

**Risk Assessment Model
for Use in Site Restoration.
Software and User Instructions**

Restoration Strategies for Radioactively Contaminated
Sites and their Close Surroundings
RESTRAT - WP4

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Summary

This technical deliverable TD 7 of the EC project RESTRAT summarizes work performed in work package WP2: "Physico-Chemical Phenomena Governing the Behaviour of Radioactive Substances" and WP4: "Risk Assessment". In WP2 an integration of the chemical speciation code MINTEQA2 (Allison et al. 1991) into the risk assessment package PRISM (Gardner et al. 1983), that performs sensitivity analysis & BIOPATH (Bergström et al. 1982), a compartmental model of contaminant transfer, was developed, tested and applied to several case studies, see also TD 2 (Brendler 1998a) and TD 5 (Brendler 1998b) of this project. Here, the respective software is delivered on an accompanying CD-ROM, together with instructions how to install and run the programs. It is aimed at a use under either the AIX 4.3.2 operating system on IBM R/6000 series computers, or under the MS-DOS system on PCs (which includes the DOS boxes of MS Windows 3.1/3.11/95/98/NT). The software package consists of the following items:

- the chemical speciation code MINTEQA2 from US EPA, with some slight modifications to accommodate special requirements from the integration into PRISM / BIOPATH. MINTEQA2 is delivered as a precompiled binaries for both afore mentioned operating systems.
- data bases to be used in conjunction with MINTEQA2, namely THERMO.DBS with thermodynamic complex stability constants for species in aqueous solutions, and HFO_DDL.DBS with surface complexation constants based on the Diffuse Double Layer model. Several entries in the version of THERMO.DBS as delivered with MINTEQA2 by EPA have been corrected, also some extensions were introduced. HFO_DDL.DBS is mainly based on the book by Dzombak and Morell (1990) about sorption on hydrous ferric oxides. All data bases are delivered in readable ASCII format.
- the input preprocessing tool CHEM2MIN, which converts input files into the format required by MINTEQA2 and PRISM. CHEM2MIN is delivered both in source code (C), and as a precompiled binary for both afore mentioned operating systems.
- the risk assessment software package PRISM / BIOPATH, consisting of two precompiled executables (PRISM1 and PRISM3) again for the two operating systems available. Due to licensing agreements it is not possible to deliver the source code for these items.
- an example for the user-defined subroutine that integrates BIOPATH into PRISM2, to be compiled together with library modules and the interface to MINTEQA2 to create an executable PRISM2. This subroutine is delivered in source code (FORTRAN77).
- several subroutines to interface PRISM / BIOPATH with MINTEQA2, delivered in source code (C).
- a set of input example files to be used to test by the integrated model, in readable ASCII format.
- further input sets for all five RESTRAT example cases: Drigg Site, Molse Nete river, Ranstad tailing site, Ravenglass estuary, and Lake Tranebärssjön.

To make use of this TD one needs access to a computer running AIX 4.3.2 or MS-DOS and a CD ROM drive.

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1. Introduction

The main objective of the overall RESTRAT project is to develop a generic methodology for the ranking of restoration techniques as a function of site and contamination characteristics. The work has been broken down into several work packages. This technical deliverable, TD 7, as required by the contract, summarizes part of the work performed in work package WP 2: Physico-chemical phenomena. There are two other technical deliverables in close connection to this report. TD 2 (Brendler 1998a) described the state-of-the-art of chemical speciation and migration modelling, leading to the conclusion that it is necessary to unfold the wide-spread K_d -concept of distribution coefficients. In TD 5 (Brendler 1998b) the focus was on concrete models for surface complexation, their application in the MINTEQA2 code (Allison et al. 1991) and the specific situation with regard to each site of the RESTRAT project. Here the underlying software will be described in more detail, together with instructions how to install and run it. On the accompanying CD-ROM all necessary software is included. The purpose is to enable other users to run the models for the various examples sites of the RESTRAT project, to allow to modify input parameters and explore the respective effects on the response functions with regard to their value and uncertainty. Furthermore, users should become acquainted with the special problems of chemical speciation, sorption and transport.

2. PRISM & BIOPATH

2.1. Short description of the PRISM-code

The PRISM-code is a generic tool for uncertainty and sensitivity analyses of any model. The code is developed at Studsvik and available on a commercial basis. PRISM consists of three main parts. Firstly in PRISM 1 random model parameters are generated, PRISM 2 evaluates the model and finally PRISM 3 is for the statistical evaluation.

2.1.1. PRISM 1

PRISM 1 generates sets of random parameter values from user defined probability density functions by using a systematic sampling method, Latin Hyper cube. As input to PRISM 1, the mean values, type of distributions, standard deviations and upper and lower limits can be given for each parameter. Necessary input depends on type of distribution of each parameter. These data are used to define probability density functions. The Latin Hyper cube method, is an efficient Monte Carlo sampling which results in random figures within the whole desired range of parameter values. Latin Hypercube sampling can give spurious correlation between parameters, however, procedures to eliminate such correlation are included in the code. In contrary, correlation given in the input between model parameters can be taken into account independent of distributions between the parameters.

