UNDP/GEF Danube Regional Project

Strengthening the Implementation Capacities for Nutrient
Reduction and Transboundary Cooperation
in the Danube River Basin

Preparation of a proposal for connection/operational link of the data collected during the Joint Danube Survey into ICPDR Information System, with particular attention to biological database

Project Component 2.2: Development of operational tools for monitoring, laboratory and information management with particular attention to nutrients and toxic substances

October 31, 2003

Prepared by: Rodeco Consulting GmbH

Authors: Jaroslav Slobodník, Astrid Schmidt-Kloiber, Juliana Adamková, Jarmila Makovinská, Birgit Vogel, Béla Csányi

Preface

The Joint Danube Survey (JDS) was carried out in August and September 2001 and provided complex information on the chemical and microbiological water quality as well as on the biodiversity in the main course of the Danube River and its major tributaries. The JDS was the most comprehensive survey ever performed in the Danube River Basin yielding information on a wide range of chemical pollutants in water, sediments, suspended solids and mussels matrices, aquatic flora and fauna and biological indicators. The survey generated data and information necessary for the ecological and chemical surface water status characterization in line with the requirements of the EU Water Framework Directive (WFD). A geo-morphological division of the Danube River Basin (DRB) was proposed and evaluated using the obtained data. The scientific outputs of the JDS were used for development of the Danube List of Priority Substances and also for the upgrade of the TNMN. Next to the printed and electronic version of the JDS Technical Report, the results were also summarized in a web-based database designed for the use by water management experts. Biological and GC-MS screening databases were established in the Danube River Basin for the first time.

The main goal of the presented part of the project was to develop a proposal for connection/operational link of the JDS data into the ICPDR Information System (DANUBIS) in order to fully utilize potential of the obtained data. A particular attention was given to the biological part of the database, with the final goal to set up a basis for regular collection of biological data for the TNMN Database in the near future. Successful implementation of the WFD requires availability of both hydrobiological and chemical data organized in a systematic way allowing experts to draw conclusions in a basin-wide scale. Having this in mind, many new ideas and inputs came either from the project team or MLIM experts during the implementation phase of this project component. Many of them were immediately used to upgrade the existing ICPDR Information System and, therefore, to see the latest version of the JDS and TNMN databases one is advised to look directly at the www.icpdr.org [Databases/New Draft Versions].

Given by the importance of the new biological and chemical parameters, which were not yet monitored within the TNMN, it is expected that the JDS and TNMN databases will be further developed in line with recommendations of the MLIM EG and this report. The results of this project component will also be provided to the DRP project outputs 1.1.6 and 1.1.7.

Table of contents

Abbreviations

JDS	Joint Danube Survey
WFD	Water Framework Directive
DRB	Danube River Basin
TNMN	Trans-National Monitoring Network
ICPDR	International Commission for the Protection of the Danube River
MLIM	Monitoring and Laboratory Information Management
EG	Expert Group
DRP	UNDP/GEF Danube Regional Project
GC-MS	Gas chromatography – mass spectrometry
LC-MS	Liquid chromatography – mass spectrometry
MS-MS	Mass spectrometry – mass spectrometry
HTG	Higher Taxonomic Group

Executive summary

Primary objective of this project component was to develop a proposal for an operational link between the JDS and TNMN databases. The project team with a help of selected MLIM experts and UNDP/GEF Information Specialist, who participated at the development of the original JDS Database, undertook an approach of on-line introduction of suggested changes/recommendations into the web-based ICPDR Information System. This gave an instant feedback on the practicality and usefulness of the JDS database upgrades and improvements. Prior to the final interlinking of databases, numerous efforts were made consisting of completion of the database for missing parameters and thorough check on the quality of stored data.

As a result recommendations for a link between the JDS and TNMN databases and harmonisation of their query templates were made and incorporated into their New Draft Versions. A proposal of the new central page on the ICPDR website comprising of all ICPDR databases (TNMN, EMIS, Bucharest Declaration Database, JDS, JDS – Investigation of the Tisa River) was drafted. During the project, the JDS Database was gradually improved and developed into the stage, that it is ready for the public use (for latest version, see www.icpdr.org [Databases/New Draft Versions]).

