

# Applying CREED criteria to national and European databases in consultancy projects

March 24, 2026

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**Leonard Osté**



Expertise:

- Natural background concentrations and bioavailability
- Prioritise contaminants of emerging concern
- Assessment of discharges
- Water and substance balances for aquatic systems



**Leonard Osté**

Environmental chemist

**We often use environmental data in our projects, from:**

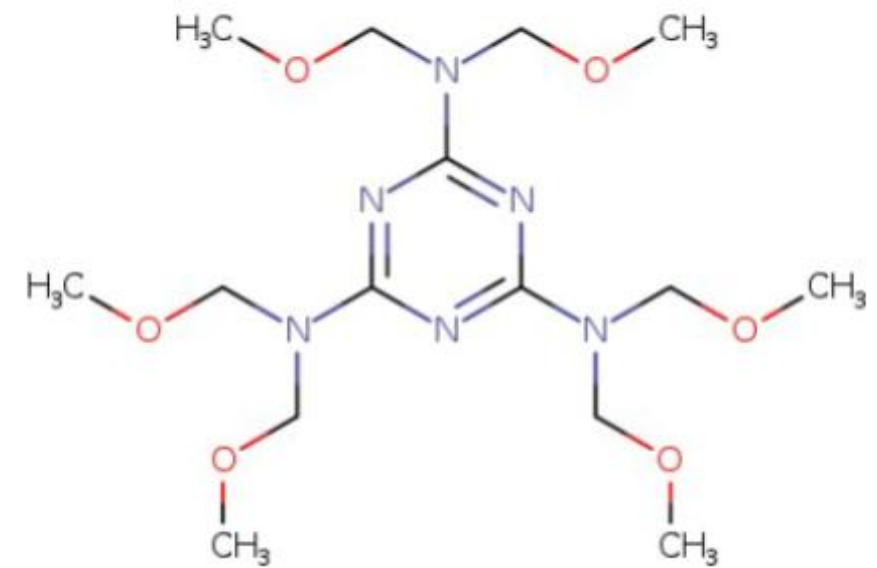
- Data producers
- National databases
- European databases



## Data from dataproducers:

- Define the purpose: to characterize the occurrence of HMMM, and, if possible, distinguishing spatial and temporal trends.
- Data received from Rijkswaterstaat (national water authority), regional water authorities and the drinking water companies (RIWA).

## Occurrence of HMMM



hexamethoxymethylmelamine

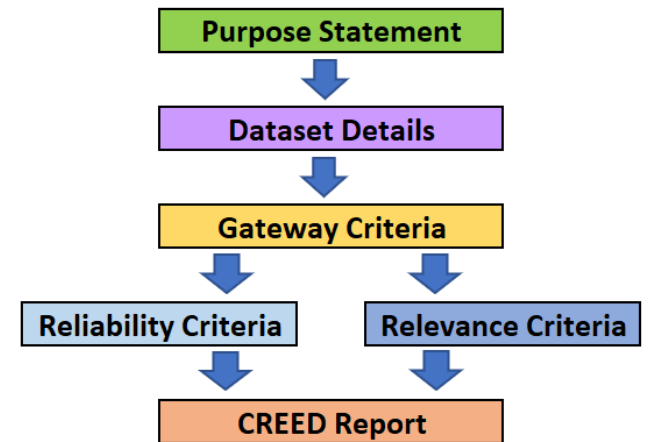
# RIWA-database export shows:

- Agency
- Location code
- Location description
- x-coordinate
- y-coordinate
- Parameter code
- Parameter description
- Unit
- CAS number
- Date/time
- Sign ( = / < / > / - )
- Value
- Validation status (empty imported / corrected)
- Suspect



## CREED Scoring Tool\* version 1.0

**Workflow** (Click buttons to enter appropriate tabs)



# Gateway

- Sampling Medium/ Matrix → surface water, because RIWA only monitors at inlet locations in rivers
- Analyte *r*
- Spatial Location *r*
- Year *r*
- Units *r*
- Data source/ Citation *r*

