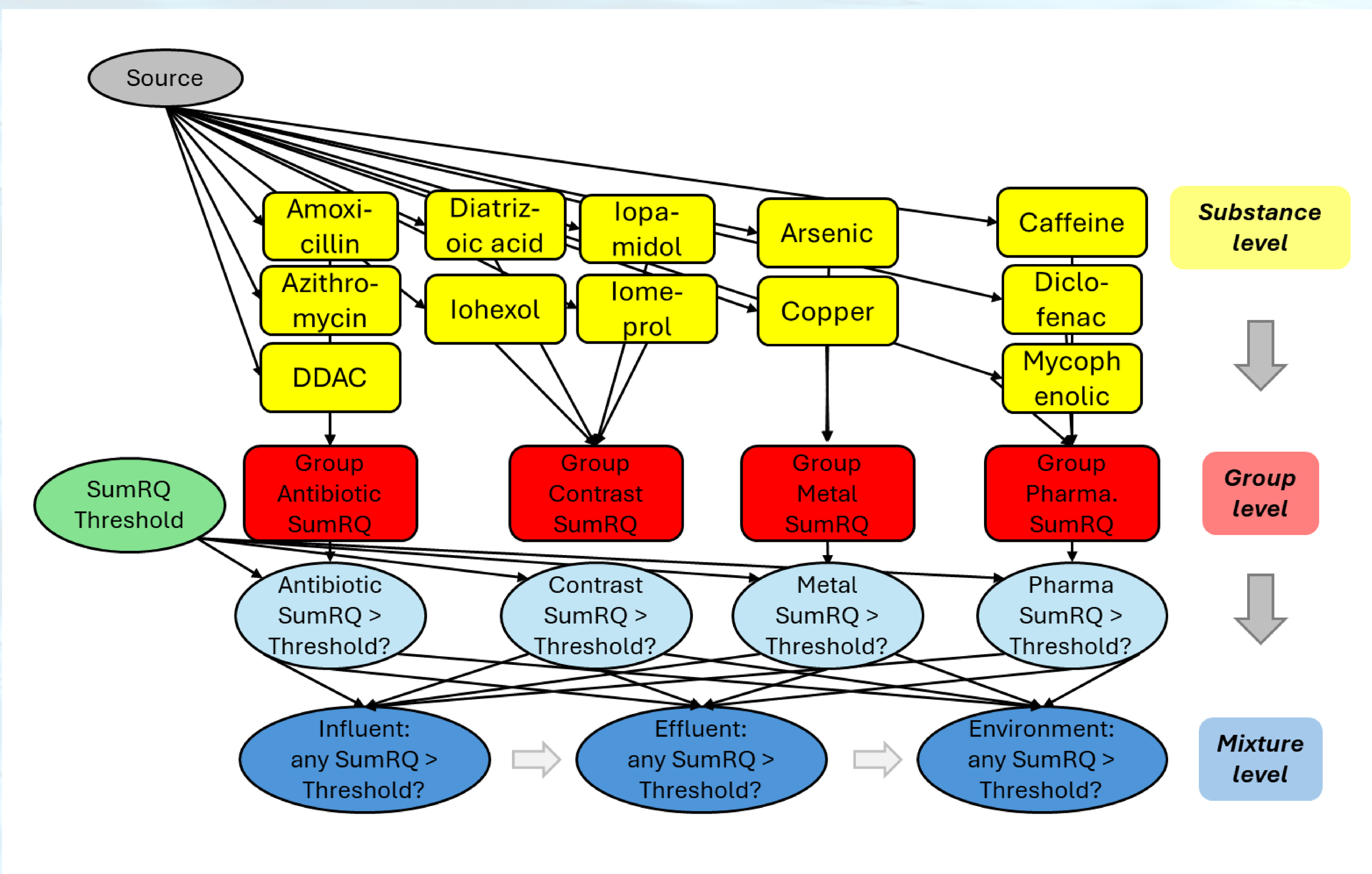
Three approaches to mixture risk:

- (1) **Sum of RQ**: based on Concentration Addition (CA) concept
- (2) **Joint P of exceedance**: based on Independent Action (IA) concept
- (3) **Integrated approach** (Fig. 2A):
  - Within groups: Sum of RQ (Fig. 2C)
  - Across groups: Joint P of any SumRQ > Threshold$_{SumRQ}$ (Fig. 2D)

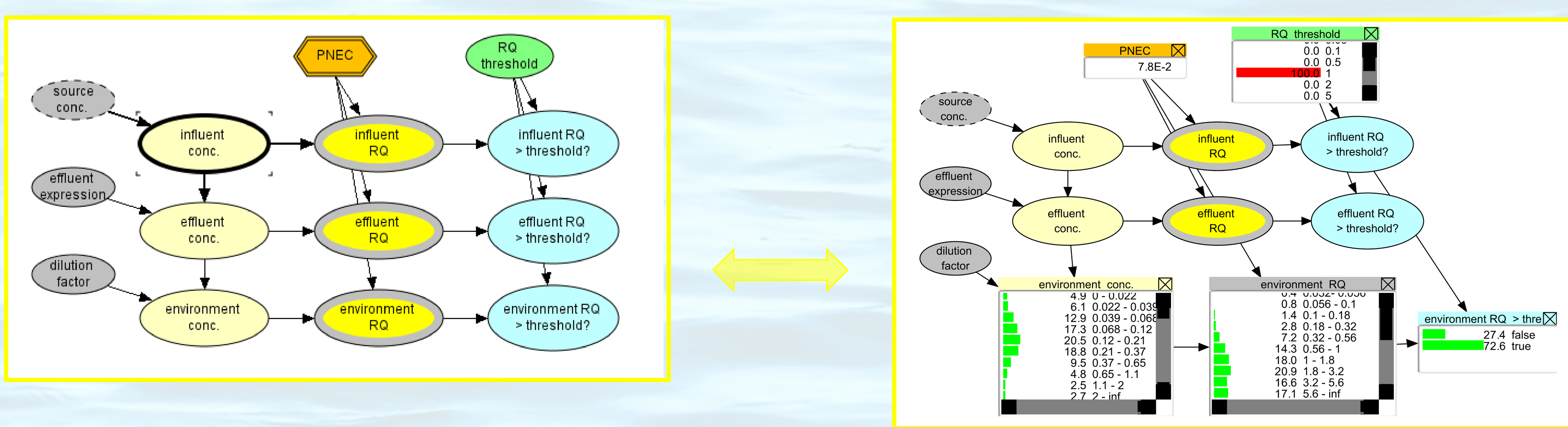
HIERARCHICAL RISK MODEL

Figure 2. Hierarchical mixture risk model: Object-oriented Bayesian network

(A) Conceptual diagram for the **Integrated approach** to mixture risk.



(B) Substance-level risk: Probability of (RQ > threshold$_{RQ}$).

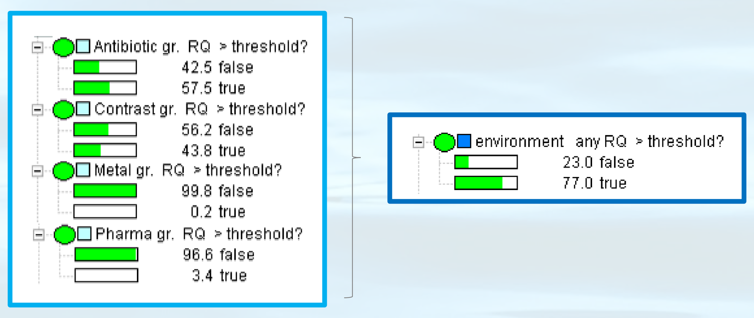


(C) Group-level risk: Probability of (SumRQ > threshold$_{SumRQ}$).