Several suggestions, which go beyond the scope of this project component, were made by the project team and MLIM experts to improve the ease-of-use of the JDS and TNMN databases. A principal upgrade and Europe-wide harmonisation of the coding system and systematic tracking of taxonomical changes in the biological part of the database was proposed in order to assure its sustainability. Also, further upgrade of the GC-MS screening part of the database was suggested to allow proper evaluation of the screening data on emerging, unknown and Danube River Basin specific pollutants as required by the WFD. A specific recommendation was made to perform similar upgrade at the JDS – Investigation of the Tisa River database, containing valuable data from survey conducted in October 2001, however, not being ready for public use in its present form.

Final goal of all the above efforts is to create a fully interlinked ICPDR Information System. This would require future harmonization of the coding system between the TNMN and EMIS databases and further development of the link between the two databases. The knowledge obtained at the development and upgrade of the JDS Database created a solid base for extension of the TNMN Database for new chemical parameters, parameters measured in other matrices than water, GC-MS screening and biological data.

1. Introduction

Joint Danube Survey (JDS) was organized by the ICPDR and took place from 13 August till 20 September 2001. The major goal was to obtain comparable, accredited information on the quality of the Danube river in its entire length. Two ships collected samples from 98 sampling sites, 74 of them on the Danube and 24 major tributaries. Among the investigated matrices were water, sediments, suspended solids and mussels. Next to chemical and microbiological determinands a wide range of biological parameters, including macrozoobenthos, phytobenthos, phytoplankton, zooplankton and macrophytes were investigated. In total, over 140 different parameters were analysed in the studied matrices by a team of international experts on the board of the ships and in seven reference laboratories. The survey generated over 40.000 results, which were stored in the web-based JDS Database. Biological and GC-MS screening databases were developed for the first time in the Danube Basin.

The results of the survey gave an overview on the ecological and chemical status of the Danube. Over 1000 biological species were found to inhabit the Danube basin and microbiological pollution profiles were constructed. Analyses of numerous chemical parameters, including EU WFD determinands, pharmaceuticals, pesticides and the screening of unknown substances were carried out for the first time. Obtained sediments, suspended solids and biological samples were stored for several years in selected institutes (VITUKI, CBC Frankfurt) to allow for follow up analyses.

The use of the obtained data was intended primarily for an upgrade of the TNMN and development of the Danube List of Priority Substances.

Among the major goals of this project component were:

- Completion of the database for missing parameters (in cooperation with the ICPDR);
- Check on the quality of data;
- Preparation of the public version of the JDS Database;
- Recommendations for a link between the JDS and TNMN databases;
- Selection of relevant database parameters and upgrade of the existing version of the JDS Database.

A close cooperation with MLIM experts was foreseen in order to achieve the project goals.

2. Description of activities and methodology used

In the course of the project, the JDS and TNMN databases were thoroughly reviewed in order to assess needs for their interlinking, future development and upgrade. Prior to the further development of the biological database its completion was proposed by the project team and ensured by the ICPDR.

Next to the project team, five MLIM experts, actively participating at the collection and storage of the JDS data in 2001 and 2002, were invited to comment on the current structure of the JDS Database. Their expertise covered all major components of the databases: (i) chemical and microbiological data, (ii) macrozoobenthos, (iii) phytobenthos, (iv) phytoplankton and zooplankton and (v) macrophytes data. Among specific tasks of the MLIM experts were:

- Thorough examination of the current version of the JDS Database and provision of comments/suggestions, whose implementation will make the database fully operational and ready to be accessible by the general public;
- Check of all data (chemical and microbiological data, macrozoobenthos, phytobenthos, phytoplankton and zooplankton and macrophytes) for correctness;
- Proposal for handling of data, which are not correct;

- Preparation of an introduction to the Chapters: "Chemical and microbiological parameters, Biological parameters – macrozoobenthos, phytobenthos, phytoplankton and zooplankton and macrophytes", which will be placed in the explanatory text of "About the database". The text should introduce in a brief and comprehensive way following:
    i. Background information on selection of measured parameters, units;
    ii. Mathematical models and calculations (if used for any of the parameters, e.g. Saprobic indeces);
    iii. Coding system;
    iv. Way of handling the data and generating reports;
- Proposal for the selection and layout of the database search parameters (if different from the current version);
- Proposal for the new coding system (if not acceptable in the current version);
- Proposal for the future direct interlinking of the biological databases of the TNMN and JDS;
- Proposal for the layout/parameters of TNMN Biological Database (if different from the current version of the JDS Database).

