

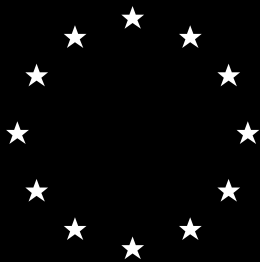
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# Documentation of the NucInfo software package in RODOS PV5.0

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**RODOS migration**  
contract

**D R A F T**  
V e r s i o n 1 . 2



**RODOS**  
REPORT

DECISION SUPPORT FOR NUCLEAR EMERGENCIES



**Documentation of the NucInfo software package in RODOS PV5.0**  
RODOS(RA1)-TN(02)-04

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## Management Summary<sup>1</sup>

Some internal and external programs in the RODOS system require information about the radionuclides that are considered during a RODOS run, and may require the radioactive half-life and other data for the selected nuclides. The program package **NucInfo** was developed to provide an interface containing such information and is described in this document.

This technical note is a part of the RODOS system documentation.

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<sup>1</sup> The work described in this report has been performed with support of the European Commission under the contract “Migration of RODOS to practical applicability for supporting decisions in operational emergency response to nuclear accidents” (RODOS migration), contract no. FIKR-CT-2000-00077

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# 1 General Information and Overview

## 1.1 General Information

### 1.1.1 Summary

The **NucInfo** (Nuclide Information) program package sets up information about the radionuclides or radionuclide compounds that are considered in a RODOS run, and some general nuclide-specific data such as the radioactive half-life.

It is part of the "Reat-time Online Decision Support System" RODOS [RODOS2000] which is developed in collaboration of different institutions in many countries of the European Union and also from other countries. The RODOS system provides information on the radiological situation to decision-makers or their advisors in the case of accidental releases from nuclear installations. Its application is possible for the near, intermediate and far distant ranges and for the short- and long-term radiological situation.

### 1.1.2 Environment

The Program package **NucInfo** for RODOS PV5.0 was developed at the Institute for Nuclear and Energy Technologies of the Forschungszentrum Karlsruhe (FZK/IKET) with support of the European Commission.

### 1.1.3 References to General Information

[RODOS2000] J. Ehrhardt, A. Weis (Editors), RODOS: Decision support system for off-site nuclear emergency management in Europe, European Commission, Report EUR19144, Nuclear science and technology series, ISBN 92-828-9773-7.

## 1.2 Overview

### 1.2.1 Background

The program system RODOS contains names, the radioactive half-life and some other data for currently 70 radionuclides or radionuclide compounds. All application-oriented RODOS calculations, however, are carried out with some subset containing less radionuclides. For example, Atmospheric Dispersion and Deposition (ADM) calculations for the near range can consider between 1 and 15 user selectable nuclides, and the far range ADM calculations between 1 and 7 nuclides user-selectable from the near range nuclides.

The **NucInfo** software was developed to control the selection of such nuclide subsets from the full set and to provide some basic nuclide information for external RODOS modules or internal RODOS procedures.

Tabelle 1 shows the names of the currently selectable radionuclides or nuclide compounds in RODOS-PV5.0. The list will be extended whenever need arises.

**Tabelle 1: Radionuclides and radionuclide compounds in RODOS-PV5.0**

(HT) <sup>2</sup> T -3x	(HTO) <sup>2</sup> TO-3x					
Na-24						
Mn-54						
Co-58	Co-60					
Kr-85m	Kr-85	Kr-87	Kr-88			
Rb-86	Rb-88					
Sr-89	Sr-90	Sr-91	Sr-92			
Y -90	Y -91					
Zr-95	Zr-97					
Nb-95						
Mo-99						
Tc-99m						
Ru-103	Ru-105	Ru-106				
Rh-105						
Ag-110m						
Sb-127	Sb-129					
Te-127m	Te-127	Te-129m	Te-129	Te-131m	Te-131	Te-132
Te-133m	Te-133	Te-134				
I -129	I -131	I -132	I -133	I -134	I -135	
Xe-133	Xe-135	Xe-138				
Cs-134	Cs-136	Cs-137	Cs-138			
Ba-140						
La-140						
Ce-141	Ce-143	Ce-144				
Pr-143						
Nd-147						
W-185	W-187					
Np-239						
Pu-238	Pu-239	Pu-240	Pu-241			
Am-241						
Cm-242	Cm-244					

The nuclide list contains:

<sup>2</sup> For the sake of the naming convention explained in Chapter 3.4.1, HT is coded as "T<sup>^</sup>-3x", and HTO as "TO-3x".