$SumRQ_{Antibiotic} = RQ_{Amoxi} + RQ_{Azith} + RQ_{DDAC}$

(D) Mixture-level risk: Joint probability of (SumRQ > threshold$_{SumRQ}$) for ANY group.

$$\text{Joint P} = 1 - (1 - P(SumRQ_{Antibiotic} > Threshold_{SumRQ})) \times (1 - P(SumRQ_{Contrast} > Threshold_{SumRQ})) \times (1 - P(SumRQ_{Metal} > Threshold_{SumRQ})) \times (1 - P(SumRQ_{Pharma} > Threshold_{SumRQ}))$$

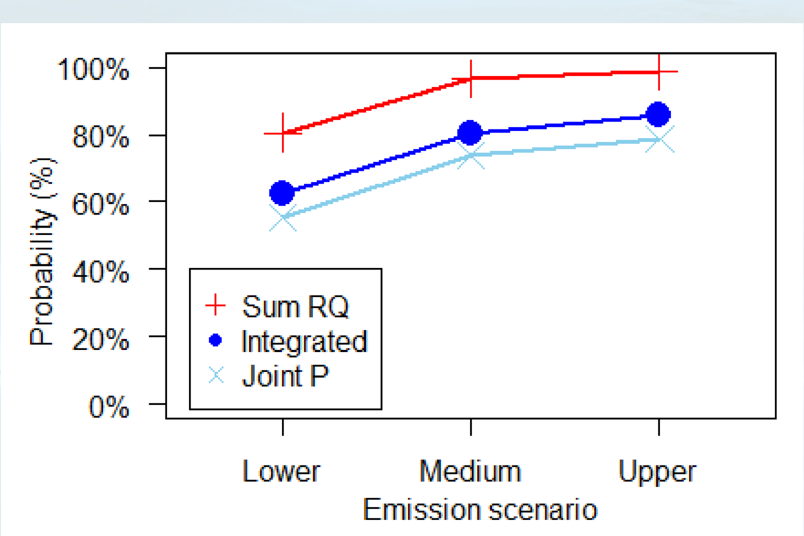


MODEL PREDICTIONS

The BN model can efficiently calculate risk for, e.g. (Fig. 3):

- The three risk levels (Fig. 2B-D)
- The 3 mixture risk approaches: SumRQ, JointP and integrated
- Scenarios of chemical emission to treatment pilot: here based on range of observed concentrations (± 10%)

Figure 3. Mixture risk predictions for pilot "FR" with emission scenarios. Threshold$_{SumRQ}$ = 2.



CONCLUSIONS AND OUTLOOK

Exploration of mixture risk predictions for MULTISOURCE pilots suggests:

- The SumRQ approach gives a stricter risk characterisation than JointP
- The integrated approach provides a compromise
- The grouping of substances enables more insights into mixture risk

Further work will address:

- Sensitivity of the model: to substance grouping, discretisation, priors, etc.
- Expansion of the model: more substances, more locations, etc.
- Diagnoistic use of the model: identify risk drivers and uncertainties
- Adaptation of the model to new projects, e.g. CEFIC-LRI ECO66 ENCORE (Poster 3.15.P-Th242)

REFERENCES

[1] MULTISOURCE pilot "FR": https://multisource.eu/raw-wastewater/.
[2] NIVA Risk Assessment database; see https://www.niva.no/source-to-outcome-predictor.
[3] HUGIN EXPERT (Bayesian network software); www.hugin.com.
[4] Moe SJ, Benestad RE & Landis WG 2022. Robust risk assessments require probabilistic approaches. *Integrated Environmental Assessment and Management* 18:1133–1134. DOI: 10.1002/ieam.4660.

MULTISOURCE

This project has received funding from the European Union's Horizon H2020 innovation action programme under grant agreement 101003527.