Assignment – Aggregate Exposure Pathway (AEP) module of the STOP

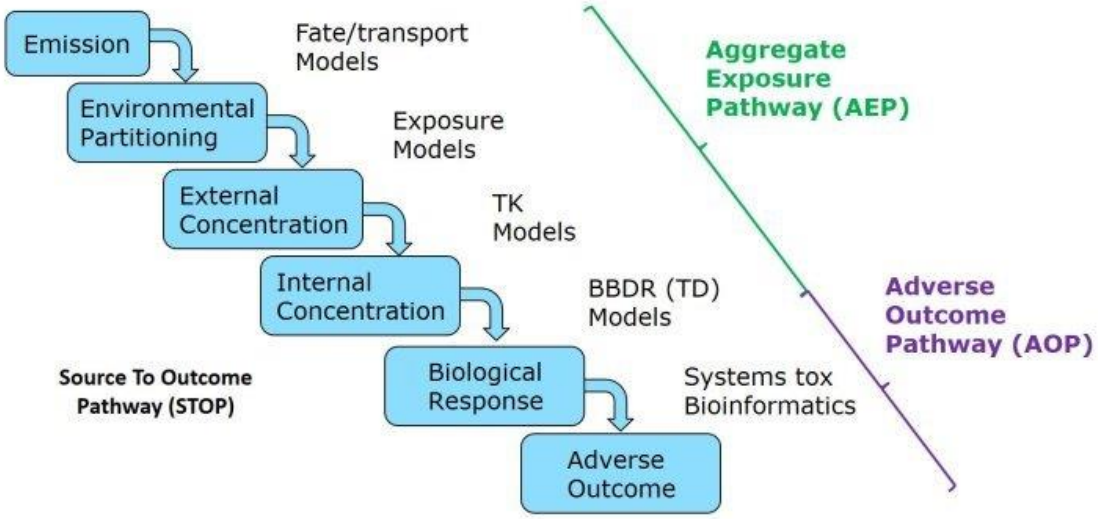

Figure1. Source to Outcome Pathway (STOP) represented by the Aggregate Exposure Pathway (AEP) and the Adverse Outcome Pathway (AOP). Abbreviations: TK-Toxicokinetic models, TD-toxicodynamic models, BBDR – Biologically based dose response models.

Assignments descriptions:

The assignment contains one theoretical and one practical (computational) task that will form the basis for discussion in the follow-up interview (2nd. Interview). The theoretical task (Task 1) is an opportunity for you to describe how your expertise and technical skillset can be used to develop the Aggregate Exposure Pathway (AEP) as one of two parts of the Source To Outcome Pathway (STOP) – see figure 1. This task should be prepared as a powerpoint presentation (maximum 10 min.) during the 2.nd interview as basis for more in-depth discussion. This task has already been provided.

The practical task (Task 2) will provide you with an opportunity to demonstrate your coding and documentation skills. In this task, you are asked to provide code, coding documentation and share this by github ahead of the interview. The candidates will have 4 working days to complete the assignment and dates for providing the last task description will be decided in consultancy with the candidates.

Task 2. Develop a miniaturized model workflow (Computational task). Develop a miniaturized workflow in R (rstudio) that import and visualize a spatio-temporal exposure data set, perform predictions of concentrations in different environmental

compartments and visualize the predictions on a map using suitable R-packages. The assignment is split into three (3) parts to allow you to solve either one, two or all subtasks (depending on your computational proficiency). Information about exposure data, prediction of external concentrations and visualization can be obtained from open literature or information provided herein (see references for some examples).

A) Import and visualize spatio-temporal exposure data

1. Import the assembly of exposure data (file: Exposure_data_AEP.xlsx) from Zenodo (https://doi.org/10.5281/zenodo.11093687) into the R (Python) environment.
2. Check the meta information in Zenodo (description) and the information provided in the xlsx sheets "README" to understand the data and relevant information to the data sets.
3. Import the datasets and integrate data (if needed).
4. Visualize the spatio-temporal data set for MCPA (STRESSOR_ID: 21) in one or more suitable figure(s) to display the spatial variance, temporal variance and spatio-temporal variance of the data.

Specifications for the spatio-temporal analysis:

The Spatio-temporal analysis of concentrations of chemicals in Freshwater (Column: MEASURED_VALUE and MEASURED_UNIT) should be performed for each location (Column: SITE_CODE) and CHEMICAL (Column: STRESSOR_NAME), and account for different sampling dates (Column: SAMPLE_DATE). The Columns "ENVIRONMENTAL_CON_ID", "ENVIRONMENTAL_COMPARTMENT", "STRESSOR_ID", CAS and INCHIKEY provide additional information for the data set.

B) Predict tissue concentrations of chemicals in fish.

1. Summarise the temporal exposure data in a table (e.g. mean, maximum, minimum, standard deviation, 5 and 95% percentile) for each location (SITE_CODE) and chemical (STRESSOR_NAME).
2. Fetch chemical properties for the chemicals using the r-package Webchem (CRAN - Package webchem (r-project.org)) or other API-supported service to perform further analysis.
3. Predict the tissue concentrations of the chemical in fish (Cf) on basis of the mean water concentration (Cw) using the following equation:

   Concentration in fish (Cf): $Cf = Cw * 10^{(0.76 \times \log P - 0.23)}$, unit: ug/kg tissue

   (Note: log P, Log KOW, XlogP refer to the same parameter)

4. Add the predicted values to the data set and display the table in a visually appealing table format. Store the data table to disk.

C) Visualize the values of Cw and Cf on a map.

1. Display the data from the table generated in the former task on a map using the geo-positioning information provided.

References

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