- LoQ is only mentioned in case of <LoQ
- LoD is not given by commercial labs

- Probably a grab sample
- Filtering is mentioned in the parameter name

# Reliability

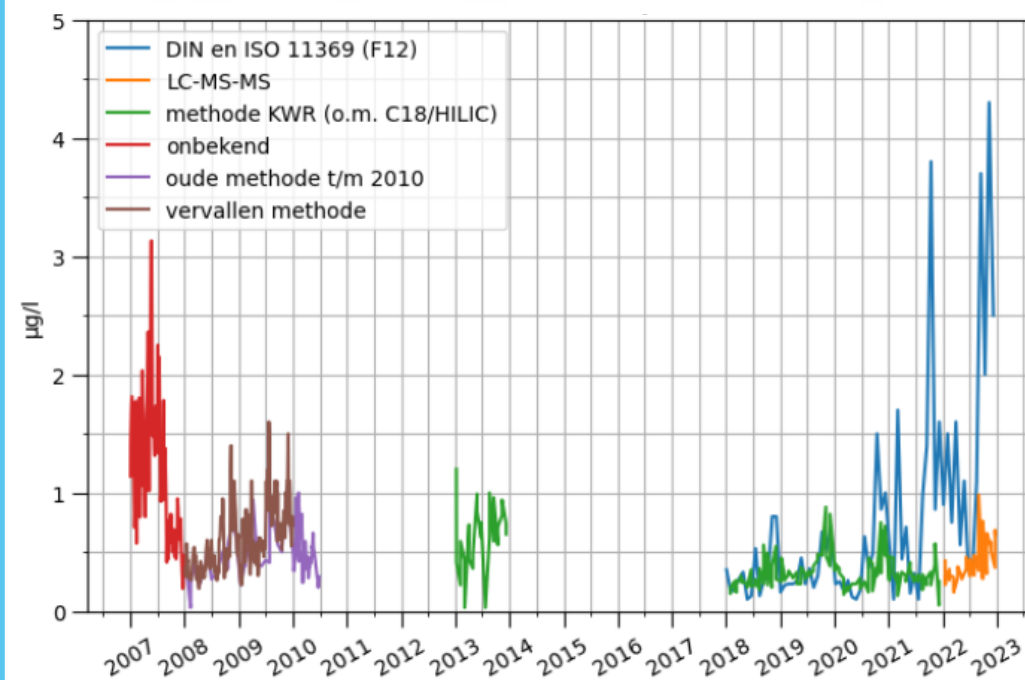
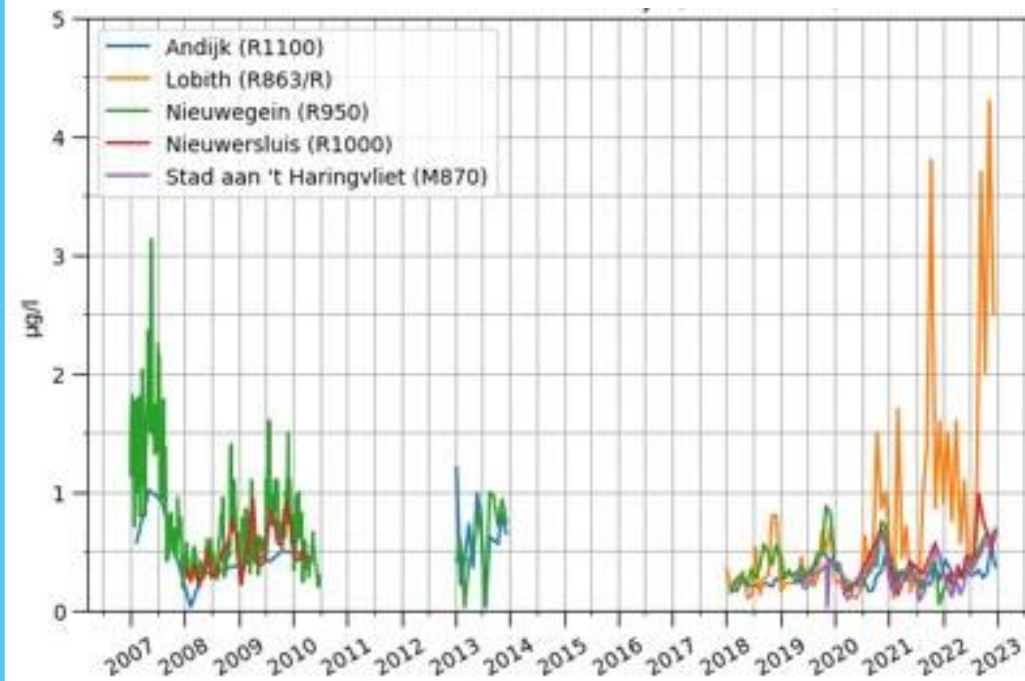


RB01	Sample Medium/ Matrix	OK
RB02	Collection Method/ Sample Type	-
RB03	Sample Handling	±
RB04	Site Location	National coördinates
RB05	Date and Time	OK
RB06	Analyte(s) Measured	OK
RB07	LOD/LOQ	±
RB08	Accreditation/ Quality Manag. System	-
RB09	Method	-
RB10	Lab Blank Contamination	-
RB11	Recovery/ Accuracy	-
RB12	Reproducibility/ Precision	-
RB13	Field QC	-
RB14	Only valid if dataset contains calculated values	-
-RB18		
RB19	Supporting Data Quality (if supporting parameters are required for the purpose)	Not necessary

This a problem

# We asked for additional information

- Between 2007 and 2023 six different methods were used, partly at the same time (see graph).
- Differences are limited, except for
  - the unknown method in the first half of 2007
  - DIN and ISO11369 (F12) from 2021, but not in the period 2018-2020.
- The differences in method and locations are difficult to separate



# Relevance HMMM

Limited number of sites (only drinking water intake) → merged with other monitoring agencies