A close cooperation was established between the project team and the Information Specialist of the UNDP/GEF Danube Regional Project at the development of the final version of the JDS Database. Majority of the proposed changes/upgrades of the JDS Database were implemented in the course of the project duration (for details, see www.icpdr.org [Databases/New Draft Versions]).

The necessity of direct interlinking of the chemical databases of the TNMN and JDS were consulted with the chemical experts from the MLIM EG.

The goals and interim results of the activities were discussed and approved at the 1st and 2nd Joint MLIM-EMIS Meetings in Vienna (3 February 2003) and Bratislava (17 September 2003), respectively. The information was also presented and approved at the MLIM EG meetings in Vienna (27 - 28 March 2003) and Bratislava (18 – 19 September 2003).

3. Results

The JDS Database consists of five major components: chemical and microbiological data, macrozoobenthos, phytobenthos, phytoplankton and zooplankton and macrophytes. Comments on the current version of the JDS Database and recommendations of individual MLIM experts are included separately below:

3.1 Biological database

3.1.1 Macrozoobenthos

General introduction

Regarding the WFD, biota is the most important component for the evaluation of the ecological quality of running water bodies. The communities investigated in rivers should include: algae, macrophytes, macrozoobenthos and fish. To describe the biological elements the following attributes have to be considered: taxa composition, abundance, and the ratio of disturbance sensitive taxa to insensitive taxa. With respect to most of the methods used to evaluate the river quality in European countries the WFD enforces a re-orientation of the monitoring procedures towards an integrative approach. Future assessment of the ecological status of water bodies considers the relationships between biota and the hydro-morphological and chemical components, instead of only documenting the biological water quality with respect to organic pollution. The current JDS database therefore serves as a valuable base for future activities in the Danube catchment area.

The evaluated part of the database focuses on benthic macro-invertebrates. Benthic invertebrates have a high indicative value, and are the most widely used indicators for water quality assessment (Rosenberg & Resh, 1993).

Aim and content of this report is to comment on the current version of the database. Main scope is turned to the structure and the handling of data for external users. For several parts suggestions for improvements are given.

Macro-invertebrate data and coding system

The coding system for benthic invertebrates is based on the Austrian Software ECOPROF (www. ecoprof.at), that was developed by the Department of Hydrobiology (BOKU, University of Natural Resources and Applied Life Sciences, Vienna; http://www.boku.ac.at/hfa). The coding system was extended for taxa that did not occur within the Austrian Taxa List (Fauna Aquatica Austriaca, Moog (ed.), 1995 and 2002). As a consequence not all taxa-codes correspond to the original ECOPROF list or any other coding system currently in use. Parallel to the ECOPROF coding system a pan-European coding system already exists, developed within the EU funded projects AQEM (www.aqem.de) and STAR (www.eu-star.at) and it is recommended to change the identity numbers to this system before going on-line with the database for the public. In order to comply only with one European taxalist it would also be useful to use taxonomy, synonymy and systematics from the AQEM and STAR taxalists, as they were already checked by taxonomical experts.

The database currently contains double entries that have to be removed.

Mathematical models and calculations

Currently available calculation parameters are:

- Abundance value per taxon;
- Number of taxa per sampling site;
- Saprobic Index per sampling site.

The Saprobic Index is based on the calculation method of Zelinka & Marvan (1961) according to the following formula:

$$SI = \frac{\sum_{i=1}^{n} s_i \cdot A_i \cdot G_i}{\sum_{i=1}^{n} A_i \cdot G_i}$$

SI Saprobic Index of the benthic community
A_i Abundance of taxon i
s_i Saprobic Value of taxon i
G_i Indication weight of taxon i
n Number of taxa

Saprobic values as compiled in the Fauna Aquatica Austriaca (Moog (ed.), 1995 and 2002) were used. The latest version of the Fauna Aquatica Austriaca is available at: www.lebensministerium.at/wasser/, sub-item "Wassergüte".

Dominance of Higher Taxonomic Groups (HTG) is currently only calculated for macrophytes and would also make sense for benthic invertebrates (and also phytobenthos).

Data handling and reports

Regarding the selection of datasets a second selection list within the benthic invertebrates is recommended. In this selection list it should additionally be possible to choose the HTG, because taxonomical specialists are mostly interested in only one taxa-group.

Default sorting of the species according to their taxagroup, family and (within the family) species alphabetically.