- All radionuclides considered in the German Risk Study Phase A [DRSA1981] (p. 17) and the German Leitfaden für LWR-Reaktoren [LEIT1995] (p. 8, 9).
- Additional radionuclides for complementation of some potentially important radioactive decay chains.
- Some activation products or other radionuclides, which may be of relevance for LWR reactors in normal operation mode or for Fast Breeder Reactors.
- The radionuclide compounds HT and HTO for fusion reactors.

The radioactive half-life data of the radionuclides contained in the database were taken from the Karlsruher Chart of the Nuclides [NUKL1995].

### *1.2.2 Objectives*

The objective of the **NucInfo** software is to provide by means of one single program package (a) information about which radionuclides or radionuclide compounds are considered in a run, (b) names, the radioactive half-life, corresponding decay constants of the selected nuclides, and (c) a cross-reference list to connect the fixdata nuclides and the selected nuclides.

### *1.2.3 Proposed Methods and Procedures*

None

### *1.2.4 Development Plan*

There existed no development plan. The first **NucInfo** software was written "top to bottom" in 1994 for the selection of near range nuclides for calculations with RODOS. In 2000 it was extended for the selection of far range nuclides. In 2002 the software was completely revised for RODOS PV5: All nuclide data were moved away from the RODOS fixdata base to files, and a part was added for the interaction with the RODOS nuclide selection Initialisation Windows to enable their use as dynamic input windows.

## 2 Operation Manual

### 2.1 Program Description

The program system RODOS contains nuclide names, the radioactive half-life and some other data for a large number of radionuclides, which are called *fixdata nuclides* in the following.

Near range Atmospheric Dispersion and Deposition calculations in RODOS are carried out with between 1 and 15 user selectable nuclides called *calculation nuclides*. Far range ADM calculations are carried out with between 1 and 7 nuclides selected from the near range nuclides and are called (by historical reason) *reduced nuclides*.

The task of **NucInfo** is to provide by means of one single program package (a) information about which nuclides are considered in a run, (b) names, the radioactive half-life and decay constant, type characterisations, and (c) a cross-reference list to make a connection between the fixdata nuclides and the nuclides used in the calculations.

*Input* to **NucInfo** is the following information

- Number and names of the fixdata nuclides.
- The radioactive half-life (in a unit best suited for humans to read).
- A type characterisation (noble gas, iodine, aerosol, special).
- Information about which nuclides shall be selected from the full set.

*Output* from **NucInfo** for the *near range nuclides* is the following information

- The total number of calculation nuclides and the number of noble gas, iodine, aerosol, and special nuclides.
- The names of the calculation nuclides.
- Their radioactive half-life in different physical units and the corresponding radioactive decay constant.
- A cross-reference list to tell which fixdata nuclide is a calculation nuclide.
- A control file containing a list of the nuclides received from the fixdata base and the calculation nuclides generated.

*Output* from **NucInfo** for the *far range nuclides* is the following information

- The total number of reduced nuclides.
- The names of the reduced nuclides.

- A cross-reference list to tell which calculation nuclide is a reduced nuclide.

A default selection for 15 calculation nuclides and 5<sup>3</sup> reduced nuclides is provided by the system. In the interactive operation mode of RODOS, the user can select other nuclides with the Initialisation Windows of RODOS [Prognosis USER GUIDE]. In the automatic operation mode of RODOS, the user cannot influence the nuclide selection at all.

## 2.2 Description of Operation Modes

The **NucInfo** software is used both in the automatic and the interactive operation mode of RODOS.

## 2.3 Connections to other RODOS Software

Program package **NucInfo** is part of the RODOS programs DIAGNOSIS and PROGNOSIS of the analysing subsystem ASY. The information generated by **NucInfo** is kept in special sections in the ASY Shared Memory. It is accessible for all external programs either directly, after NucInfo generated the information, or indirectly, after the corresponding Shared Memory sections have been filled using RODOS load instructions for the respective archived information.

## 2.4 Help Functions

Help functions are neither available nor foreseen. For trouble-shooting see Chapter 4.2.2.