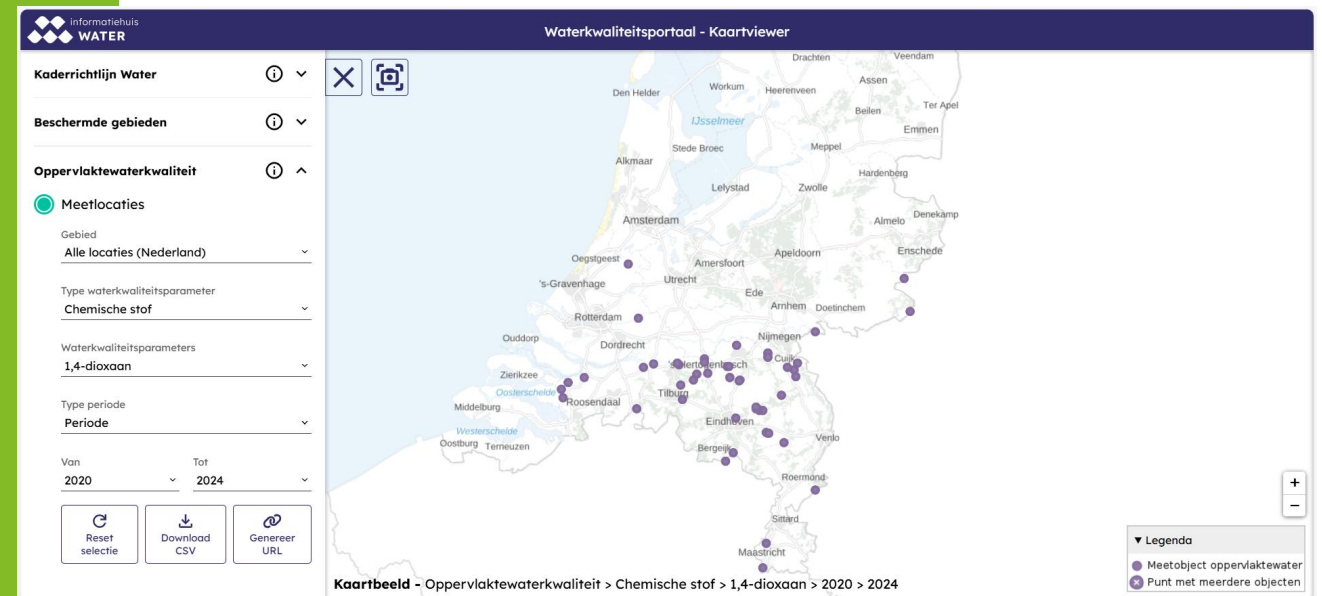
No.	Title	Criterion	Option in database?	Project?
RV01	Sample Medium/ Matrix	Was the sampling medium/matrix appropriate?	OK	+
RV02	Collection Method/ Sample Type	Was the sample collection method adequate?	?	-
RV03	Study Area	Were the study area and number of locations sampled suitable?	OK	±
RV04	Site Type	Was the rationale for selection of sampling locations provided and was it suitable?	OK	+
RV05	Sampling Timespan	Were the samples collected over a time scale that was appropriate?	OK	+
RV06	Sampling Frequency	Over the timespan, was the sampling frequency appropriate?	OK	+
RV07	Temporal Conditions	Were conditions during sampling events documented and relevant?	no	-
RV08	Analyte	Was/were the reported analyte(s) appropriate for the given purpose?	OK	+
RV09	Sensitivity/ LOD/ LOQ	Was the method sensitive enough?	OK	+
RV10	Summary Statistics Type	Were the summary statistics provided appropriate?	Yes (not needed)	+
RV11	Supporting Parameters	Were all supporting parameters provided that were needed?	OK	+



# Data from national databases

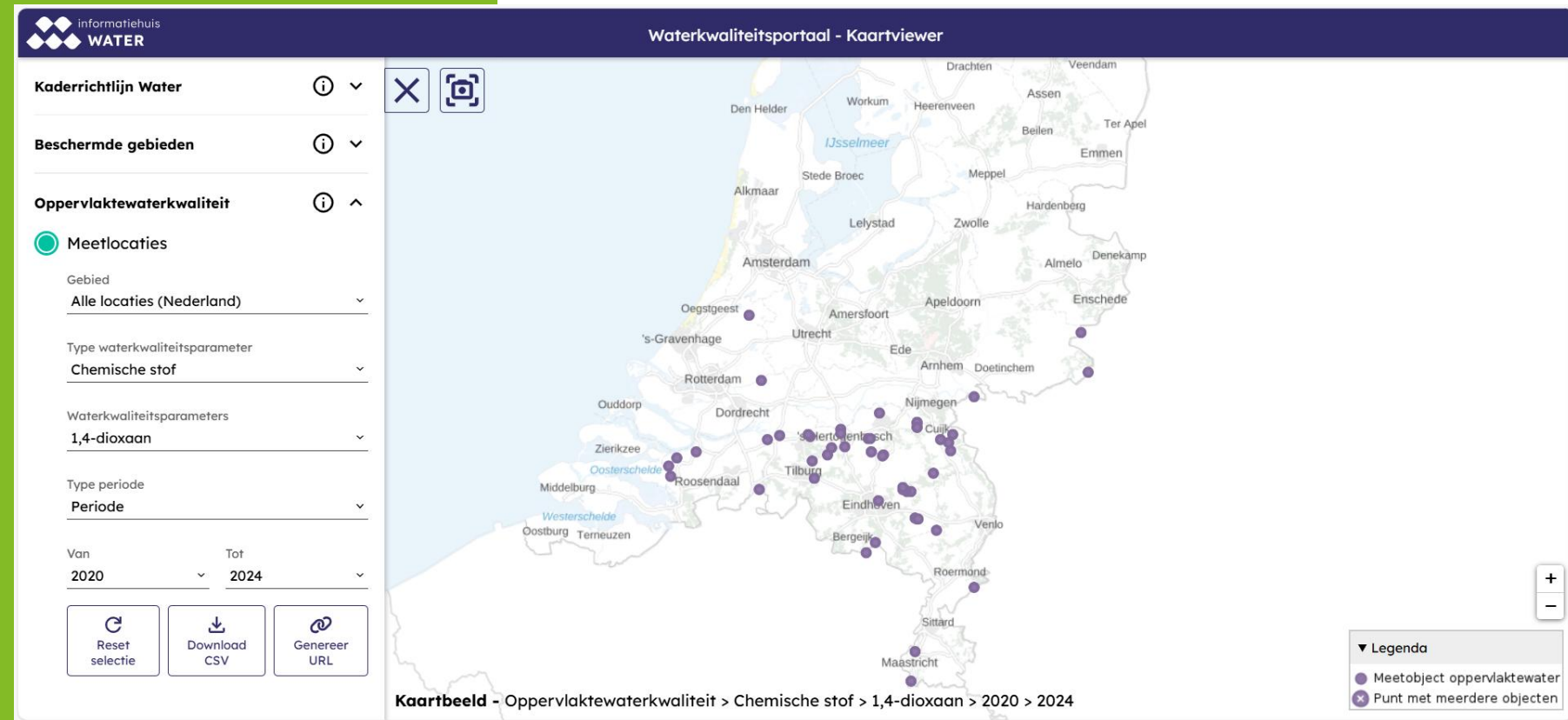
Water quality data is collected in national databases in the Netherlands:

- Surface water
- Discharge water of WWTP
- Rainwater / road run off water



# Dutch Surface water Quality portal

- Contains all surface water quality measurements in the Netherlands (yearly update)



