DANMARKS OG GRØNLANDS GEOLOGISKE UNDERSØGELSE **RAPPORT 2025/37**

Groundwater chemistry data for status, risk, and trend analyses related to the fourth River Basin Management Plan (Vandområdeplan 4)

Documentation report

Denitza D. Voutchkova & Lærke Thorling

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GEUS

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G E U S

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1. Summary

1.1 Dansk resume

Denne rapport dokumenterer udarbejdelsen af grundvandskemiske datasæt til den fjerde vandområdeplan 2027-2032 (Vandområdeplan 4, VP4). Data er primært til brug i risiko-, tilstands- og trendvurderinger i VP4 for grundvandets kemiske tilstand. Derudover er data målrettet brug til vurderinger af kemiske påvirkninger fra vandindvinding, i den kvantitative tilstandsvurdering. Dette arbejde er gennemført som en del af projektet "*Etablering af kemiske grunddata til Vandområdeplan IV*", finansieret af Styrelsen for Grøn Arealareallægning og Vandmiljø (SGAV, 2025).

Formålet med rapporten er at tjene som detaljeret teknisk dokumentation for dataforberedelsen og de mange valg, der skal træffes under dataforberedelsen. Derfor beskrives detaljerne for følgende dataforberedelsestrin 1) udtræk fra Jupiter-databasen, 2) rensning inklusive forskellige kvalitetskontroller og filtreringsprocedurer, 3) aggregering til **årsmiddelværdi (AM)** og **periodemiddel for årsmiddelværdi (MAM)**, 4) formatering af leverancer (dataprodukter).

Dataprodukterne er grupperet i fem leverancer og er tilgængelige i Voutchkova (2026):

1) metadata på indtagsniveau,
2) renset datasæt på prøveniveau,
3) aggregerede datasæt for AM på indtagsniveau,
4) aggregerede datasæt for MAM på indtagsniveau,
5) udfyldte skabeloner til rapportering til EU.

Leverance 1 og 2 er de datasæt, der bruges til at forberede leverance 3, 4 og 5. De kan derudover bruges til fremtidigt arbejde med trends og andre VP4-opgaver, der endnu ikke er defineret, og til andre projekter med fokus på grundvandskvalitet. Leverance 2 kan bruges til specifikke kvalitetskontroller af data, herunder ved manuelle statusvurderinger eller til at udvikle metoder til trendvurdering med fokus på data på prøveniveau (i stedet for årligt aggregerede data). Formålet med Leverance 3 er at levere data til trendvurderinger i VP4 baseret på AM-aggregering. Leverance 4 skal anvendes i risiko- og tilstandsvurderingerne i VP4, mens leverance 5 er målrettet den delmængde af data, der er skal indgå i for EU-rapporteringen.

Da datasættene vil blive brugt til forskellige formål, er den relevante dataperiode forskellig. Der er ingen begrænsning i dataperioden for leverance 2 og 3, og derfor inkluderer disse datasæt alle tilgængelige kvalitetssikrede data for de udvalgte parametre i Bilag B. Perioden for leverance 4 og 5 er begrænset til 2019-2024 (inklusive begge år), hvilket er den relevante periode for VP4-tilstandsvurderinger. Desuden er leverancerne opdelt i parametergrupper for at lette den praktiske anvendelse af data i de VP4-relaterede opgaver. Leverance 1-4 inkluderer data for alle indtag uanset om det er knyttet til en grundvandforekomst eller ej.

Leverance 5 inkludere kun indtag som er knyttet til en grundvandsforekomst (som ønsket af SGAV).

1.2 English summary

This report documents the preparation of groundwater chemistry datasets for the fourth River Basin Management Plan 2027-2032 (Vandområdeplan 4, VP4), to be used primarily in the qualitative risk, status, and trend assessments. Additionally, some of the data could support the quantitative status assessments regarding groundwater quality impacts from abstraction. The work presented here is part of the project "*Etablering af kemiske grunddata til Vandområdeplan IV*", funded by The Danish Agency for Green Transition and Aquatic Environment (Styrelsen for Grøn Arealomlægning og Vandmiljø, SGAV, 2025).

The purpose of the report is to serve as a technical documentation for the data-preparation including a detailed account of all decisions taken in this process. Therefore, the following data-preparation steps are described here: 1) extraction from Jupiter database, 2) cleaning including various quality checks and filtering procedures, 3) aggregation with **annual mean (AM)** and **mean annual mean (MAM)**, 4) formatting of deliverables (data-products).

The data-products are grouped in five deliverables and are available from the GEUS Dataverse (Voutchkova, 2026), including:

1) well-screen meta-data,
2) clean dataset at sample level,
3) aggregated dataset(s) with AM at well-screen level,
4) aggregated dataset(s) with MAM at well-screen level,
5) filled templates for reporting to EU.

Deliverables 1 and 2 are the datasets used for preparing the rest of the deliverables. They can be used potentially for future work with trends or other not yet defined VP4-tasks or even other projects focusing on groundwater quality. Deliverable 2 could potentially be used for specific quality checks during manual status assessments, or for developing trend-assessment techniques using sample-level data (instead of annually aggregated data). The purpose of Deliverable 3 is to provide data for trend assessments in VP4 based on AM aggregation. Deliverable 4 is to be used in the risk and status assessments in VP4, while deliverable 5 includes the subset relevant to EU reporting.

Because the datasets will be used for different purposes, the relevant data-period differed. There was no restriction for Deliverables 2 and 3, thus these datasets include all available quality assured data for the target parameters. While the period was restricted for Deliverables 4 and 5 to 2019–2024 (including both years), which is the relevant period for VP4 status assessment. Furthermore, the deliverables are split into parameter groups to facilitate future use in the VP4-related tasks. Deliverables 1 to 4 include data for both well-screens with and without association to groundwater body. Deliverable 5 includes only well-screens with association to groundwater body, as requested by SGAV.

2. Introduction

This work is part of the project "*Etablering af kemiske grunddata til Vandområdeplan IV*", funded by The Danish Agency for Green Transition and Aquatic Environment (Styrelsen for Grøn Arealomlægning og Vandmiljø, SGAV, 2025).

The scope of this report is to document the preparation of groundwater chemistry datasets to be used further in relation to the fourth River Basin Management Plan 2027-2032 (Vandområdeplan 4, abbreviated VP4). The datasets described here will be primarily used in the qualitative risk, status, and trend assessments in VP4, but may also support other VP4 tasks.

The work-process is visualised in Figure 1. This report describes the following steps of the data-preparation:

1. Extraction from Jupiter database,
2. Data-cleaning procedures, including calculation of sample-related variables,
3. Data-aggregation,
4. Data-formatting (according to specification provided from SGAV)

The work described here is based on a detailed work-description (Step 0) prepared by GEUS, that included an overview of methods used in various projects related to the previous River Basin Management Plan (Vandområdeplan 3, abbreviated VP3). This was needed, as in the VP3-related work, specific datasets were extracted, cleaned, and aggregated for individual VP3 projects (e.g. status assessment for pesticides, nitrate, trace-elements, etc.). The aim in the current project was to reduce repetitive work and streamline the data-preparation tasks. The detailed work-description was approved by SGAV (after revisions) and was followed here.

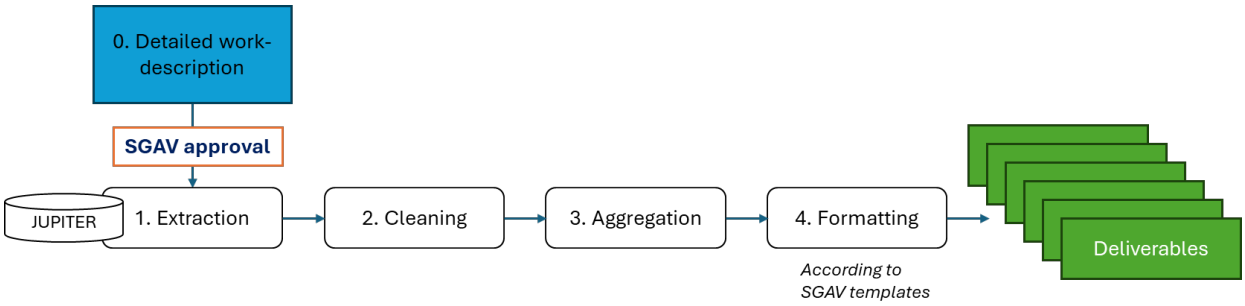

Figure 1 Diagram visualising the work process for "Etablering af kemiske grunddata til Vandområdeplan IV"; Here we document the actual work done in steps 1-4 and overview the deliverables.

2.1 Definitions

The following definitions are used in this report:

- ***Well-screen*** – a sampling point. Here the unique identification number referring to the well and well-screen ID in the Jupiter database are used (BORID_INDTAGSID). The DGU numbers and the well-screen numbers are also available in the datasets

as part of the meta-data but are not used as unique identifying numbers, because the empty spaces within the DGU number format can be problematic when using with some programs.

- ***Analysis*** – a single laboratory or field measurement for a parameter of interest, e.g. a chloride analysis at a specific well-screen and date. It refers to a single value (a row) in the long-format datasets. In the Jupiter database each analysis has a unique identifying number (ANALYSEID).
- ***Sample*** – a specific groundwater sample, analysed for at least one parameter of interest. Here the unique sample identification number from Jupiter is used (PROEVEID).
- ***Groundwater body*** – The Water Framework Directive defines a groundwater body in Article 2.12: "Body of groundwater" means a distinct volume of groundwater within an aquifer or aquifers (EU, 2000). Danish groundwater bodies comprise of one or more aquifers from the National Water Resource Model (DK-model) and are delineated by Troldborg et al. (2023). Here, we use the updated groundwater bodies (version VP4, n = 2049).
- ***AM*** – annual mean for specific parameter at a specific well-screen
- ***MAM*** - mean of the annual means for a specific period, here the VP4 data-period is relevant (2019–2024, incl. both years)
- ***Raw data*** – dataset(s) extracted from Jupiter database. See section 3 for summary of the data-extraction procedure (including preliminary quality assurances and filtering) and section 9 for the Data-request that was followed during data-extraction (section 9 is in Danish). This data is not directly suitable for use in related to VP4 tasks but is used for producing the deliverables (data-products), described in this report.

3. Data-extraction from Jupiter

The data-extraction procedure followed the request (see Appendix A, section 9, in Danish). Relevant Jupiter fields or codes are capitalized and provided in parentheses throughout the report. The produced datafiles are shown in *"italic"* and quotation marks.

The **raw data** was extracted from Jupiter on 25/26 August 2025:

- "*vp4-grunddata-raadata-24092025.dsv*" – includes all chemical analyses for the target parameters; There were 11,145,930 rows (individual chemical analyses) and 35 columns. There were 88,393 unique well-screens (BORID_INDTAGSID), 467,447 samples (PROEVEID), and 974 parameters (STOFKODE).
- "*vp4-grunddata-redox-25092025.dsv*" – includes the redox-type relevant data for each well-screen

Both files are column-separated text files, with encoding Cp1252, and comma (",") for decimal separator. The decimal separator was converted to full stop (".") and it is further consistently used throughout this report and in all deliverables.

The quality assurance and filtering procedures described in this section (see below) were done during the data-extraction from Jupiter database, therefore changes are possible only if a new data-extraction is made. The raw data is a result of the procedure provided in section 9 (in Danish). A summary in English follows here:

- **Parameters**: see list in Appendix B (section 10). Conversion of units and parameters was carried out if necessary, following the rules used in Jupiter. Except for waterworks wells (DATATYPE = "VF"), for all other well-types, only samples filtered at the field were included for the parameters Al, As, Ba, Pb, Cd, Cu, Cr, Hg, Ni, Sr, Zn, Fe, Mn. The exception for waterworks wells was made because the codes for filtering are not used consistently in Jupiter or the samples are rarely filtered in the field for this type of wells. Due to the large abstraction of water, the waterworks wells are not expected to be affected by suspended matter.
- **Period:** unrestricted. Note that although the target period for VP4 is 2019-2024, the period was not limited at data-extraction to ensure that the data can be used also for trend assessments where potentially longer time-series are needed.
- Only the attributes "<" (below detection limit) and " " (empty, i.e. detected) were allowed, as in VP3, because a check showed that there were no new analyses with attribute "B" (quantified).
- All analyses with zero or negative concentrations were excluded. Except for dissolved oxygen, where 0 values were allowed, because for this parameter, 0 is not a lab. reporting error, but the instrumental result.
- All analyses that were not approved by the data-owner (based on the quality assurance, Jupiter-field) were excluded. Thus, only samples with status "approved" were included in the dataset. This filtering procedure is relevant to old data (from before the administrative reform), as currently unapproved data is not uploaded to Jupiter database.
- The analyses for well-screens that were rebuilt, so the physical properties of the screen were changed (but the ID number was not changed), were marked. Further

filtering based on this was done during the data-cleaning procedures (section 4, Table 1).
- The analyses for dug wells (brønd) were marked. Further filtering based on this was done during the data-cleaning procedures (section 4, Table 1).
- Duplicates (i.e. same sample Id and same result) were excluded.

The **PFAS-sum4**, PFAS-sum12, and **PFAS-sum22** were calculated at data-extraction following the description in Appendix A (section 9.5). See section 4.5 for further details on the quality assurance of PFAS sums.

The **datatypes** on well-screen level (DATATYPE) were also assigned at the data-extraction following the description in section 9.2.4 of Appendix A. The request was that each well-screen should be assigned a (single) datatype. In summary, the following datatypes were defined, in this specific **order**:

1. **GRUMO** – well-screens from the national groundwater monitoring programme, which should all have a GRUMO-identification number.
2. **VF** – well-screens in waterworks wells, if
    a. the latest code indicates that it is public waterworks (VIRKSOMHEDSTYPE "V1", "V2", or "M42"
    b. AND the well-screen's latest use/purpose indicated waterworks (FORMAAL "V" or "VV")
3. **DEPOT** – well-screens used for point-sources pollution monitoring.
    a. at least one sample is marked with project that indicates it
    b. OR if the data-owner is a Region.
4. **DEPOT (øvrige)** – same as DEPOT, but if the data-owner is not a Region.
5. **Grundvandskortlægning** – well-screens from the national groundwater mapping programme. Assigned, if the sample purpose for all samples is with the code "GEBKOR" (groundwater mapping programme).
6. **ANDET** – all other well-screens that were not classified in the previous steps

Importantly, the data type is determined from samples in the period 2019–2024, as this is the relevant period to VP4 risk and status assessments. However, since the data-period is not restricted, in the dataset are included also older chemical analyses from well-screens that are either no longer sampled or are closed. For these well-screens there are no samples in the period 2019–2024, thus only the conditions that are not sample-specific could be used. Conditions 3., 4., and 5. require sample-level information, thus well-screens lacking such information can only be classified as GRUMO, VF or ANDET (ANDET includes all other than GRUMO or VF well-screens that did not have data in 2019–2024).

The **redox state** of each well-screen was also determined as part of the data-extraction, and it is based on the raw data with additional filtering criteria (see section 9.3 Appendix A). The standard redox algorithm was used*, see* section 9.3, Appendix A (*Hansen & Thorling 2018, Geovejledning 6).* The redox was determined based on the latest sample with all needed parameters (NO_3, SO_4, Fe, DO) in the period 2010–2024. This period was longer than the relevant VP4 period (2019–2024), to allow for more well-screens to be classified.

Additional specific data-extraction of well-screens was made from Jupiter on 11 September 2025. This was used for **coupling between well-screens and groundwater bodies** (input file: "*intake2gwb.csv*"). The difference in the data-extraction dates for this input file and the rest of the raw data is inconsequential, as the VP4 relevant period is 2019–2024. This input file is part of another deliverable in the same project ("*Etablering af kemiske grunddata til Vandområdeplan IV*"), so it is not discussed further here. Further details are provided in (Troldborg, L. 2025).

4. Data-cleaning procedures

The raw data went through various data-quality checks and filtering to assure the highest possible quality of the data and to minimize bias. Table 1 lists the procedures in their order of execution and provides information on the number of analyses, samples, and well-screens left after the procedure. Specific field names from the raw data and Jupiter codes are used in Table 1.

Table 1 Overview of data-cleaning procedures. Number of analyses, samples and well-screens after the procedure are provided; for procedures where data was filtered out, the numbers of excluded analyses, samples and well-screens is provided in parenthesis and negative sign. For procedures that did not include filtering, no numbers are provided.

#	Procedure	Number after the procedure AND (number excluded during the procedure)		
		Analyses	Samples	Well-screens
	Raw data (974 parameters)	11,145,930	467,447	88,393
1.	Exclude samples with wrong sampling date (format also changed to Date); excluded analyses with sampling year 1 and 217, thus the data was from 1890-2025. The relevant period will be chosen at the aggregation step.	11,143,256 (-2,674)	467,373 (-74)	88,391 (-2)
2	Exclude samples taken before the well-screen was rebuilt, but the ID number was kept the same. Filtering based on UDELADES_GRUNDET_OMBYG_D. Removing column after filtering.	11,110,347 (-32,909)	465,636 (-1,737)	88,375 (-16)
3	Exclude analyses associated with dug wells (BRØND). Removing column after filtering.	11,082,666 (-27,681)	464,011 (-1,625)	87,749 (626)
4	Add a field “GROUP”, indicating which sub-project (group) is the parameter part of (see **section 4.1**). This was needed, so parameter-specific procedures can be carried out. No data-exclusion at this step. Note, that the Jupiter ‘stofgrupper’ were modified according to SGAV specifications.	11,082,666	464,011	87,749
5	Add a field “KORT_NAVN” to use for further grouping. Used for PFAS and MFS (see **section 4.1**). This was needed, so parameter-specific procedures can be carried out. No data-exclusion at this step.	11,082,666	464,011	87,749
6	Check if the selected parameters are classified in accordance with provided feedback by SGAV (see **section 4.1**). Three specific checks were resulting in excluding analyses for few parameters, details are provided in section 4.1.	11,082,657 (-9)	464,011 (0)	87,749 (0)
7	Check for zero-values. Zero values are only present for dissolved oxygen (**DO,** STOFKODE 50), and PFAS sum-4, sum-12, and sum-22, as expected. There are 2080 samples with DO = 0 mg/l. No action is required at this step. Check for negative values – no negative values; no action required.	11,082,657	464,011	87,749
8	Remove obvious errors in reported **pH**. The range of pH in the dataset was different depending on datatype but ranged	11,082,428 (-229)	463,999 (-12)	87,744 (-5)

	from 0.02 to 74000 (both values obvious reporting errors); Excluded pH values: > 15 - all reporting errors irrespective of data type > 9 – for all except for DEPOT, DEPOT (øvrige), as higher pH is possible for these 2 datatypes. < 3 – for all except DEPOT, DEPOT (øvrige), as lower pH is possible for these 2 datatypes due to pollution.			
9	Exclude **PFAS** analyses with sampling years 2000 or 2001 (reporting errors in the sampling year, same as in the PFAS project[1]). The PFAS data starts in 2012.	11,082,185 (-243)	463,998 (-1)	87,744 (0)
10.	Exclude **TFA** analyses for 2023 in GRUMO wells (same condition as in PFAS project, known erroneous data for TFA in the GRUMO well-screens for 2023)	11,082,039 (-146)	463,925 (-73)	87,744 (0)
11.	For **PFAS**, old data is excluded depending on datatype (same condition as in the PFAS project). Therefore, in the dataset are kept: - For GRUMO and VF: only data for the period 2021-2025 (incl. both years), except for TFA. For TFA all data except the excluded at step 10 is kept in the dataset. - For all other datatypes – all data from step 10 is included	11,049,620 (-32,419)	463,542 (-383)	87,744 (0)
12.	Exclude values < LOD with a high LOD (see **section 4.2**)	9,453,293 (-1,596,327)	459,771 (-3,771)	87,243 (-501)
13.	Check for double reporting of stereoisomers (relevant to **pesticides**). See **section 4.3** for details.	9,453,293	459,771	87,243
14.	Add “SUB” and “SUB_sum” fields, containing the substituted values which are to be used further for calculation of sample-based variables (**IG, FG, sum pest, sum chl. Solvents, s**ee **section 4.4)**, and for aggregation. SUB should be used for individual parameters, SUB_sum for calculating the sum-parameters (sum pesticides and sum chlorinated solvents). See **section 4.2** for details about SUB and SUB_sum.	9,453,293	459,771	87,243
15.	Calculate sample-based variables (**IG, FG, sum pest, sum chl. solvents**)., see **section 4.4 for methodology.** A separate table is made with the sample-based variables, which is linked to the clean dataset in step 18 (see below).	-	-	-
16.	QA/QC on the **sum-PFAS**. See **section 4.5** Exclude sum-PFAS that do not meet the quality criteria. Revise LOD, LOQ, SUB, SUB_sum, for sum-PFAS (9004, 9012, 9022), so LOD and LOQ ignored (0 value), SUB and SUB_sum = MAENGDE (as calculated at data-extraction).	9,452,520 (-773)	459,769 (-2)	87,243 (0)
17.	Export incomplete dataset for internal GEUS use. It includes MAENGDE, SUB, SUB_sum, but without the additional meta-data and the calculated sample-based variables from step 15. "*incomplete_clean_dataset_20250926.rds/csv*"	9,452,520	459,769	87,243
18.	Calculate sample-mean for all parameters (for samples with replicate analysis) and **join with the sample-based variables** (from 15.) Export file for further use during aggregation: “*sample_mean_20250926.rds/csv*”	10,072,064 (+619,544) [2]	459,769	87,243

[1] Refers to the project ‘*Udvikling af metode til kemisk tilstandsvurdering af de danske grundvandsforekomster for PFAS*’ 2024-2025 (see Albers et al. (2025))

[2] Here number of analyses refers to number of values (rows), which could be either a sample-mean for a specific parameter, or the sample-based variables from procedure 15. There is a positive sign because the sample-based variables were added to the dataset, so the total number of values in the dataset increased.