---

<sup>3</sup> The limitation to 5 default far range nuclides stems from one of the models for the far range atmospheric dispersion.

### 3 Functional Specification and Data Specification Documents

In this Chapter, program, subroutine and variable names are written in capital letters, and file names between the brackets "<>".

#### 3.1 Overview

##### 3.1.1 Software Organisation and Program Inventory

Tabelle 2 shows the program inventory of **NucInfo**. The entry subroutines SETNUK and SETNUK\_RED are called from the input module of ASY. SETNUK calls all other subroutines of the program package.

**Tabelle 2: Program inventory of NucInfo**

file	content	type/task
PAR_NUCLS	PAR_NUCLS	Include-file with parameter statements
SHM_NUCLS	SHM_NUCLS	Include-file for Shared Memory
<i>calculation nuclides</i>		
setnuk.ff	SETNUK	SETUP OF CALCULATION NUCLIDES FOR RODOS NEAR RANGE MODELS
setnuk.ff	SETNUK_FIXNUK	READ RODOS FIXDATA NUCLIDES
setnuk.ff	SETNUK_DFLNUK	READ DEFAULT SETTING FOR RODOS NEAR RANGE NUCLIDES
setnuk.ff	SETNUK_WINDOW	A-USER DYNAMIC INITIALISATION WINDOWS
setnuk.ff	SETNUK_BUSER	B-USER INTERFACE
<i>reduced calculation nuclides</i>		
setnuk_red.ff	SETRED	SETUP OF REDUCED CALCULATION NUCLIDES FOR RODOS FAR RANGE MODELS
setnuk_red.ff	SETRED_DFLNUK	READ DEFAULT SETTING FOR RODOS FAR RANGE NUCLIDES
setnuk_red.ff	SETRED_WINDOW	A-USER DYNAMIC INITIALISATION WINDOWS

##### 3.1.2 File Inventory

Tabelle 3 shows the file inventory of **NucInfo**.

File <in.NuclideData> contains radioactive half-lives and type characterisation flags for an arbitrary number of nuclides. File <in.FixDataNuclides> contains the number and names of fixdata

nuclides, and files <in.CalculaNuclides> and <in.FarRangeNuclides> the number and names of the default calculation nuclides for the near and far range, respectively. The file structure and contents are explained in Chapter 6.

All three files reside in directory <~rodos/roextern/data/sourceterm/setup/>

**Tabelle 3: File inventory of NucInfo**

file name	file content	type
in.NuclideData	nuclide data	input
in.FixDataNuclides	number and names of fixdata nuclides	input
in.CalculaNuclides	number and names of the default calculation nuclides for the near range	input
in.FarRangeNuclides	number and names of the default calculation nuclides for the far range	input

## 3.2 Data and Interface Description

### 3.2.1 Input Data

Almost all input data for **NucInfo** are read from files, which are described in Chapter 6.

A steering flag called INUDFL, which tells whether the run is carried out with default or user calculation nuclides for the near range, must be set via Assign-File.

A steering flag called IREDFL, which tells whether the run is carried out with default or user reduced calculation nuclides for the far range, must be set via Assign-File.

### 3.2.2 Output Data

All output data from **NucInfo** reside in Shared Memory.

### 3.2.3 Description of NucInfo Shared Memory

In RODOS, the instructions for defining the Shared Memory, the loading of data into it or archiving of data from it, and of assigning values to Shared Memory variables are contained in separate files for different programs. **NucInfo** is not a RODOS program of its own but part of another RODOS program, which means that the corresponding instructions are not contained in separate files, but are part of the files of the other program (for example ALSMCdiag, QuickProgn).

#### 3.2.3.1 Shared Memory Definition

In the Shared Memory, the output variables from **NucInfo** are distributed over several data classes, which represent FORTRAN common blocks. The definition of each variable consists of two lines:

- The first line contains the name of the variable, the dimensions of the array, the type of the variable, upper and lower range for the values of the variable ("0:0" means that no ranges are set), and the physical unit;
- The second line contains a description of the variable.

The statements for the RODOS DefineEditor are listed below.