2.1.2. PRISM 2

PRISM 2 evaluates model predictions for each set of parameter values from PRISM1 and produces input files for the statistical analyses performed in PRISM 3. Any model which can be executed from a FORTRAN program can be analysed by PRISM, the input and output from the model must be able to read from this module, for example as text files.

2.1.3. PRISM 3

PRISM 3 statistically evaluates and summarises the joint set of model parameters and model predictions. The general statistics for the distribution of each parameter and the response of the model to this distribution contain the following:

- the arithmetic mean
- the standard deviation
- the coefficient of variation
- the geometric mean
- the percentiles (5, 25, 50, 75, and 95 %)
- the five highest values and the five lowest values, respectively

Correlations analysis between the model parameters and responses as well as between responses are also obtained. Two correlations coefficients are calculated: firstly, the simple Pearson correlation coefficient and secondly Spearman R which is the correlation of the ranked values of the parameters and model responses. Associated with each correlation coefficient is percent COVAR. This represents the percent variance that one variable accounts for in another variable or response. In cases of correlated model parameters and responses, percent COVAR indicates the amount of variability of the model response explained by the variability of that model parameter.

The regression procedures are used to obtain the relationship between model parameters and model uncertainties. The selection of parameters to be entered into the regression analysis is chosen among those which have the greatest improvement in the sum of squares of regression. Default values are given in the code but may be changed if chosen.

The output from PRISM 3 consists of all statistic information (intercept, slopes and mean values) required to write the regression equation for the relationships between model parameters and response. In these calculations the relative contribution to the total uncertainty from each parameter is also obtained. This means that simple analytical equations can be used to characterise the relationships between total doses and each exposure pathway.

2.2. Short description of the BIOPATH code

The BIOPATH code (formerly a separate program, now closely integrated as the subroutine **users.for** into PRISM 2) calculates the distribution of a radioactive nuclide in a compartment system, i.e. the concentration as a function of time, after releases in one or more compartments. The amount of the activity of a specific nuclide may be the result of release of that nuclide into one or several compartments, during some periods of time, or it may be generated by decay of one or more nuclides and their transfer between compartments. Of course, also initial inventories can be set for any compartment. The program calculates the activity distribution (solves the linear differential equation system) for a nuclide during the specified time period. The result is then further processed to obtain doses to man.

The time steps for which the solution is written out, are determined at the calculation for the first nuclide. For the other nuclides, interpolation is performed if the times at which the activity is calculated do not agree with the times for the first nuclide. For each nuclide one or more sets of input data may be given in order to control the calculations during different time intervals. In that way it is possible to use different solution methods, step sizes etc., not only for different nuclides, but also for the same nuclide during different time periods.

2.2.1. Mathematical theory

It is assumed that the system contains **N** compartments. During calculation **N+1** compartments are then needed where the additional compartment acts as the receiver of the outflow. The amount of activity for a nuclide, as a function of the time, can be obtained by solving the following system of linear differential equations:

$$y_i'(t) = \sum_{j=1}^N a_{ij} \cdot y_j(t) + g_i(t) - \lambda \cdot y_i(t) , \quad i = 1, N; \quad (1)$$

or with vector notation:

$$Y'(t) = A \cdot Y(t) + G(t) - \Lambda Y(t) \quad (2)$$

where **Y** is an **N**-element vector, in which **y_i(t)** is the amount of activity in compartment **i** at time **t**. **A** is a **N**·**N** matrix, where the matrix element **a_{ij}** expresses the transfer rate of activity from compartment **j** to

compartment i . For $i \neq j$ the numbers a_{ij} are called the transfer coefficients. Λ describes the radioactive decay. \mathbf{G} is an N -element vector, where $g_i(t)$ is the rate of release into compartment i of the nuclide, at time t . The matrix \mathbf{A} can also be time-dependent. The source term \mathbf{G} is specified by input data, or is a function of previous calculations for parent nuclides, or may be the sum of both.

2.2.2. Solution methods

The program can use different methods to solve a linear equation system. These methods can be combined in a run if wanted. It means that different methods can be used for different time spans, for the separate nuclides. Below follows a short description of the method LINDIF, which is implemented by default.

LINDIF is a semianalytical solution method. It uses the EISPACK matrix calculation package to get the eigen values and eigen vectors of the coefficient matrix. When the eigen values are obtained the solution can be achieved. For a detailed description see Forssén 1977 and Smith et al. 1974.

In the theory the solution given by LINDIF is exact, but only if the source term \mathbf{G} is constant. In the general case, where the source term is not constant (for example if \mathbf{G} is a result of a parent decay), the function \mathbf{G} may be approximated by a stepwise constant function, and the solution can be recalculated at the time of each change. Another problem with this method appears for stiff differential equation systems, because the rounding errors in the computer may give too big contributions. This will occur if the magnitudes of the eigen values of the coefficient matrix vary too much.