19.	Prepare (clean) meta-data for the well-screens and add to the dataset. These include redox type, groundwater body, etc. identification numbers for EU. See **section 6.2** Exported file for further use: "*metadata_20250926.rds/csv*"	-	-	87,243
20.	**Export complete clean dataset (based on sample mean)** to be used further for aggregation. Note that samples for **GRUMO wells without INDTAGSID (or INDTAGSNR) are excluded** from this dataset. These samples are taken during well-drilling and not relevant to the assessment. See **section 6.3** for details.	**10,068,898** [3] (-3,166)	**459,513** (-256)	**87,206** (-37)

4.1 Parameters: grouping and quality checks

The parameters included here were grouped, so various filtering and cleaning procedures specific to a type of parameter can be carried out. The grouping is as in Appendix B (see section 10).

In **procedure 4** (Table 1) the following parameters (STOFKODE provided, same as Stancode) were grouped by the project they will be used in. The new field "GROUP" includes:

- "sporstoffer" – 267, 270, 271, 274, 279, 318, 300, 319, 326, 331, 353;
- "salte_etc" – 240, 280, 308, 59, 312, 297, 321, 356, 324, 75, 50, 13, 261, 335, 1167, 322;
- "nitrat" – 246;
- "mfs" – 83, 85, 86, 374, 378, 379, 380, 383, 386, 543, 868, 1076, 1171, 202, 215, 218, 400, 401, 449, 404, 407, 408, 409, 410, 411, 412, 413, 414, 426, 166, 483, 211, 217, 207, 209;
- "pfas" – 1255, 2908, 1599, 2923, 1259, 2912, 1260, 2913, 1261, 2914, 2932, 1262, 2915, 2933, 1264, 2917, 1265, 2918, 1266, 2919, 1267, 2920, 1597, 2921, 2230, 2925, 1256, 2909, 2930, 1598, 2922, 2910, 1257, 2931, 2231, 2926, 1258, 2911, 2232, 2927, 2233, 2928, 2234, 2929, 1263, 2916, 2934, 1603, 2924, 9004, 9022, 2251, 9012);
- "pest" – all other STOFKODE from Jupiter group 50, that were not already included in the groups above;

In **procedure 5** (Table 1), the following parameters were further grouped. The new field "KORT_NAVN" was used for further grouping of:

- "pfas" – used because there were two or three STOFKODE used for the same parameter (linear or sum). The grouping is the same as in the PFAS project[4]:
  - "PFBA" – 1255, 2908
  - "PFHxS" – 1256, 2930, 2909
  - "PFOS" – 1257, 2931, 2910
  - "PFDS" – 1258, 2911
  - "PFHxA" – 1259, 2912
  - "PFHpA" – 1260, 2913
  - "PFOA" – 1261, 2932, 2914
  - "PFNA" – 1262, 2933, 2915
  - "PFOSA" – 1263, 2934, 2916
  - "PFDA" – 1264, 2917
  - "PFUnDA" – 1265, 2918

[3] Here analyses refers to a value (sample-mean for a parameter or sample-based calculated variable), i.e. single row in the dataset.
[4] Refers to the project '*Udvikling af metode til kemisk tilstandsvurdering af de danske grundvandsforekomster for PFAS*' 2024-2025 (see Albers et al. (2025))

    - "PFDoDA" – 1266, 2919
    - "PFTrDA" – 1267, 2920
    - "PFBS" – 1597, 2921
    - "PFHpS" – 1598, 2922
    - "PFPeA" – 1599, 2923
    - "6:2 FTS" – 1603, 2924
    - "PFPeS" – 2230, 2925
    - "PFNS" – 2231, 2926
    - "PFUnDS" – 2232, 2927
    - "PFDoDS" – 2233, 2928
    - "PFTrDS" – 2234, 2929
    - "TFA" – 2251.
- "mfs" – used because there was additional grouping in Appendix B for these parameters, so specific procedures can be carried out (e.g. calculate sample sum for chlorinated solvents):
    - "chl.solvents_etc" – 83, 85, 86, 374, 378, 379, 380, 383, 386, 543, 868, 1076, 1171
    - "btxn" – 202, 215, 218, 400, 401, 449
    - "phenoler" – 404, 407, 408, 409, 410, 411, 412, 413, 414, 426
    - "water_soluble" – 483, 211, 217
    - "cyanides" – 207, 209
    - "mtbe" – 166

In **procedure 6** (Table 1), we checked if parameters were correctly classified, in accordance with provided clarifications from SGAV (see Appendix E, section 13) on parameters, included in group 50 in Jupiter (classified as pesticides), but part of the MFS group for VP4. The following three checks were made (by STOFKODE and if needed KORT_NAVN or GROUP):

- Are 407, 409, 410, 408, 4011, 412, 413, 414, 426 included in "phenoler" ("mfs")?
    - Yes, no action needed
- Are 415, 416, 418, 524, 424, 421, 422, 423, 861, 420, 1322, 1323, 1324, 1325, 417, 768, 419, 767, 769, 770, 287, 427, 523, 397, 764, 2050, 2049, 103, 140, 168, 172 included in "pest"?
    - Yes, no action needed
- Are 4888, 903, 1806, 870, 871, 0872, 0873, 0874, 201, 1973, 2051, 2897, 0575, 0576, 0577, 0763, 1205, 1550, 1551, 1552, 1559 excluded from "pest"?
    - No, five of these parameters were present in the dataset (1550, 1551, 1552, 1559, 1973), but there are only 9 analyses (3 samples, for 3 well-screens) all below limit of detection (< LOD). Therefore, the analyses for these parameters (1550, 1551, 1552, 1559, 1973) were excluded from the dataset.

4.2 Handling analyses below limit of quantification (<LOQ)

All values below limit of quantification (LOQ) are substituted before aggregation. The substitution is as follow:

- For individual compounds: < LOQ = ½ LOQ, where LOQ = 3*max(LOD); max(LOD) is the highest allowed LOD
- For sums: < LOQ = 0

This follows the same substitution rules as in VP3 projects. Specifically, in two of the VP3 projects (Sporstoffer and Salte), a rule about the highest acceptable LOQ was introduced, according to which the highest LOQ ≤ TV*30%. This rule originates from "Analysekvalitetskravdirektivet, artikel 4 stk 1":

"Medlemsstaterne stiller som mindstekrav til alle anvendte analysemetoder, at deres måleusikkerhed er højst 50 % (k = 2) ved værdien af det pågældende miljøkvalitetskrav, og at deres kvantifikationsgrænse er 30 % af værdien af det pågældende miljøkvalitetskrav eller lavere."

The maximum allowed LOD in this project was selected during step 0 (Figure 1, Detailed work description) based on provided overview for each parameter. The LODs have changed through time for most parameters, so additionally time-series of used LODs was prepared showing that high LODs were present primarily in the old data (early 1980-90s).The maximum allowed LODs were selected considering that if the LOQ is high, then a lot of actual measurements would be censored (substituted with ½ LOQ), but on the other hand, if the maximum allowed LOD is too low, a lot of analyses with values < LOD (with high LOD) will be excluded from the dataset.

The handling of analyses < LOQ was done for all parameters simultaneously. For this, first an additional column LOD was added to the dataset. LOD contains the maximum allowed LOD for each parameter. Overview of the maximum allowed LODs per parameter (or group of parameters) is provided in Appendix C (section 11, Table C1). Additional parameter-specific details on the maximum allowed LODs are provided below.

Then, the values < LOD with high LODs (above the max allowed one) were excluded from the dataset (ATTRIBUT = "<" and MEANGDE > LOD).

Lastly, the substituting of values < LOQ was done by adding new columns (SUB and SUB_sum) to the dataset:

- SUB, when MAENGDE < LOQ = ½ LOQ, otherwise = MAENGDE
- SUB_sum when MAENGDE < LOQ = 0, otherwise = MAENGDE

PFAS

Maximum allowed LODs for PFAS are as in the PFAS project[5] as follow:

- **0.001 µg/L** for PFOA, PFNA, PFHxS, PFOS (TV=0.002 µg/L).
- **0.05 µg/L** for the rest of the PFAS. Same as in PFAS project, except for TFA

In the PFAS project, there was an exemption for TFA, as no high LOD was set and no values < LOD with high LOD were excluded (there was no substitution <LOQ, only <LOD). Here we have selected a maximum allowed LOD, so we could substitute all < LOQ with ½ LOQ without censoring large amounts of data (representing samples with detected PFAS). The most frequent LOD for TFA is 0.05 µg/L (see Figure C1), so max LOD was also set to 0.05 µg/L. For the rest of the PFAS parameters the most frequent LODs are 0.001 µg/L and 0.0003 µg/L.

[5] Refers to the project '*Udvikling af metode til kemisk tilstandsvurdering af de danske grundvandsforekomster for PFAS*' 2024-2025, see Albers et al. (2025).

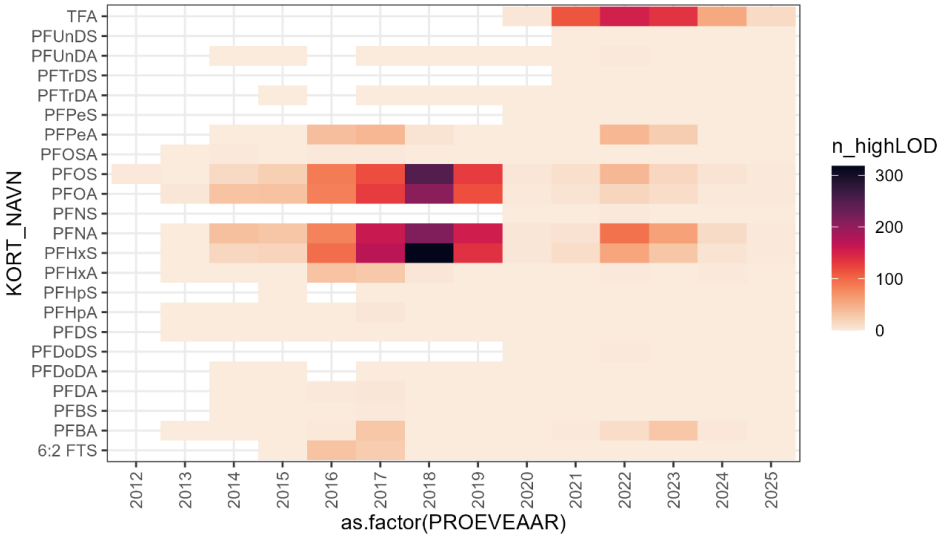

Figure 2 Distribution of values <LOD with high LOD (> 0.001 µg/L for the four PFAS with low TV and 0.05 µg/L for the rest) per year and PFAS parameter

Pesticides

The maximum allowed LOD in the dataset, for all parameters from the pesticides group is **0.01 µg/L**. No distinction was made between parameters, as all parameters are also with the same TV (0.1 µg/L).

MFS

The maximum allowed LODs for MFS (VP4) are compared to the maximum allowed LODs from VP3 (Table 2). The argumentation for selection of slightly different maximum allowed LODs is provided as well in Table 2. This difference is in the selected precision, and it is not consequential. While argumentation for the selection for VP4 is provided here, no such argumentation could be found in the documentation for the data-preparation as part of VP3-MFS, which was reviewed during step 0 of the process (Figure 1) and discussed with SGAV.

Table 2 Comparison of maximum allowed limit of detection (max LOD) for VP3 and VP4 (this dataset) for the following groups of MFS parameters

Group of parameters	KORT_NAVN	Max LOD (VP3)	Max LOD (VP4)	Argumentation
Chlorinated solvents	chl.solvents_etc [1]	0.1001	0.1	LOQ = 30% of TV (TV = 1 ug/l, LOQ = 0.3 ug/l)
Vinyl-chloride	chl.solvents_etc	0.02002	0.02	Analysekvalitetsbekendtgørelsen [3]
BTEXN	btxn	0.1001	0.1	LOQ = 30% of TV (TV = 1 ug/l, LOQ = 0.3 ug/l)
Phenol-compouds	phenoler	0.05005	0.05	LOQ = 30% of TV (TV = 0.5 ug/l, LOQ =0.15 ug/l)
MTBE	mtbe	0.5005	0.5	LOQ = 30% of TV (TV = 5 ug/l, LOQ = 1.5 ug/l)
Water-soluble	water_soluble	1.005	1	LOQ = 30% of TV (TV = 10 ug/l, LOQ = 3 ug/l)
Cyanid, total	cyanides [2]	5.005	5	LOQ = 30% of TV (TV = 50 ug/l, LOQ = 15 ug/l)
Cyanid, syreflygtigt	cyanides [2]	2.002	2	LOQ = 30% of TV (TV = 20 ug/l, LOQ = 6 ug/l)

[1] note that vinyl chloride has its own max LOD

[2] note that the two compounds in this group have compound-specific max LOD

[3] the current one at the time was BEK nr 811 af 19/06/2024

pH

There are 10 analyses for pH with ATTRIBUT = "<" (below LOD) with values in the range 2-7.5. For pH there should not be data < LOD, as this does not allow for proper classification. All analyses with ATTRIBUT = "<" should be excluded. Thus, here we give a value 0 in the LOD field, so all analyses with ATTRIBUT "<" and MEANGDE > LOD are excluded.

Calcium (Ca), sodium (Na), chloride (Cl)

This step should not be relevant for Ca, Na, and Cl, as usually in Danish groundwater these parameters are always detected (i.e. above the LOD). However, there could be reporting errors in Jupiter, where "<" was used in ATTRIBUTE erroneously. Thus, here we have excluded all analyses < LOD for Ca, Na, Cl. As with pH, the LOD value for Ca, Na, Cl was set to 0, so the same condition can be used across the entire dataset. Overview of number of analyses <LOD with LOD range for:

- Ca: n=46 with LOD in the range 0.5-200 mg/l (0.5, 20, 200 most frequently)
- Cl: n=44 with LOD in the range 0.1-67 mg/l (0.5 and 1 most frequently)
- Na: n=18 with LOD in the range 0.01-175 mg/l (1 and 0.1 most frequently)

Ammonium and NVOC

The maximum LODs for ammonium and NVOC allowed in this dataset (VP4) differ from those used in VP3. For ammonium, we used previously 0.257 mg/l in VP3, while in VP4 the maximum allowed LOD is 0.005 mg/l. For NVOC, previously we used 0.2 mg/l, while now for VP4 we use 0.1 mg/l. For both parameters, the maximum LODs that are used here (VP4) are according to the requirements listed for groundwater in the "Analysekvalitetsbekendtgørelsen" (BEK nr 811 af 19/06/2024 was the current version at the time of assessment).

4.3 Checks for stereoisomers

Here we check how many samples have both the sum and the active stereoisomer reported for the same sample. This check is relevant for the following parameters metalaxyl and metalaxyl-M, dichlorprop and dichlorprop-P, mechlorprop and mechlorprop-P. In the samples where both codes are used, only one of the parameters should be used in the sum-pest to avoid double-counting. In these cases, only metalaxyl (692), dichlorprop (841), and mechlorprop (843) should be used. The check revealed that there are:

- 1801 samples (PREOVEID) with both measurements for metalaxyl and metalaxyl-M (692, 1543).
- 3 samples (PROEVEID) with both measurements for dichlorprop and dichlorprop-P (841, 2034).
- 266 samples (PREOVEID) with both measurements for mechlorprop and mechlorprop-P (843, 2039).

The difference from VP3 is that here we use only metalaxyl (692), dichlorprop (841), and mechlorprop (843) when the stereoisomers are also reported for the same sample. This was not done in VP3, as each parameter (STOFNR) was treated as individual compound. This resulted in potential double-counting when calculating sum-pesticides.

4.4 Calculating sample-based variables

All sample-based variables were calculated separately and then joined together using BORID_INDTAGSID, PROEVEID, PROEVEDATO, PROEVEAAR. The following STOFKODEs were defined here:

- 9000 for sum pesticides (STOFNAVN “sum_pest”). In total 160,094 samples
- 9001 for sum chlorinated solvents (STOFNAVN “sum_chl_solv”). In total 108,176 samples
- 9002 for the weathering degree index (STOFNAVN “FG”). In total 166,967 samples
- 9003 for the ion exchange index (STOFNAVN “IG”). In total 184,356 samples.

At least one of these sample-based variables were calculated for 339,162 samples (PROEVEID) at 73,511 well-screens. Detail on the calculations are provided below.

4.4.1 Weathering degree

The weathering degree index (in Danish: forvitningsgrad, FG, (Hansen & Thorling, 2018)) is calculated using the formula:

$$FG = 2 \times \frac{\left(\frac{Ca^{2+}}{40.1}\right) + \left(\frac{Mg^{2+}}{24.3}\right)}{\left(\frac{HCO_3^-}{61.0}\right)}$$

Where FG is the weathering index calculated for each sample, where all Ca, Mg, and HCO3 were simultaneously measured. All concentrations are in mg/L and are converted to molar concentrations. The substitute value (SUB) was used when calculating the index.

4.4.2 Ion exchange

The ion exchange index (in Danish: ionbytningsgrad, IG, (Hansen & Thorling, 2018) is calculated using the formula:

$$IG = \frac{\left(\frac{Na^+}{23.0}\right)}{\left(\frac{Cl^-}{35.5}\right)}$$

Where IG is the ion exchange index calculated for each sample, where both Na and Cl were simultaneously measured. The concentrations are in mg/L and converted to molar concentrations. The substitute value (SUB) was used when calculating the index.

4.4.3 Pesticides sum

The procedure below was followed for calculating sum-pesticides:

1. Only the analyses from GROUP “pest” (pesticides) were selected,
2. For samples where both isomers were reported for:

a. mechlorprop, only the STOFKODE 843 was included (STOFKODE 2039 excluded)
b. dichlorprop, only the STOFKODE 841 was included (STOFKODE 2034 excluded)
c. metalaxyl, only the STOFKODE 692 was included (STOFKODE 1543 excluded)

3. A sample mean was calculated from the SUB_sum (substituted <LOQ = 0); although this step was included in the code, to avoid double-counting of replicates in the sum, it turned out that there were no duplicates based on BORID_INDTAGSID, PROEVEID, PROEVEAAR, PROEVEDATO, STOFKODE, STOFNAVN. Thus, here the sample mean = SUB_sum.
4. For each sample (PROEVEID, PROEVEDATO, PROEVEAAR) and each well-screen (BORID_INDTAGSID) a sum of all values (sample-mean from step 3.) was calculated.

4.4.4 Chlorinates solvents sum

The procedure was like that for pesticides:

1. Only the analyses in the GROUP “mfs” and sub-group chlorinated solvents (KORT_NAVN “chl.solvents”) were selected
2. A sample mean was calculated from SUB_sum (substituted < LOQ = 0). As with pesticides, there were no duplicates in this sub-set. Therefore, at this step sample mean = SUB_sum.
3. For each sample (PROEVEID, PROEVEDATO, PROEVEAAR) and each well-screen (BORID_INDTAGSID) a sum of all values (sample-mean from step 3.) was calculated

4.5 QA/QC on sum PFAS

The quality assurance and quality check (QA/QC) procedure for sum-PFAS, described below, was developed in the project: *‘Udvikling af metode til kemisk tilstandsvurdering af de danske grundvandsforekomster for PFAS*’ 2024-2025 and it is followed here as well.

In the initial calculation of the sums during data-extraction (Appendix A, section 9), sums were calculated only if certain minimum of parameters were analysed per sample (as a quality assurance):

- **Minimum 2 parameters for PFAS-4 sum** (the parameters included in PFAS-4 are: "PFOS", "PFOA", "PFNA", "PFHxS")
- **Minimum 5 for PFAS-12 sum** (the parameters included in PFAS-12 are: "PFOS", "PFOA", "PFNA", "PFHxS", "PFBS", "PFOSA", "6:2 FTS", "PFBA", "PFPeA", "PFHxA", "PFDA", "PFHpA")
- **Minimum 13 for PFAS-22** (the parameters included in PFAS-22 are: "PFBS", "PFHxS", "PFOS", "PFOSA", "6:2 FTS", "PFBA", "PFPeA", "PFHxA", "PFHpA", "PFOA", "PFNA", "PFDA", "PFPeS", "PFHpS", "PFNS", "PFDS", "PFUnDS", "PFDoDS", "PFTrDS", "PFUnDA", "PFDoDA", "PFTrDA")

In the data-cleaning procedures, some analyses <LOD with high LOD (step 11, Table 1) could have been excluded. Thus, the same quality assurance conditions were used here to check if there are still minimum 2, 5, or 13 parameters analysed per sample, for each of the existing sums. This check was performed for each sample.

For all samples, where the conditions were not met for a specific sum (sum-4, sum-12, sum-22), the sum was corrected by substituting the sum-value with NA (i.e. excluding the sum from the dataset).

4.6 Outliers

The cleaning of the dataset has known limitations regarding outliers. Outliers are single values that are very different from the rest of the analyses for a specific well-screen and parameter. Such outliers could be due to reporting errors in the concentration (the actual value), the unit, or the attribute (few examples discussed in the next paragraphs).