**Sections for fixdata nuclides (Postfix "SD" stands for "StammDaten")**

```
CNUKSD:
  CISOTOP [1:7][1:100] Char (0:0) ---
  'Nuclide names (fixdata/StammDaten nuclides)';
  CISOTYP [1:4][1:100] Char (0:0) ---
  'Deposition type (noble gas/iodine/aerosol/special)';
  CRHLISO [1:1][1:100] Char (0:0) ---
  'Phys. unit for RHLISO in DNUKSD';
END CLASS
DNUKSD:
  ISONUK [1:100] Integer (0:0) ---
  'Cross-reference between fixdata and calc. nuclides';
  ISOYES [1:100] Integer (0:0) ---
  'Flag to select calc. nuclides from fixdata nuclides';
  NISOT [] Integer (0:0) ---
  'Total number of nuclides (fixdata/StammDaten)';
  RHLISO [1:100] Real (0:0) CRHLISO
  'Radioactive half-lives';
  ZzDNUKS [] Real (0:0) ---
  'Alignment-Correction';
END CLASS
```

**Sections for near range nuclides ((Postfix "PD" stands for "ProgrammDaten"))**

```
CNUKPD:
  CNUDFL [1:7][1:15] Char (0:0) ---
  'Default near range calculation nuclides';
  CNUKL [1:7][1:15] Char (0:0) ---
  'Names of near range calculation nuclides';
  CRHALFX [1:1][1:15] Char (0:0) ---
  'Phys. unit for RHALFX in DNUKPD';
  ZzCNUKPD [1:7] Char (0:0) ---
  'Alignment-Correction';
END CLASS
DNUKPD:
  INUDFL [1:2] Integer (0:0) ---
  'Run with default (1 0) or user (0 1) near range nu.';
  NAERO [] Integer (0:0) ---
  'Number of aerosol nuclides in NNUKL';
  NIODS [] Integer (0:0) ---
  'Number of iodine nuclides in NNUKL';
  NNOBL [] Integer (0:0) ---
  'Number of noble gas nuclides in NNUKL';
  NNUKL [] Integer (0:0) ---
  'Total number of calculation nuclides';
```



```

NSPCL [] Integer (0:0) ---
'Number of special nuclides in NNUKL';
RADEC [1:15][1:5] Real (0:0) 1/(s,m,h,d,a)
'Radioactive decay constants (ln2/rad.half-life)';
RHALF [1:15][1:5] Real (0:0) (s,m,h,d,a)
'Radioactive half-lives';
RHALFX [1:15] Real (0:0) CRHALFX
half-lives (nice format for printout)';
END CLASS

```

**Sections for far range nuclides (Postfix "RE" stands for "Reduced")**

```

CNUKRE:
  CREDFL [1:7][1:15] Char (0:0) ---
  'Default near range calculation nuclides';
  CNURED [1:7][1:15] Char (0:0) ---
  'Names of reduced far range calculation nuclides';
  ZzNUKRE [1:7] Char (0:0) ---
  'Alignment-Correction';
END CLASS

DNUKRE:
  IREDFL [1:2] Integer (0:0) ---
  'Run with default (1 0) or user (0 1) far range nuc.';
  IREDNU [1:15] Integer (0:0) ---
  'Flag array for reduced calculation nuclides';
  MXXRED [] Integer (0:0) ---
  'Maximum number of reduced calculation nuclides';
  NNURED [] Integer (0:0) ---
  'Actual number of reduced calculation nuclides';
END CLASS

```

**Section for near range nuclides for the RODOS graphics manager (Postfix "GO" stands for "GraphikOberfläche")<sup>4</sup>**

```

CNUKGO:
  CNUGRF [1:8][1:15] Char (0:0) ---
  'Calculation nuclides names for graphics';
END CLASS

```

### 3.2.3.2 Loading

To run **NucInfo**, start-up values for variables INUDFL and IREDFL must be loaded from a RODOS Assign-File.

For assessing the information provided by **NucInfo**, programs that are part of the analysing subsystem ASY of RODOS need to do nothing, because all information is already contained in the Shared Memory. Programs that are not part of ASY need to load the required sections of the Shared Memory from the program data archive of an ASY run.

### 3.2.3.3 Archiving

The complete section of the Shared Memory used by **NucInfo** is archived.

### 3.2.3.4 Assignment of Data

---

<sup>4</sup> This re-assignment of the calculation nuclide names must be done because the graphics system requires the nuclide names as 8 character variables and not as the 7 character variables used elsewhere.