2.3. Contact Address

Further information about PRISM and BIOPATH can be received from

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3. MINTEQA2

The chemical speciation software MINTEQA2 (Allison *et al.* 1991) is called a “geochemical assessment model for environmental systems” by its authors. It is distributed by the US Environmental Protection Agency (EPA), Center of Exposure Assessment Modeling. The software is based on the well-known MINEQL code (Westall *et al.* 1976).

The software has the following features:

- computation of chemical speciation for the homogeneous aqueous phase or for mixed phase systems, including simultaneous consideration of various minerals and a gas atmosphere;
- fixed activities (bulk mineral, indefinite atmosphere etc.) can be defined;
- it can also handle redox reactions;
- sorption phenomena can be dealt with by means of seven different sorption models, incorporating three surface complexation models (SCM): the Diffuse Double Layer model, the Constant Capacitance model and the Triple Layer model;
- it is available in source code format (FORTRAN77) with special adaptations to UNIX systems and the MS-DOS operating system for PCs. These system-dependent parts are rather small, so porting of the software to even other computer systems should be straightforward;
- an external thermodynamic data base (with its own proprietary format) is distributed together with the software, including some sorption data and organic compounds;
- there is a separate user interface program for interactive creation of data input files (problem description files) available.

Its main limitations are the lack of a kinetic mode, the missing ability to handle solid solutions, and shortcomings in scope, quality and documentation of the internal thermodynamic data base. The latter of course can be overcome by setting up an own data base, or at least by carefully checking and correcting of the one accompanying MINTEQA2. Also the convergence of the numerical algorithm for the solution of the mass equilibria equation system is not always guaranteed. This is especially the case where the default master species for an element is actually not present in measurable amounts in the real system under investigation. An example is the modelling of systems under reducing conditions containing uranium. The pre-set master species for uranium is the uranyl cation, which at redox potentials below 50 mV is hardly present. Numerical convergence can be drastically improved by delivering starting estimates for such basic species of at least two orders of magnitude close to their real free concentration. Occasionally another peculiarity can be observed when a mineral is marked as excluded from consideration that is not the thermodynamical stable one in the defined chemical system. Here it may become necessary to also exclude the more stable minerals containing the same element as the excluded one.

4. Software distribution on CD

4.1. File categories

The software distribution as made available in this TD, i.e., on the accompanying CD-ROM, consists of four types of files: They are either ready-to-use executables, source code files, data bases to be used by the program package, or auxiliary files (tools, documentation etc.). Here, *executables* for two operating systems are included on the CD:

- the AIX operating system (AIX version 4.3.2), which is a UNIX dialect most often found on IBM computers such as the RS/6000 series;
- the MS-DOS operating system from Microsoft, which runs on PCs, and is also available as part of the various MS Windows versions (3.1 / 3.11 / 95 / 98 / NT). Notably, the software has been tested under the DOS box of MS Windows 4.0.

According to their purpose the various files of this software distribution can also be grouped into the following categories:

- **PRISM 1 & PRISM 3:** Due to licensing agreements the source code is not openly accessible, only precompiled executables are delivered by Studsvik Eco&Safety AB for both afore mentioned operating systems.
- **PRISM 2:** Again, the source code is not openly accessible, so only precompiled executables for AIX and MS-DOS are delivered by Studsvik Eco&Safety AB. Whereas PRISM1 and PRISM3 are independent from a specific application model, PRISM2 incorporates routines that reflects the particularities of the risk assessment model under consideration. Actually, this is done inside the **BIOPATH** module. To set up the radionuclide transfer model, a user-defined FORTRAN77 subroutine must be written. This subroutine will be called by PRISM2, and will call the chemical speciation software via an extra interface. Subsequently, it must be compiled together with the PRISM2 object modules and the interface modules to the chemical speciation software MINTEQA2 (see below) to create an executable PRISM2. Thus, for each application case a separate PRISM2 executable is put onto the CD. For a better understanding of the model principles, examples for such BIOPATH routines as FORTRAN sources codes are also accessible from the CD.
- **Interface to chemical speciation:** Several subroutines to couple PRISM / BIOPATH with MINTEQA2, which means the computing of K_a values (see TD 2, Brendler 1999a), are delivered in C source code on the CD.
- **MINTEQA2:** To compute the chemical speciation, the code MINTEQA2 from U.S. EPA is used, with some slight modifications to accommodate special requirements from the integration into PRISM / BIOPATH. The respective FORTRAN77 sources are open in principle, but to make the software installation as easy as possible, on the CD only two precompiled executables for both AIX and MS-DOS are included: one for the speciation modelling itself, and another to perform data base operations.
- **CHEM2MIN:** This is the input preprocessing tool, which converts input files into the format required by MINTEQA2 and PRISM. It is delivered on the CD both in C source code, and as a precompiled executable for the AIX OS and for MS-DOS.
- **Data Bases:** Several data bases are to be used in conjunction with MINTEQA2. The most important ones are THERMO.DBS with thermodynamic complex stability constants for species in aqueous solutions, and HFO_DDL.DBS with surface complexation constants based on the Diffuse Double Layer model. Several entries in the version of THERMO.DBS as delivered with MINTEQA2 by EPA have been corrected, also some extensions were introduced. HFO_DDL.DBS was especially created for this RESTRAT project and contains data for anion and cation sorption on hydrous ferric oxides (Dzombak and Morell 1990). Other data bases included in this distributions are ALK.DBS,