Concerning the output options, it would improve readability, if identical columns could be skipped and written instead in the caption of the displayed table.

The additional display of the AQEM/STAR 8 letter shortcode within the result output would be of a value, because such a code might often be used for further analysis.

In the current version of the database JDS and ITR data are presented together: in case of entering overlapping river km values on the Danube and the Tisa (i.e. 0-500), JDS and subsequently ITR data will appear on the screen – databases should be separated.

All biological databases (macrozoobenthos, phytobenthos, phytoplankton, zooplankton, macrophytes) should use the same structure and queries.

Proposal for the layout/parameters of TNMN Biological Database

Concerning the report generation page it could be considered to choose more than only one parameter within "determinand". For practical use it would be comfortable to have related calculations displayed together, e.g. number of taxa AND Saprobic Index. Further, it would make sense to extend the calculated parameters by the dominance of higher taxonomic groups (HTG).

Regarding the output, the sampling site could be complemented by the river kilometre. It is recommended to add the previously defined query elements in the caption text of the displayed table.

General conclusions

The available databases are already well established and publishable for further public use. Generally a common design and layout for all different databases within the ICPDR web-page should be considered.

3.1.2 Phytobenthos

General introduction

The JDS phytobenthos data consists of the groups of Cyanophyceae, Bacillariophyceae (Diatomophyceae), Chrysophyceae, Bangiophyceae, Chlorophyceae, Charophyceae, Xanthophyceae, Zygnematophyceae. Organisms of the group of Bryophyta were not identified. Quantitative data are in the form of estimation of the relative abundance (scale 1 -5).

Background database for phytobenthic organisms was based on the list compiled within the "Development of a Preliminary Set of Danube River Basin Ecosystem Indicators, Preparation of a Concept for Monitoring Ecological Status of Significant Impact Areas and Wetlands" in "Review of the Bioindicators Study in Yugoslavia" (ICPDR, 2000) and (ii) software ECOPROF that was developed by the Department of Hydrobiology (BOKU, University of Natural Resources and Applied Life Sciences, Vienna, Austria).

Phytobenthos data and coding system

Basically, the problem of synonyms and new taxa names should be solved. This relates mainly to the diatoms, where new taxa and new combinations of the taxa are published frequently in connection to the new development in this field, e.g., techniques using electron microscopy.

New taxa can be added to the database easily (using new code). Renamed taxa should be connected to the previous ones to keep continuity with old and new data.

From time to time (e.g. every five years) the database should be revised by the experts for the individual group of organisms to provide about mentioned changes.

The use of certain determination keys for individual groups of organisms would be useful (e.g. Susswasserflora von Mitteleuropa, Gustav Fischer Verlag). This is important mainly from the point of view of future upgrade of the TNMN Database for biological parameters.

Sorting the species could be arranged first according to their taxa-group, then according to the family and finally the species alphabetically including synonyms.

In connection to the proposal of EN standard for the benthic diatoms (pr 13946: Rutin sampling and pre-treatment of benthic diatoms from rivers; pr 14407: Identification and enumeration of benthic diatoms from rivers) also relative abundance should be included (instead of estimation the scale 1-5) and/or some transfer between this different quantitative data should be done.

Mathematical models and calculations

Currently available calculation parameters are:

- Abundance value per taxa;
- Number of taxa per sampling site;
- Saprobic Index per sampling site.

The Saprobic Index is based on the calculation method of Zelinka & Marvan (1961) according to the following formula:

$$SI = \frac{\sum_{i=1}^{n} s_i \cdot A_i \cdot G_i}{\sum_{i=1}^{n} A_i \cdot G_i}$$

SI	Saprobic Index of the benthic community
A_i	Abundance of taxon i
s_i	Saprobic Value of taxa i
G_i	Indication weight of taxa i
n	Number of taxa

3.1.3 Macrophytes

After a thorough examination of the database concerning the biological parameter macrophytes the following should be further integrated:

General suggestions

The macrophyte database still demands some improvements/corrections concerning species terminology. Related changes were suggested. The following categories for changes were created:

a) Corrections concerning terminology mistakes;

b) Species, which were not collected during JDS but were collected in general in the Danube River. It should be mentioned within the database where these data stem from (probably from Pall & Janauer (1998) Macrophyte Inventory of the Danube River);

c) Species which do not exist – need to be deleted;

d) Species, which were initially missing in database - to be added.