The unit conversion (ENHED) was handled during data-extraction following well-accepted rules used with Jupiter data. However, if ENHED was wrongly reported, then the value (MAENGDE) would be converted wrongly (multiplied by the conversion factor). For example, a lab-measurement for As was 1 µg/L, but the unit was wrongly reported to Jupiter as mg/l (i.e. lab result reported as 1 mg/l). The standard unit for As in Jupiter is µg/L, so the mg/L is converted at data-extraction to µg/L. This changes the reported value from 1 mg/l to 1000 µg/L, but the As concentration measured at the lab was 1 µg/L, i.e. 1000 times lower. Usually, such mistakes due to wrongly reported units can easily be spotted, because there are few orders of magnitude difference. However, it is more difficult for parameters where the concentration distribution varies also with few orders of magnitude. In those cases, individual time-series need to be examined. In the current dataset there are also data from wells monitoring point-source pollution, where the concentrations of pollutants are much higher than they would be in GRUMO or waterworks wells. Thus, fast evaluation of unit errors was not possible. Such errors are not very frequent, but they exist. Further evaluation should be based on the time-series for a specific pollutant at a specific location (well-screen) and considering the DATATYPE, but this is not part of this project.

Due to numerous reporting errors in the electrical conductivity (konduktivitet), most probably due to wrong reporting of the unit, we have decided to exclude it from the parameter list, thus conductivity cannot be used in VP4-related work.

Another known reporting error in the MEANGDE field is when “,” is used instead of “.”, or the “.” was not entered by mistake. For example, instead of reporting 1.0 µg/L it was reported 10 µg/L. These errors in the reported value (MAENGDE) are hard to spot, as there could also be correct measurements with the same concentration (within the normal range). Such errors could be identified also by examining the time-series for a specific parameter and location. This has not been done in the current project.

4.7 Recommendations

Considering the limitations listed in the previous section, we recommend the following:

- When using the aggregated datasets (AM or MAM) in VP4, we recommend critical assessment on a case-by-case basis of suspiciously high values. This assessment could be done by double-checking the time-series in the clean dataset.
- Future method-development should include testing and developing of parameter-specific algorithms for automated outlier detection where the DATATYPE is considered.

5. Aggregation

The aggregation in VP4 (like in VP3) is based on the mean of the annual means (MAM). The calculation proceeded in the following order:

1) Annual mean (AM) for each parameter at each well-screen – this is needed for the next step, but also as a separate deliverable for future trend analysis
2) Mean annual mean (MAM) – it will be used for risk and status assessment; only the annual data for the VP4 period (2019-2024) were included.

The relevant periods for specific tasks in VP4 are provided in Table 3.

Table 3 Relevant sampling period for specific tasks in VP4; AM – annual mean, MAM – mean of the annual means

Sampling period	Datasets and purpose
2019-2024 (incl. both years)	Aggregated datasets for status and risk assessment (MAM)
Not restricted	Clean and aggregated datasets for trends (AM)

Appendix B (section10) provides an overview of which parameters must be aggregated with AM and MAM. Several parameters were marked with "no" under aggregation with AM or MAM in the request from SGAV: Ba, Sr, Ca, F, HCO_3, Fe, Mg, CH_4, Na, NVOC, O_2, pH, P_{tot}, SO_4, H_2S, Mn. However, some of these were aggregated nevertheless, as GEUS needed the input for other VP4 related tasks (see next paragraph).

Finally, **aggregated data is available for** the following parameters:

- All parameters from the GROUPs "pest", "nitrate", "mfs", "pfas", "sporstoffer"
- From GROUP "Salte og øvrige" only the parameters: NH_4, Cl, NVOC, pH (STOFKODE 240, 297, 75, 13)

Aggregation for the rest of the parameters should be included in future specific VP4 projects.

In the aggregated datasets are included both the well-screens with and without association with a groundwater body for the parameters listed above. Data for all parameters from Appendix B (section10) is available in the clean dataset (at PROEVEID) for all well-screens irrespective if they are associated with a groundwater body or not.

6. Description of deliverables

6.1 Overview

Table 4 lists the project deliverables. These are the data-products resulting of the cleaning and aggregation procedures described in this report. They are available from the GEUS Dataverse (Voutchkova, 2026).

The main file format is comma-separated values (.csv) with comma as separator (“,”) and full stop as decimal (“.”). Additionally, the files were exported as R dataset (.rds) for direct use in R.

Table 4 Overview of deliverables and report section where more details are provided about the specific deliverable; Data available from GEUS Dataverse (Voutchkova, 2026)

Deliverables		Section	File names
1	Well-screen meta-data	6.2	“metadata_complete_20251002.rds/csv”
2	Clean dataset	6.3	"clean_dataset_with_metadata_20251002.rds/csv"
3	Aggregated dataset(s), including annual mean concentrations (AM, unrestricted period)	6.4	"AM_pest_20251002.rds/csv" "AM_pfas_20251002.rds/csv " "AM_nitrate_20251002.rds/csv " "AM_mfs_20251002.rds/csv " "AM_other_20251002.rds/csv "
4	Aggregated dataset(s), including mean annual mean concentrations (MAM, VP4 period)	6.5	"MAM_pest_20251002.rds/csv " "MAM_pfas_20251002.rds/csv " "MAM_nitrate_20251002.rds/csv " "MAM_mfs_20251002.rds/csv " "MAM_other_20251002.rds/csv "
5	Filled EU templates	6.6	1 file for “Skabelon for indtag – Målestationsniveau grunddata”: “EU_table_wellscreens.rds/csv” 49 files for “Skabelon for indtag – Målestationsniveau Parameter”: EU_table_STOFNAVN.csv”

Note that the specific ‘work-files’ needed for the detailed assessments in individual projects should be prepared within the specific project. The clean and the aggregated (AM, MAM) datasets can be used for these purposes. Therefore, the clean and aggregated datasets are provided in long-format which is easier to use in programming environments. Further details on the content of the deliverables are provided in the specific sub-section.

The files from the fifth deliverable were according to the EU templates provided by SGAV (Appendix D, section 12).

6.2 Meta-data for all well-screens (Deliverable 1)

The following meta-data (Table 5) is prepared for all well-screens with at least one lab. analysis for the included parameters. These meta-data were joined with all other deliverables but are also provided as a separate file.

Thus, the complete meta-data file includes information about **87,243 well-screens**. Note that not all of them have a well-screen ID or a link to groundwater body, and some have chemical sample(s) with sampling date outside the VP4 data-period. Since all chemical data will be used either for the risk assessments or for the trend analysis, the complete meta-data file is exported from R for future use.

Table 5 Well-screen meta-data (Deliverable 1)

Name	Meaning
Meta-data also included in VP3:	
BORID_ INDTAGSID	Unique identification number (ID) for each well-screen combining BORID and INDTAGSID, used for joining different tables.
BORID	Well identification number (numeric)
INDTAGSID	Well-screen identification number (numeric)
DGUNR	Well number (text)
INDTAGSNR	Well-screen number, used on the GEUS homepage (differs sometimes from INDTAGSID)
INDTAG_BUND	Depth to well-screen bottom (m below terrain)
INDTAG_TOP	Depth to well-screen top (m below terrain)
BORINGSDYBDE	Well depth (m below terrain)
XUTM32EUREF89	Projected X coordinate in 32 EUREF 89
YUTM32EUREF89	Projected Y coordinate in 32 EUREF 89
TERRAENKOTE	Terrain elevation at the well (m above sea level)
DATATYPE	Datatype in the format: ANDET, VF, GRUMO, DEPOT, "DEPOT (øvrige)", "Grundvandskortlægning" (see Appendix A for definition)
GVF	Groundwater body ID in the format: “dkmj_16_ks” (updated, for VP4)
GVMAG	Groundwater aquifer ID in the format: “dkmj_ks2_1059” (updated, for VP4)
REDOXVANDTYPE	Redox type: A, B, C, D, X, Y or empty (NA) (see Appendix A for definition)
LOOP	Well-screens form the LOOP program (“yes”, NA)
New meta-data included in VP4 (due to EU reporting needs, see section 6.6 and Appendix D)”	
Grundvandsforekomst	EU-ID for the groundwater body in the format: “DK110_dkmj_1106_ks”
euMonitoringSiteCode	EU-ID for well-screens in the format: “DK201-3854-1” (DGUNR and INDTAGSNR)
euProgrammeCode	Information about the monitoring program for the intake. Includes: DKGRUMO, DKLOOP, DKVandforsyning, DKGEBKOR, DKForurening, DKOevrige Based on DATATYPE (and LOOP Id numbers)
chemicalMonitoring	Information on whether the well-screen is used for chemical monitoring (Yes/No). All well-screens in this dataset: Yes
investigativeMonitoring	Based on **euProgrammeCode:** Yes for DKGEBKOR, DKForurening; No for DKGRUMO, DKLOOP, DKVandforsyning, DKOevrige
surveillanceMonitoring	Based on **euProgrammeCode:** Yes for DKGRUMO, DKLOOP, DKVandforsyning, DKOevrige; No for DKGEBKOR, DKForurening
wellSpring	For all well-screens it should have the value “Well”
Depth	For all well-screens “Unknown”

Name	Meaning
quantitativeMonitoring	Information on whether the well-screen is used for quantitative monitoring (monitoring of ground water level); the field is left empty, as the information is not currently available.

An overview of some aspects of the meta-data is provided here with focus on the different DATATYPEs and the definitions of the new EU meta-data for well-screen classification.

Table 6 shows the number of well-screens per category for the datatype (DATATYPE) and the classification based on the fields from the EU template: euProgrammeCode, chemicalMonitoring, investigativeMonitoring, surveillanceMonitoring (see Appendix D).

Table 6 Well-screens classified according to EU templates (incl. the fields euProgrammeCode, chemicalMonitoring, investigativeMonitoring, surveillanceMonitoring), see Table 5 and Appendix D for definitions; n - number of well-screens

DATATYPE	euProgramme-Code	chemi-calMonitor-ing	investigative-Monitoring	surveillance-Monitoring	n
ANDET	DKLOOP	Yes	No	Yes	391
ANDET	DKOevrige	Yes	No	Yes	53,179
DEPOT	DKForurening	Yes	Yes	No	24,146
DEPOT (øvrige)	DKForurening	Yes	Yes	No	219
GRUMO	DKGRUMO	Yes	No	Yes	2,675
Grundvandskortlægning	DKGEBKOR	Yes	Yes	No	85
VF	DKVandforsyning	Yes	No	Yes	6,548

Note that there are 85 “DKGEBKOR” well-screens. This is because only the well-screens with samples in the VP4 period (2019-2024) can be classified as the DKGEBKOR (Grundvandkortlægning) type. As explained previously (see section 3), this DATATYPE class is based on information at sample level, so if there were no samples in the VP4 period, this classification could not be made. This means that all well-screens with only old samples (before 2019) are classified as ANDET.

As mentioned previously, all well-screens that had at least one analysis for the target parameters were included in the meta-data file; this included also the samples associated only with a well number but without well-screen number. The meta-data table was prepared at step 19 of the cleaning procedures (Table 1) and so it includes also wells (BORID_INDTAGSID) for which INDTAGSID is NA (or INDTAGSNR is NA). Based on this overview the final step of the cleaning procedure was added (step 20, Table 1), where samples associated only with BORID (INDTAGSID is empty) were excluded from the clean dataset for GRUMO well-screens. For GRUMO wells it is known that these samples are taken during well-establishment (drilling), so they are not relevant to the VP4 as they cannot be associated with a specific well-screen (depth of sampling). However, it should be noted that most of the samples associated with only BORID are for ANDET or DEPOT well-screens (Table 7). These are kept in the clean and aggregated datasets, because the reason for the missing well-screen number is unknown. These samples are assigned to different unique numbers (BORID_INDTAGSID), where the INDTAGSID is empty. For example, BORID_INDTAGSID: “77_” is used for the samples that are without INDTAGSID, but all other samples for this well

are associated with INDTAGSID = 1, so they are associated with the BORID_INDTAGSID: “77_1”, as the well-screen number is provided explicitly.

Table 7 Number of well-screens (BORID_INDTAGSID), where the INDTAGSID was missing (empty)

DATATYPE	euProgrammeCode	Missing INDTAGSID (n)	Action
ANDET	DKLOOP	0	
ANDET	DKOevrige	3,289	Kept in dataset
DEPOT	DKForurening	673	Kept in dataset
DEPOT (øvrige)	DKForurening	0	
GRUMO	DKGRUMO	37	Excluded at step 20 (Table 1)
Grundvandskortlægning	DKGEBKOR	0	
VF	DKVandforsyning	0	

There were also 6,723 well-screens not associated with a groundwater body (Table 8), note that the GRUMO wells without INDTAGSID are included in this overview. Further overviews are provided in the respective sections for the clean and aggregated datasets.

Table 8 Well-screens not associated with groundwater body (GVF)

DATATYPE	euProgrammeCode	Missing GVFnr (n)
ANDET	DKLOOP	0
ANDET	DKOevrige	5,470
DEPOT	DKForurening	1,199
DEPOT (øvrige)	DKForurening	6
GRUMO	DKGRUMO	37
Grundvandskortlægning	DKGEBKOR	0
VF	DKVandforsyning	11

6.3 Clean dataset (Deliverable 2)

The clean dataset includes all analyses for the target parameters, that have passed our quality assurance (after step 20, Table 1). The well-screen meta-data is also included, see Table 5 for well-screen meta-data content. Table 9 lists the additional information included in the clean dataset.

This deliverable can be used further for trend-analyses, natural background level estimation or other purposes, as there is no period restriction. It also allows for outlier detection or exclusion at sample-level (see section 4.6 for limitations in our data-cleaning procedures).

Table 9 Clean dataset contents (Deliverable 2), all other meta-data from Table 5 is also in this deliverable.

Name	Meaning
BORID_ INDTAGSID	Unique identification number (ID) for each well-screen combining BORID and INDTAGSID, used for joining different tables.
PROEVEID	Unique identification number for the sample
PROEVEAAR	Sampling year (based on PROEVEDATO)
PROEVEDATO	Sampling date in the format “YYYY-MM-DD”

Name	Meaning
GROUP	Grouping of chemical parameters: "pest", "salte_etc", "nitrate", "mfs", "pfas", "sporstoffer" (see Table 1)
STOFKODE	Unique identification number for the chemical parameter (stancode)
STOFNAVN	Name of the parameter
KORT_NAVN	Short names for the PFAS and grouping of MFS (see Table 1)
value	Sample mean for the parameter
CASNUMBER	CAS number (as in Parameterlisten)
EUNAME	EU name of the chemical parameter (as in Parameterlisten)
ENHED	Unit (for value): 1 – mg/l, 20 – µg/l, 3 – unitless (pH)

Table 10 shows the number of well-screens that are included in the clean dataset, i.e. have at least one analysis. Note that the ANDET group contains all well-screens without samples in the VP4 data-period that were not GRUMO or VF type. It cannot be distinguished between ANDET and DEPOT without information at sample-level for the purpose of sampling.

Table 10 Number of well-screens (BORID_INDTAGSID) with at least one analysis for a target parameter per parameter GROUP and DATATYPE, included in the clean dataset, for the total period.

DATATYPE	euProgrammeCode	Well-screens with data per GROUP (n)					
		mfs	nitrate	pest	salte_etc	sporstoffer	pfas
ANDET	DKLOOP	57	381	155	383	42	NA
ANDET	DKOevrige	31,540	19,026	17,685	31,246	5,009	4,165
DEPOT	DKForurening	19,860	3,661	11,230	6,708	3,924	9,990
DEPOT (øvrige)	DKForurening	155	131	123	176	65	120
GRUMO	DKGRUMO	1,948	2,425	2,245	2,636	2,115	943
Grundvandskortlægning	DKGEBKOR	41	85	85	85	38	2
VF	DKVandforsyning	4,921	6,336	6,430	6,522	6,366	3,487
total		58,522	32,047	37,953	47,756	17,559	18,707

Table 11 shows the number of samples in the clean dataset per parameter GROUP and DATATYPE. Note that not all parameters within a GROUP are analysed for each sample. Further, a more detailed overview should be provided within specific projects.

Table 11 Number of samples (PROEVEID) per parameter GROUP and DATATYPE, included in the clean dataset, for the total period.

DATATYPE	euProgramme-Code	Samples with data per GROUP (n)					
		mfs	nitrate	pest	salte_etc	sporstof-fer	pfas
ANDET	DKLOOP	385	2,1457	2,193	25,322	271	NA
ANDET	DKOevrige	59,849	57,652	47,491	115,631	7,120	5,516
DEPOT	DKForurening	42,551	7,246	16,173	16,202	4,399	11,733
DEPOT (øvrige)	DKForurening	1,835	1,440	326	3,460	339	279
GRUMO	DKGRUMO	16,999	47,412	33,093	65,126	15,572	1,856
Grundvandskortlægning	DKGEBKOR	67	126	183	142	42	7
VF	DKVandforsyning	26,106	37,074	67,389	67,912	42,677	7,921
total		147,792	172,407	166,848	293,794	70,420	27,312

6.4 Aggregated dataset with annual means (AM, Deliverable 3)

The annual mean aggregated files were requested so they can be directly used in trend analysis, thus the period is not restricted to the VP4 data-period. The specific period of interest should be selected in the specific follow-up projects.

Five datasets were prepared based on GROUP of parameters (to be used in different VP4 projects), where the parameter GROUPs were: “nitrate”, or “pest”, or “pfas”, or “mfs”, and the rest (“other”). The “other” dataset includes all parameters from GROUP “sporstoffer” and the parameters NH_4, Cl, NVOC, pH (STOFKODE 240, 297, 75, 13) as these may be relevant with respect to estimating natural background levels.

All files contain the well-screen meta-data (content description in Table 5) and the additional information is in Table 12.

Table 12 Aggregated datasets (Deliverable 3), all other meta-data from Table 5 is also in this deliverable

Name	Meaning
BORID_ INDTAGSID	Unique identification number (ID) for each well-screen combining BORID and INDTAGSID, used for joining different tables.
PROEVEAAR	Sampling year (based on PROEVEDATO)
GROUP	Grouping of chemical parameters: "pest", "salte_etc", "nitrate", "mfs", "pfas", "sporstoffer" (see Table 1)
STOFKODE*	Unique identification number for the chemical parameter (stancode)
STOFNAVN*	Name of the parameter
KORT_NAVN	Short names for the PFAS and grouping of MFS (see section 4.1)
AM	Annual mean concentration (see unit in ENHED)
CASNUMBER**	CAS number (as in Parameterlisten)
EUNAME**	EU name of the chemical parameter (as in Parameterlisten)
ENHED	Unit (for value): 1 – mg/l, 20 - µg/l, 3 – unitless (pH)

* STOFKODE and STOFNAVN are not included for PFAS because KORT_NAVN is used instead, combining multiple STOFNR.

** The CASNUMBER and EUNAME are as provided in Parameterlisten at the time of data-extraction.

Table 13 provides an overview of well-screen number in the “other” group per DATATYPE. For number of well-screens for “mfs”, “nitrate”, “pest”, and “pfas”, see the clean dataset overview (Table 10). Below is overview for the dataset including the rest of the parameters.

Table 13 Number of well-screens in the parameter group “other”; the number of well-screens for the rest of the groups in this dataset is as in Deliverable 2 (Table 10)

DATATYPE	euProgrammeCode	Well-screens (n) in “other”
ANDET	DKLOOP	383
ANDET	DKOevrige	31,133
DEPOT	DKForurening	9,059
DEPOT (øvrige)	DKForurening	176
GRUMO	DKGRUMO	2,636
Grundvandskortlægning	DKGEBKOR	85
VF	DKVandforsyning	6,518
total		49,990

6.5 Aggregated dataset with mean annual means (MAM, Deliverable 4)

The aggregated datasets with MAM were requested, so they can be used in the risk and status assessments for VP4. The period was restricted to the VP4 data-period (2019-2024, incl. both years), so only AM values from this period were aggregated (with a mean). Both well-screens with and without association with groundwater bodies (GVF) were included, as requested. Only the well-screens associated with GVF are relevant to the status assessment and EU reporting for VP4, however those not associated with a specific groundwater body could be used in a risk assessment or specific detailed (manual) evaluation. For further details on aggregation, see section 5.

Five datasets were prepared based on GROUP to be used in different VP4 projects, where GROUP was “nitrate”, “pest”, “pfas”, “mfs”, and the rest (“other”). The “other” dataset includes all parameters from GROUP “sporstoffer” and the parameters NH_4, Cl, NVOC, pH (STOFKODE 240, 297, 75, 13), as these may be relevant in the risk and/or status assessment for trace elements (or other related tasks).

All files contain the well-screen meta-data (content description in Table 5) and the additional information is in Table 14.

Table 14 Aggregated datasets (Deliverable 4), all other meta-data from Table 5 is also in this deliverable

Name	Meaning
BORID_ INDTAGSID	Unique identification number (ID) for each well-screen combining BORID and INDTAGSID, used for joining different tables.
GROUP	Grouping of chemical parameters: "pest", "salte_etc", "nitrate", "mfs", "pfas", "sporstoffer" (see Table 1)
STOFKODE*	Unique identification number for the chemical parameter (stancode)
STOFNAVN*	Name of the parameter
KORT_NAVN	Short names for the PFAS and grouping of MFS (see Table 1)
MAM	Mean annual mean (MAM) concentration (see unit in ENHED)
CASNUMBER**	CAS number (as in Parameterlisten)
EUNAME**	EU name of the chemical parameter (as in Parameterlisten)
ENHED	Unit (for value): 1 – mg/l, 20 - µg/l, 3 – unitless (pH)

* STOFKODE and STOFNAVN are not included for PFAS because KORT_NAVN is used instead, combining multiple STOFNR.

** The CASNUMBER and EUNAME are as provided in Parameterlisten at the time of data-extraction.

In total, there are 34,228 well-screens (BORID_ INDTAGSID) with a MAM value for at least one of the included parameters. Table 15 shows how many well-screens have data for specific group of parameters, and the number of those well-screens that are associated with a groundwater body. It should be noted that for the ‘mfs’ group 67% of the well-screens that have MAM value for at least one of the ‘mfs’ parameters are not associated with a groundwater body. For the rest of the parameter GROUPs the percentages were between 72% and 84% (Table 15). Most of the well-screens without association to a groundwater body are the DEPOT type (euProgrammeCode: DKForurening). This data could be used either within a risk assessment framework or at the detailed manual status assessments for specific groundwater bodies.