ANALYT.DBS, COMP.DBS, COMPLIG.DBS and ERROR.DBS. For more details about their purpose and usage please refer to the MINTEQA2 manual, which is also included on the CD (see below). All these data bases are delivered in readable ASCII format. Two of them must be converted to a special binary format before MINTEQA2 can make use of them. This conversion has already been made, the respective binary data files THERMO.UNF and TYPE6.UNF are included on the CD. If one likes to introduce further changes to THERMO.DBS or TYPE6.DBS, they must afterwards be converted to the binary format by means of **xunfrmtx.exe**.

- **Further Input Sets:** for all five RESTRAT example cases (Drigg Site, Molve Nete river, Ranstad tailing site, Ravenglass estuary, and Lake Tranebärssjön) the input data sets for the base case (no restoration) are also included.
- **Miscellaneous:** MINTEQA2.WP is the manual for MINTEQA2, in *WordPerfect for DOS 4.2* format, and there is also a makefile script delivered for the installation of the whole software package. Furthermore, PostScript versions of two other related RESTRAT Technical Deliverables 2 and 5 (they were already referred to in this document before) are copied to the CD. Finally, this document itself is included as PDF, Postscript, and WordPerfect 6.1 File.

4.2. Comprehensive file list and directory structure

The above mentioned files (input examples, data bases, source code, executables, and auxiliary files) are stored on the CD in a specific directory structure. This structure is also the recommended one for any installation of the whole software package on a computer.

subdirectory AIX:

prism1	PRISM1 executable
prism3	PRISM3 executable
xminteqx.exe	MINTEQA2 executable (speciation computation)
xunfrmtx.exe	MINTEQA2 executable (data base format converter)
chem2min	Input file preprocessor for MINTEQA2 / PRISM (executable)
THERMO.UNF	MINTEQA2 thermodynamic data file (binary)
TYPE6.UNF	MINTEQA2 solids data file (binary)

subdirectory PC:

prism1.exe	PRISM1 executable
prism3.exe	PRISM3 executable
xminteqx.exe	MINTEQA2 executable (speciation computation)
xunfrmtx.exe	MINTEQA2 executable (data base format converter)
chem2min.exe	Input file preprocessor for MINTEQA2 / PRISM (executable)
cwsdpmi.exe	DOS memory allocator to be used together with chem2min.exe (executable)
THERMO.UNF	MINTEQA2 thermodynamic data file (binary)
TYPE6.UNF	MINTEQA2 solids data file (binary)

subdirectory SRC:

*.c ; *.h	C sources for the MINTEQA2 / PRISM coupling interface and for the CHEM2MIN input preprocessing software. Their mutual relationship is given in appendices A and B.
USERS	subdirectory containing the various <i>users.f</i> model setups (FORTRAN77 sources) for all five RESTRAT example cases.

subdirectory DATA:

THERMO.DBS	MINTEQA2 thermodynamic data file (ASCII)
TYPE6.DBS	MINTEQA2 solids data file (ASCII)

HFO_DDL.DBS	MINTEQA2 Diffuse Double Layer SCM data base for hydrous ferric oxides
ALK.DBS	MINTEQA2 alkalinity data base
ERROR.DBS	List of internal MINTEQA2 error messages
ANALYT.DBS	Temperature dependencies of log k reaction constants
COMP.DBS	List of MINTEQA2 chemical components
COMPLIG.DBS	MINTEQA2 data base for composite ligands (with DOM - dissolved organic matter)
<i>subdirectory DOCS:</i>	
MINTEQA2.WP	Manual for MINTEQA2, in <i>WordPerfect for DOS 4.2</i> format
database.txt	Description of the main thermodynamic data base THERMO.DBS (ASCII)
TD2_4.ps	RESTRAT TD 2 (Postscript)
TD5_2.ps	RESTRAT TD 5 (Postscript and PDF)
Readme.*	This document (Postscript, PDF, and WordPerfect 6.1)
<i>subdirectory DRIGG:</i>	base case input sets for RESTRAT example case Drigg Site
<i>subdirectory MOL:</i>	base case input sets for RESTRAT example case Molse Nete river
<i>subdirectory TAIL:</i>	base case input sets for RESTRAT example case Ranstad tailing site
<i>subdirectory RAVEN:</i>	base case input sets for RESTRAT example case Ravenglass estuary
<i>subdirectory LAKE:</i>	base case input sets for RESTRAT example case Lake Tranebärssjön

5. Detailed installation guide

5.1. General arrangements

There are certain software and hardware requirements for the compilation of the **PRISM / BIOPATH / MINTEQA2** package under various operating systems. A special problem here is the mixed language programming and the large memory needed to address data blocks. Mixed language programming requires the use of two compilers, that creates object code in the same internal format, so that the modules can really co-operate, exchange data, and be linked together to form one binary executable. Whereas this demand is easy to fulfil on any UNIX system (because binary-compatible FORTRAN and C compilers are regarded as standard on such systems), the situation is more difficult on PC systems. Therefore, in a first stage the software and hardware environment was set to the UNIX system available to one of the authors, the AIX OS, version 4.3.2. Later, the whole software package was ported to the MS-DOS system to widen the range of applicability. On request, also a version for the ConvexOS 11 can be supplied by the corresponding author.