- Abbreviation P. within the column GENUS should always be changed to POTAMOGETON.
- The Higher Taxonomic Group CHLOROPHYTA/CHAROPHYCEAE shows a mismatched Group Code. Therefore, the current Group Code should be changed from H (phytobenthos) to F (macrophytes). If the biological parameter group Phytobenthos also includes the Higher Taxonomic Group CHLOROPHYTA/CHAROPHYCEAE both Group Codes H and F need to be included in the database.

Coding system

The used coding system is reasonable (consecutive numbering) and can therefore stay unchanged. Therefore, no further suggestion concerning a new coding system is made.

Proposal for selection and layout of database search parameters

The database is well structured and intuitive to use. Generating reports is easy. Following suggestions are made:

- So far the database enables a report generation using SPECIES or SPECIES CODES. It would be very useful to additionally enable an inquiry using the FAMILY/HIGHER TAXONOMIC GROUP level. This option would be reasonable for all biological parameter groups;

- After a report was generated and when clicking the option BACK TO FORM it would be useful if the content of the last used inquiry were not erased out of the database mask.

Proposal of layout/parameters of TNMN biological database / interlinking

Possible combination of determinants would be useful and reasonable in order to achieve complex reports.

Introductory text for macrophyte chapter

The objective of the Joint Danube Survey concerning the collection and evaluation of macrophytes was to gain comparable and reliable information by applying uniform, standardised methodologies. JDS provided a unique, first time opportunity to gain an overview of aquatic plant growth for the entire course of the Danube River.

Within the frame of the Joint Danube Survey macrophytes (aquatic plants) were collected on both banks of the Danube River. Although the tributaries were searched for macrophytes on both banks, the collection results were integrated into one single sample due to the smaller size of tributaries providing very consistent abiotic habitat conditions for the whole river transect. Adding seven further investigation sites to the original JDS sampling programme, a total of 180 sites (both banks of Danube and tributaries) were investigated for macrophytes. At each site a longitudinal stretch between 0.2 and 5 river km was sampled for aquatic plants.

Each collected species was associated to one of six species groups: 1) Bryophyta, 2) Chlorophyta, 3) Spermatophyta (higher plants) - submerged Rhizophytes, 4) Spermatophyta - free floating and floating leafed plants, 5) Spermatophyta - amphibious plants and 6) Spermatophyta – Helophytes. These species groups and their relevant species are included in the present JDS Database. Reports providing information on macrophytes can be generated via species names or species codes. To investigate on a species code number a separate list with all collected species plus their corresponding code is provided in the database. The coding is based on consecutive numbering of species.

Further, the available database includes Relative Plant Mass (RPM, Pall & Janauer 1995) calculations, which were based on plant mass estimations (Kohler 1978) on a five–level scale (Equation 1). The Relative Plant Mass, weighted for the mass of each species or group of species and the stretches of species occurrence, indicates dominant and sub dominant species within each sampled reach in relation to the overall plant mass in the relevant reach. Additionally, the database contains the calculated dominance of each Higher Taxonomic Group (Equation 2).

$$RPM(\%) = \frac{\sum_{i=1}^{n} (M_1^3 * L_i) * 100}{\sum_{j=1}^{k} \left[\sum_{i=1}^{n} (M_{ji}^3 * L_i) \right]}$$

Equation 1: Relative Plant Mass (RPM), Li=length of reach i; Mi=estimated plant mass of a species for a reach; j=different plant species.

$$Do\min anceHTGx = \frac{NumberTaxaHTGx * 100}{TotalTaxaNumber}$$

Equation 2: Dominance of each Higher Taxonomic Group (HTG)

References

Pal, K. & Janauer G.A. (1995): Die Makrophytenvegetation von Flussstauen am Beispiel der Donau zwischen Fluss-km 2552 und 2511,8 in der Bundesrepublik Deutschland. Arch.Hydrobiol.Suppl. 101, Large Rivers 9/2, 91-109

Kohler, A. (1978): Methoden der Kartierung von Flora und Vegetation von Süßwasserbiotopen. Landschaft und Stadt, 10:23-85

3.1.4 Phytoplankton and zooplankton

General

Regarding the WFD, aquatic biota is the most important component for the evaluation of the ecological status of running water bodies. Although zooplankton does not occur among the biological elements investigated in rivers (such as algae, macrophytes, benthic invertebrates, and fish) the involvement of this group of organisms is inevitably important, especially on the middle and lower Danube sections and on the large Danube tributaries, as well.