Assign values for **NucInfo** must be set in the RODOS Assign-File of the program of which **NucInfo** is a part. The following settings are necessary for proper operation:

- Variable **INUDFL** (near range nuclides, "X" means not relevant):

```

RUN WITH DEFAULT NUCLIDES WITHOUT USER INTERFACE:
--> INUDFL (1) = -1 ..... INUDFL (2) = X
RUN WITH RODOS A-USER INTERFACE:
--> INUDFL (1) = +1 .AND. INUDFL (2) = 0 TAKE DEFAULT NUCLIDES
--> INUDFL (1) = 0 .AND. INUDFL (2) = 1 TAKE USER      NUCLIDES
RUN WITH RODOS B-USER INTERFACE:
--> INUDFL (1) = X ...   INUDFL (2) = X
    
```

- Variable **IREDFL** (far range nuclides, "X" means not relevant):

```

RUN WITH DEFAULT NUCLIDES WITHOUT USER INTERFACE:
--> IREDFL (1) = -1 ..... IREDFL (2) = X
RUN WITH RODOS A-USER INTERFACE:
--> IREDFL (1) = +1 .AND. IREDFL (2) = 0 TAKE DEFAULT NUCLIDES
--> IREDFL (1) = 0 .AND. IREDFL (2) = 1 TAKE USER      NUCLIDES
    
```

### 3.3 Module Description

As **NucInfo** is not a RODOS module on its own right and consists only of a few subroutines, more details than in Chapter 3.1.1 are not given.

### 3.4 Using the Information Provided by NucInfo

#### 3.4.1 Names of Radionuclides and Radionuclide Compounds

NucInfo itself and other programs using the information provided by NucInfo recognise radionuclides or radionuclide compounds by their name. Names not of interest or not recognisable are skipped or ignored.

To ensure common understanding, the names must obey strict naming rules that are collected in Tabelle 4. All names currently implemented in RODOS are listed in Tabelle 1.

**Tabelle 4: Spelling rules for NucInfo names**

char.	content	spelling rules
1,2	<p><i>chemical elements:</i> names as in periodic tables</p> <p>-----</p> <p>chemical compounds, or any other type</p>	<p>chemical element: 2-character element : 1st char. upper case, 2nd char. lower case char. 1-character element : 1st char. upper case, 2nd char. blank character.</p> <p>-----</p> <p>symbolic name: no constraint on upper/lower case characters; however, for 1-character names the 2nd character must be the blank character.</p>

3	hyphen	the minus-sign "-"
4,5,6	nucleon number of radionuclide	Right-adjusted. Missing figures to the left must be filled with the blank character.
7	additional information	no restriction; for instance - the blank character; - the lower case "m" for metastable states; - the lower case "x" for unclassifiable entries.

### 3.4.2 Sequence of Fixdata Nuclides

Variable NISOT gives the total number of fixdata nuclides. The 1...NISOT radionuclides or radionuclide compounds appear in the sequence defined by the arrangement of the nuclides in the fixdata nuclide definition file <in.FixDataNuclides>.

### 3.4.3 Near Range Calculation Nuclides Delivered by NucInfo

How many (NNUKL) and which (CNUKL) near range calculation nuclides are present in a run depends on the selection made by the user; the current maximum number is 15. NNOBL, NIODS, NAERO, NSPCL count the number of noble gas, iodine, aerosol and special nuclides among the calculation nuclides, and the sum (NNOBL+NIODS+NAERO+NSPCL) equals NNUKL. *Please note that one, two, or three of the counters NNOBL, NIODS, NAERO, NSPCL can be zero, but not all four: NucInfo guarantees that at least one calculation nuclide is present.*

The sequence of near range calculation nuclides in all nuclide-dependent arrays is made up by NucInfo in a way particularly suited for the ADMs. This sequence is shown in Tabelle 5.

**Tabelle 5: Sequence of near range nuclides delivered by NucInfo**

type	array elements
noble gases	1 ... NNOBL
iodine isotopes	NNOBL+1 ... NNOBL+NIODS
aerosols	NNOBL+NIODS+1 ... NNOBL+NIODS+NAERO
specials	NNOBL+NIODS+NAERO+1 ... NNOBL+NIODS+NAERO+NSPCL=NNUKL

### 3.4.4 Far Range Calculation Nuclides Delivered by NucInfo

How many (NNURED) and which (CNURED) far range calculation nuclides are present in a run depends on the selection made by the user;

the current maximum number is 7<sup>5</sup>. Please note that NNURED can also be zero!