Under any computer operating system, the very first step will be the creation of a project root directory, called, e.g., **RESTRAT**. This directory then must be added to the environment variable specifying the path to all the executable programs, normally called **path** or **PATH**. Then the installation steps for each part of the software package will follow subsequently as described below. For details how to create directories, set appropriate file permissions, copy files etc. please ask your local system administrator.

In case that one intends to make modifications or additions to the MINTEQA2 thermodynamic database, a guide how to do that is found in the MINTEQA2 manual. For a re-compilation of the data base, namely **THERMO.UNF** and **TYPE6.DBS**, the executable **xunfrmtx.exe** is needed, which otherwise is not required by the **PRISM/BIOPATH/MINTEQA2** package.

Remarks to the PC version (MS-DOS):

- the executables **prism1**, **prism2**, **prism3** and **chem2min** have to have also the file name extension **“.exe”**;
- because MS-DOS restricts filenames to 8 character plus 3 characters extension, the input files **model.chem** and **minteq.template** are renamed to **model.chm** and **minteq.tmp**, respectively;
- all input files from the **DATA**, **DRIGG**, **MOL**, **TAIL**, **RAVEN** and **LAKE** subdirectories of the CD-ROM are shared by the AIX and MS-DOS version. However, the rules in these systems to indicate an end of a line are different: Whereas AIX only uses a Linefeed (LF) for the end of a line, MS-DOS requires both a Linefeed (LF) and a Carriage Return (CR) character at this place. Thus, files from AIX look under MS-DOS just as one huge line. This will cause problems to some MS-DOS programs. A very easy way to overcome it is to load such files into the MS-DOS editor with the command “*edit filename*” and then just save the file. This will add all missing CR characters.

5.2. Installation of **PRISM & BIOPATH, MINTEQA2 and CHEM2MIN** and test runs

The following actions must be performed to properly install the **PRISM** code:

- copy **prism1** and **prism3** from the CD-ROM (from either the AIX or PC subdirectory, depending on the selected platform) into the project root directory;
- copy **xminteq.exe**, **xunfrmtx.exe** and **chem2min** from the CD-ROM into the project root directory, in case of the MS-DOS version also the file **cwsdpmi.exe** must be copied;

- copy all the necessary thermodynamic data files for MINTEQA2 from the CD-ROM (subdirectory DATA) into the project root directory: THERMO.DBS, HFO_DDL.DBS, TYPE6.DBS, ALK.DBS, ANALYT.DBS, COMP.DBS, COMPLIG.DBS and ERROR.DBS;
- copy THERMO.UNF and TYPE6.UNF from the CD-ROM (from either the AIX or PC subdirectory) into the project root directory.

5.3. Test runs

Now test runs can be performed successively. The following explanations are based on the application case Molse Nete river, they have to be applied respectively to the other example sites also to be found on the CD.

When the installation processes as described below are all finished successfully, six executable programs should exist in the project directory: **prism1**, **prism2**, **prism3**, **chem2min**, **xunfrmtx.exe**, and **xminteqx.exe**. In case of the MS-DOS version, also **cwsdpmi.exe** must be there. Under AIX, all of them should have the execution-permission for the user (can be set by the UNIX command *chmod 755 **). The executable **xminteqx.exe** will be called automatically from inside **prism2**, **xunfrmtx.exe** is not required at this stage.

There are three different modes the PRISM/BIOPATH/MINTEQA2 package can be used. The first one is identical to the original, pure PRISM/BIOPATH model without any chemical speciation. The second one is a two-phase approach: First, just K_d distribution values are computed using PRISM/BIOPATH, which afterwards have to be incorporated into the old PRISM/BIOPATH model. The third mode is the fully integrated one, where the computation of K_d values is performed in parallel to the BIOPATH calculations. All three approaches are dealt with in the next sections.

5.3.1. Run of the pure (old) PRISM/BIOPATH approach

- go to the MOL subdirectory;
- copy the example input files **PRISM1*.BIO** and **PRISM2*.BIO** into the project directory and rename them there to **PRISM1.INP** and **PRISM2.INP**, respectively. The asterisk * stands for the radionuclide of interest, in case of the Molse Nete river site, e.g., Cobalt, Americium and Plutonium input files are available;
- copy the executable **PRISM2BIO** into the project directory (from either the AIX or PC subdirectory) and rename it there to **prism2** (or **prism2.exe**, see above);
- copy the example input file **PRISM3.INP** into the project directory;
- go to the project directory.