Table 15 Number of well-screens in the aggregated dataset with mean annual means (MAM) per DATATYPE and parameter group. In the column "GVF" is indicated if the overview includes all well-screens (with and without association with groundwater body, Y+N) or only the well-screens with association with groundwater body (Y); NA – not available

DATATYPE	euProgramme-Code	GVF	Well-screens with data per GROUP (n)					
			nitrate	pest	salte_etc	mfs	spor-stoffer	pfas
ANDET	DKLOOP	Y+N	92	51	92	NA	NA	NA
		Y	13	7	13	NA	NA	NA
ANDET	DKOevrige	Y+N	1,619	1,786	1,902	986	179	969
		Y	1,345	1,544	1,555	818	112	861
DEPOT	DKForurening	Y+N	3,179	11,013	5,949	19,617	3,784	9,905
		Y	2,132	6,606	3,790	11,919	2,140	6,051
DEPOT (øvrige)	DKForurening	Y+N	106	113	165	137	50	118
		Y	83	95	132	104	42	99
GRUMO	DKGRUMO	Y+N	1,336	1,184	1,342	1,102	1,059	826
		Y	1,189	1,040	1,195	968	924	730
Grundvands-kortlægning	DKGEBKOR	Y+N	85	85	85	38	35	2
		Y	77	77	77	33	31	2
VF	DKVandforsyn-ing	Y+N	5,614	6,008	5,923	3,114	5,889	3,336
		Y	5,241	5,581	5,507	2,934	5,475	3,120
Total well-screens		Y+N	12,031	20,240	15,458	24,994	10,996	15,156
		Y	10,080	14,950	12,269	16,776	8,724	10,863
		Y (%)	**83.8%**	**73.9%**	**79.4%**	**67.1%**	**79.3%**	**71.7%**

6.6 EU templates (Deliverable 5)

Two templates with instructions for formatting and content for EU reporting were provided by SGAV (Appendix D).

Template "Målestationsniveau grunddata"
This template includes the meta-data for only the well-screens (n= 23,451) that are:

- included in the aggregated MAM datasets (only within VP4 data-period), AND
- are with data for at least one of the parameters with threshold values (Appendix B, section 10), AND
- are associated with a groundwater body.

Therefore, this template does not include all well-screens from Deliverable 4, but a subset that is relevant to the qualitative risk and status assessments for VP4.

The following meta-data were included in this table (as per the EU template): "Grundvandsforekomst", "euMonitoringSiteCode", "euProgrammeCode", "chemicalMonitoring", "quantitativeMonitoring", "investigativeMonitoring", "surveillanceMonitoring", "wellSpring", "Depth" (see Table 5 for description). Note that the "quantitativeMonitoring" needs to be filled later, when the information about which well-screens are used also for quantitative monitoring is available.

To facilitate this, we have also kept in the table the following identification numbers for well-screens: "BORID_INDTAGSID", "BORID", "INDTAGSID", "DGUNR", "INDTAGSNR".

Template "Målestationsniveau Parameter"
This template was filled out based on the clean dataset, with the following restrictions:

- only analyses from the VP4 period were included AND
- only for the parameters with thresholds from Appendix B (section 10), but for pesticides only sum-pesticides, and for PFAS only sum-4 and sum-22.
- only for well-screens affiliated with GVF

The following meta-data were included in this table (as per Appendix D, section 12): Grundvandsforekomst, euMonitoringSiteCode, gwPollutantCode, gwPollutantOther, ChemicalMatrix, ChemicalPurpose, Frequency, Cycle, LastMonitored. In addition, the identification numbers were also kept in the tables (when relevant), so the "ChemicalPurpose" field can be revised later when it is clear if it is used also for trend analysis: "BORID_INDTAGSID", "STOFKODE", "STOFNR". For details on these meta-data see Table 5. Below are provided details about the parameter-specific meta-data: Frequency, Cycle, LastMonitored, gwPollutantCode, gwPollutantOther.

Frequency is the frequency of measurements in the well-screen per year (mean number per year within the years with measurements) for a specific parameter in the VP4 data-period 2019-2024. Only round numbers between 1-365 are accepted. Therefore, the frequency was rounded in R based on the standard IEC 60559, where rounding off a 5 follows the rule '*go to the even digit*'. Example, 2.5 is rounded to 2, while 3.5 is rounded to 4. This is only an issue for the exact 5, if the number is 2.51 it is rounded to 3 (as expected) and if 3.51 is rounded to 4.
For example, if there was 1 sample for 2019, 3 samples for 2020, and 4 samples for 2024, then the Frequency is calculated as follow:

Frequency = (1+3+4)/3 = 2.667 ≈ 3

Since the Frequency is calculated only for years with measurements there are some peculiarities in the results. For example, Frequency = 3 also if 3 samples were taken every year, i.e.

Frequency = (3+3+3+3+3+3)/6 = 3

Similarly, Frequency = 1, when there is:

- one sample every year in the period. This is the standard case, where there was a regular sampling in the VP4 period (with 1 sample taken every year). In this case, the Frequency = (1+1+1+1+1+1)/6 = 1
- a single sample in only one year (no other measurements). This is because the frequency for that year will be 1, and for all other years (without data) will not be available (NA). So, in this case Frequency = (1)/1 = 1
- or a single sample in only some years and no samples in the rest of the years in the period.

Thus, the Frequency should be used together with Cycle (see below).

Cycle is the monitoring cycle – mean number of years between sampling years. The acceptable values are 0, 1, 2, 3, 4, 5, 6, 12, 18, -9999. It is calculated as difference between the sampling years. For example, if there were measurements in 2019, 2021, 2024, then we calculate difference between the sampling years (2021-2019 = 2, 2024-2021=3), then the Cycle is calculated as follow:

Cycle = (2+3)/2 = 2.5 ≈ 2 (rounding rule the same as described for Frequency).

For those well-screens where cycle could not be calculated, -9999 is used. This is for example the case where there was only one measurement in the VP4 period. For example, if there was only one measurement in 2019, it is not possible to calculate difference in sampling years, as there is only one sampling year.

If there was only one sample for a specific parameter at a specific well-screen, then Cycle = -9999 and Frequency = 1. Therefore, the Cycle and Frequency together could provide a better idea, if there was indeed only one sample within one year or one sample every year in the VP4 period.

LastMonitored – latest sampling year for the specific parameter in format YYYY.

gwPollutantCode is the same as “EU-navn (WISE)” (here EUNAVN) from the Parameterlisten (DMP, https://parameterlisten.miljoeportal.dk/parameter/cc5e28f9-b6f8-413d-9ec9-1adc406eb0cb), so it was used as a starting point to create a link between STOFNR (stancode) and the “EU-navn (WISE)”. It was quality assured that the gwPollutantCode is in the list with codes, provided by SGAV. Where there was missing information, the gwPollutantCode was added based on the provided list from SGAV. For the parameters not in the provided list, “EEA_00-00-0 Other” was used, as per template. In that case, gwPollutantOther was filled out. The code "EEA_00-00-0 - Other parameter" was given to sum pesticides, sum chlorinated solvents, sum pfas-4 and sum pfas-22. See Table C2 (Appendix C, section 11) for overview of gwPollutantCode corresponding to the specific STOFNR.

gwPollutantOther was used for those parameters where gwPollutantCode was ”EEA_00-00-0 Other”. It is in the format “CAS number – Parameter name”. SGAV provided additional list with gwPollutantOther for sum pesticides, sum chlorinated solvents, sum pfas-4 and sum pfas-22 (See Table C2, Appendix C, section 11).

Table C2 (section 11) provides overview of the used gwPollutantCode, gwPollutantOther, STOFKODE, and STOFNAVN with number of well-screens with data for the specific parameter. Note that these are only the well-screens associated with a groundwater body.

Figure 3 shows an example of Frequency, Cycle, and LastMonitored for two of the parameters: nitrate and sum PFAS-22 to illustrate that there are parameter-specific differences in data-availability.

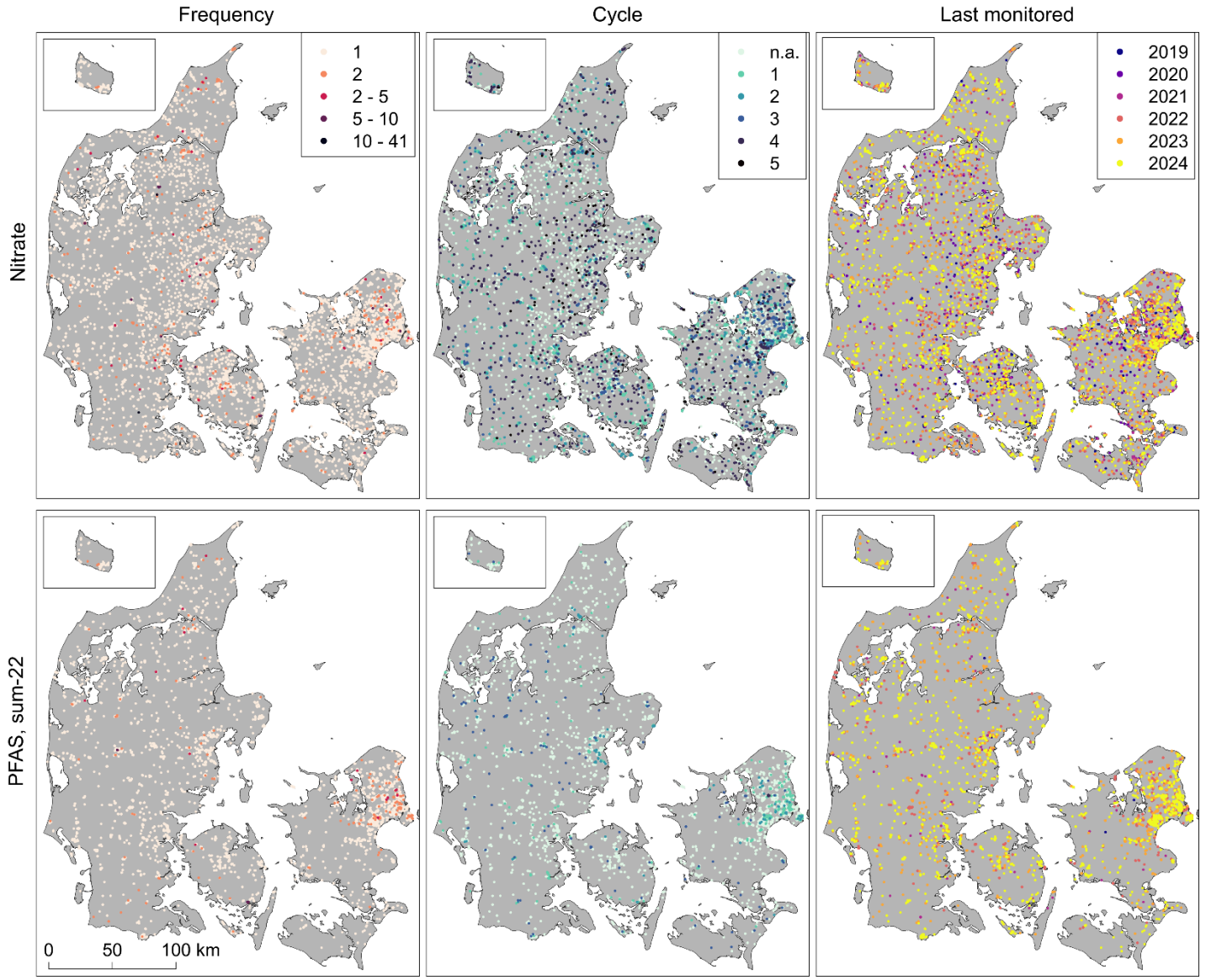

Figure 3 Example of Frequency, Cycle, and LastMonitored for two parameters: nitrate and sum PFAS-22

7. References

Albers, C.N., Voutchkova, D., Thorling, L., Lund, O.B. Fjordbøge, A.S. (2025) Udvikling af metode til kemisk tilstandsvurdering af de danske grundvandsforekomster for PFAS. Udkast til rapport, GEUS.

EU (2000) The Water Framework Directive 2000/60/EC. https://eur-lex.europa.eu/eli/dir/2000/60/oj (accessed 5 Jan 2026)

Hansen, B. & Thorling, L. (2018) Kemisk grundvandskortlægning. GEO-VEJLEDNING 2018/2. Særudgivelse fra GEUS. https://data.geus.dk/pure-pdf/Geovejledning%202018-2.pdf

Troldborg, L., Møller, I. B., & Sandersen, P., (2023). Revision af grundvandsforekomster: Opsamling på erfaringer fra arbejde med kvalitativ tilstandsvurdering. GEUS. Danmarks og Grønlands Geologiske Undersøgelse Rapport Bind 2023 Nr. 49 https://doi.org/10.22008/gpub/34716

Troldborg, L. (2025) Revision af indtagskoblingen til grundvandsforekomster. GEUS-notat 06-VA-2025-05.

Voutchkova, D. (2026) Groundwater chemistry data for the fourth River Basin Management Plan (Vandområdeplan 4), https://doi.org/10.22008/FK2/IHVDXL, GEUS Dataverse, V1

8. Acknowledgements

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9. Appendix A: Data-request (in Danish)

In Danish: “Dataudtræk VP4 grunddata 2025”

LTS, DV/Rev 22 Sep. 2025

9.1 Formål

Udtrækket skal anvendes i projektet "*Etablering af kemiske grunddata til Vandområdeplan IV*" (SGAV, 2025), hvor GEUS udarbejder ét datasæt, der skal bruges til alle VP4-relaterede projekter for grundvandsforekomsternes kemiske tilstand (inklusive risiko-, tilstands- og trendvurderinger) og som understøttende information til den kvantitative tilstandsvurdering for VP4.
Detaljerne om hvilke data og metadata, der skal inkluderes i Jupiter-udtrækket, findes nedenfor. Beskrivelsen er baseret på PFAS-metode til tilstandsvurdering (2024).

9.2 Udtræk af rådata for forskellige stoffer i grundvand

9.2.1 Format

Jupiter-udtrækket med rådata:

- Et **lang-format** datasæt udarbejdes, hvor hver analyseparameter får sin egen linje.
- Filnavn: VP4-grunddata-raadata-dato
- Dokumenttype: tekst (semikolon-separeret fil, med decimal ”,”)
- Tomme felter: tomme, ikke udfyldt

Herudover, en tabel med tjek af hvor mange prøver, der er med attribut “A” (ikke påvist), “B” (påvist), “C” (spor) (https://data.geus.dk/tabellerkoder/koder.html?codetype=754) og information om kvantificeringsgrænsen for de relevante stoffer. **Resultaterne viser, at der er ikke indberettet analyser med attribut B, efter der blev åbnet op for denne mulighed sidste år.** Filtrering for attribut (se 2.2) behøver ikke at blive ændret og er som i VP3.

9.2.2 Søgekriterier og filtrering

- Stoffer:
    - se **Appendix B (”Appendix_B.xlsx”) for alle stoffer som inkluderes,**
        - **for PFAS se også Bilag 1 og 2 (her); listen skulle blive det same som i Appendix_B.xlsx) og i PFAS-projektet**
        - **for pesticider: alle i Jupiter gruppe 50, filtreres i datarensningstrinnet.**
- Parametre som er indberettet med anden parameter, men omregnes:
    - Hovedbestanddele: 242 omregnes til 240; 313 omregnes til 312; 247, 248, og 251 omregnes til 246; 262 omregnes til 261; 334 omregnes til 335; 342 og 343 omregnes til 1167. Parameteren 59 udtrækkes og **omregnes ikke**.

- Pesticider: 287, 91, 635 og 637 omregnes **ikke** manuelt.

- Periode: **ubegrænset**
- Attribut ud for mængde må være kun ”<” eller uden attribut (tom).
- Mængden må ikke være ”0” eller negativ, **bortset fra oxygen Indhold** (STANCODE 50)
- Analysens kvalitetssikringsfelt må ikke være 4, 5, 6, 8, 12, 13,14 eller 15 (betyder ”afvist”).
- Prøvens status skal være blank, 2, 4, 6, 8, 10 eller 14 (betyder ”godkendt”).
- Hvis et givet indtag er ombygget i perioden, skal der i den senere dataanalyse kun anvendes data for den del af perioden, der ligger efter ombygningen og dette markeres derfor. Ombygning kan identificeres, hvis der er indtag med forskellig indtag top eller bund, men med samme boringsindtags-nr., brug start/slut data på filteret).
- Hvis boringen er en brønd, markeres dette, genbrug algoritme fra vandområdeplanerne.
- Forkerte enheder som kan omregnes, omregnes for alle stoffer (eksempel: pesticider med enhed 1 omregnes til enhed 20).
- **Bortset fa VF**, for all andre typer inkluderes kun feltfiltrerede prøve (”2. filtreret i felten” og ”4. filtreret”) for stofferne:

Stof	STANCODE
Aluminium (Al)	267
Arsen (As)	270
Barium (Ba)	271
Bly (Pb)	274
Cadmium (Cd)	279
Kobber (Cu)	318
Chrom (Cr)	300
Kviksølv (Hg)	319
Nikkel (Ni)	326
Strontium (Sr)	331
Zink (Zn)	353
Jern (Fe)	312
Mangan (Mn)	322

HCO3, Ca, Mg er ikke inkluderet i listen på baggrund af et overblik over mængde af analyser fra vandforsyningsboringer der bliver (ikke) filtreret:

STOF	STANCODE	FILTRERING	ANTAL	MAX_INDDATO
Calcium	280	Andet	13	19-12-00 12:08
		Filtreret	211	14-05-25 23:07
		Filtreret i felten	8220	27-06-25 14:58
		Filtreret i laboratoriet	710	03-12-14 20:54
		Ikke filtreret	**39406**	13-08-25 16:04
		Ikke oplyst	26870	28-11-19 9:51
			11864	08-08-25 17:05
Hydrogencarbonat	59	Andet	15	19-12-00 12:08
		Filtreret	133	28-11-19 11:08
		Filtreret i felten	6767	27-06-25 14:58
		Filtreret i laboratoriet	740	25-01-16 11:10
		Ikke filtreret	**40442**	13-08-25 16:04
		Ikke oplyst	27363	28-11-19 9:51
			10371	08-08-25 17:05
Magnesium	321	Andet	14	19-12-00 12:08
		Filtreret	205	14-05-25 23:07
		Filtreret i felten	8129	27-06-25 14:58

STOF	STANCODE	FILTRERING	ANTAL	MAX_INDDATO
		Filtreret i laboratoriet	677	03-12-14 20:54
		Ikke filtreret	**39288**	13-08-25 16:04
		Ikke oplyst	26668	28-11-19 9:51
			11837	08-08-25 17:05

- Dubletter forkastes (analyser samme prøveID, og samme resultat for alle parametre).

9.2.3 Disse felter udtrækkes:

- Anlæg
  - Virksomhedsstype (anvendes til at identificere VV)
- Boring
  - BORID
  - DGU nr.
  - Boringsdybde
  - X-UTM32EUREF89
  - Y-UTM32EUREF89
  - Terrænkote (z-koordinat)
  - BOR_FORMAAL (gerne lang tekst)
  - BOR_ANVENDELSE
- Indtag
  - Grundvandsforekomst
  - Magasin
  - Indtags nr.
  - Indtags ID
  - GRUMO nr. (8 cifret)
  - Indtagsbund (m u.t.)
  - Indtagstop (m u.t.)
  - Anvendelse
  - Bjergart (kalk, ler, sand osv.) brug algoritmen i GRUMO-udtrækket det er hovedkomponent
  - For indtag uden oplysninger om indtagstop anvendes en kobling i de tilfælde, hvor der er tale om hårde bjergarter som kalk, og granit, med udgangspunkt i Lars Troldborgs liste og algoritmen i GRUMO-udtrækket til BORTEK.
- Prøve
  - Dataejer
  - Projekt
  - PrøveID
  - Prøveår
  - Prøve dato
  - Stofkode
  - Stofnavn
  - Laboratorie
  - Mængde
  - Detektionsgrænse
- Parameterlisten
  - Stofkode (stankode)
  - CAS nummer – eksempel format: ”7440-38-2”
  - EU-navn (WISE) – eksempel format: ”CAS_7440-38-2 - Arsenic and its compounds”

PFAS-sum4, PFAS-sum12 og PFAS-sum22 beregnes som i PFAS projektet (se Bilag 2 nedenfor). Pseudo_Stofkoder genereres for PFAS-sum4, PFAS-sum12 og PFAS-sum22.

9.2.4 Datatyper på indtagsniveau.

Alle indtag skal tilskrives én datatype. Vi har behov for, at det er på indtagsniveau til dette projekt. Derudover vil vi gerne skelne mellem regionens data og andre punktkildedata. Vi ønsker også indtag, der kun er anvendt til gebyrkortlægning identificeret, da de som oftest vil have høj kvalitet og er uden indvinding.
Dette betyder ift. GRUMO -udtrækket at vi underopdeler DEPOT-kategorien og andet-kategorien.
Der indsættes kolonne med datatype direkte i udtrækket.