There is no fixed arrangement of the far range nuclides: If NNURED is greater than 1, array CNURED simply contains the names of the 1...NNURED nuclides as they come in. It may even be possible that the sequence is different when the far range nuclides were selected with the RODOS Initialisation Windows or the RODOS B-User interface, respectively (at present this matter is not finally settled). So the only way to identify individual far range nuclides is "by name".

### 3.4.5 Cross-Reference between Fixdata and Near Range Calculation Nuclides

The array ISOYES contains the selection flag, which tells for each fixdata nuclide if it is selected as a calculation nuclide. If this is so, the cross-reference array ISONUK gives its address in the calculation nuclides arrays, if not, ISONUK is zero for the corresponding fixdata nuclide.

In FORTRAN for instance, this information can be utilised with the following construction:

```
DO ## ISO=1,NISOT {"Loop over all fixdata nuclides ISO"}
  IF(ISOYES(ISO).GT.0) THEN
    INU=ISONUK(ISO)
    {"This fixdata nuclide ISO is a calculation nuclide with calculation
    nuclide number INU"}
  ELSE
    {"This fixdata nuclide ISO is not a near range calculation nuclide"}
  END IF
## CONTINUE
```

## 3.5 Description of Runs

First, a PROGNOSIS or DIAGNOSIS run must be carried out to produce NuInfo data. Any other program can then use this information in the way described in Chapter 3.2.3.2.

---

<sup>5</sup> The code allows up to 15 far range nuclides. The limitation to 7 (set by variable MXXRED) stems from one of the models for the far range atmospheric dispersion.

## 4 Program Maintenance, Integration and Test Plan

### 4.1 Operating Environment

#### 4.1.1 Program Language

**NucInfo** is written in FORTRAN 77. Program development was on a HP Workstation Series 9000-7xx with UNIX operation system HPUX-10.20 and HPUX F77 compiler.

There are a few extensions to standard FORTRAN 77:

- FORTRAN include statements for including files with definitions of parameters, variables etc.
- Use of the compiler \$alias-directive for coupling to RODOS procedures written in C.
- Use of the compiler \$NOSTANDARD SYSTEM directive to enable the use of the FORTRAN library subroutines DATE and TIME.
- Names can be longer than 6 characters.
- In a few places, lower case characters are used.

#### 4.1.2 Programming Conventions

None.

#### 4.1.3 Support Software

**NucInfo** uses procedures written in C for communication with the RODOS Initialisation Windows (win\_request) and for sending messages to the RODOS screen during a run (errorMessage).

### 4.2 Maintenance Procedures

#### 4.2.1 Verification Procedures

The software of **NucInfo** is inspected routinely for proper performance.

#### 4.2.2 Error Correction Procedures

**NucInfo** performs several checks, and, in case of a problem, reports the nature of the problem.

Loading errors or wrong entries in the input files can cause problems. Such "installation errors" do not allow proper performance and lead to an error stop. The respective problem is recorded in the "RODOS run protocol" which is written on disk but not accessible with the RODOS graphics.

Errors can also be caused by the user selection of near or far range nuclides. Such "user input errors" are detected by the **NucInfo** subroutine interacting with the Initialisation Windows. During program

execution, a message explaining the problem is flashed on the screen, and the window in which the error was made is popped up again for another attempt of the user.

#### **4.3 Test Plan and Test Analysis Report**

In the initial test phase in 1994 and after all subsequent extensions, tests were made to ascertain that the task performs correctly. Since **NucInfo** is in use no errors were detected at FZK or reported by external users.

## 5 Model Description

**NucInfo** performs the following tasks.

- Checks of validity of input nuclide information.
- Checks of the selection of near and far range calculation nuclides.
- Reorganisation and cross-referencing of nuclide arrays.
- Transformation of radioactive half-life data into different units.
- Calculation of the radioactive decay constants ( $\ln 2/\text{rad. half-life}$ ) in different units of time.

All these tasks are straightforward and simple and need no further explanations.

## 6 Description of Input Files

File <in.FixDataNuclides> contains the number and names of all RODOS fixdata nuclides. The files <in.CalcNuclides> and <in.FarRangeNuclides> contain the number and names of the default calculation nuclides for the near and for the far range, respectively. File <in.NuclideData> contains the radioactive half-life and a type characterisation flag for an arbitrary number of nuclides.