The executables **prism1**, **prism2**, and **prism3** can now be run successively. After each step the newly created output files (most of them being input files for the next step) should be checked carefully. The following output files should be created in the course of this first test run:

- **PRISM1.OUT** (records the execution progress of **PRISM1**, all generated parameter sets and their internal correlation matrices) and **PRISM1.RSL** (binary parameter matrix to be used in **PRISM2**) after executing **PRISM1**;
- **PRISM2.OUT** (records just the problem dimensions), and **PRISM2.RSL** (binary file to record all input-response vectors from **PRISM2**, is used by **PRISM3** for statistical evaluation) after executing **PRISM2**;
- **PRISM3.OUT** (extensive sensitivity analysis) and **PRISM3.TBL** (abridged sensitivity analysis) after executing **PRISM3**.

5.3.2. Run of the simplified K_d assessment approach

- go to the MOL subdirectory;
- copy the example input files **PRISM1.KD** and **PRISM2.KD** into the project directory and rename them there to **model.box** and **PRISM2.INP**, respectively;
- copy the input file **chem*.inp** into the project directory and rename it there to **model.chem**. The asterisk * stands for the radionuclide of interest, in case of the Molsse Nete river site, e.g., Cobalt, Americium and Plutonium input files are available;
- copy the executable **PRISM2KD** into the project directory and rename it there to **prism2[.exe]**;
- copy the example input file **PRISM3.INP** into the project directory;
- go to the project directory.

After the executable **chem2min** has been run, successive calls to **prism1**, **prism2**, and **prism3** follow. In addition to the above explained output files, this test version creates:

- **dim.chem** (problem dimension file to be used by the interface modules), **minteq.template** (template with all physico-chemical parameters for **MINTEQA2**), and **PRISM1.INP** (input file for **PRISM1**) after executing **chem2min**;
- **PRISM2.LOG** (records the **MINTEQA2** return codes and all computed K_d values, for monitoring purposes only, e.g., post-mortem analysis) after executing **prism2**, this only works under AIX.

5.3.3. Run of the fully integrated approach

- go to the MOL subdirectory;
- copy the example input files **PRISM1*.BIO** and **PRISM2*.ALL** into the project directory and rename them there to **model.box** and **PRISM2.INP**, respectively. The asterisk * stands for the radionuclide of interest, in case of the Molsse Nete river site, e.g., Cobalt, Americium and Plutonium input files are available;
- copy the input file **chem*.inp** into the project directory and rename it there to **model.chem**. The selected radionuclide must be the same as in the **PRISM1*.BIO** file;
- copy the executable **PRISM2ALL** into the project directory and rename it there to **prism2[.exe]**;
- copy the example input file **PRISM3.INP** into the project directory;
- go to the project directory.

After the executable **chem2min** has been run, successive calls to **prism1**, **prism2**, and **prism3** follow. The proceeding of the test run is exactly as described in the previous section.

