For our Environment



Second Global Round Table on PRTRs, Madrid Verification of Data Quality within the PRTR Process Chain in Germany

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Index

1 LEGAL BACKGROUND

2 PRTR PROCESS CHAIN IN GERMANY

3 QA LEVELS

4 CONCLUSION

1 Legal background for QA/ QC

E-PRTR regulation and German act on PRTR

- both operator and competent authorities responsible at different stages for data assurance
- at operator level: completeness, coherence, reliability
- at authority level: checks via comparison with other data (data submitted to authorities on different reporting obligations, permit data, time series etc.)
- \rightarrow act: not defined how data checks have to be done

2 PRTR process chain in Germany



Data flow

2 PRTR process chain in detail



- formal correctness
- syntactic correctness xml schema
- semantic correctness additional tools
 - ex. NACE vs. activities
 - ex. release vs. accidential release
- scientific/ technical plausibility external tools
 - outlier problems (comparison, time series)
 - causal connections

CONCEPT OF BUBE TESTS

- integrated in business logic of BUBE (Java application)
- covers all BUBE modules (PRTR + LCP + emission declaration)
- 2 test stages at operator level
 - direct support via UI where possible (lists, data types)
 - complete test prior to submission of data to competent authority
- flexible configuration (stored in db)
- error level configuration error / warning
- configurations possible at level of federal state – different levels of strictness – different levels data quality



Selected emission factors (EF) in BUBE since 2014*/ 2015 for UWWTP

Pollutant	No. (Annex II E-PRTR)	EF in mg/pop. equiv.*a	PRTR-threshold for releases to water in kg/a	size of plant (pop. equiv.) with PRTR- threshold being potentially reached based on EF
Pb*	23	64	20	196,078
Cd*	18	18	5	500,000
Ni*	22	716	20	54,794
Hg*	21	0.91	1	10,000,000
DEHP	70	91	1	30,303
Diuron	37	11.4	1	250,000
Isoproturon	67	6.8	1	500,000

important: - average for all German UWWTP, provide basis for quality checks (warning)

- <u>threshold</u> Annex I E-PRTR: 100.000 pop. equiv.

Work on <u>future</u> inclusion of:

Atrazine, Benzo(b)fluoranthene, Benzo(g,h,i)perylene, Fluoranthene, Nonylphenol, Octylphenols, Pentachlorophenol, Simazine, Tributyltin, Trichloromethane

QA at German PRTR database

- 2 quality assurance stages
- directly checking xml-files
- additional checks and transformations during input into database
- transfer to presentation module (<u>www.Thru.de</u>)
- conversion to EU-xml file

Test suite for xml-transfer format

- providing quick response to Federal States
- in-house development
- written in scripting language (TCL)
- based on software test tools (tcltest)
- an error a missing test
- XPath selection on DOM-tree
- flexible and quick addition of tests
 - complete test ~ 25 LOC, ~ 15 nearly unchanging
- possible combination with other data pools (UWWTD, LCP) for plausibility checks

```
variable SETUP {}
variable CLEANUP {unset testNodes}
# kommunale Kläranlage hat immer Freisetzung und nicht
Abwasserverbringung
set testID xml2-7.7
set testDesc {Test kommunale Kläranlage mit Abwasserverbringung?}
tcltest::test $testID $testDesc -setup {
# xml2-_testgruppe.laufende_Nummer
    set res 0
# Betriebe mit Freisetzungen Abwasser
    set testNodes [$::root selectNodes {//p_betrieb
[p_vabw_Relation/p_vabw]}]
  -body {
# body
foreach betrieb $testNodes {
    set taetigkeiten [$betrieb getElementsByTagName NRPRTR]
# loop ueber taetigkeiten JH 20.2
     foreach t $taetigkeiten {
         set taet [$t asText]
         if {$taet eq {5.f}} {
# kommunale Kläranlage
              set Inr 0
# ids fuers logging
             set IDNode [$betrieb getElementsByTagName KENNNR]
set nameNode [$betrieb getElementsByTagName NAME1]
# jetzt die Verbringungen_Abwasser holen
              set vNodes [$betrieb getElementsByTagName p_vabw]
              foreach p_vabw $vNodes {
# Initialisierung aller relevanten Testvariablen
                   set logstring [logEntryStart $IDNode $testID $nameNode
$testDesc $lnr]
                   incr lnr
                   set stoffnrN [$p_vabw getElementsByTagName STOFFNR]
                  if {[string length $stoffnrN]} {
    set stoffnr [$stoffnrN asText]
} else {set stoffnr "FEHLEND"}
lfputs [append logstring [logEntryEnd f "'Verbringung
Abwasser' für [dict get $stoff_info $stoffnr -name] gemeldet."]] 0
                   incr<sup>-</sup>res
         }
    }
set res [expr {$res == 0} ]
} -cleanup $CLEANUP -result {1}
```