- Indtaget anses for at være ”GRUMO”, når der er et tilknyttet GRUMO-nummer
- Ellers er indtaget ”VF” (Vandforsyningsboring), hvis
    - Indvindingsanlæggets seneste virksomhedstype var ”V01”, ”V02” eller ”M42”
    - Og boringens seneste anvendelse (sekundært formål) var ”V” eller ”VV”.
- Ellers er indtaget ”DEPOT”, hvis mindst en prøves projekt indikerer dette eller hvis dataejer er Region. Der skelnes mellem ”DEPOT” (regionsdata= region er dataejer) og ”DEPOT (øvrige)”.
- Ellers er indtaget ”Grundvandskortlægning”, hvis prøveformål for alle prøver er GEBKOR.
- Ellers er indtaget som værende af datatypen ”ANDET”.

Denne opdeling kræver at der søges på disse niveauer

- Anlæg
    - Anlægstype
- Boring
    - Formål
    - BORID
    - Indtags ID
    - GRUMO nr.
    - Anvendelse
- Prøve, alle prøver i perioden 2019-2024:
    - Projekt
    - Dataejer

Datatyperne er baseret på prøve i perioden 2019-2024. Hvis der er indtag i datasetet, uden prøver i perioden, så datatypen er GRUMO, VF, eller ANDET (disse datatyper er ikke på prøveniveau, men for hver indtag).

9.3 Redoxvandtype (separat datasæt).

9.3.1 Formål

Der skal beregnes redoxvandtyper, som vi efterfølgende kan flette med det aggregerede datasæt.

Dataudtrækket fra punkt 2.kan bruges og **søgekriterierne og filtreringen fra 2.2** er også relevante her.
Derudover, skal analyser med attribut "<" **og** MÆNGDE højere end de specifikke værdier udelukkes før redoox-algorimen køres:

- Nitrat 0.3 mg/l (attribute "<" og MAENGDE > 0.3)
- Sulfat 0.5 mg/l (attribute "<" og MAENGDE > 0.5)
- Jern 0.01 mg/l (attribute "<" og MAENGDE > 0.01)
- Ilt 0.1 mg/l (attribute "<" og MAENGDE > 0.1)

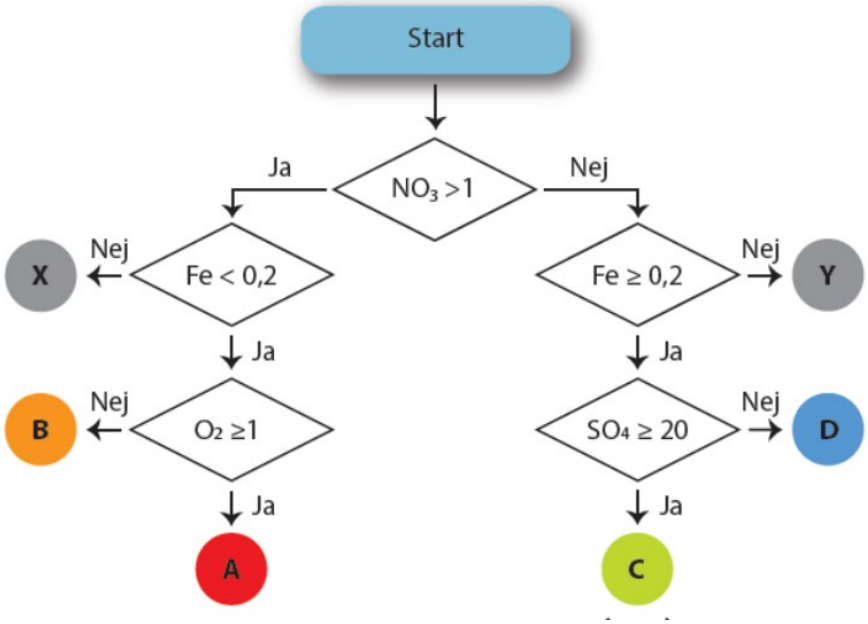
9.3.2 Etablering af datasæt

Der udarbejdes en datafil (VP4-grunddata-redox-dato) med dette indhold:
Periode: **2010-2024**
Kolonner i udtrækket, hvor hver række repræsenterer et indtag:

- BORID
- Indtags ID
- DGU nr.
- Indtag nr.
- X-UTM32EUREF89
- Y-UTM32EUREF89
- Prøvedato (for seneste analyse med sammenhørende værdier for nitrat, sulfat, ilt og jern)
- Nitrat (seneste værdi)
- Sulfat (seneste værdi)
- Jern (seneste værdi)
- Ilt (seneste værdi)
- Nitrat (middelværdi 2010-2024)
- Sulfat (middelværdi 2010-2024)
- Jern (middelværdi 2010-2024)
- Ilt (middelværdi 2010-2024)
- Redoxvandtype, Beregnet værdi baseret på seneste værdi med sammenhørende værdier: se næste afsnit. Samme algoritme som i vandområdeplan 3.

9.3.3 Redoxvandtyper

Redoxvandtyper beregnes efter algoritmen i figur 1.
Redoxvandtypen beregnes på basis af seneste analyse med samtidige værdier for nitrat, ilt, jern og sulfat. Hvis dette ikke er muligt, beregnes det på basis af gennemsnitskoncentrationen for perioden 2010-2024. Dvs, gennemsnits beregninger anvendes kun, når der ikke er en prøve inden for den udtrukne periode, med data for alle parametre (nitrat, ilt, jern og sulfat samtidigt.



Figur 1. Algoritme for beregning af redoxvandtyper (Hansen og Thorling, Geovejledning 6, 2018).

9.4 Bilag 1: PFAS-stoffer (stofgruppe 110, perfluorerede stoffer)

Fra PFAS-projektet "Udvikling af metode til kemisk tilstandsvurdering af de danske grundvandsforekomster for PFAS 2024-2025".
Datahåndteringen og metoder til aggregering m.m. er identiske med dem som blev fast lagt i projektet *'Udvikling af metode til kemisk tilstandsvurdering af de danske grundvandsforekomster for PFAS*', der gennemføres i 2024-25.
PFAS omfatter i denne sammenhæng **alle stoffer i stofgruppe 110** (se nedenfor), dog undtaget koder med "inklusiv precursor" i stofnavn[6].
Stofnr. 2251 (Trifluoreddikesyre) er inkluderet i udtrækket, selvom det pt. er noteret i anden stofgruppe i Jupiter-databasen.
Sumværdierne for 4, 12, og 22 PFAS er inkluderet i udtrækket, efter metode som beskrevet i Bilag 2. Der skal være:

- mindst 2 stoffer for at beregne PFAS4,
- mindst 5 stoffer for at beregne PFAS12,
- mindst 13 stoffer for at beregne PFAS22.

Sumværdierne er inkluderet i datasættet med stofnavn (PFAS-sum4, PFAS-sum12, PFAS-sum22) en ekstra kolonne i udtrækket for hver sumværdi med dét antal stoffer, som har indgået i sumberegningen.

[6] Koder med "inklusiv precursor" i stofnavn er ikke stofspecifikke, men relaterer til en særlig oxidationsmetode ("TOP"), som forsøger at fange eventuelle precursorer, som kan omdannes til det respektive stof over tid. En sådan uspecifik måling er ikke velegnet til tilstandsvurdering.

Stancode	Stofnavn
Beregnet	PFAS-Sum4
Beregnet	PFAS-sum12
Beregnet	PFAS-sum22
1255	PFBA (Perfluorbutansyre)
1256	PFHxS (Perfluorhexansulfonsyre)
1257	PFOS (Perfluoroktansulfonsyre)
1258	PFDS (Perfluordecansulfonsyre)
1259	PFHxA (Perfluorhexansyre)
1260	PFHpA (Perfluorheptansyre)
1261	PFOA (Perfluoroktansyre)
1262	PFNA (Perfluornonansyre)
1263	PFOSA (Perfluoroktansulfonamid)
1264	PFDA (Perfluordecansyre)
1265	PFUnDA (Perfluorundecansyre)
1266	PFDoDA (Perfluordodecansyre)
1267	PFTrDA (Perfluortridecansyre)
1386	Perfluorooctan sulfonyl fluorid
1596	Perfluortetradecansyre (Lineær)
1597	PFBS (Perfluorbutansulfonsyre)
1598	PFHpS (Perfluorheptansulfonsyre)
1599	PFPeA (Perfluorpentansyre)
1600	Perfluor-3,7-dimethyloctansyre
1601	7H-Perfluorheptansyre
1602	2H,2H-Perfluor-decansyre
1603	6:2 FTS (1H,1H,2H,2H-Perfluoroctansulfonsyre)
1604	2H,2H,3H,3H-Perfluorundecansyre
1605	1H,1H,2H,2H- Perfluordecansulfonsyre
1606	1H,1H,2H,2H- Perfluorhexansulfonsyre
1609	1H,1H,2H,2H-Perfluorhexanol
1610	1H,1H,2H,2H-Perfluoroctanol (lineær)
1611	1H,1H,2H,2H-Perfluordecanol (lineær)
1612	1H,1H,2H,2H-Perfluordodecanol
1613	n-Methyl-perfluoroctansulfonamid
1614	n-Ethyl-perfluoroctansulfonamid
1615	n-Methyl-perfluoroctansulfonamidethanol
1616	n-Ethyl-perfluoroctansulfonamidethanol
1832	Perfluorhexadecansyre (Lineær)
1833	n-Ethylperfluoroctan-sulfonamid-eddikesyre
1834	n-Methylperfluor-octansulfonamid-eddikesyre
1835	Perfluoroctansulfonamid-eddikesyre
1895	Perfluor-4-ethylcyclohexan sulfonsyre
1896	Perfluor-1-ethylcyclohexan sulfonat
2162	Perfluoroheptansyre inklusiv precursor
2163	Perfluoroctansyre inklusiv precursor
2164	Perfluornonansyre inklusiv precursor
2165	Perfluorbutansulfonsyre inklusiv precursor
2166	Perfluorhexansulfonsyre inklusiv precursor
2167	Perfluoroctansulfonsyre inklusiv precursor
2168	Perfluordecansulfonsyre inklusiv precursor
2169	Perfluoroctansulfonamid inklusiv precursor
2170	Perfluorhexansyre inklusiv precursor
2171	Perfluorbutansyre inklusiv precursor
2172	Perfluorheptansulfonsyre inklusiv precursor
2173	Perfluorundecansyre inklusiv precursor
2174	Perfluortetradecansyre inklusiv precursor
2175	Perfluorpentansyre inklusiv precursor
2176	Perfluordecansyre inklusiv precursor
2177	6:2 Fluortelomer sulfonsyre inklusive precursor
2178	Perfluordodecansyre inklusiv precursor
2179	Perfluortridecansyre inklusiv precursor
2182	8:2 Fluortelomer sulfonsyre inklusiv precurser
2189	HFPO-DA (GenX)
2230	PFPeS (Perfluorpentansulfonsyre)
2231	PFNS (Perfluornonansulfonsyre)
2232	PFUnDS (Perfluorundecansulfonsyre)

Stancode	Stofnavn
2233	PFDoDS (Perfluordodecansulfonsyre)
2234	PFTrDS (Perfluortridecansulfonsyre)
2555	9-Chlorhexadecafluor-3-oxanonan-1-sulfonsyre
2556	11-Chloreicosafluor-3-oxaundecan-1-sulfonsyre
2571	4:2 Fluortelomer sulfonsyre inklusiv precursor
2572	Perfluor-3,7-dimethyloctansyre inklusiv precursor
2573	7H-Perfluorheptensyre inklusiv precursor
2574	n-Methylperfluoroctansulfonamid inklusiv precursor
2575	n-Ethyl-perfluoroctansulfonamid inklusiv precursor
2576	n-Methyl-perfluoroctansulfonamidethanol inklusiv precursor
2577	n-Ethyl-perfluoroctansulfonamidethanol inklusiv precursor
2578	Perfluorhexadecansyre inklusiv precursor
2579	Perfluoroctansulfonamid-eddikesyre inklusiv precursor
2595	Perfluoroctadecansyre (Lineær)
2596	10:2 Fluorotelomer sulfonsyre
2597	perfluor-2,5-dimethyl-3,6-dioxanonansyre
2598	Perfluorbutansulfonamid
2599	3:3 Fluortelomercarboxylsyre
2600	Nonafluor-3,6-dioxaheptansyre
2601	Perfluor(2-ethoxyethan)sulfonsyre
2602	3-Perfluorheptylpropansyre
2603	Perfluor-4-methoxybutansyre
2604	Perfluor-3-metoxypropansyre
2605	3-Perfluorpentylpropansyre
2606	Perfluorhexansulfonamid
2607	Dodecafluor-3H-4,8-dioxanonanoat (lineær)
2751	Trifluormethansulfonsyre
2758	Perfluorpentansulfonsyre incl. precursor
2759	Perfluordodecansulfonsyre incl. precursor
2885	Perfluor([5-methoxy-1,3-dioxolan-4-yl]oxy)eddikesyre
2908	Perfluorbutansyre (sum forgrenet og lineær)
2909	Perfluorhexansulfonsyre (sum forgrenet og lineær)
2910	Perfluoroctansulfonsyre (sum forgrenet og lineær)
2911	Perfluordecansulfonsyre (sum forgrenet og lineær)
2912	Perfluorhexansyre (sum forgrenet og lineær)
2913	Perfluorheptansyre (sum forgrenet og lineær)
2914	Perfluoroctansyre (sum forgrenet og lineær)
2915	Perfluornonansyre (sum forgrenet og lineær)
2916	Perfluoroctansulfonamid (sum forgrenet og lineær)
2917	Perfluordecansyre (sum forgrenet og lineær)
2918	Perfluorundecansyre (sum forgrenet og lineær)
2919	Perfluordodecansyre (sum forgrenet og lineær)
2920	Perfluortridecansyre (sum forgrenet og lineær)
2921	Perfluorbutansulfonsyre (sum forgrenet og lineær)
2922	Perfluorheptansulfonsyre (sum forgrenet og lineær)
2923	Perfluorpentansyre (sum forgrenet og lineær)
2924	6:2 Fluortelomersulfonsyre (sum forgrenet og lineær)
2925	Perfluorpentansulfonsyre (sum forgrenet og lineær)
2926	Perfluornonansulfonsyre (sum forgrenet og lineær)
2927	Perfluorundecansulfonsyre (sum forgrenet og lineær)
2928	Perfluordodecansulfonsyre (sum forgrenet og lineær)
2929	Perfluortridecansulfonsyre (sum forgrenet og lineær)
2930	Perfluorhexansulfonsyre (lineær)
2931	Perfluoroctansulfonsyre (lineær)
2932	Perfluoroctansyre (lineær)
2933	Perfluornonansyre (lineær)
2934	Perfluoroctansulfonamid (lineær)
2936	Perfluortetradecansyre (sum forgrenet og lineær)
2937	Perfluorhexadecansyre (sum forgrenet og lineær)
2938	Perfluoroctadecansyre (sum forgrenet og lineær)
2939	1H,1H,2H,2H-Perfluoroctanol (sum forgrenet og lineær)
2940	1H,1H,2H,2H-Perfluordecanol (sum forgrenet og lineær)
2941	Dodecafluor-3H-4,8-dioxanonanoat (sum forgrenet og lineær)

9.5 Bilag 2: Stoffer som indgår i udtrækkenes PFAS-sumberegninger

Fra PFAS-projektet "Udvikling af metode til kemisk tilstandsvurdering af de danske grundvandsforekomster for PFAS 2024-2025".

Generelt om sum-beregningerne:

Inden beregning af summer oprettes en tabel med rådata, som indeholder analyser udtrukket efter søgekriterierne i udtræksbeskrivelsen.

Rådata er renset for dubletter (flere analyser af samme stofparameter i samme prøve) efter disse kriterier: Hvis alle analyser har samme attribut, tages gennemsnit af alle analyser. Hvis der er både påviste og ikke-påviste værdier, tages kun gennemsnit af de påviste.

Da det siden marts 2024 eller deromkring er blevet muligt at indberette analyser af "samme" stof med både de gamle stofparametre (som bruges i GRUMO) og nye mere præcise stofparametre, har vi været nødt til at lave en prioritering, da der kan være indberettet begge dele på samme prøver. Vi har lavet en tabel (se nederst) til at registrere hvilke stofparametre der hører til stofgrupperne og hvilken prioritering de har fået. Hovedreglen er, at stofparametrene af 'sum forgrenet og lineær' prioriteres højest, derefter 'lineær' og til sidst dem man ikke rigtig ved om er det ene eller andet (disse koder er lukket fra foråret 2024).

For at summerne beregnes, skal der være mindst 2 stoffer for at beregne PFAS4, mindst 5 stoffer for at beregne PFAS12 og mindst 13 stoffer for at beregne PFAS22 og mindst 17 stoffer for at beregne PFAS24. PFAS24 er i øvrigt bare en almindelig sum og ikke som PFOA-ækvivalenter.

Sum 22:

Sum af PFBS (perfluorbutansulfonsyre), PFHxS (perfluorhexansulfonsyre), PFOS (perfluoroktansulfonsyre), PFOSA (perfluoroktansulfonamid, 6:2 FTS (6:2 fluorotelomersulfonsyre), PFBA (perfluorbutansyre), PFPeA (perfluorpentansyre), PFHxA (perfluorhexansyre), PFHpA (perfluorheptansyre), PFOA (perfluoroktansyre), PFNA (perfluornonansyre), PFDA (perfluordecansyre), PFPS (Perfluorpentansulfonsyre), PFHpS (Perfluorheptansulfonsyre), PFNS (Perfluornonansulfonsyre), PFDS (Perfluordecansulfonsyre), PFUnS (Perfluorundecansulfonsyre), PFDoS (Perfluordodecansulfonsyre), PFTrS (Perfluortridecansulfonsyre), PFUnDA (Perfluorundecansyre), PFDoDA (Perfluordodecansyre), PFTrDA (Perfluortridecansyre).

Sum12:

Sum af PFBS, PFHxS, PFOS, PFOSA, 6:2 FTS, PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA.

Sum4:

Sum af PFOS, PFOA, PFNA, PFHxS.

Tabel. Prioritering af stofkoder til beregning af summer. ”Sum_Parameter” er Stancode for stoffet (parameteren). ”Sum_Parameter_Prio” er den prioritering der er givet til de forskellige koder for samme stof, skulle der være analyser for flere af disse i samme prøve.

SUM_GROUP	SUM_PARAMETER	SUM_PARAMETER_NO	**SUM_PARAMETER_PRIO**	**NAVN**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	2909	1	**1**	**PFHxS (Perfluorhexansulfonsyre (sum forgrenet og lineær))**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	2930	1	**2**	**PFHxS (Perfluorhexansulfonsyre (lineær))**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	1256	1	**3**	**PFHxS (Perfluorhexansulfonsyre)**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	2910	2	**1**	**PFOS (Perfluoroctansulfonsyre (sum forgrenet og lineær))**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	2931	2	**2**	**PFOS (Perfluoroctansulfonsyre (lineær))**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	1257	2	**3**	**PFOS (Perfluoroktansulfonsyre)**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	2914	3	**1**	**PFOA (Perfluoroctansyre (sum forgrenet og lineær))**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	2932	3	**2**	**PFOA (Perfluoroctansyre (lineær))**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	1261	3	**3**	**PFOA (Perfluoroktansyre)**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	2915	4	**1**	**PFNA (Perfluornonansyre (sum forgrenet og lineær))**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	2933	4	**2**	**PFNA (Perfluornonansyre (lineær))**
PFAS sum af PFOA, PFOS, PFNA, PFHxS	1262	4	**3**	**PFNA (Perfluornonansyre)**
PFAS sum af 12	2909	1	**1**	**PFHxS (Perfluorhexansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 12	2930	1	**2**	**PFHxS (Perfluorhexansulfonsyre (lineær))**
PFAS sum af 12	1256	1	**3**	**PFHxS (Perfluorhexansulfonsyre)**
PFAS sum af 12	2910	2	**1**	**PFOS (Perfluoroctansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 12	2931	2	**2**	**PFOS (Perfluoroctansulfonsyre (lineær))**
PFAS sum af 12	1257	2	**3**	**PFOS (Perfluoroktansulfonsyre)**
PFAS sum af 12	2914	3	**1**	**PFOA (Perfluoroctansyre (sum forgrenet og lineær))**
PFAS sum af 12	2932	3	**2**	**PFOA (Perfluoroctansyre (lineær))**
PFAS sum af 12	1261	3	**3**	**PFOA (Perfluoroktansyre)**
PFAS sum af 12	2915	4	**1**	**PFNA (Perfluornonansyre (sum forgrenet og lineær))**
PFAS sum af 12	2933	4	**2**	**PFNA (Perfluornonansyre (lineær))**
PFAS sum af 12	1262	4	**3**	**PFNA (Perfluornonansyre)**
PFAS sum af 12	2908	5	**1**	**PFBA (Perfluorbutansyre (sum forgrenet og lineær))**
PFAS sum af 12	1255	5	**2**	**PFBA (Perfluorbutansyre (lineær))**
PFAS sum af 12	2912	6	**1**	**PFHxA (Perfluorhexansyre (sum forgrenet og lineær))**
PFAS sum af 12	1259	6	**2**	**PFHxA (Perfluorhexansyre (lineær))**
PFAS sum af 12	2913	7	**1**	**PFHpA (Perfluorheptansyre (sum forgrenet og lineær))**
PFAS sum af 12	1260	7	**2**	**PFHpA (Perfluorheptansyre (lineær))**
PFAS sum af 12	2916	8	**1**	**PFOSA (Perfluoroctansulfonamid (sum forgrenet og lineær))**
PFAS sum af 12	2934	8	**2**	**PFOSA (Perfluoroctansulfonamid (lineær))**
PFAS sum af 12	1263	8	**3**	**PFOSA (Perfluoroktansulfonamid)**
PFAS sum af 12	2917	9	**1**	**PFDA (Perfluordecansyre (sum forgrenet og lineær))**
PFAS sum af 12	1264	9	**2**	**PFDA (Perfluordecansyre (lineær))**
PFAS sum af 12	2921	10	**1**	**PFBS (Perfluorbutansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 12	1597	10	**2**	**PFBS (Perfluorbutansulfonsyre (lineær))**
PFAS sum af 12	2923	11	**1**	**PFPeA (Perfluorpentansyre (sum forgrenet og lineær))**
PFAS sum af 12	1599	11	**2**	**PFPeA (Perfluorpentansyre (lineær))**
PFAS sum af 12	2924	12	**1**	**6:2 FTS (6:2 Fluortelomersulfonsyre (sum forgrenet og lineær))**