# Gateway

- Sampling Medium/ Matrix *r*
- Analyte *r*
- Spatial Location *r*
- Year *r*
- Units *r*
- Data source/ Citation *r*

- LoQ is only mentioned in case of <LoQ
- LoD is not given by commercial labs

- Option available in the database

# Reliability



RB01	Sample Medium/ Matrix	OK
RB02	Collection Method/ Sample Type	-
RB03	Sample Handling	OK
RB04	Site Location	OK
RB05	Date and Time	OK
RB06	Analyte(s) Measured	CAS / Aquo-code
RB07	LOD/LOQ	±
RB08	Accreditation/ Quality Manag. System	-
RB09	Method	-
RB10	Lab Blank Contamination	-
RB11	Recovery/ Accuracy	-
RB12	Reproducibility/ Precision	-
RB13	Field QC	-
RB14	Only valid if dataset contains calculated values	-
-RB18		
RB19	Supporting Data Quality (if supporting parameters are required for the purpose)	Optional as separate records

No fields to fill

# Relevance

Relevance really depends on the purpose!

No.	Title	Criterion	Option in database?	Used?
RV01	Sample Medium/ Matrix	Was the sampling medium/matrix appropriate?	OK	+
RV02	Collection Method/ Sample Type	Was the sample collection method adequate?	OK	-
RV03	Study Area	Were the study area and number of locations sampled suitable?	OK	depends
RV04	Site Type	Was the rationale for selection of sampling locations provided and was it suitable?	OK	Depends
RV05	Sampling Timespan	Were the samples collected over a time scale that was appropriate?	OK	Depends
RV06	Sampling Frequency	Over the timespan, was the sampling frequency appropriate?	OK	Depends
RV07	Temporal Conditions	Were conditions during sampling events documented and relevant?	no	
RV08	Analyte	Was/were the reported analyte(s) appropriate for the given purpose?	OK	+
RV09	Sensitivity/ LOD/ LOQ	Was the method sensitive enough?	OK	Varies per substance
RV10	Summary Statistics Type	Were the summary statistics provided appropriate?	no	
RV11	Supporting Parameters	Were all supporting parameters provided that were needed?	OK	+



# Discussion with the Dutch water quality portal

Our wishes:

- Field for addition information on the analytical method, at least the name of the laboratory and the protocol used by the lab.
- Field for addition information on the sampling method (type of sample, depth, protocol used).
- Separate field for the LoQ, also if the value is >LoQ

The database manager is willing to discuss these wishes with water managers. It would be an advantage if European organisations like EEA adopt CREED.



# Example of an international database: NORMAN

The screenshot shows the NORMAN EMPODAT Database search page. At the top, there is a navigation bar with the NORMAN logo and links for NORMAN WEBSITE, NORMAN DATABASE SYSTEM, REST API, HOME, and LOGIN. Below the navigation bar, there are links for SEARCH, STATISTICS, and DCT DOWNLOAD. The main heading is "NORMAN EMPODAT Database - Chemical Occurrence Data". A search bar is present with the text "Search".

**Search options**

All the selected criteria must comply  At least one of the selected criteria must comply

If no criteria is selected, the result of search will be the overall database.

**Search criteria**

Country: Antarctica, Austria, Belgium, Black Sea - open sea area, Bulgaria, Croatia

Ecosystems/matrices: Surface water - Sea water, Surface water - River water, Surface water - Lake water, Surface water - Transitional water, Surface water - Coastal water, Surface water - Territorial (marine) water

Sampling site/station: [Empty text box]

Note: hold down the ctrl/cmd button to select multiple options.

- [NORMAN EMPODAT Database - Chemical Occurrence Data](#)
- Search per country, date, substance and compartment (surface water, sediment, wastewater, etc.),



# Reliability



RB01	Sample Medium/ Matrix	Surface water River/Lake/Sea, waste water, sediment
RB02	Collection Method/ Sample Type	no
RB03	Sample Handling	Sample preparation method
RB04	Site Location	Internat. Coordinates, name, km, depth
RB05	Date and Time	OK
RB06	Analyte(s) Measured	Name / CAS / StdInCHIKey / NORMANSusDatID
RB07	LOD/LOQ	Seperate columns for LOD and LOQ
RB08	Accreditation/ Quality Manag. System	Field for accreditation of the lab, the method, interlab.studies,
RB09	Method	Fields for analytical method and whether it is a standardised method
RB10	Lab Blank Contamination	Field for blank checking
RB11	Recovery/ Accuracy	field for correction of recovery
RB12	Reproducibility/ Precision	+
RB13	Field QC	-
RB14 – RB18	Only valid if dataset contains calculated values	Option individual/average/etc
RB19	Supporting Data Quality (if supporting parameters are required for the purpose)	Extra field in the record available for salinity, DOC, hardness

Fraction  
(total, diss)



# Wrap up NORMAN



- Extensive database, suitable for gold level (except for sampling method)
- Many fields were empty.