6. References

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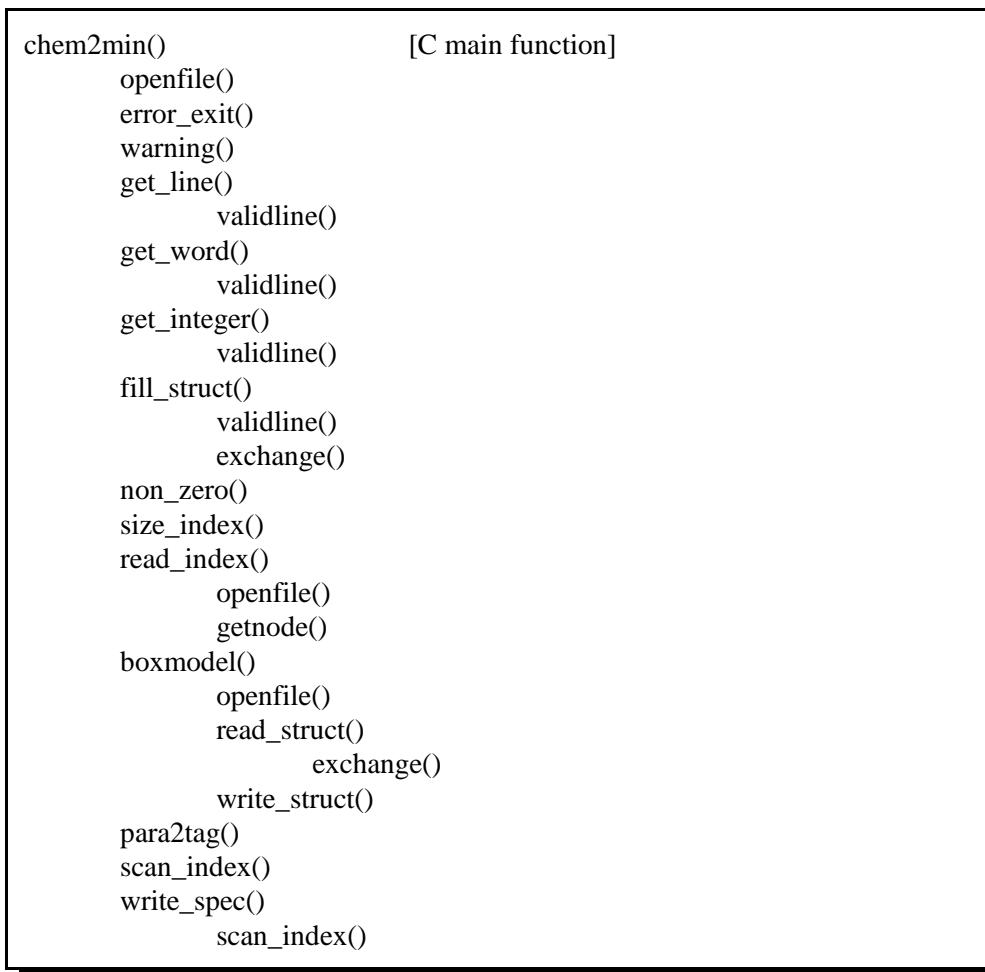
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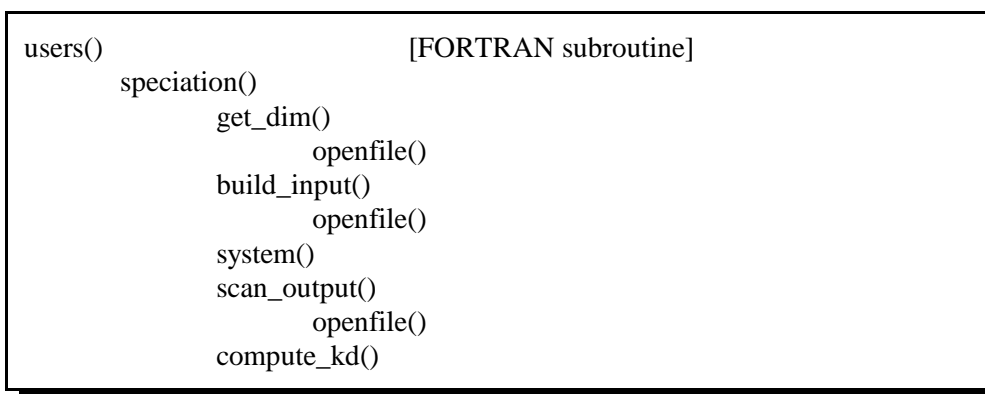
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Appendices

Appendix A: Call tree for CHEM2MIN (input file preprocessor)



Appendix B: Call tree for PRISM2 (speciation interface)



Appendix C: Installation makefile for the integrated PRISM / BIOPATH / MINTEQA2 software on a UNIX computer (without all comment lines, but they are retained on the CD version)

```
SPECMOD=      -DMINTEQA2
CFLAGS=       -O $(SPECMOD)

DIR_LIB=      ../PRISM/lib
VPATH=        ./RCS

LIB_PR2=      $(DIR_LIB)/prism2_lib.a $(DIR_LIB)/prism_lib.a
LIB_SPC=      $(DIR_LIB)/minteq_lib.a

SRC_0=        openfile.c validline.c exchange.c
OBJ_0=        $(SRC_0:.c=.o)

SRC_N=        get_line.c get_word.c get_integer.c size_index.c \
              warning.c error_exit.c
OBJ_N=        $(SRC_N:.c=.o)

SRC_1=        chem2min.c para2tag.c boxmodel.c non_zero.c \
              read_index.c scan_index.c write_spec.c \
              getnode.c fill_struct.c read_struct.c write_struct.c
OBJ_1=        $(SRC_1:.c=.o)

SRC_2=        speciation.c get_dim.c build_input.c scan_output.c compute_kd.c
OBJ_2=        $(SRC_2:.c=.o)

SRC_F=        users.f
OBJ_F=        $(SRC_F:.f=.o)

HDR=          prism.h messages.h

OBJ_C2M=      $(OBJ_0) $(OBJ_N) $(OBJ_1)
OBJ_LIB=      $(OBJ_0) $(OBJ_2)
OBJ_USR=      $(OBJ_F)

$(OBJ_1):     $(HDR)
$(OBJ_2):     $(HDR)

$(LIB_SPC):   $(OBJ_LIB)
              ar r $@ $(OBJ_LIB)
              ranlib $@ $(LIB_PR2)

chem2min:     $(OBJ_C2M)
              cc -o $@ $(OBJ_C2M) -lm

prism2:       $(LIB_PR2) $(OBJ_USR) $(LIB_SPC)
              fc -o $@ $(LIB_PR2) $(OBJ_USR) $(LIB_SPC)

test1:        chem2min
              $? ; less minteq.template PRISM1.INP ; prism1 ; less PRISM1.OUT

test2:        prism2
              $? ; less MININ.DAT MINOUT.OUT

.IGNORE:
```