3 QA levels - Test suite for xml-transfer format

```
variable SETUP {}
variable CLEANUP {unset testNodes}
# kommunale Kläranlage hat immer Freisetzung und nicht Abwasserverbringung
set testID xml2-7.7
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tcltest::test $testID $testDesc -setup {
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    set res 0
# Betriebe mit Freisetzungen Abwasser
    set testNodes [$::root selectNodes {//p_betrieb[p_vabw_Relation/p_vabw]}]
} -bodv {
# body
foreach betrieb $testNodes {
    set taetigkeiten [$betrieb getElementsByTagName NRPRTR]
# loop ueber taetigkeiten JH 20.2
    foreach t $taetigkeiten {
        set taet [$t asText]
        if \{\text{staet eq } \{5,f\}\}
# kommunale Kläranlage
            set Inr 0
# ids fuers logging
            set IDNode [$betrieb getElementsByTagName KENNNR]
            set nameNode [$betrieb getElementsByTagName NAME1]
# jetzt die Verbringungen_Abwasser holen
            set vNodes [$betrieb getElementsByTagName p_vabw]
            foreach p_vabw $vNodes {
# Initialisierung aller relevanten Testvariablen
                set logstring [logEntryStart $IDNode $testID $nameNode $testDesc $lnr]
                incr lnr
                set stoffnrN [$p_vabw getElementsByTagName STOFFNR]
                if {[string length $stoffnrN]} {
                set stoffnr [$stoffnrN asText]
} else {set stoffnr "FEHLEND"}
                Ifputs [append logstring [logEntryEnd f "'Verbringung Abwasser' für [dict get $stoff_info $stoffnr -name]
                gemeldet."]] 0
                incr res
            }
        }
    }
}
set res [expr {$res == 0} ]
} -cleanup $CLEANUP -result {1}
```

Verification of Data Quality within the PRTR Process Chain in Germany

3 QA levels

Ergebnis Überprüfung Datei NI_2012_Korr1.xml

24. September 2014

Fehlermeldungen

Es liegen keine Meldungen vor

Warnungen

Ergebnis Betrieb Name vertraulich ID 03-03-03000244840; KennNr. 03-03-03000244840

 Test: Pflichtfelder zu p_vabf bei gefährlichem Abfall vollständig? Warnung. Vertraulichkeit fÃ1¼r ALAND und Schutzgrund vorhanden; aber EU-Problem

Ergebnis Betrieb DOW Deutschland Anlagengesellschaft; KennNr. 03-03-03030273580

- Test: Pflichtfelder zu p_vabf bei gef\u00e4hrlichem Abfall vollst\u00e4ndig? Warnung. Vertraulichkeit f\u00e41\u00e4r ALAND und Schutzgrund vorhanden; aber EU-Problem
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Hinweise insbes. mögliche Ausreisser

Ergebnis Betrieb Salzgitter Flachstahl GmbH; KennNr. 03-01-01211092310

 Test: Branche 1.c - keine Freisetzungen von 'Quecksilber in Luft' aus Verbrennungsanlagen? (ab 400000 t CO2 ist auch eine Quecksilbermeldung zu erwarten) Hinweis. CO2 = 7980000.0000 t. Unter Annahme von mittleren Verhältnissen wäre für diese Anlage ein Quecksilberwert von etwa 192 kg/a realistisch.

Test results

- pdf document
- errors
- warnings
 - -expected emissions
 - missing
 - -confidentiality
- potential outliers

Outlier tests – Hg

- PRTR data not normally distributed, not easy to check for potential outliers, missing releases ...
- data on facility size/ gross power not mandatory in E-PRTR + German PRTR
- assumption: some parameters closely related to size of a plant

LCP power plant >50 MW = PRTR 1.c (thermal power stations + combust. installations >50 MW) \rightarrow CO2 emission very closely related to size of a facility (gross power) received from LCP reporting (R=0.92)

- ightarrow CO2 emission used as alternative to determine size of facility
- \rightarrow relation Hg/CO2 nicely linear, esp. for lignite, but too few facilities \rightarrow <u>used only for</u> <u>hard coal</u>
- indicator for Hg releases \rightarrow >0.04 kg Hg/1.000 t CO2 possible statistical outlier \rightarrow >400 kt CO2/a \rightarrow Hg release should be reported

Outlier tests – Ni

similar method used for UWWTP – size of plant derived from reporting to UWWTD \rightarrow size of plant and TOC closely related (R=0.82)

- ightarrow TOC used as alternative to determine size of UWWTP
- \rightarrow relation Ni/TOC nicely linear
- indicator for Ni releases: \rightarrow >0.001 Ni/TOC \rightarrow Ni is potential outlier

 \rightarrow >55 t TOC \rightarrow Ni release should be reported

both relations (Hg/CO2 + Ni/TOC) established in BUBE to check on both potential outliers and missing releases

at **EU level**:

research of ETC on cross pollutant relations: 174 relations between different pollutants established on releases to air, not yet installed at EEA QA validation tool \rightarrow future work

4 Conclusions and recommendations

Experiences

- fixed contents required at beginning of reporting period
- check as early as possible in the process chain
- early strictness is important bottle neck at the beginning, not at the end
- use flexible and easy-to-expand tools along the chain
- use different tools for different tasks be pragmatic and flexible
- corrections must be integrated in the base data set (feedback channel)

Thank you!

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German Environment Agency - www.uba.de German PRTR - www.thru.de

Umwelt 🌍 Bundesamt