# Conclusions

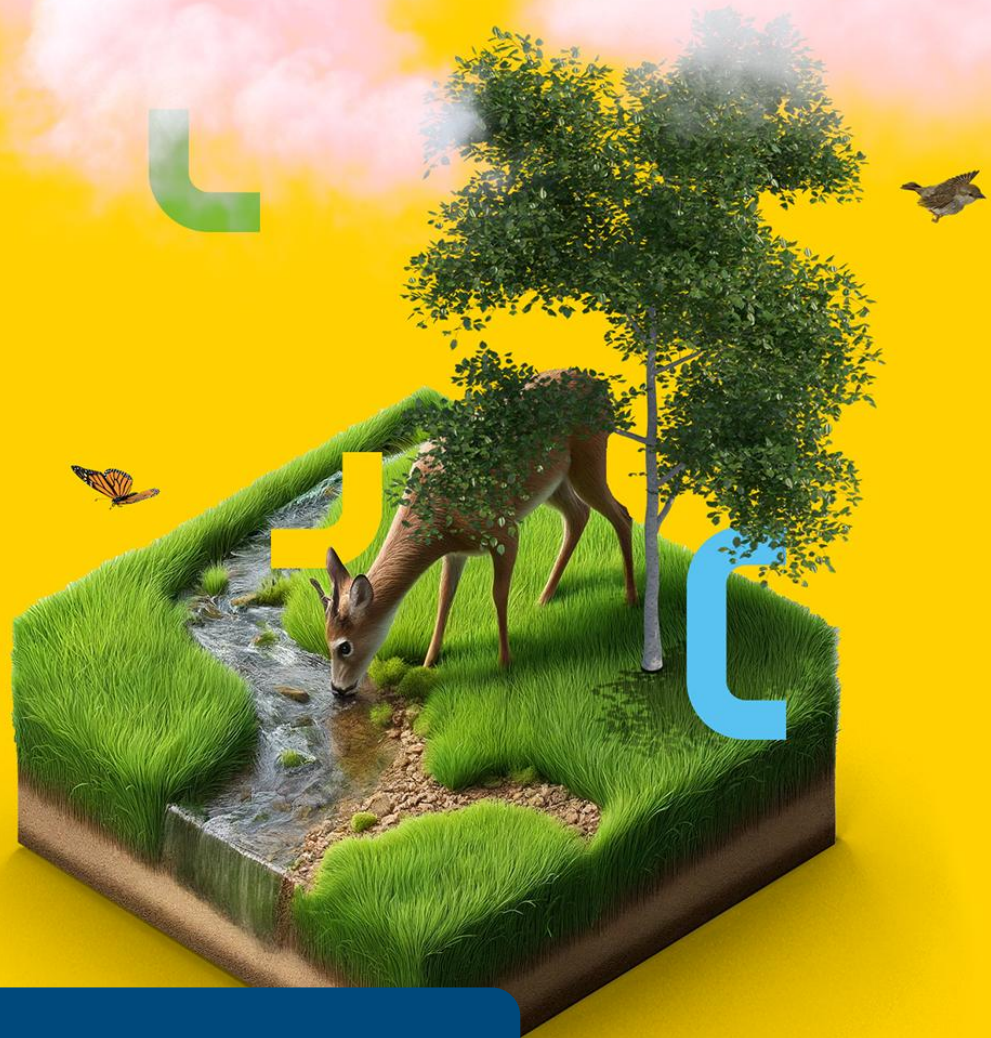
- **CREED supports a critical review of data and also to contact data suppliers for additional information.**
- **Silver level is ok for operational projects; gold is recommended for scientific studies**
- **Critical information which is often lacking is:**
  - **method/lab/sample treatment**
  - **Separate field for LOD/LOQ**
- **Pay within CREED more attention to the fraction analysed**



# Recommendations

- Elaborate CREED criteria one step further to recommended database fields for silver and gold level.
  - Promote universal analyte ID's. INCHI-key's?
  - Define site locations (at least international coordinates)
- Try to get CREED implemented in important database managers: European agencies (EEA), drinking water sector (EurEaux).
- What if gateway criteria are met, but silver not
- Create an icon/logo to show that database managers met CREED criteria.





**Thank you**

# A CREED example

Repurposing exposure data -  
an example for aquatic metals  
modelling

Stephen Lofts [stlo@ceh.ac.uk](mailto:stlo@ceh.ac.uk)

24/03/2026



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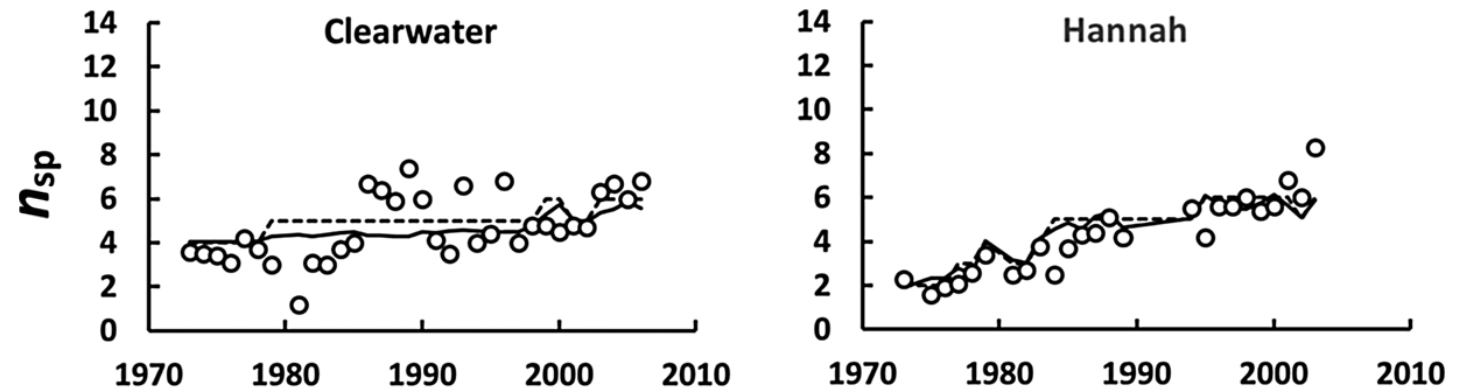
# Contents

- The research question
- Choice of dataset and why
- CREED evaluation of the datasets
- Processing of the dataset
  - Requirements – sampling site level
  - Requirements – sample level
  - Infilling process
- Outcomes
- Summary and conclusions

## The research question

WHAM- $F_{\text{TOX}}\beta$

A model of the impacts of acidity and metals (Mn, Ni, Cu, Zn, Cd, Pb) on aquatic biodiversity



Tipping E, Lofts S, Keller W (2021). Aquatic Toxicology, 231, 105708. DOI: <https://doi.org/10.1016/j.aquatox.2020.105708>.