The JDS Database contains also quantitative data on phytoplankton and zooplankton. Phytoplankton abundance is given in individual number/l, zooplankton abundance is given in individual number/100 l.

Use of the database

The user first has to select or determine one of the "Location" items in any particular combination, country, river stretch or sampling site(s) could be selected. Second step is to select "Biological data" from the "Determinand" dropdown list, and, either Phytoplankton or Zooplankton from the "Group" dropdown list. The possibility to search for particular species is provided by the database, as well.

The data can be sorted out or grouped for further analysis according to the following parameters:

Higher Taxonomic Group	Family	Genus Species	Author	Sampling Site	Determinand Name	Value	Unit	River km	Species Code

General comments

Phytoplankton and zooplankton data of the JDS Database were tested and controlled in order to reveal possible and/or evident mistakes. As a result, it can be generally stated that there is no evident mistake among the data on phytoplankton and zooplankton. The database is well established and ready to be used by general public.

Specific comments

The search results on the screen are limited to 50 rows – should be adjusted to higher (unlimited) number.

Sorting out data according to "Value" should be enabled.

If a data set consisting of several hundreds of rows is created, there is no option to go back directly to the original query panel – should be added.

Concerning the "Determinand" name it could be advised that instead of "*Zooplankton - Total Number of Individuals*" only "*Zooplankton - Number of Individuals*" should be used because the total number includes all individual numbers of zooplankton at a given sampling site, whereas this particular values mean only the number of the given species. The same is true for phytoplankton.

A default view on the result of the database search should be given: the most important columns being "Sampling site", "River km", "Genus species" and "Value". Other columns could be selectable as "Additional information".

Names of the sampling sites in a given country should be written also in the national language.

The query options as selected by the user should be maintained when searching the database (not set to default).

3.2 Chemical and microbiological data

General comments

JDS microbiological data in surface water and chemical data in surface waters, sediments and suspended solids have been reviewed from the point of view of (i) logical relations between couples or groups of the measured determinands, (ii) theoretically *allowed* ranges of values that can occur in water samples and (iii) limits of detection. Found errors are reported among the *Specific comments*. It can be generally stated that, taken into account the number of measurements done within the JDS, the extent of erroneous data is low. Majority of inconsistencies were found in surface water samples.

There is a need for the central page at the ICPDR Information System for accessing of all (public and expert) databases.

An idea of "expandable" database, which can store data from all future surveys and investigations in the major tributaries is welcome. This should not be limited only to „major tributaries", but to all survey activities done within the ICPDR countries in the future, even if it would be concerned only to limited stretches of the Danube River.

Missing possibility of selection of several (choice of the database user) locations at the same time.

Missing possibility of selection of several (choice of the database user) determinands at the same time.

Recommendations for a link between the JDS and TNMN databases

The JDS data should be linked to TNMN data from the same (or closest sampling site) via button "SHOW TNMN Database" – using river km.

It is recommended that in the first step the nearest TNMN locations would appear – closest station up the JDS site and the closest station below the JDS site, with basic information such as the TNMN code of the station and river km. However, a possibility to show more than two stations on the screen should be given due to the following:

- Some stations are included in TNMN by both neighbouring countries, therefore at one river km data from two stations are reported;
- Some stations have three sites in one profile (at one location) – left, middle and right.

Having a choice of TNMN stations, the user could then select the sampling site of interest for further data search/export.

As regards the linking of all databases (including EMIS database, especially when data on the priority and other relevant substances will be collected by both TNMN and EMIS) – the coding of determinands in EMIS and TNMN databases should be harmonized.

Specific comments

In the current TNMN Database (DANUBIS) - if statistical characteristics are calculated, the "zero" values represent actual value of "below limit of detection" (LOD) and should be included in calculations (not to calculate with the "zero" value). This method of data processing is used in the current ICPDR publications. The proposal is to include in the JDS Database also the option "CALCULATIONS USING VALUES BELOW LOD" with three possibilities:

1. Calculation with value of LOD;
2. Calculation with half of the LOD value;
3. Calculation with "zero" value.

This would give a possibility to select appropriate type of data processing according to specific needs of the report.

The option of selecting data from the TNMN database on the basis of analytical methods might be deleted.