PFAS sum af 12	1603	12	**2**	**6:2 FTS (1H,1H,2H,2H-Perfluoroctansulfonsyre (lineær))**
PFAS sum af 22	2909	1	**1**	**PFHxS (Perfluorhexansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	2930	1	**2**	**PFHxS (Perfluorhexansulfonsyre (lineær))**
PFAS sum af 22	1256	1	**3**	**PFHxS (Perfluorhexansulfonsyre)**
PFAS sum af 22	2910	2	**1**	**PFOS (Perfluoroctansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	2931	2	**2**	**PFOS (Perfluoroctansulfonsyre (lineær))**
PFAS sum af 22	1257	2	**3**	**PFOS (Perfluoroktansulfonsyre)**
PFAS sum af 22	2914	3	**1**	**PFOA (Perfluoroctansyre (sum forgrenet og lineær))**
PFAS sum af 22	2932	3	**2**	**PFOA (Perfluoroctansyre (lineær))**
PFAS sum af 22	1261	3	**3**	**PFOA (Perfluoroktansyre)**
PFAS sum af 22	2915	4	**1**	**PFNA (Perfluornonansyre (sum forgrenet og lineær))**
PFAS sum af 22	2933	4	**2**	**PFNA (Perfluornonansyre (lineær))**
PFAS sum af 22	1262	4	**3**	**PFNA (Perfluornonansyre)**
PFAS sum af 22	2908	5	**1**	**PFBA (Perfluorbutansyre (sum forgrenet og lineær))**
PFAS sum af 22	1255	5	**2**	**PFBA (Perfluorbutansyre (lineær))**
PFAS sum af 22	2912	6	**1**	**PFHxA (Perfluorhexansyre (sum forgrenet og lineær))**
PFAS sum af 22	1259	6	**2**	**PFHxA (Perfluorhexansyre (lineær))**
PFAS sum af 22	2913	7	**1**	**PFHpA (Perfluorheptansyre (sum forgrenet og lineær))**
PFAS sum af 22	1260	7	**2**	**PFHpA (Perfluorheptansyre (lineær))**
PFAS sum af 22	2916	8	**1**	**PFOSA (Perfluoroctansulfonamid (sum forgrenet og lineær))**
PFAS sum af 22	2934	8	**2**	**PFOSA (Perfluoroctansulfonamid (lineær))**
PFAS sum af 22	1263	8	**3**	**PFOSA (Perfluoroktansulfonamid)**
PFAS sum af 22	2917	9	**1**	**PFDA (Perfluordecansyre (sum forgrenet og lineær))**
PFAS sum af 22	1264	9	**2**	**PFDA (Perfluordecansyre (lineær))**
PFAS sum af 22	2921	10	**1**	**PFBS (Perfluorbutansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	1597	10	**2**	**PFBS (Perfluorbutansulfonsyre (lineær))**
PFAS sum af 22	2923	11	**1**	**PFPeA (Perfluorpentansyre (sum forgrenet og lineær))**
PFAS sum af 22	1599	11	**2**	**PFPeA (Perfluorpentansyre (lineær))**
PFAS sum af 22	2924	12	**1**	**6:2 FTS (6:2 Fluortelomersulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	1603	12	**2**	**6:2 FTS (1H,1H,2H,2H-Perfluoroctansulfonsyre (lineær))**
PFAS sum af 22	2911	13	**1**	**PFDS (Perfluordecansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	1258	13	**2**	**PFDS (Perfluordecansulfonsyre (lineær))**
PFAS sum af 22	2918	14	**1**	**PFUnDA (Perfluorundecansyre (sum forgrenet og lineær))**
PFAS sum af 22	1265	14	**2**	**PFUnDA (Perfluorundecansyre (lineær))**
PFAS sum af 22	2919	15	**1**	**PFDoDA (Perfluordodecansyre (sum forgrenet og lineær))**
PFAS sum af 22	1266	15	**2**	**PFDoDA (Perfluordodecansyre (lineær))**
PFAS sum af 22	2920	16	**1**	**PFTrDA (Perfluortridecansyre (sum forgrenet og lineær))**
PFAS sum af 22	1267	16	**2**	**PFTrDA (Perfluortridecansyre (lineær))**
PFAS sum af 22	2922	17	**1**	**PFHpS (Perfluorheptansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	1598	17	**2**	**PFHpS (Perfluorheptansulfonsyre (lineær))**
PFAS sum af 22	2925	18	**1**	**PFPeS (Perfluorpentansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	2230	18	**2**	**PFPeS (Perfluorpentansulfonsyre (lineær))**
PFAS sum af 22	2926	19	**1**	**PFNS (Perfluornonansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	2231	19	**2**	**PFNS (Perfluornonansulfonsyre (lineær))**

PFAS sum af 22	2927	20	**1**	**PFUnDS (Perfluorundecansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	2232	20	**2**	**PFUnDS (Perfluorundecansulfonsyre (lineær))**
PFAS sum af 22	2928	21	**1**	**PFDoDS (Perfluordodecansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	2233	21	**2**	**PFDoDS (Perfluordodecansulfonsyre (lineær))**
PFAS sum af 22	2929	22	**1**	**PFTrDS (Perfluortridecansulfonsyre (sum forgrenet og lineær))**
PFAS sum af 22	2234	22	**2**	**PFTrDS (Perfluortridecansulfonsyre (lineær))**

10. Appendix B: Target parameters

The target parameters were decided in step 0 (Figure 1), based on initial request provided by SGAV and revised by GEUS (adding few additional relevant parameters).
The following abbreviations are used in the table below:

- TV – threshold value for VP4
- GVF (VP3) – here refers to the groundwater body-specific threshold values defined in VP3
- MAM – mean annual mean
- AM – annual mean
- RTT – risk, status, trends (dk: Risiko, tilstand og trends)
- Q – supporting parameter for quantitative assessment (dk: Kvantitativ støtteparameter)
- FG – weathering degree (dk: Forvitringsgrad)
- R – parameters used in the redox algorithm or other supplementary redox-sensitive parameters (e.g. Mn)
- IG – ion exchange (dk: Ionbytningsgrad)
- O – supporting parameter for the surface water assessments (in relation to groundwater-surface water interactions, dk: overfladevand)
- NBV – national background levels, relevant to trace elements only
- Y – yes
- N – no
- ChlS – chlorinated solvents and degradation products (dk: Chlorerede opløsningsmidler og nedbrydningsprodukter)

GROUP	Parameter (Jupiter name)	Reason	TV			Filtered in the field	Aggregation		STANCODE = STOFNR	Note
			national	unit	GVF (VP3)		MAM	AM		
Sporstoffer	Aluminium (Al)	RTT	100	µg/l	Y	Y	Y	Y	267	
	Arsen (As)	RTT	5	µg/l	Y	Y	Y	Y	270	
	Barium (Ba)	Q	-	-	-	Y	N	N	271	
	Bly (Pb)	RTT	1	µg/l		Y	Y	Y	274	
	Cadmium (Cd)	RTT	0.5	µg/l	Y	Y	Y	Y	279	
	Kobber (Cu)	RTT	100	µg/l		Y	Y	Y	318	
	Chrom (Cr)	RTT	25	µg/l		Y	Y	Y	300	
	Kviksølv (Hg)	RTT	0.1	µg/l		Y	Y	Y	319	
	Nikkel (Ni)	RTT	10	µg/l	Y	Y	Y	Y	326	

GROUP	Parameter (Jupiter name)	Reason	TV			Filtered in the field	Aggregation		STANCODE = STOFNR	Note
			national	unit	GVF (VP3)		MAM	AM		
	Strontium (Sr)	Q	-	-		Y	N	N	331	
	Zink (Zn)	RTT	100	µg/l		Y	Y	Y	353	
Salte og øvrige	Ammonium (NH4)**	RTT	2.0	mg/l			Y	Y	240	
	Calcium (Ca)	FG	-	-			N	N	280	
	Fluorid (F)	Q	-	-			N	N	308	
	Hydrogencarbonat (HCO3)	Q (FG)	-	-			N	N	59	
	Jern (Fe)	R	-	-		Y	N	N	312	
	Chlorid (Cl)	RTT, Q (IG)	250	mg/l			Y	Y	297	
	Magnesium (Mg)	FG	-	-			N	N	321	
	Methan (CH4)	R	-	-			N	N	356	
	Natrium (Na)	Q (IG)	-	-			N	N	324	
	NVOC (non-volatile organic carbon)	NBV, RTT	-	-			N	N	75	
	Oxygen indhold (DO)	R	-	-			N	N	50	
	pH	NBV, RTT	-	-			N	N	13	
	Phosphor, total-P (Ptot)	O	-	-			N	N	261	
	Sulfat (SO4)	R	-	-			N	N	335	
	Svovlbrinte (sulfid) (H2S)	R	-	-			N	N	1167	
	Mangan (Mn)	R	-	-		Y	N	N	322	
Nitrat	Nitrat (NO3)	RTT	50	mg/l			Y	Y	246	
Pesticider	**Jupiter, stofgruppe 50 (Pesticider)**	RTT	0.10	µg/l			Y	Y	**xxx**	Jupiter group 50
	Sum - pesticider	RTT	0.50	µg/l			Y	Y	**9000**	Section 4.4.3
MFS	Cis-1,2-dichlorethylen	RTT	1	µg/l			Y	Y	83	ChlS
	1,1-Dichlorethylen	RTT	1	µg/l			Y	Y	85	ChlS
	Trans-1,2-dichlorethen	RTT	1	µg/l			Y	Y	86	ChlS
	Trichlormethan (old: Chloroform)	RTT	1	µg/l			Y	Y	374	ChlS
	Tetrachlormethan	RTT	1	µg/l			Y	Y	378	ChlS
	Tetrachlorethylen	RTT	1	µg/l			Y	Y	379	ChlS
	Trichlorethylen	RTT	1	µg/l			Y	Y	380	ChlS
	1,1,1-trichlorethan	RTT	1	µg/l			Y	Y	383	ChlS
	Dichlormethan	RTT	1	µg/l			Y	Y	386	ChlS
	Chlorethan	RTT	1	µg/l			Y	Y	543	ChlS
	1,1-Dichlorethan	RTT	1	µg/l			Y	Y	868	ChlS
	1,2-Dichlorethan	RTT	1	µg/l			Y	Y	1076	ChlS
	Vinylchlorid	RTT	0.2	µg/l			Y	Y	1171	ChlS
	Sum - chlorerede opløsningsmidler og nedbrydnings-produkter	RTT	3	µg/l			Y	Y	**9001**	ChlS, section 4.4.4
	Naphthalen	RTT	1	µg/l			Y	Y	202	BTEXN
	Benzen	RTT	1	µg/l			Y	Y	215	BTEXN
	Toluen	RTT	1	µg/l			Y	Y	218	BTEXN

GROUP	Parameter (Jupiter name)	Reason	TV			Filtered in the field	Aggregation		STANCODE = STOFNR	Note
			national	unit	GVF (VP3)		MAM	AM		
	o-Xylen	RTT	1	µg/l			Y	Y	400	BTEXN
	m+p-Xylen	RTT	1	µg/l			Y	Y	401	BTEXN
	Ethylbenzen	RTT	1	µg/l			Y	Y	449	BTEXN
	Phenol	RTT	0.5	µg/l			Y	Y	404	Phenoler
	3-Methylphenol	RTT	0.5	µg/l			Y	Y	407	Phenoler
	2,3-Dimethylphenol	RTT	0.5	µg/l			Y	Y	408	Phenoler
	2-Methylphenol	RTT	0.5	µg/l			Y	Y	409	Phenoler
	4-Methylphenol	RTT	0.5	µg/l			Y	Y	410	Phenoler
	3,4-Dimethylphenol	RTT	0.5	µg/l			Y	Y	411	Phenoler
	3,5-Dimethylphenol	RTT	0.5	µg/l			Y	Y	412	Phenoler
	2,6-Dimethylphenol	RTT	0.5	µg/l			Y	Y	413	Phenoler
	2,4-Dimethylphenol	RTT	0.5	µg/l			Y	Y	414	Phenoler
	2,5-Dimethylphenol	RTT	0.5	µg/l			Y	Y	426	Phenoler
	Methyl-tert-butylether (old: MTBE)	RTT	5.0	µg/l			Y	Y	166	MTBE
	Diethylether	RTT	10	µg/l			Y	Y	483	Vandopløselige stoffer
	2-propanol	RTT	10	µg/l			Y	Y	211	Vandopløselige stoffer
	Methyl-isobutylketon	RTT	10	µg/l			Y	Y	217	Vandopløselige stoffer
	Cyanid, total	RTT	50	µg/l			Y	Y	207	Cyanider
	Cyanid, syreflygtigt	RTT	20	µg/l			Y	Y	209	Cyanider
PFAS	PFBA (Perfluorbutansyre (lineær))	RTT	-	-			Y	Y	1255	
	PFBA (Perfluorbutansyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2908	
	PFPeA (Perfluorpentansyre (lineær))	RTT	-	-			Y	Y	1599	
	PFPeA (Perfluorpentansyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2923	
	PFHxA (Perfluorhexansyre (lineær))	RTT	-	-			Y	Y	1259	
	PFHxA (Perfluorhexansyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2912	
	PFHpA (Perfluorheptansyre (lineær))	RTT	-	-			Y	Y	1260	
	PFHpA (Perfluorheptansyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2913	
	PFOA (perfluoroctansyre)	RTT	-	-			Y	Y	1261	
	PFOA (Perfluoroctansyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2914	
	PFOA (Perfluoroctansyre (lineær))	RTT	-	-			Y	Y	2932	
	PFNA (perfluornonansyre)	RTT	-	-			Y	Y	1262	
	PFNA (Perfluornonansyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2915	
	PFNA (Perfluornonansyre (lineær))	RTT	-	-			Y	Y	2933	
	PFDA (Perfluordecansyre (lineær))	RTT	-	-			Y	Y	1264	
	PFDA (Perfluordecansyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2917	
	PFUnDA (Perfluorundecansyre (lineær))	RTT	-	-			Y	Y	1265	
	PFUnDA (Perfluorundecansyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2918	
	PFDoDA (Perfluordodecansyre (lineær))	RTT	-	-			Y	Y	1266	
	PFDoDA (Perfluordodecansyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2919	

GROUP	Parameter (Jupiter name)	Reason	TV			Filtered in the field	Aggregation		STANCODE = STOFNR	Note
			national	unit	GVF (VP3)		MAM	AM		
	PFTrDA (Perfluortridecansyre (lineær))	RTT	-	-			Y	Y	1267	
	PFTrDA (Perfluortridecansyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2920	
	PFBS (Perfluorbutansulfonsyre (lineær))	RTT	-	-			Y	Y	1597	
	PFBS (Perfluorbutansulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2921	
	PFPeS (Perfluorpentansulfonsyre (lineær))	RTT	-	-			Y	Y	2230	
	PFPeS (Perfluorpentansulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2925	
	PFHxS (perfluorhexansulfonsyre)	RTT	-	-			Y	Y	1256	
	PFHxS (Perfluorhexansulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2909	
	PFHxS (Perfluorhexansulfonsyre (lineær))	RTT	-	-			Y	Y	2930	
	PFHpS (Perfluorheptansulfonsyre (lineær))	RTT	-	-			Y	Y	1598	
	PFHpS (Perfluorheptansulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2922	
	PFOS (Perfluoroctansulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2910	
	PFOS (perfluoroctansulfonsyre)	RTT	-	-			Y	Y	1257	
	PFOS (Perfluoroctansulfonsyre (lineær))	RTT	-	-			Y	Y	2931	
	PFNS (Perfluornonansulfonsyre (lineær))	RTT	-	-			Y	Y	2231	
	PFNS (Perfluornonansulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2926	
	PFDS (Perfluordecansulfonsyre (lineær))	RTT	-	-			Y	Y	1258	
	PFDS (Perfluordecansulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2911	
	PFUnDS (Perfluorundecansulfonsyre (lineær))	RTT	-	-			Y	Y	2232	
	PFUnDS (Perfluorundecansulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2927	
	PFDoDS (Perfluordodecansulfonsyre (lineær))	RTT	-	-			Y	Y	2233	
	PFDoDS (Perfluordodecansulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2928	
	PFTrDS (Perfluortridecansulfonsyre (lineær))	RTT	-	-			Y	Y	2234	
	PFTrDS (Perfluortridecansulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2929	
	PFOSA (Perfluoroktansulfonamid)	RTT	-	-			Y	Y	1263	
	PFOSA (Perfluoroctansulfonamid (sum forgrenet og lineær))	RTT	-	-			Y	Y	2916	
	PFOSA (Perfluoroctansulfonamid (lineær))	RTT	-	-			Y	Y	2934	
	6:2 FTS (1H,1H,2H,2H-Perfluoroctansulfonsyre (lineær))	RTT	-	-			Y	Y	1603	
	6:2 FTS (6:2 Fluortelomersulfonsyre (sum forgrenet og lineær))	RTT	-	-			Y	Y	2924	
	SUM PFAS-4	RTT	0.002	µg/l			Y	Y	9004	Sections 3 and 4.5
	SUM PFAS-22	RTT	0.1	µg/l			Y	Y	9022	Sections 3 and 4.5

GROUP	Parameter (Jupiter name)	Reason	TV			Filtered in the field	Aggregation		STANCODE = STOFNR	Note
			national	unit	GVF (VP3)		MAM	AM		
	TFA	RTT	9	µg/l			Y	Y	2251	Organisk mikroforurening
	SUM PFAS-12	(RTT)	-	-			Y	Y	9012	Sections 3 and 4.5

11. Appendix C: Other large tables and figures

Table C1 Maximum limit of detection (LOD)

GROUP	KORT_NAVN	STOFKODE	STOFNAVN	Max LOD
sporstof-fer		267	Aluminium	0.5
		270	Arsen	0.03
		271	Barium	1
		274	Bly	0.03
		279	Cadmium	0.003
		300	Chrom	0.03
		318	Kobber	0.03
		319	Kviksølv	0.001
		326	Nikkel	0.03
		331	Strontium	1
		353	Zink	0.5
salte_etc		13	pH	0
		50	Oxygen indhold	0.1
		59	Hydrogencarbonat	3
		75	Ikke flygtigt organisk kulstof	0.1
		240	Ammoniak+ammonium	0.005
		261	Phosphor, total-P	0.01
		280	Calcium	0
		297	Chlorid	0
		308	Fluorid	0.05
		312	Jern	0.01
		321	Magnesium	0.3
		322	Mangan	0.02
		324	Natrium	0
		335	Sulfat	0.5
		356	Methan	0.01
		1167	Svovlbrinte (sulfid)	0.02
pfas	6:2 FTS	1603	6:2 Fluortelomersulfonsyre (lineær)	0.05
	6:2 FTS	2924	6:2 Fluortelomersulfonsyre (sum forgrenet og lineær)	0.05
	PFBA	1255	Perfluorbutansyre (lineær)	0.05
	PFBA	2908	Perfluorbutansyre (sum forgrenet og lineær)	0.05
	PFBS	1597	Perfluorbutansulfonsyre (lineær)	0.05
	PFBS	2921	Perfluorbutansulfonsyre (sum forgrenet og lineær)	0.05
	PFDA	1264	Perfluordecansyre (lineær)	0.05
	PFDA	2917	Perfluordecansyre (sum forgrenet og lineær)	0.05
	PFDS	1258	Perfluordecansulfonsyre (lineær)	0.05
	PFDS	2911	Perfluordecansulfonsyre (sum forgrenet og lineær)	0.05
	PFDoDA	1266	Perfluordodecansyre (lineær)	0.05
	PFDoDA	2919	Perfluordodecansyre (sum forgrenet og lineær)	0.05
	PFDoDS	2233	Perfluordodecansulfonsyre (lineær)	0.05
	PFDoDS	2928	Perfluordodecansulfonsyre (sum forgrenet og lineær)	0.05
	PFHpA	1260	Perfluorheptansyre (lineær)	0.05
	PFHpA	2913	Perfluorheptansyre (sum forgrenet og lineær)	0.05
	PFHpS	1598	Perfluorheptansulfonsyre (lineær)	0.05
	PFHpS	2922	Perfluorheptansulfonsyre (sum forgrenet og lineær)	0.05
	PFHxA	1259	Perfluorhexansyre (lineær)	0.05
	PFHxA	2912	Perfluorhexansyre (sum forgrenet og lineær)	0.05
	PFHxS	1256	Perfluorhexansulfonsyre	0.001
	PFHxS	2909	Perfluorhexansulfonsyre (sum forgrenet og lineær)	0.001