Research aim: to apply this model to English rivers, using the Environment Agency freshwater chemistry (*and biodiversity*) datasets

## The Environment Agency dataset

- Regulator dataset for surface waters in England
- Available online for 2000 onwards (accessible via API)
- Multiple sample types e.g. freshwaters (rivers/streams), WwTP effluent, minewaters
- *MULTIPLE PURPOSES e.g. WFD compliance, targeted survey*
- ~19,000 sample locations, ~7000 determinands
- Sampling locations typically display:
  - A range of sampling timelines
  - Variations over time in analytes

Aim: to filter sample locations for a minimum number of **suitable** samples for chemical modelling.  
Suitability criteria: minimum number of samples having **essential** determinands measured and **optional** determinands estimatable

# CREED evaluation

## Purpose statement:

To generate chemical quality data suitable for processing with the WHAM-FTOX $\beta$  model for the purpose of calibrating and testing this model against metal/acidity mixture impacts on freshwater macroinvertebrates.

Purpose Summary Table (optional)		Fully Met (FM)	Partly Met (PM)
Enter thresholds for "Partly Met" (minimum information required) and "Fully Met" (optimal information) to fit the assessment purpose. Thresholds can be specific or general, depending on how important a criterion is to the user for the assessment purpose. Also, users can choose not to enter any threshold(s) for "Partly Met", if they want a yes/no decision.			
RV1	The sampling medium/matrix was appropriate for the given purpose.	Must be surface freshwater	N/A
RV2	The sample collection method (e.g., grab, depth- and width-integrated, discrete, composite, or time-integrated samples, or continuous monitoring) was adequate for the given purpose.	N/A	N/A
RV3	The study area and number of locations sampled was suitable for the given purpose.	No limit within dataset extent	N/A
RV4	The rationale for selection of sampling locations was provided and it is suitable for the given purpose.	Any surface freshwater	N/A
RV5	The samples were collected over a time scale that was appropriate for the given purpose.	No limit	N/A
RV6	Over the timespan, the sampling frequency was appropriate for the given purpose.	Location by location assessment	N/A
RV7	Conditions during sampling events were documented and relevant for the given purpose (e.g., baseflow, storm events, planned/unplanned discharges, etc.).	N/A	N/A
RV8	The analyte(s) reported was/were appropriate for the given purpose.	pH,temp,DOC,metals,majors,alk	Minimum pH, DOC, metals
RV9	The method was sensitive enough for the given purpose (i.e., the LOD and/or LOQ were below the benchmarks or metrics to which concentrations in the dataset will be compared).	N/A	N/A
RV10	The summary statistics provided (e.g., median, geometric mean, arithmetic mean, percentiles) were appropriate for the given purpose.	N/A	N/A
RV11	All supporting parameters that were needed to achieve the given purpose were provided.	Spatial location coordinates	N/A

## CREED evaluation II

- Nature of dataset → evaluation for relevance depends on determinands available AND capability for ‘infilling’ of data gaps
- Relevance evaluation is **site and sample-specific**.
- Initially, define two sets of model variables: **essential** and **optional**.
- **Essential:** pH, DOC, dissolved concentrations of metals: Mn, Ni, Cu, Zn, Cd, Pb
  - We also require dissolved Al – this can be modelled if not measured
- **“Optional”:** temperature, dissolved concentrations of Na, Mg, K, Ca, Cl, NO<sub>3</sub>, SO<sub>4</sub>
  - Some data on these variables required – see later
- We also want to evaluate whether there may be **non-metal stresses** at sites
  - No evidence of other stresses → data usable for model **fitting**
  - Evidence of other stresses → not usable for fitting, potentially usable for evaluation

## CREED evaluation III

- We also want to evaluate whether there may be **non-metal stresses** at sites
  - No evidence of other stresses → data usable for model **fitting**
  - Evidence of other stresses → data not usable for model fitting, but may be usable for evaluation if desired
- **Criterion:** all relevant WFD criteria must be Pass/High/Good at the site (if a WFD classification site) or at the nearest downstream classification site, for all classification years
  - Phosphate, ammonia, dissolved oxygen, BOD, temperature
  - Specific chemicals (other than our metals of interest)
- Conservative, but (relatively) straightforward
- All classification data are available online