List of discovered inconsistencies in the results of analyses of surface water:

- Ptotal < P-PO4 at the JDS stations No. 67, 73, 74, 82, 84 and 87;
- Measured value of concentration of N_{org} is lower than indicated limit of detection for this determinand at the JDS stations No. 12 and 17;
- Limits of detection are not listed for ammonium-N, nitrate-N, nitrite-N and orthophosphate-P;
- pH 0 is reported at the JDS stations No. 58, 69, 74, 84 and 87;
- conductivity is reported as „zero“ value at the JDS station No. 58;
- Concentrations of several "total" concentrations of metals is lower than "dissolved" concentrations in the same sample: Al (stations 29, 37, 70), As (35 samples, probably in the range of uncertainty of the analysis, larger differences at stations No. 43), Cd (six samples, probably in the range of uncertainty of the analysis), Co (stations No. 24 and 42), Pb (station No. 2), Zn (31 samples, large differences at stations No. 01, 02).

List of discovered inconsistencies in the results of analyses of organic micropollutants:

- Measured value of 4-para-nonylophenol was lower than its limit of detection at the JDS station No. 05.

It is proposed that all erroneous data should be flagged with an explanatory note describing the problem (special section as in the TNMN database).

3.3 GC-MS screening database

Experience from building GC-MS databases in the Netherlands and the Slovak Republic was used at the development of the current version of the GC-MS component of the JDS Database. In order to improve the current structure, the search query template consisting of (at least) following parameters was proposed:

- Characteristic ions: BP, P1, P2, P3, P4 [BP - base peak m/z, P – ion m/z]
- Match factor [Given by the library search]
- CAS Number [Identification number of the compound in the CAS registry]
- MW [Molecular weight]
- Chemical formula
- Compound name

The query using "Characteristic ions" should allow for searching all ions in all fields (BP, P1-4) if typed in the field P1-4. If typed in "BP" field, only base peaks should be searched. "Match factor" should give hits for all values "equal" and "higher than" the typed in number (0-100).

Databases using mass spectral information (obtained mostly by the GC-MS or LC-MS(MS) techniques) are at present the major source of information on unknown, emerging and river basin specific pollutants. Therefore inclusion of the GC-MS screening data into the ICPDR Information System is highly recommended.

Further development of the GC-MS database should focus on the following:

- Availability of the raw GC-MS spectra of both tentatively identified and unknown substances in order to allow for their future identification;
- Organisation of the raw GC-MS spectra in the Danube Basin Spectral Library;
- Harmonisation of methodologies using at the (GC-MS) screening projects in the ICPDR countries and related trainings of experts responsible for data processing;
- Harmonisation of methodologies used for semi-quantitative evaluation of GC-MS data.

The structure of the database should allow for future extensions using LC-MS and LC-MS-MS data on substances, which are not amenable to GC analysis.

3.4 Hydro-morphology

The JDS resulted also in a proposal of the hydro-morphological division of the Danube basin, which are essential at evaluation of the ecological status of the river. The database was upgraded to be able to sort out data automatically within the individual hydro-morphological reaches as proposed by Vogel et al.

4. Recommendations and assessment of needs

The work of the project team and MLIM experts resulted in a significant improvement of the existing version of the JDS Database. Still, several recommendations were made to improve the current version of the ICPDR Information System, which go beyond the scope of this project component. A summary of major suggestions is given below:

ICPDR Information System

- Development of a central page for all ICPDR databases;
- Subdivision of the databases into:
  - Emission sources – EMIS Database;
  - Water quality – TNMN Database, Bucharest Declaration Database, Surveys – JDS, JDS-Investigation of the Tisa River;
  - Water quality/Surveys - expandable for data from similar (to be organised) surveys on all major tributaries/stretches of the Danube;
  - Water quality/Surveys – expandable for data from national surveys.
- ALL DATABASES TO BE ACCESSIBLE BY GENERAL PUBLIC
  - Each of the database users to be identified by providing basic information on his/her name, organisation, coordinates and intended use of the database;
- Improvement/upgrade of the JDS – Investigation of the Tisa River Database in the same way as the JDS Database.

Welcome page of the JDS and TNMN databases
Should allow selection of options “Search the database” and “About the database” (to be developed: information on sampling sites, parameters, matrices, laboratories, how to work with the data, assumptions and calculation models used).

Interlinking of the JDS and TNMN Databases

- TNMN Database should use the same structure (layout/coding) as the JDS Database;
- Currently, only a link from the JDS Database to the TNMN database was established, the TNMN Database should have the same option.