	PFHxS	2930	Perfluorhexansulfonsyre (lineær)	0.001
	PFNA	1262	Perfluornonansyre	0.001
	PFNA	2915	Perfluornonansyre (sum forgrenet og lineær)	0.001
	PFNA	2933	Perfluornonansyre (lineær)	0.001
	PFNS	2231	Perfluornonansulfonsyre (lineær)	0.05
	PFNS	2926	Perfluornonansulfonsyre (sum forgrenet og lineær)	0.05
	PFOA	1261	Perfluoroctansyre	0.001
	PFOA	2914	Perfluoroctansyre (sum forgrenet og lineær)	0.001
	PFOA	2932	Perfluoroctansyre (lineær)	0.001
	PFOS	1257	Perfluoroctansulfonsyre (sum forgrenet og lineær)	0.001
	PFOS	2910	Perfluoroctansulfonsyre (sum forgrenet og lineær)	0.001
	PFOS	2931	Perfluoroctansulfonsyre (lineær)	0.001
	PFOSA	1263	Perfluoroctansulfonamid	0.05
	PFOSA	2916	Perfluoroctansulfonamid (sum forgrenet og lineær)	0.05
	PFOSA	2934	Perfluoroctansulfonamid (lineær)	0.05
	PFPeA	1599	Perfluorpentansyre (lineær)	0.05
	PFPeA	2923	Perfluorpentansyre (sum forgrenet og lineær)	0.05
	PFPeS	2230	Perfluorpentansulfonsyre (lineær)	0.05
	PFPeS	2925	Perfluorpentansulfonsyre (sum forgrenet og lineær)	0.05
	PFTrDA	1267	Perfluortridecansyre (lineær)	0.05
	PFTrDA	2920	Perfluortridecansyre (sum forgrenet og lineær)	0.05
	PFTrDS	2234	Perfluortridecansulfonsyre (lineær)	0.05
	PFTrDS	2929	Perfluortridecansulfonsyre (sum forgrenet og lineær)	0.05
	PFUnDA	1265	Perfluorundecansyre (lineær)	0.05
	PFUnDA	2918	Perfluorundecansyre (sum forgrenet og lineær)	0.05
	PFUnDS	2232	Perfluorundecansulfonsyre (lineær)	0.05
	PFUnDS	2927	Perfluorundecansulfonsyre (sum forgrenet og lineær)	0.05
	TFA	2251	Trifluoreddikesyre	0.05
		9004	SUM PFAS-4	0.05
		9012	SUM PFAS-12	0.05
		9022	SUM PFAS-22	0.05
nitrate		246	Nitrat	0.3
mfs	btxn	202	Naphthalen	0.1
	btxn	215	Benzen	0.1
	btxn	218	Toluen	0.1
	btxn	400	o-Xylen	0.1
	btxn	401	m+p-Xylen	0.1
	btxn	449	Ethylbenzen	0.1
	chl.solvents_etc	83	Cis-1,2-dichlorethylen	0.1
	chl.solvents_etc	85	1,1-Dichlorethylen	0.1
	chl.solvents_etc	86	Trans-1,2-dichlorethen	0.1
	chl.solvents_etc	374	Trichlormethan	0.1
	chl.solvents_etc	378	Tetrachlormethan	0.1
	chl.solvents_etc	379	Tetrachlorethylen	0.1
	chl.solvents_etc	380	Trichlorethylen	0.1
	chl.solvents_etc	383	1,1,1-trichlorethan	0.1
	chl.solvents_etc	386	Dichlormethan	0.1
	chl.solvents_etc	543	Chlorethan	0.1
	chl.solvents_etc	868	1,1-Dichlorethan	0.1
	chl.solvents_etc	1076	1,2-Dichlorethan	0.1
	chl.solvents_etc	1171	Vinylchlorid	0.02
	cyanides	207	Cyanid, total	5
	cyanides	209	Cyanid, syreflygtigt	2
	mtbe	166	Methyl-tert-butylether	0.5
	phenoler	404	Phenol	0.05
	phenoler	407	3-Methylphenol	0.05
	phenoler	408	2,3-Dimethylphenol	0.05
	phenoler	409	2-Methylphenol	0.05

	phenoler	410	4-Methylphenol	0.05
	phenoler	411	3,4-Dimethylphenol	0.05
	phenoler	412	3,5-Dimethylphenol	0.05
	phenoler	413	2,6-Dimethylphenol	0.05
	phenoler	414	2,4-Dimethylphenol	0.05
	phenoler	426	2,5-Dimethylphenol	0.05
	water_soluble	211	2-propanol	1
	water_soluble	217	Methyl-isobutylketon	1
	water_soluble	483	Diethylether	1
pest		All other included STOFKODE (n=845) from group 50		0.01

Figure C1 Overview of frequency of use of specific limits of detection for PFAS parameters

Table C2 Overview of parameters, their CAS number and the used gwPollutantCode and gwPollutantOther, as used for the EU tables

STOFKODE	STOFNAVN	CASNUMBER	EUNAME = gwPollutantCode	gwPollutantOther	n
83	Cis-1,2-dichlorethylen	156-59-2	CAS_156-59-2 - Cis-1,2-dichloroethene		11596
85	1,1-Dichlorethylen	75-35-4	CAS_75-35-4 - 1,1-dichloroethene		11296
86	Trans-1,2-dichlorethen	156-60-5	CAS_156-60-5 - trans-1,2-dichloroethene		11453
166	Methyl-tert-butylether	1634-04-4	CAS_1634-04-4 - MTBE		1738
202	Naphthalen	91-20-3	CAS_91-20-3 - Naphthalene		12228
207	Cyanid, total	57-12-5	CAS_57-12-5 - Free cyanide		1925
209	Cyanid, syreflygtigt	74-90-8	* "EEA_00-00-0 - Other parameter"	“CAS_74-90-8 - Hydrogen cyanide”	440
211	2-propanol	67-63-0	* "EEA_00-00-0 - Other parameter"	“CAS_67-63-0 - 2-Propanol”	40
215	Benzen	71-43-2	CAS_71-43-2 - Benzene		13316
217	Methyl-isobutylketon	108-10-1	* "EEA_00-00-0 - Other parameter"	“CAS_108-10-1 - Methyl isobutyl ketone”	46
218	Toluen	108-88-3	CAS_108 -88 -3 - Toluene		12238
240	Ammoniak+ammonium	14798-03-9	CAS_14798-03-9 - Ammonium		10089
246	Nitrat	14797-55-8	CAS_14797-55-8 - Nitrate		10080
267	Aluminium	7429-90-5	CAS_7429-90-5 - Aluminium and its compounds		1674
270	Arsen	7440-38-2	CAS_7440-38-2 - Arsenic and its compounds		7006
274	Bly	7439-92-1	CAS_7439-92-1 - Lead and its compounds		3144
279	Cadmium	7440-43-9	CAS_7440-43-9 - Cadmium and its compounds		3039
297	Chlorid	16887-00-6	CAS_16887-00-6 - Chloride		10156
300	Chrom	7440-47-3	CAS_7440-47-3 - Chromium and its compounds		3140
318	Kobber	7440-50-8	CAS_7440-50-8 - Copper and its compounds		3133
319	Kviksølv	7439-97-6	CAS_7439-97-6 - Mercury and its compounds		1459
326	Nikkel	7440-02-0	CAS_7440-02-0 - Nickel and its compounds		8450
353	Zink	7440-66-6	CAS_7440-66-6 - Zinc and its compounds		3148
374	Trichlormethan	67-66-3	CAS_67-66-3 - Trichloromethane		12510
378	Tetrachlormethan	56-23-5	CAS_56-23-5 - Carbon tetrachloride		10875
379	Tetrachlorethylen	127-18-4	CAS_127-18-4 - Tetrachloroethylene		12134
380	Trichlorethylen	79-01-6	CAS_79-01-6 - Trichloroethylene		12159
383	1,1,1-trichlorethan	71-55-6	CAS_71-55-6 - 1,1,1-trichloroethane		12495
386	Dichlormethan	75-09-2	CAS_75-09-2 - Dichloromethane		9460
400	o-Xylen	95-47-6	CAS_95 -47 -6 - O -xylene		11741
401	m+p-Xylen		* “EEA_33-18-1 - Meta xylene + para xylene”		11751
404	Phenol	108-95-2	CAS_108 -95 -2 - Phenol		2109

STOFKODE	STOFNAVN	CASNUMBER	EUNAME = gwPollutantCode	gwPollutantOther	n
407	3-Methylphenol	108-39-4	* "EEA_00-00-0 - Other parameter"	“CAS_108-39-4 - 3-Methylphenol”	2385
408	2,3-Dimethylphenol	526-75-0	* “CAS_526-75-0 - 2,3-dimethyl-phenol”		2391
409	2-Methylphenol	95-48-7	* “CAS_95-48-7 - 2-methyl-phenol”		2435
410	4-Methylphenol	106-44-5	* “CAS_106-44-5 - 4-methyl-phenol”		2178
411	3,4-Dimethylphenol	95-65-8	* “CAS_95-65-8 - 3,4-dimethyl-phenol”		2229
412	3,5-Dimethylphenol	108-68-9	* “CAS_108-68-9 - 3,5-dimethyl-phenol”		2202
413	2,6-Dimethylphenol	576-26-1	* “CAS_576-26-1 - 2,6-dimethyl-phenol”		2412
414	2,4-Dimethylphenol	105-67-9	* “CAS_105-67-9 - 2,4-dimethyl-phenol”		2415
426	2,5-Dimethylphenol	95-87-4	* “CAS_95-87-4 - 2,5-dimethylphenol”		2401
449	Ethylbenzen	100-41-4	CAS_100-41-4 - Ethylbenzene		12171
483	Diethylether	60-29-7	* "EEA_00-00-0 - Other parameter"	“CAS_60-29-7 - Diethyl ether”	46
543	Chlorethan	75-00-3	CAS_75-00-3 - Chloroethane		9609
868	1,1-Dichlorethan	75-34-3	CAS_75-34-3 - 1,1-dichloroethane		9915
1076	1,2-Dichlorethan	107-06-2	CAS_107-06-2 - 1,2-dichloroethane		11499
1171	Vinylchlorid	75-01-4	CAS_75-01-4 - Chloroethene (vinylchloride)		10778
9000	sum_pest		"EEA_00-00-0 - Other parameter"	“Group of pesticides”	14038
9001	sum_chl_solv		* "EEA_00-00-0 - Other parameter"	“Group of 13 chlorinated solvents: CAS_127-18-4; CAS_79-01-6; CAS_156-59-2; CAS_156-60-5; CAS_75-35-4; CAS_75-01-4; CAS_71-55-6; CAS_75-34-3; CAS_107-06-2; CAS_56-23-5; CAS_67-66-3; CAS_75-09-2; CAS_75-00-3”	12693
9004	SUM PFAS-4		* "EEA_00-00-0 - Other parameter"	“Group of 4 PFAS: CAS_355-46-4; CAS_1763-23-1; CAS_335-67-1; CAS_375-95-1”	9114
9022	SUM PFAS-22		* "EEA_00-00-0 - Other parameter"	" “Group of 22 PFAS: CAS_355-46-4; CAS_1763-23-1; CAS_335-67-1; CAS_375-95-1; CAS_375-22-4; CAS_307-24-4; CAS_375-85-9; CAS_754-91-6; CAS_335-76-2; CAS_375-73-5; CAS_2706-90-3; CAS_27619-97-2; CAS_335-77-3; CAS_2058-94-8; CAS_307-55-1; CAS_72629-94-8; CAS_375-92-8; CAS_2706-91-4; CAS_68259-12-1; CAS_749786-16-1; CAS_79780-39-5; CAS_791563-89-8”	6202

* revised, missing in Parameterlisten

12. Appendix D: EU templates

Provided by SGAV

NOTAT

Styrelsen for Grøn Arealomlægning og Vandmiljø

Hav- og Vandmiljø
J.nr. 2025 - 7576
Ref. CGREV
Den 4. marts 2025

Skabelon for indtag – Målestationsniveau grunddata

Beskrivelse af datakolonner i skabelon for grunddata for målestationer/indtag til grundvandsdatabase

Kolonner der udfyldes af dataleverandør:

Grundvandsforekomst - Der anvendes EU-ID for grundvandsforekomsten. Denne er i formatet DKxxx_dkmx_xxxx_xx (DK110_dkmj_1106_ks).

euMonitoringSiteCode - der anvendes EU-ID for boringsindtagene, der er tilknyttet en grundvandsforekomst, og som anvendes til kemisk eller kvantitativ risiko-og/eller tilstandsvurdering til BA4/VP4.
Denne er i formatet DKxxx-xxxx-y (DK201-3854-1), hvor y svarer til indtagsnr.

euProgrammeCode - Angivelse af hvilket overvågningsprogram, boringsindtaget er del af:

DKGRUMO	*- Indtag der er en del af det nationale overvågningsprogram for vand og natur, NOVANA, undtagen LOOP-indtag*
DKLOOP	*- Grundvandsprøver fra landovervågningsprogrammet (LOOP)*
DKVandforsyning	*- Indtag tilknyttet indvinding af drikkevand fra almene vandværker (virksomhedstyperne V01 og V02 i Jupiterdatabasen)*
DKGEBKOR	*- Indtag fra grundvandskortlægningen*
DKForurening	*- Vandprøver af datatypen 'depot' fra forureningsundersøgelser i henhold til jordforureningsloven*
DKOevrige	*- Øvrige indtag med enten kemidata eller indvindingsdata*

chemicalMonitoring - anvendes boringsindtaget til kemisk monitering? *(Yes, No)*

quantitativeMonitoring - anvendes boringsindtaget til kvantitativ monitering (monitering af oppumpede vandmængder? *(Yes, No)*

investigativeMonitoring - Udfyldes kun for indtag med "Yes" for **chemicalMonitoring**. Der tages udgangspunkt i indtagstyper fra **euProgrammeCode**:

DKGRUMO	*- No*
DKLOOP	*- No*
DKVandforsyning	*- No*
DKGEBKOR	*- Yes*
DKForurening	*- Yes*
DKOevrige	*- No*

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surveillanceMonitoring - anvendes boringsindtaget til kemisk monitering? *(Yes, No)*
Udfyldes kun for indtag med "Yes" for **chemicalMonitoring**:

DKGRUMO	*- Yes*
DKLOOP	*- Yes*
DKVandforsyning	*- Yes*
DKGEBKOR	*- No*
DKForurening	*- No*
DKOevrige	*- Yes*

wellSpring - For alle indtag angives *Well*

Depth – Angiver hvilket grundvandslag i grundvandsforekomsten vandprøven udtages fra. *Der udfyldes med "Unknown" for alle indtag. (Charlotte Greve: "Denne kolonne udfyldes ved indtagskoblingen")*

Upper – Indtag i øverste magasin i grundvandsforekomst med flere overlejrende magasiner
Medium – Indtag i midterste magasin i grundvandsforekomst med flere overlejrende magasiner
Lower – Indtag i nederste magasin i grundvandsforekomst med flere overlejrende magasiner
Mixed – Indtag over xx meter
Unknown – For alle andre indtag

Kolonner der udfyldes af SGAV ved efterbehandling:

ecologicalMonitoring – alle udfyldes med *Not applicable*

operationalMonitoring - Anvendes boringsindtaget til operationel monitering? *(Yes, No)*
Udfyldes kun for indtag med "Yes" for **chemicalMonitoring**, og *"DKGRUMO"* i **euProgrammeCode**. Besvares ud fra lister fra SGAV Overvågning over indtag med operationel overvågning

programmeName – Nemt forståeligt engelsk navn på overvågningsprogrammet, der reflekterer formålet, f.eks. Overvågning eller operationel.

DKGRUMO	*- National groundwater monitoring program*
DKLOOP	*- Open land monitoring program*
DKVandforsyning	*- Public drinking water monitoring program*
DKGEBKOR	*- Groundwater mapping*
DKForurening	*- Pollution investigation*
DKOevrige	*- Other chemical or quantitative monitoring*

programmeReference - En reference eller link til dokumenter med relevant information for overvågningsprogrammet, som er angivet i **euProgrammeCode.** Der anvendes oversigten nedenfor over referencer eller links for hver af de forskellige indtags-/datatype:

DKGRUMO

DKLOOP
DKVandforsyning
DKGEBKOR
DKForurening

DKOevrige

NOTAT

Styrelsen for Grøn Arealomlægning og Vandmiljø

Hav- og Vandmiljø
J.nr. 2025 - 7576
Ref. CGREV
Den 4. marts 2025

Skabelon for indtag – Målestationsniveau Parameter

Beskrivelse af datakolonner i skabelon for parameterdata for målestationer/indtag til grundvandsdatabase.

Der skal dannes separate ark for hver parameter der udtrækkes data for. For pesticider kun pesticider samlet og for PFAS kun for hhv. PFAS-4 og PFAS-22 samlet.

Kolonner der udfyldes af dataleverandør:

Grundvandsforekomst - Der anvendes EU-ID for grundvandsforekomsten. Denne er i formatet DKxxx_dkmx_xxxx_xx (DK110_dkmj_1106_ks).

euMonitoringSiteCode - der anvendes EU-ID for boringsindtagene, der er tilknyttet en grundvandsforekomst, og som anvendes til kemisk risiko- og/eller tilstandsvurdering til BA4/VP4. Denne er i formatet DKxxx-xxxx-y (DK201-3854-1), hvor y svarer til indtagsnr.

gwPollutantCode – EU-stofkode (CAS eller EEA) – se Bilag 1 - gwPollutantCode - EU's liste over CAS-numre

gwPollutantOther – Hvis **gwPollutantCode er *"EEA_oo-oo-o Other"*** udfyld CAS nummer og navn af stoffet.

ChemicalMatrix - Udfyldes med "Water"

ChemicalPurpose - anvendes data fra indtaget til tilstandsvurdering, trendberegning eller begge dele?

Status	*- indtaget anvendes til tilstandsvurdering*
Trend	*- indtaget anvendes til trendberegning*
Both	*- indtaget anvendes til både tilstandsvurdering og trendberegning*

Frequency – Frekvensen af målinger i indtaget pr. år (gennemsnitligt antal målinger pr. år indenfor måleår).
Tilladte værdier: Kun hele tal mellem 1-365.

Cycle – Moniteringscyklus for indtaget (Gennemsnitligt antal år imellem måleår).
Tilladte værdier: 0, 1, 2, 3, 4, 5, 6, 12, 18, -9999

LastMonitored - Årstal for den seneste måling for det specifikke stof i indtaget i formatet YYYY.

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13. Appendix E: Clarification of debatable pesticide compounds to be included in VP4

This appendix presents the communication between GEUS and SGAV regarding which specific compounds should be moved from Jupiter group 50 (i.e. “pesticides”) to the MFS group for VP4.

This communication occurred during step 0 (Table 1) of the process, when a detailed work-description was prepared for approval by SGAV.

GEUS required further clarification, as in the project description (see contract, file: *“Aftale 2, Kemiske parametre.xlsx”*), in the part including which parameters should be extracted from Jupiter, under “pesticides” it was provided a note that group 50 (of Jupiter) should be used. However, during VP3, some of the phenol-compounds, part of group 50, were excluded from pesticides and included instead in the MFS assessments. GEUS requested clarification from SGAV on which specific parameters should be included in which group. This has a relevance for calculating the sum-pesticides, for example. It was decided to revisit the issue, as during VP3 only some of the phenol-compounds were moved to MFS (not all of them).

SGAV provided feedback via e-mail (with two attached files). These were exported as pdfs and are added to this report as a part of this appendix, as they provide argumentation on which specific parameter should be included/excluded in the pesticides or MFS groups in the data-products described in this report.

The following 3 pdf files were added to the next pages:

1. Email from Charlotte Greve (SVAV) from 15 Aug 2025 with subject “Afklaring af diskutable pesticider, der skal indgå til VP4 (SGAV Id nr.: 12766450)
2. Attachment 1 to the email, including a commented by SGAV version of Appendix G from the detailed work-description sent previously to SGAV for approval. In the e-mail this file is referred to as Appendix G. It includes a note prepared by Anders Risbjerg Johnsen on 25 June 2025 with title “*Gennemgang af udvalgte biocidstoffer til tilstandsvurdering*”. Anders Johnsen is the person responsible for defining group 50 of Jupiter in respect to which compounds are pesticides.
3. Attachment 2 to the email, including a fast check prepared by Anders Johnsen on the number of analyses for the compounds that were not included in VP3.

Based on this, **procedure 6** (Table 1) was carried out to ensure that the instructions provided by SGAV were indeed followed. The details regarding this procedure were provided in section 4.1.

Outlook

Afklaring af diskutable pesticider, der skal indgå til VP4 (SGAV Id nr.: 12766450)

From Charlotte Greve <cgrev@sgav.dk>
Date Fri 8/15/2025 3:08 PM
To Lærke Thorling <lts@geus.dk>; Denitza Voutchkova <dv@geus.dk>
Cc Tine Ørbæk Nielsen <tinon@sgav.dk>; Luc Taliesin Eisenbrückner <lueis@sgav.dk>

2 attachments (99 KB)

VP4 Biocider analyser antal arj.xlsx; Appendix G ARJ Gennemgang af biocidstoffer til tilstandsvurdering inkl SGAVs kommentarer.pdf;

Kære Lærke og Denitza

Vi har kigget på appendix G omkring diskutable biocidstoffer fra gruppe 50 i Jupiter (pesticidlisten) for at se på, hvilke af stofferne der skal indgå i VP4 som pesticider eller evt. som øvrige MFS, og som derfor skal med i dataudtrækket etc. Tine har også haft en lang snak med Anders Johnsen omkring en del af stofferne og Anders har lavet vedhæftede excel-liste, der viser antallet af analyser i Jupiter for de stoffer, der ikke indgik i VP3. for mange af dem er der ikke eller kun få analyser i Jupiter, og dermed udelades de. Nogle stofgrupper skal indgå til VP4 - ikke som pesticider, men som øvrige MFS (phenol-gruppen), som de også gjorde til VP3.