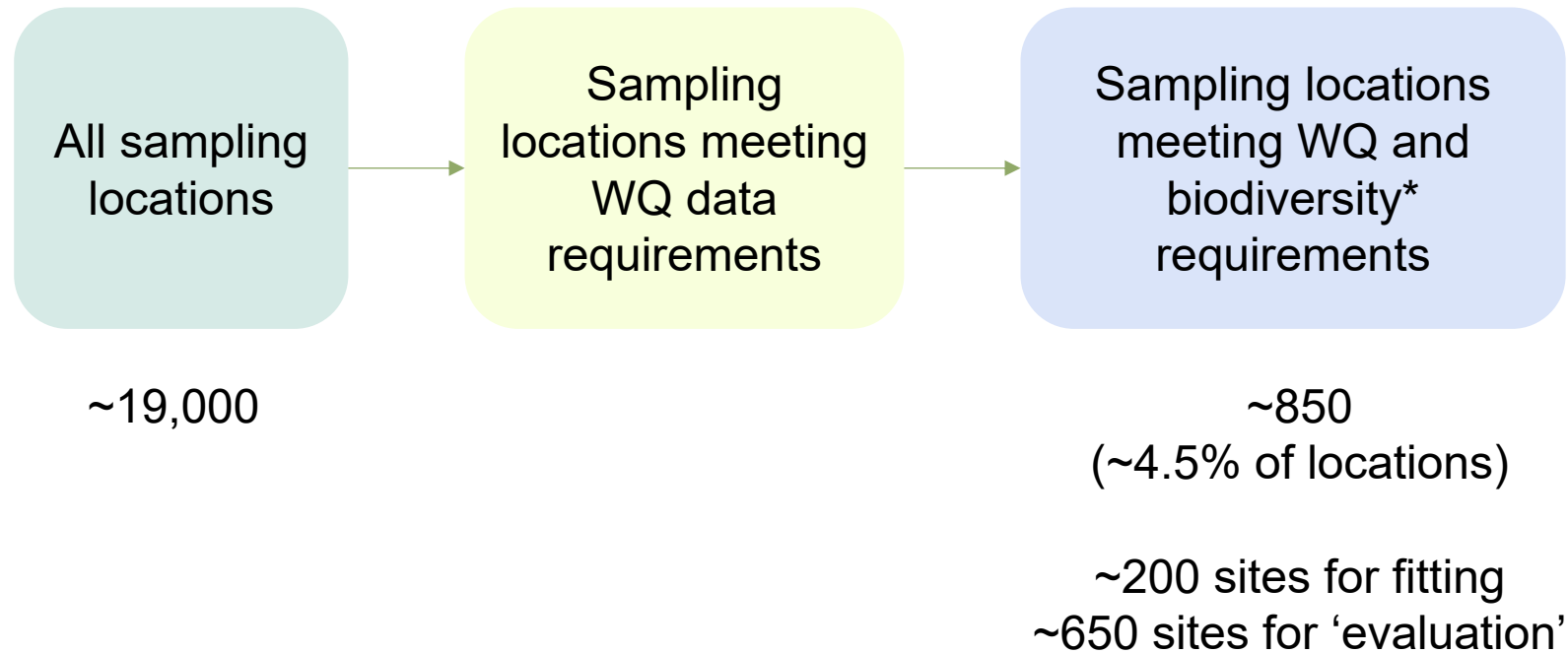
## Summary of infilling procedure

- sites pre-filtered to those having a minimum number of samples meeting the **essential** data requirements
- all data infilling done using only data from the sampling site

	Substitution	Regression	Averaging	Global regression
temperature		✓		
dissolved Na	total Na	✓	✓	✓
dissolved Mg	total Mg	✓	✓	✓
dissolved K	total K	✓	✓	✓
dissolved Ca	total Ca	✓	✓	
dissolved Fe	x	✓	✓	
dissolved Cl	-	✓	✓	✓
dissolved NO <sub>3</sub>	total NO <sub>3</sub> , dissolved N <sub>ox</sub> , total N <sub>ox</sub>		✓	
dissolved SO <sub>4</sub>	total SO <sub>4</sub>	✓	✓	✓
alkalinity	-	✓	✓	✓

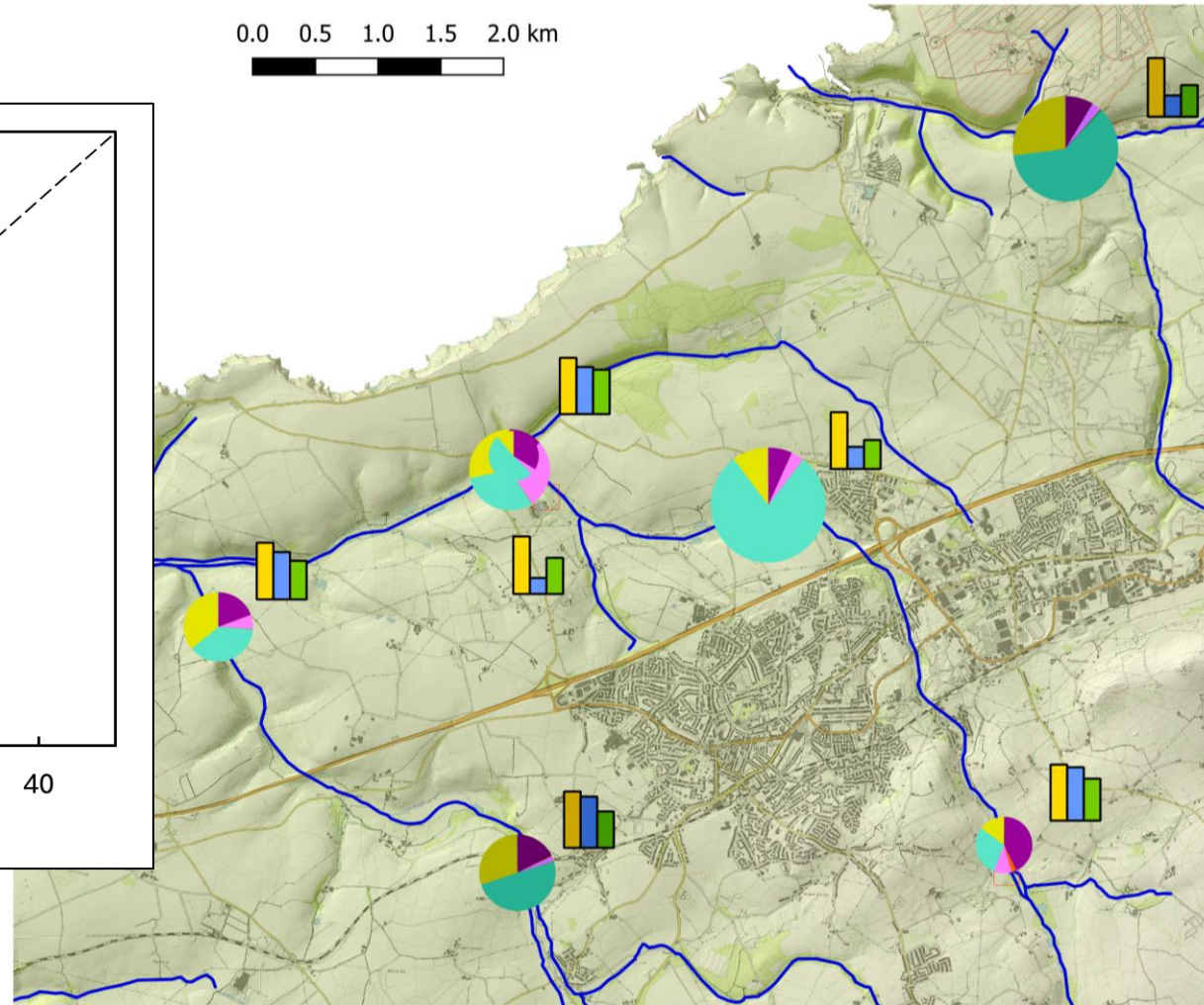
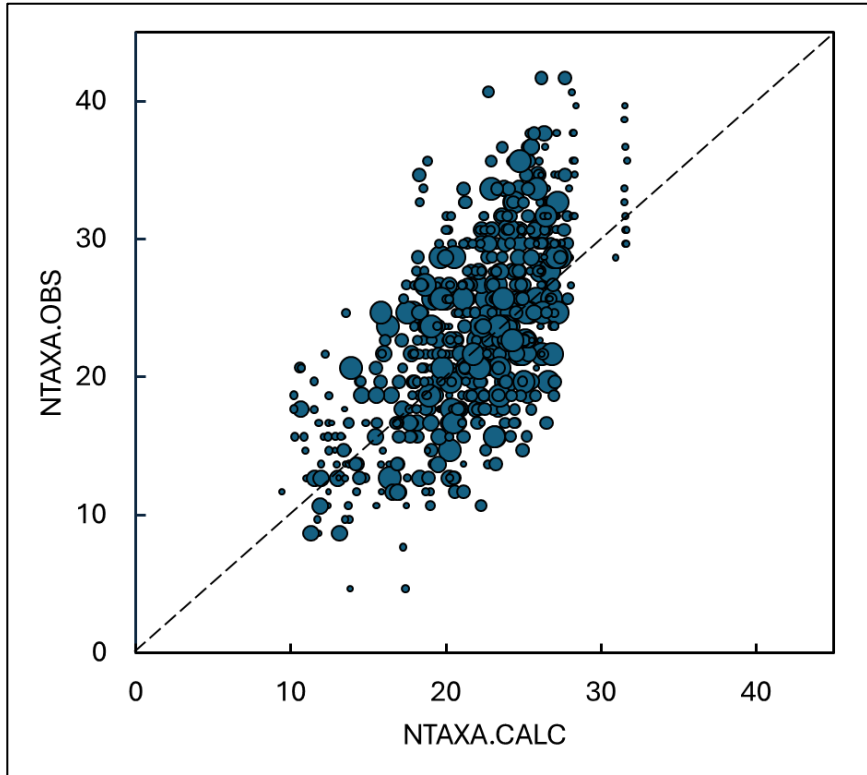
## Outcomes