Appendix D: Installation makefile for the integrated PRISM / BIOPATH / MINTEQA2 software under MS-DOS

```
#####
# FILE:      makefile
#
# TASK :    Build the CHEM2MIN or CHEM2EQ preprocessing program,
#           and the complete PRISM2 program.
#           The original target system is AIX OS, an IBM UNIX derivative.
#           Here, the makefile is adapted to a PC / MS-DOS environment:
#           a) GCC (DJGPP) for creating "chem2min"
#           b) Metaware High C/C++ for the C-Modules for prism2
#           c) Lahey F90 for the Fortran77 modules for prism[123]
#           The makefile itself can be run by these make utilities:
#           GNU make 3.75, Borland make 3.7 Lahey make 5.31
#           Work is performed as part of the RESTRAT EU project.
#
# AUTHOR :  Dr. Vinzenz Brendler
#           Research Center Rossendorf Inc., Institute of Radiochemistry
#
# VERSION : Revision: 1.2                      Date: 1999/08/25
#####

# Flags to include debugging output (on several levels) and to select
# the right speciation module (MINTEQA2 or EQ3/6)
SPECMOD=      -DMINTEQA2
#SPECMOD=      -DDEBUG=2 -DMINTEQA2

# Compiler and compiler options
CFLAGS=       -O $(SPECMOD)
CC=           gcc
HCC=          hc386
FFLAGS=       -inln
FC=           lf90

# Directory containing standard PRISM2 object files and libraries,
# also the speciation interface libraries
DIR_LIB=      ../PRISM/lib
VPATH=        ./SOURCES
HCDIR=        C:\HIGHC
LHDIR=        C:\LF90\LIB

# PRISM2 standard object files and libraries
LIB_PR2=      $(DIR_LIB)/p2_lib.a $(DIR_LIB)/ps_lib.a

# Library containing object files for the PRISM2 speciation part
# LIB_SPC=     $(DIR_LIB)/eq36_lib.a
LIB_SPC=      $(DIR_LIB)/mint_lib.a

# Metaware High C/C++ runtime libraries
LIB_HC=       $(HCDIR)/flat/hc386.lib $(HCDIR)/flat/hc387.lib

# Metaware High C/C++ interface module
OBJ_HC=       $(LHDIR)/hc330.obj

# General utility source files, not requiring prism.h
SRC_0=        openfile.c valid_ln.c exchange.c
OBJ_0=        $(SRC_0:.c=.o)

# Source files for CHEM2MIN not requiring prism.h
SRC_N=        get_line.c get_word.c get_int.c size_ind.c \
              warning.c error_ex.c
OBJ_N=        $(SRC_N:.c=.o)
```

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```
# Source files for CHEM2MIN requiring prism.h
SRC_1=      chem2min.c para2tag.c boxmodel.c non_zero.c \
            read_ind.c scan_ind.c write_sp.c \
            getnode.c fill_str.c read_str.c write_st.c
OBJ_1=      $(SRC_1:.c=.o)

# Source files for PRISM2 speciation part, most requiring prism.h
SRC_2=      $(SRC_0) speciatn.c get_dim.c build_in.c scan_out.c comp_kd.c
OBJ_2=      $(SRC_2:.c=.obj)

# Source file for PRISM2 (BIOPATH setup and link to speciation)
SRC_F=      users.f
OBJ_F=      $(SRC_F:.f=.obj)

# Common global headers for PRISM2 and CHEM2MIN / CHEM2EQ
HDR=        prism.h messages.h

# Sets of object files for the various sub-projects
OBJ_C2M=    $(OBJ_0) $(OBJ_N) $(OBJ_1)
OBJ_LIB=    $(OBJ_2)
OBJ_USR=    $(OBJ_F)

##### Start of make dependencies #####

# Source files dependent on prism.h
$(OBJ_1):   $(HDR)

$(OBJ_2):   $(HDR)

# Library of object files for building PRISM2 speciation part
$(LIB_SPC): $(OBJ_LIB)
            386LIB $@ -replace $(OBJ_LIB)

#-----
# The suffix list and implicit dependence rules must be newly defined
# because every make utility has its own defaults
.SUFFIXES:
.SUFFIXES: .exe .obj .o .c .f .h

.c.o:
            $(CC) $(CFLAGS) -c $<

.c.obj:
            $(HCC) $(CFLAGS) -c $<

.f.obj:
            $(FC) $(FFLAGS) -c $<

chem2min:   # Build executable CHEM2MIN with GNU C/C++ compiler
chem2min:   $(OBJ_C2M)
            $(CC) -o $@.exe $(OBJ_C2M) -lm

prism2:     # Build executable PRISM2 with Metaware High C/C++ compiler
prism2:     $(LIB_PR2) $(OBJ_USR) $(LIB_SPC) $(OBJ_HC) $(LIB_HC)
            $(FC) -OUT $@.exe $(OBJ_USR) $(OBJ_HC) -LIB $(LIB_PR2) $(LIB_SPC)
            $(LIB_HC)

#-----
# Do not stop after a make step failed
.IGNORE:
```