Ud fra vedhæftede oversigt fra Anders over biocidstoffer m/u analyser, har Tine lavet følgende beskrivelse af, hvad der skal udtrækkes til grunddata:

- Cresoler (methylphenoler): Alle stoffer indgår, som i VP3, som del af "Øvrige MFS"
- Xylenoler (dimethylphenoler): Stofferne 0408, 0411, 0412, 0413, 0414, 0426 indgår som i VP3 som del af "Øvrige MFS". Øvrige stoffer har ingen eller kun få analyser og indgår derfor ikke.
- Chlorcresoler (chlormethylphenoler): Alle stoffer indgår, som i VP3, som en del af "Pesticider"
- Chlorphenoler: Alle stoffer listet under denne skal indgå som del af "Pesticider" til VP4, da der er analyser på samtlige stoffer og vil være nedbrydningsprodukter fra biocidanvendelse.
- Aldehyder: Formaldehyd indgår, som i VP3, som en del af "Pesticider". Glutaraldehyd har ingen analyser i Jupiter og ikke indgår derfor ikke til VP4. : Acetaldehyd har samlet fra 1988-d.d. 107 analyser, men primær anvendelse er jf appendix G ikke biocid, hvorfor den ikke medtages som del af "Pesticider". Inddragelse som eget stof under "Øvrige MFS" kan overvejes, men umiddelbart er der for få analyser til at kunne gennemføre en valid tilstandsvurdering.
- Parabener: Stofferne medtages ikke, da der ikke er nogen analyser for nogen af stofferne i Jupiter.
- Thiazolinoner: Stoffet 2049 indgik til VP3 i "Pesticider". Til kommende VP4 skal stoffet 2049 indgå i "Pesticider" sammen med stofferne 764 og 2050, der har en del analyser i Jupiter. Stofferne 1973, 2051 og 2897 medtages ikke, da der ikke er nogen analyser for nogen af stofferne i Jupiter.

- Organiske tin forbindelser: 0103: dibutyltin, 0140: monobutyltin, 0168: tributyltin og 0172: triphenyltin indgår, som i VP3, som en del af "Pesticider". For de øvrige stoffer er der ingen analyser i Jupiter, hvorfor stofferne ikke medtages.

- Organiske kviksølvforbindelser: Disse stoffer medtages ikke, da de vil høre under en eventuelt tilstandsvurdering for kviksølv.

Jeg har også vedhæftet appendix G med tilknyttede kommentarer til stofferne.

Med hensyn til de 6 pesticider med drikkevandskrav lavere end 0,10 µg/l - dem I har tilføjet med gult til appendix B - så skal alle stofferne med til VP4 som pesticider med grundvandskvalitetskravet 0,10 µg/l.

I har også fremhævet MFS'erne Trichlormethan (Chloroform), Naphalen, og TFA. Jeg er usikker på, hvorfor de er fremhævet med gult, men de skal alle indgå i VP4, og skal dermed i dataudtrækket. I må sige til, hvis der er nogle spørgsmål til stofferne. De skal indgå med tærskelværdier svarende til dem, I har skrevet i kolonne D.

Jeg håber dette giver tilstrækkeligt svar på jeres forespørgsel, men ellers ved I, hvor I kan finde os ;o)
Rigtig god weekend

Venlig hilsen

Charlotte Greve
AC tekniker | Vandmiljø
+45 23 72 15 39 | cgrev@sgav.dk

Ministeriet for Grøn Trepart
Styrelsen for Grøn Arealomlægning og Vandmiljø | Lerchesgade 35 | 5000 Odense C | Tlf. +45 33 95 80 00 | mail@sgav.dk

Gennemgang af udvalgte biocidstoffer til tilstandsvurdering, **25. juni 2025 (arj)**

Medmindre andet er anført, er følgende stoffer i gruppe 50:

Cresoler (methylphenoler)

0409: 2-methylphenol**.** Biocidanvendelse fx i beton og produkter lavet af fibercement (Lupsea et al, 2014, Miljøstyrelsen 2020). Cresol er på biociddirektivets annex 1 over aktivstoffer.

0410: 4-methylphenol. Biocidanvendelse fx i beton og produkter lavet af fibercement (Lupsea et al, 2014, Miljøstyrelsen 2020). Cresol er på biociddirektivets annex 1 over aktivstoffer. Dannes også naturligt i rådnende dyrekadavre (doi:10.1016/j.forsciint.2009.03.034 og https://doi.org/10.1016/j.wasman.2018.03.009)

0407: 3-methylphenol. Cresol er på biociddirektivets annex 1 over aktivstoffer, 3-methylcresol nævnes også specifikt på annex 1 som m-cresol, indgik i 2021 massescreening men efter fund klassificerede MST stoffet som ikke-pesticid, er ikke i gruppe 50.

Xylenoler (dimethylphenoler)

0201: xylenoler er på biociddirektivets annex 1. Enkeltstoffer er i gruppe 50 men 0201 er ikke i gruppe 50 da det er en uspecifik sumgruppe. I forbindelse med massescreeningerne ønskede MST de enkelte dimethylphenoler i gruppe 50.

0408: 2,3-dimethylphenol. Xylenoler er på biociddirektivets annex 1.

0411: 3,4-dimethylphenol. Xylenoler er på biociddirektivets annex 1.

0412: 3,5-dimethylphenol. Xylenoler er på biociddirektivets annex 1.

0413: 2,6-dimethylphenol. Xylenoler er på biociddirektivets annex 1.

0414: 2,4-dimethylphenol. PPDB: Also known as: 2,4-xylenol; 2,4-DMP; hydroxy-o-xylene; m-xylenol. A fungicide and disinfectant with a variety of agricultural uses as well as many industrial applications. Xylenoler er på biociddirektivets annex 1.

0426: 2,5-dimethylphenol**.** Xylenoler er på biociddirektivets annex 1.

4888: 2-ethylphenol. PubChem: “4-Ethylphenol is contained in the xylenol fraction boiling between ca. 205 and 225 °C obtained from tar phenols”, dette må også gælde 2-ethylphenol som dermed hører under xylenoler på biociddirektivets annex 1.

1722: 2,3,5-trimethylphenol. Ikke I gruppe 50, vurderes hovedsageligt at stamme fra olieforurening, men muligvis også biocidanvendelse.

1815: 2,4,6-trimethylphenol. Ikke I gruppe 50, vurderes hovedsageligt at stamme fra olieforurening, men muligvis også biocidanvendelse.

Summary of Comments on Appendix G ARJ Gennemgang af biocidstoffer til tilstandsvurdering inkl SGAVs kommentarer.pdf

Page: 1

Number: 1 Author: b063024 Subject: Kom. til tekst Date: 15-Aug-25 1:08:21 PM +02'00'

Stofferne skal ikke indgå som pesticid til VP4, men alle skal indgå som øvrige MFS (phenoler).
Var også del af øvrige MFS (phenoler) til VP3.

Number: 2 Author: b063024 Subject: Kom. til tekst Date: 15-Aug-25 9:22:07 AM +02'00'

Skal ikke indgå til VP4 (da det er en sumværdi)

Number: 3 Author: b063024 Subject: Kom. til tekst Date: 15-Aug-25 1:12:42 PM +02'00'

Stofferne skal ikke indgå som pesticid til VP4, men som øvrig MFS (phenoler).
Var også del af øvrige MFS (phenoler) til VP3.

Number: 4 Author: b063024 Subject: Fremhæv Date: 15-Aug-25 1:12:18 PM +02'00'

Stofferne skal ikke indgå til VP4, da stofferne enten har ingen eller kun få analyser

1. Chlorcresoler (chlormethylphenoler)

Ifølge Liste over drikkevandskvalitetskriterier (2023) har chlorphenoler, bortset fra pentachlorphenol et kvalitetskrav i drikkevand på 0,1. Listen definerer ikke chlorphenoler og det vides derfor ikke om chlorphenoler også omfatter chlormethylphenolerne.

0415: 4-chloro-2-methylphenol (4-chloro-2-cresol; 2-methyl-4-chlorophenol), nedbrydningsprodukt fra herbiciderne mecoprop og MCPA.

0416: 6-chlor-2-methylphenol (2-methyl-6-chlorphenol), nedbrydningsprodukt fra 2,6-MCPP der er en synteseforurening i mecoprop svarende til 2,6-DCPP som er på drikkevandsbekendtgørelsens obligatoriske liste selvom det er en synteseforurening i dichlorprop og ikke et aktivstof. Desuden er 6-chlor-2-methylphenol en chlorocresol og dermed sandsynlig biocidanvendelse i tekniske chlorcresolblandinger som er på biociddirektivets annex 1

0418: 4,6-dichloro-2-methylphenol (2,4-dichloro-6-methylphenol), ikke i PPDB men ifølge PubChem nedbrydningsprodukt fra tolclofos-methyl, hvilket er meget sandsynligt når man ser strukturen og sammenligner med nedbrydning af de andre phenoxysyrer. Desuden en chlorocresol som sandsynligvis har været til stede i tekniske blandinger af chlorcresoler, dvs. sandsynlig biocidanvendelse; chlorocresoler er nævnt på biociddirektivets annex 1

0524: 4-chlor-3-methylphenol, chlorcresol, indgik i MSTs massescreening 2019 og 2020. ECHA substance infocard: approved for use as a biocide in the EEA and/or Switzerland, for: human hygiene, disinfection, veterinary hygiene, product preservation, preservation of fibres, leather, rubber, or polymers, preservation for working / cutting fluids. Chlorcresol er på biociddirektivets annex 1

2. Chlorphenoler

0424: Pentachlorphenol (PCP) er på biociddirektivets annex 1, kravværdi i drikkevandsbekendtgørelsen er 0,01. Pentachlorphenol har været anvendt til træbeskyttelse (facader, plankeværker, stolper, og jernbanesveller) samt som herbicid (ifølge PPDB) dog uden registreret herbicidanvendelse i DK. Teknisk PCP kan indeholde andre chlorphenoler fx op til 120 g/kg i de senest tilladte anvendelser (Miljøstyrelsen, 2009). Disse lettere chlorphenoler har med stor sandsynlighed bidraget til produkternes biocidvirkning. PCP kan yderligere nedbrydes til lettere chlorphenoler under anoxiske forhold i grundvandet. Ifølge Liste over drikkevandskvalitetskriterier har chlorphenoler, bortset fra pentachlorphenol et kvalitetskrav i drikkevand på 0,1.

0421: 2,3,4,6-tetrachlorphenol. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

0422: 2,3,5,6-tetrachlorphenol. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

0423: 2,3,4,5-tetrachlorphenol. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

0861: 2,4,5-trichlorophenol er ifølge PPDB et aktivstof og et nedbrydningsprodukt fra herbicidet 2,4,5-T. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

0420: 2,4,6-trichlorophenol er på biociddirektivets annex 1. Sandsynlig biprodukt og nedbrydningsprodukt i PCP.

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Number: 1 Author: b063024 Subject: Kom. til tekst Date: 15-Aug-25 12:58:21 PM +02'00'

Alle stofferne skal indgå som pesticider til VP4.
De indgik også som pesticider til VP3.

Number: 2 Author: b063024 Subject: Kom. til tekst Date: 15-Aug-25 12:56:56 PM +02'00'

Alle stofferne skal indgå som pesticider til VP4 og alle med kravværdien 0,10 µg/l.
De fleste indgik også som pesticider til VP3. Dem der ikke var med skyldes sandsynligvis manglende data.

1322: 2,3,4-trichlorphenol. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

1323: 2,3,5-trichlorphenol. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

1324: 2,3,6-trichlorphenol. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

1325: 3,4,5-trichlorphenol. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

0417: 2,4-dichlorophenol. Nedbrydningsprodukt fra herbiciderne 2,4-D og 2,4,5-T. Nedbrydningsprodukt fra biocidet triclosan. Sandsynligt biprodukt og nedbrydningsprodukt fra PCP.

0768: 2,5-dichlorphenol. Nedbrydningsprodukt fra 2,4,5-T (Al-Fathi, 2019). Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

0419: 2,6-dichlorphenol. Nedbrydningsprodukt fra synteseurenheden 2,6-DCPP. 2,6-dichlorphenol har været på drikkevandsbekendtgørelsens pesticidliste i næsten alle år. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

0767: 2,3-dichlorphenol. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

0769: 3,4-dichlorphenol. Nedbrydningsprodukt fra 2,4,5-T (Al-Fathi, 2019). Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

0770 3,5-dichlorphenol. Sandsynligt biprodukt og nedbrydningsprodukt i PCP.

0287: 2-chlorphenol. Ifølge ppdb nedbrydningsprodukt fra fluoxastrobin, ingen godkendte produkter i bekæmpelsesmiddeldatabasen, men i udlandet brugt som bejdsemiddel fx til raps. Sandsynligvis nedbrydningsprodukt fra dichlorprop og 2,4-D.

0427: 4-chlorophenol. Nedbrydningsprodukt fra fx herbiciderne 2,4-D (PPDB), og 2,4,5-T (Al-Fathi, 2019). Ifølge PPDB også nedbrydningsprodukt fra fungicidet triadimenol og derfor sandsynligvis også triadimefon-metabolit, idet triadimenol kan omdannes til triadimefon. Muligt biprodukt og nedbrydningsprodukt i PCP.

0523: 3-chlorphenol. Nedbrydningsprodukt fra 2,4,5-T (Al-Fathi, 2019). Muligt biprodukt og nedbrydningsprodukt i PCP.

Aldehyder

0397: Formaldehyd. Er på biociddirektivets annex 1. Må formodes at komme fra biocidanvendelse, når det findes i grundvandet i det åbne land, fx anvendelse i klovbade med formalin som sælges i 1000L palletanke. Skal kravværdien være 0,1 eller 50 (drikkevandskriteriet)?

0903: Glutaraldehyd (glutaral). Er på biociddirektivets annex 1.

1806: Acetaldehyd. Ifølge PPDB nedbrydningsprodukt fra metaldehyd, men også mange industrielle anvendelser. Er ikke på biociddirektivets annex 1. Ikke gruppe 50.

Parabener

Biocider til konservering.

Page: 3

Number: 1 Author: b063024 Subject: Kom. til tekst Date: 15-Aug-25 1:05:41 PM +02'00'

Skal indgå som pesticid til VP4, med kravværdien 0,10 µg/l.
Indgik også som pesticid til VP3 med kravværdien 0,10 µg/l.

Number: 2 Author: b063024 Subject: Fremhæv Date: 15-Aug-25 1:02:05 PM +02'00'

Skal ikke indgå til VP4, da der ikke findes analyser i Jupiter. Indgik heller ikke til VP3.

Number: 3 Author: b063024 Subject: Fremhæv Date: 15-Aug-25 1:05:10 PM +02'00'

Vurderes ikke at stamme fra pesticid-/biocidanvendelse, og skal ikke indgå som pesticid til VP4.
Skal heller ikke indgå til VP4 som øvrig MFS, da der kun er få analyser i Jupiter.
Indgik heller ikke til VP3.

Number: 4 Author: b063024 Subject: Fremhæv Date: 15-Aug-25 1:21:58 PM +02'00'

Stofferne skal ikke indgå til VP4, da der ikke er nogle analyser i Jupiter.
Indgik heller ikke til VP3.

0870: methylparaben

0871: ethylparaben

0872: propylparaben

0873: butylparaben

0874: benzylparaben

Thiazolinoner

Biocider til konservering.

0764: dichloroctylisothiazolinon

1973: 2-octyl-4-isothiazolin-3-on

2050: 2-methyl-2H-isothiazol-3-on

2049: 1,2-benzisothiazolin-3-on

2051: Benzisothiazol

2897: 2-methyl-1,2-benzothiazol-3(2H)-on

Organiske tin forbindelser

Nogle er på biociddirektivets annex 1, andre er nedbrydningsprodukter.

0103: dibutyltin

0140: monobutyltin

0168: tributyltin

0172: triphenyltin

0575: tributyltinacetat

0576: tributyltinnaphthalen

0577: tributyltinoxid

0763: monophenyltin

1205: tiphenyltin

1550: monooctyltin

1551: dioctyltin

1552: tricyclohexyltin

1559: tetrabutyltin

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Number: 1 Author: b063024 Subject: Kom. til tekst Date: 15-Aug-25 1:21:51 PM +02'00'
Stoffet skal indgå som pesticid til VP4.
Indgik ikke til VP3.

Number: 2 Author: b063024 Subject: Fremhæv Date: 15-Aug-25 1:21:45 PM +02'00'
Stoffet skal ikke indgå som pesticid til VP4, da der ikke er nogle analyser i Jupiter.
Indgik heller ikke til VP3.

Number: 3 Author: b063024 Subject: Kom. til tekst Date: 15-Aug-25 1:22:18 PM +02'00'
Stoffet skal indgå som pesticid til VP4.
Indgik ikke til VP3.

Number: 4 Author: b063024 Subject: Kom. til tekst Date: 15-Aug-25 1:20:36 PM +02'00'
Stoffet skal indgå som pesticid til VP4.
Indgik også som pesticid til VP3.

Number: 5 Author: b063024 Subject: Fremhæv Date: 15-Aug-25 1:22:41 PM +02'00'
Stoffet skal ikke indgå som pesticid til VP4, da der ikke er nogle analyser i Jupiter.
Indgik heller ikke til VP3.

Number: 6 Author: b063024 Subject: Fremhæv Date: 15-Aug-25 1:22:53 PM +02'00'
Stoffet skal ikke indgå som pesticid til VP4, da der ikke er nogle analyser i Jupiter.
Indgik heller ikke til VP3.

Number: 7 Author: b063024 Subject: Kom. til tekst Date: 15-Aug-25 1:24:57 PM +02'00'
Stofferne skal indgå som pesticider til VP4.
Indgik også som pesticider til VP3.

Number: 8 Author: b063024 Subject: Fremhæv Date: 15-Aug-25 1:26:17 PM +02'00'
Stofferne skal ikke indgå som pesticid til VP4, da der ikke er nogle analyser i Jupiter.
Indgik heller ikke til VP3.

Organiske kviksølvforbindelser

Er ikke på biociddirektivets annex 1. Kan i varierende grad have været brugt som bejdse og konservering.

571: diethylkviksølv. Er ikke i gruppe 50

572: dimethylkviksølv. Er ikke i gruppe 50

573: diphenylkviksølv. Er ikke i gruppe 50

1542: methylkviksølv. Er ikke i gruppe 50

Number: 1 Author: b063024 Subject: Fremhæv Date: 15-Aug-25 1:27:26 PM +02'00'
Stofferne skal ikke indgå til VP4.
De indgik heller ikke til VP3

STANCODE	Navn	Grænseværdi	Gruppe	BK	GRUMO	LOOP	DEPO (=punktkilde	Andre	Total
1816	2-ethylphenol	0.1 µg/l	50 - Pestici						
1722	2,3,5-trimethylphenol		40 - Organi	12					12
1815	2,4,6-trimethylphenol		40 - Organi						
422	2,3,5,6-Tetrachlorphenol	0.1 µg/l	50 - Pestici	978	591		146	23	1738
1322	2,3,4-Trichlorphenol	0.1 µg/l	50 - Pestici	49			30	1	80
1323	2,3,5-Trichlorphenol	0.1 µg/l	50 - Pestici	49			6	1	56
1324	2,3,6-Trichlorphenol	0.1 µg/l	50 - Pestici	49			6	1	56
1325	3,4,5-Trichlorphenol	0.1 µg/l	50 - Pestici	50	250		11	1	312
287	2-Chlorphenol	0.1 µg/l	50 - Pestici	283			55	7	345
523	3-Chlorphenol	0.1 µg/l	50 - Pestici	43			37	1	81
903	Glutaraldehyd	0.1 µg/l	50 - Pestici						
1806	Acetaldehyd		40 - Organi	43			64		107
870	Methylparaben	0.1 µg/l	50 - Pestici						
871	Ethylparaben	0.1 µg/l	50 - Pestici						
872	Propylparaben	0.1 µg/l	50 - Pestici						
873	Butylparaben	0.1 µg/l	50 - Pestici						
874	Benzylparaben	0.1 µg/l	50 - Pestici						
764	Dichloroctylisothiazolinon	0.1 µg/l	50 - Pestici	7	495		3	15	520
1973	2-Octyl-4-isothiazolin-3-on	0.1 µg/l	50 - Pestici	1					1
2050	2-Methyl-2H-isothiazol-3-on	0.1 µg/l	50 - Pestici	1	247		9		257
2051	Benzisothiazol	0.1 µg/l	50 - Pestici						
2897	2-Methyl-1,2-benzothiazol-3(2H)-on	0.1 µg/l	50 - Pestici						
575	Tributyltinacetat	0.1 µg/l	50 - Pestici						
576	Tributyltinnaphthalen	0.1 µg/l	50 - Pestici						
577	Tributyltinoxid	0.1 µg/l	50 - Pestici						
763	Monophenyltin	0.1 µg/l	50 - Pestici						
1205	Diphenyltin	0.1 µg/l	50 - Pestici						
1550	Monooctyltin	0.1 µg/l	50 - Pestici	2					2
1551	Dioctyltin	0.1 µg/l	50 - Pestici	2					2
1552	Tricyclohexyltin	0.1 µg/l	50 - Pestici	2					2
1559	Tetrabutyltin	0.1 µg/l	50 - Pestici	2					2

Antal analyser er siden 1988-01-01 og formål alene bestemt vha. prøvens projekt, dvs. der er ikke taget højde for boringsformål eller boringsanvendelse.

Danish Ministry of Climate,
Energy and Utilities

DANMARKS OG GRØNLANDS GEOLOGISKE UNDERSØGELSE **RAPPORT 2025/37**

Groundwater chemistry data for status, risk, and trend analyses related to the fourth River Basin Management Plan (Vandområdeplan 4)

Documentation report

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GEOLOGICAL SURVEY OF DENMARK AND GREENLAND
DANISH MINISTRY OF CLIMATE, ENERGY AND UTILITIES

G E U S