Data retrieval, evaluation and infilling all automated in R – a necessity for such a large dataset



\* not discussed here

# Results summary



## Contributions to $F_{TOX}$

- H
- Al
- Mn
- Ni
- Cu
- Zn
- Cd
- Pb

## Invertebrates

- reference NTAXA
- observed NTAXA
- modelled NTAXA

## Summary and conclusions

- “Repurposing” a dataset
  - Complex requirements
    - multiple variables for modelling; minimum number of samples per location
    - dataset with variations in determinands over locations and time
  - Schema for selecting **individual sites and samples**
    - **Essential** and **optional** variables
    - Basic minimum requirements – variables and number of samples per site
    - **Infilling** of optional variables following a defined system

Relevance applies at the level of sampling location and sample, not only at dataset



What Next?  
Where might we go from here?

Adam Peters



# Welcome



- Klimisch and CREED are widely used in regulatory focused risk assessments
- Application of CREED in retrospective risk assessments
  - » Some papers already published where CREED has been applied
- CREED can be used to ensure that future datasets are more widely applicable
- There may be aspects of CREED that require adaptation or refinement as its use increases

# Quality Assessment



- Are there any other aspects of risk assessments where more formalised assessments of reliability and relevance would be beneficial?
- Environmental fate testing?
  - » How can you compare field measurements to the results of standardised OECD test methods?
- Modelled data?
- Ecological data?

# Applications of CREED



Contents lists available at [ScienceDirect](#)

## Environmental Research

journal homepage: [www.elsevier.com/locate/envres](http://www.elsevier.com/locate/envres)



[Check for updates](#)

### Trend analysis of environmental concentrations of Bisphenol A in European waters and sediments

Chesney Swansborough <sup>a</sup>, Javier Soto <sup>a</sup>, Imogen Shapland <sup>a,1</sup>, Christopher B. Hughes <sup>a,2</sup>, Elaine Jennings <sup>a,\*</sup>, Margaret McArdle <sup>b</sup>, Ellen Mihaich <sup>c</sup>, Evelyn Majoris <sup>d</sup>, Michael Bunge <sup>e</sup>

## Environmental Science Advances




### COMMENT

[View Article Online](#)  
[View Journal](#) | [View Issue](#)



Cite this: *Environ. Sci.: Adv.*, 2025, 4, 2034

Comment on “Why there is no evidence that pyridine killed the English crabs” by A. T. Ford, M. F. Fitzsimons and C. Halsall, *Environ. Sci.: Adv.*, 2024, 3, 1385, DOI: <https://doi.org/10.1039/D4VA00006D>

Adam Peters \*

# Application of CREED



- CREED is already being used in practice
- Originally focused on monitoring data
  - » Inclusion of other media, soil, sediment, biota
  - » Limited consideration of atmospheric data
- Explicit reporting of limitations for particular applications
- Greater experience may identify problems or areas for refinement

# Environmental Fate



- Studies are straightforward to assess if they follow standardised OECD guidelines
- Lots of published studies based on measurements from the field
- How should they be assessed?
- How do they compare to standards tests?
- What are their limitations?



wca

[wca-consulting.com](http://wca-consulting.com)