

Supplemental Materials for the paper: Pesticides pollution of small streams in Germany

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1 Data Cleaning

Each of more than 30 datasets have been cleaned and homogenized separately, before combining in a common database. Cleaning steps comprised (Figure 1.1 gives a graphical overview).

1. Structure: Structure has been adjusted to the database structure.
2. Coordinates: Coordinates have been transformed to a common Coordinate Reference System (DHDN / 3-Grad Gauss-Krüger Zone 3 (EPSG:31467) and duplicates merged.
3. Chemicals: Chemical names and identifiers have been unified using the webchem package (Szöcs, 2016).
4. Identifiers: Unique identifiers have been assigned.
5. Units: All concentrations have been converted to $\mu\text{g}/\text{L}$. Values below limit of quantification have been set to zero.
6. Other meta-data: meta-data has been standardised.
7. Temporal resolution: The temporal resolution of the database is 1 day. Data below this resolution has been aggregated by maximum.
8. Validity Checks: Simple rules for validity checks have been implemented (e.g. no negative concentrations).

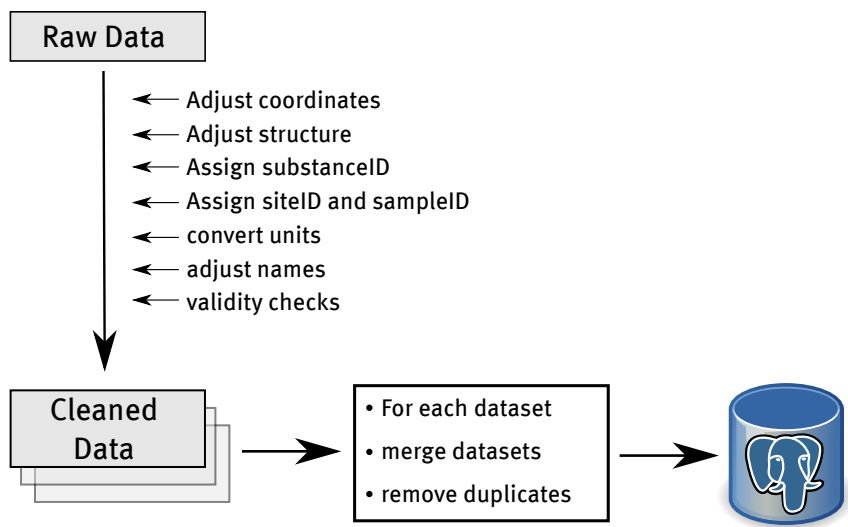


Figure 1.1: Overview on data cleaning steps. After cleaning data has been stored in a relational spatial PostgreSQL database.

2 Overview on compiled data

Table 2.1: Overview on chemical samples. Only data from running waters and grab sampling is shown.

state ^a	begin	end	no. sites	no. samples	no. compounds ^b
BW	2005-01-03	2014-10-02	118	4569	127
BY	2006-04-19	2013-12-18	19	297	157
HE	2007-01-15	2014-12-18	68	2512	144
MV	2005-03-08	2014-12-17	135	1535	227
NI	2014-03-24	2014-10-13	3	17	226
NW	2005-01-11	2015-01-22	1320	10985	204
RP	2005-01-05	2013-12-18	44	1277	278
SH	2005-04-26	2014-11-26	273	1419	180
SL	2005-01-03	2013-12-09	6	420	57
SN	2005-01-02	2013-12-18	917	17052	173
ST	2005-01-10	2015-03-25	46	712	93
TH	2005-01-31	2014-12-10	100	1441	76
Total	2005-01-02	2015-03-25	3049	42236	484

^a: Abbreviation according to ISO 3166-2:DE .

^b: Including metabolites.

Bibliography

Szőcs, E. (2016). webchem: webchem v0.1.0. DOI: 10.5281/zenodo.46930.