Biological databases

- Using the JDS Database structure and coding for establishment of the TNMN Biological Database;
- Coding:
  - Change/upgrade of the JDS codes taking into account work of expert groups at the EU level (e.g., AQEM project);
  - Incorporation of taxonomical changes according to AQEM;
  - Introduction of a shortcode for species (8 letter code) and different national codes and a table of current synonyms;
- Using special (non-Excel) data collection sheets (e.g., adjusted AQEM-DIP programme);
- Dominance of Higher Taxonomic Groups (HTG) should be calculated for macrozoobenthos, phytobenthos and macrophytes;

- A selection tree "HTG – Families – Species" should be a query option in biological databases;
- Upgrades and introduction of data into each part of the biological database (macrozoobenthos, phytobenthos, macrophytes, zooplankton, phytoplankton) should be taken care of by several institutions /team of experts.

GC-MS screening databases

- Using the JDS Database structure for establishment of the TNMN GC-MS Screening Database;
- Upgrade of the existing database structure to facilitate storage of the raw GC-MS spectra of both tentatively identified and unknown substances in order to allow for their future identification;
- Systematic evaluation of data by a separate institution/team of experts in order to gain information on unknown, emerging and Danube River Basin specific pollutants.

5. Conclusions

The JDS Database was completed for the missing parameters and quality of all stored data was thoroughly checked. During the project, the database was gradually improved and developed into the stage, that it is ready for the public use. Recommendations for a link between the JDS and TNMN databases and harmonisation of their query templates were made and incorporated into the New Draft Versions of both databases. A proposal of the new central page on the ICPDR website comprising of all ICPDR databases was made.

Despite the current version of the JDS Database (www.icpdr.org [Databases/New Draft Versions] is fully usable by both experts and general public, several suggestions, which go beyond the scope of this project component, were made by the project team and MLIM experts to improve its ease-of-use. A principal upgrade and Europe-wide harmonisation of the coding system and systematic tracking of taxonomical changes in the biological part of the database was proposed in order to assure its sustainability. Also, further upgrade of the GC-MS screening part of the database was suggested to allow proper evaluation of the screening data on emerging, unknown and Danube River Basin specific pollutants as required by the WFD. A need has arisen to perform similar upgrade at the JDS – Investigation of the Tisa River database, which is not ready for public use in its present form.

Final goal of all the above efforts is to create a fully interlinked ICPDR Information System. This would require future harmonization of the coding system between the TNMN and EMIS databases and further development of the link between the two databases. The knowledge obtained at the development and upgrade of the JDS Database created a solid base for extension of the TNMN Database for new chemical parameters, parameters measured in other matrices than water, GC-MS screening and biological data. Here, it should be seriously considered that systematic feeding of databases with data, check on their correctness and upgrade of parameters in line with scientific developments and experience gained at the implementation of the WFD can be accomplished only by a dedicated team of experts.

6. References

Referred web-pages:

- www.aqem.de
- http://www.boku.ac.at/hfa/profil/benthosoekologie.htm
- www.ecoprof.at
- www.eu-star.at
- www.lebensministerium.at/wasser/; sub-item "Wassergüte"

Moog, O. (ed) (1995): Fauna Aquatica Austriaca – A Comprehensive Species Inventory of Austrian Aquatic Organisms with Ecological Notes. Federal Ministry for Agriculture and Forestry, Wasserwirtschaftskataster Vienna: loose-leaf binder.

Rosenberg, D. M. & V. H. Resh (eds) (1993): Freshwater Biomonitoring and Benthic Macroinvertebrates. Chapman & Hall, New York.

Zelinka, M. & Marvan, P. (1961): Zur Präzisierung der biologischen Klassifikation der Reinheit fließender Gewässer. Arch. Hydrobiol. 57: 389-407.

Vogel B., JDS Technical Report, ICPDR, September 2002.

Pal, K. & Janauer G.A. (1995): Die Makrophytenvegetation von Flussstauen am Beispiel der Donau zwischen Fluss-km 2552 und 2511,8 in der Bundesrepublik Deutschland. Arch.Hydrobiol.Suppl. 101, Large Rivers 9/2, 91-109.

Kohler, A. (1978): Methoden der Kartierung von Flora und Vegetation von Süßwasserbiotopen. Landschaft und Stadt, 10:23-85.