All files reside in directory

- <~rodos/roextern/data/sourceterm/setup/>

### 6.1 File <in.FixDataNuclides>

Tabelle 6 shows the top and bottom part of file <in.FixDataNuclides>. The file structure is simple:

The first line contains the number of radionuclides or radionuclide compounds contained in the file (integer number with 3 digits, right adjusted, value between 1 and 100).

All following lines contain

- The number of the nuclide position in the file (integer with 3 digits, right adjusted).
- The colon (some internal RODOS procedure needs that).
- The name of the radionuclide(-compound) as shown in Tabelle 1.

**Tabelle 6: Part of the file <in.FixDataNuclides>**

70
1:T - 3x
2:TO- 3x
3:Na- 24
4:Mn- 54
5:Co- 58
6:Co- 60
7:Kr- 85m
8:Kr- 85
9:Kr- 87
10:Kr- 88
.....
.....
.....
67:Pu-241
68:Am-241
69:Cm-242
70:Cm-244



The order of nuclides in the file does not have functional relevance for **NucInfo**. However, the order determines the readability of the file by humans, the appearance of the fixdata nuclides in the RODOS Initialisation Windows and the RODOS B-User interface, and due to the latter also the sequence of nuclides in the files for the default near and far range nuclides. Therefore, new nuclides should be placed at appropriate positions in the file and not just dumped at the end. A stand-alone program (FORTRAN program FixNuks) exists that will update the nuclide number and renumber the nuclides in the file, so that work needs not to be done by hand.

## 6.2 File <in.CalculaNuclides>

Tabelle 7 shows file <in.CalculaNuclides>. The file structure is very simple:

The first line contains the number of radionuclides or radionuclide compounds contained in the file (integer number with 2 digits, right adjusted, value between 1 and 15).

All following lines contain the name of the radionuclide as shown in Tabelle 1.

**Tabelle 7: File <in.CalculaNuclides>**

15
Kr- 88
Rb- 88
Sr- 89
Sr- 90
Zr- 95
Te-132
I -131
I -132
I -133
I -135
Xe-133
Xe-135
Cs-134
Cs-137
Ba-140

### ATTENTION

The nuclides **MUST APPEAR IN THE ORDER THEY HAVE IN FILE** <~rodos/roextern/data/sourceterm/setup/in.FixDataNuclides>.

This is a vital condition for the RODOS B-User interface and is checked at run time of RODOS. Violation leads to a program stop with the message "installation error".

### 6.3 File <in.FarRangeNuclides>

Tabelle 8 shows file <in.FarRangeNuclides>. The file structure is very simple:

The first line contains the number of radionuclides or radionuclide compounds contained in the file (integer number with 2 digits, right adjusted, value between 1 and 15).

All following lines contain the name of the radionuclide as shown in Tabelle 1.

**Tabelle 8: File <in.FarRangeNuclides>**

5
Zr- 95
Te-132
I -131
Xe-133
I -133
Cs-137

#### ATTENTION

The nuclides **MUST APPEAR IN THE ORDER THEY HAVE IN FILE** <~rodos/roextern/data/sourceterm/setup/in.FixDataNuclides>. This is a vital condition for the RODOS B-User interface.

Please note also, that for the far range nuclides, **NO MORE THAN ONE IODINE NUCLIDE CAN BE SPECIFIED**<sup>6</sup>.

Both condition are checked at run time of RODOS. Violation leads to a program stop with the message "installation error".

---

<sup>6</sup> This limitation stems from one of the models for the far range atmospheric dispersion.

### 6.4 File <in.NuclideData>

Tabelle 9 shows the top part of file <in.NuclideData>. Explanations follow after the Table.

**Tabelle 9: Top part of the file <in.NuclideData>**

```

=====
NCOMM = 15 ***** number of comment lines to follow *****
-----
C. Landman/FZK ***** file in.NuclideData ***** Version 25.09.2002
=====
Rad. half-life from [Karlsruher Nuklidkarte. Hrsg: Forschungszentrum
Karlsruhe, Technik und Umwelt (November 1995)].
-----
Natuerl. Nuklide p=primordial | k=kosmisch_erzeugt | z=Zerfallsreihe
-----
The deposition types of T-3x and TO-3x are set to AERO, because the
current ADMS need this so. It should be SPCL, though.
=====
-----
pro.   Name   rad. half-   depo   Comments
num.       life & unit code
-----
001 H - 3    1.2323E+01 a XXXX k beta-
001 T - 3x   1.2323E+01 a AERO
001 TO- 3x   1.2323E+01 a AERO
004 Be- 7    5.3290E+01 d XXXX k
004 Be- 10   1.6000E+06 a XXXX beta-(no_gamm)
006 C - 14   5.7300E+03 a XXXX k beta-(no_gamm)
011 Na- 22   2.6030E+00 a AERO
011 Na- 24   1.4960E+01 h AERO
014 Si- 32   1.7200E+02 a XXXX beta-(no_gamm)
015 P - 33   2.5340E+01 d XXXX beta-(no_gamm)
018 Ar- 41   1.8300E+00 h XXXX
019 K - 40   1.2800E+09 a XXXX p beta- el.capt beta+
020 Ca- 47   4.5400E+00 d XXXX
021 Sc- 44m  2.4400E+00 d XXXX
021 Sc- 44   3.9200E+00 h XXXX
021 Sc- 46   8.3820E+01 d XXXX
021 Sc- 47   3.3500E+00 d XXXX
021 Sc- 48   4.3670E+01 h XXXX
023 V - 48   1.5970E+01 d XXXX
023 V - 49   3.3000E+02 d XXXX no_gamm
024 Cr- 51   2.7700E+01 d XXXX
025 Mn- 52m  2.1000E+01 m AERO
025 Mn- 52   5.6000E+00 d AERO
025 Mn- 53   3.7000E+06 a AERO no_gamm
025 Mn- 54   3.1220E+02 d AERO
025 Mn- 56   2.5800E+00 h AERO
026 Fe- 52   8.2700E+00 h XXXX
026 Fe- 55   2.7300E+00 a XXXX no_gamm

```

The first line in file <in.NuclideData> is a comment line.

The second line contains the number of comment lines to follow in the file header (8 arbitrary characters, integer number with 5 digits (right adjusted), followed by arbitrary comment characters).

Then follow NCOMM comment lines.

Then follows for each nuclide one line with data:

- The proton number of the pure radionuclide or of the radionuclide in a compound.
- The name of the radionuclide(-compound). If the name is contained in file <in.FixDataNuclides>, the name from the file must be used. If the name is not contained in the file, a name according to the naming convention in Chapter 3.4.1 must be made up. In the latter case, this name is cogent if the nuclide will later be added to the fixdata nuclides.
- The radioactive half-life and the physical unit for the radioactive half-life (exactly in the format shown in the Table; allowed notations for the physical unit are "s", "m", "h", "d", "a" for second, minute, hour, day, year, this is checked by **NucInfo!**).
- A code for the deposition property for the Atmospheric Dispersion and Deposition models.
  - If the radionuclide(-compound) is not contained in file <in.FixDataNuclides>, the code is meaningless (represented by XXXX in the Table).
  - If the radionuclide(-compound) is contained in file <in.FixDataNuclides>, only four values are allowed: "AERO" for aerosol<sup>7</sup> - type deposition property, "IOD" for all iodine nuclides(-compounds)<sup>8</sup>, "NOBL" for noble gas - type deposition property (in other words, no deposition), "SPECL" for a deposition type not fitting into the above scheme.
- An arbitrary comment.

The number radionuclides or radionuclide compounds in the file and their order is completely arbitrary. However, to maintain good readability of the file by humans, new nuclides should be placed at appropriate positions in the file and not just dumped at the end.

---

<sup>7</sup> "Aerosol" means here fission products released to the atmosphere as solid or liquid suspensions in air via a carrier (e.g. CsI, NaOH etc.).

<sup>8</sup> The distinction between elementary iodine, organically bound iodine and iodine in aerosol form is made elsewhere in RODOS.

## 7 References

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**[NUKL1995]** Karlsruher Nuklidkarte. Hrsg: Forschungszentrum Karlsruhe, Technik und Umwelt (November 1995).

**[Prognosis USER GUIDE]** User Guide of the Prognosis Models in RODOS

## 8 Index

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Far range nuclide, definition of ~, *Chapter 2.1*

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