NUCLEAR SAFETY INSTITUTE OF RUSSIAN ACADEMY OF SCIENCES

IBRAE RAN

New MELCOR 2.1 Code Features

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Outline

- CF-TF from restart:
  - Goal;
  - Modifications of input;
  - Changes in output;
  - Testing.
- Activity calculations
  - Model;
  - Modifications of input;
  - Output data on activity values;
  - Testing.

ИБРАЭ

CF-TF from restart

- MELCOR code has the ability to stop a calculation at any time, to modify some parameters in the input file and to continue the calculation using the restart file.
- A very limited capability of modifying a control function using a restart file has been accessible in MELCOR code (user could only change min and max control function values).
- There was no capability to change TFs from restart.
- The following capabilities have been added to MELCOR 2.1:
  - the user is allowed to change any CF and TF parameters from the restart;
  - new CFs and TFs can be set from the restart.

General remarks

- Newly set TFs and CFs are added to the end of the list (Attention when working with control functions!).
- User may change the type of an existing control function (with name identical to one in MELGEN) but it means that all records for the control function must be input.

Changes in the CF input

- Record formats are identical in both cases: for MELGEN input and for MELCOR input.

```
! ***********MELCOR input *****************
Program MELCOR
!********** Block: CF data**************************
CF_INPUT ! CF package start record
!*     1 - Number of Control Functions added from the restart
CF_ID 'MyTestCF'    TAB-FUN    ! CFNAME  CFTYPE
CF_SAI        1.0     0.0     0.0
CF_MSC   'AppliedPower'
CF_ARG   1 ! NARG CHARG          ARSCAL          ARADC
                  1 EXEC-TIME       1.0             0.0
END Program MELCOR data
```

Changes in the TF input

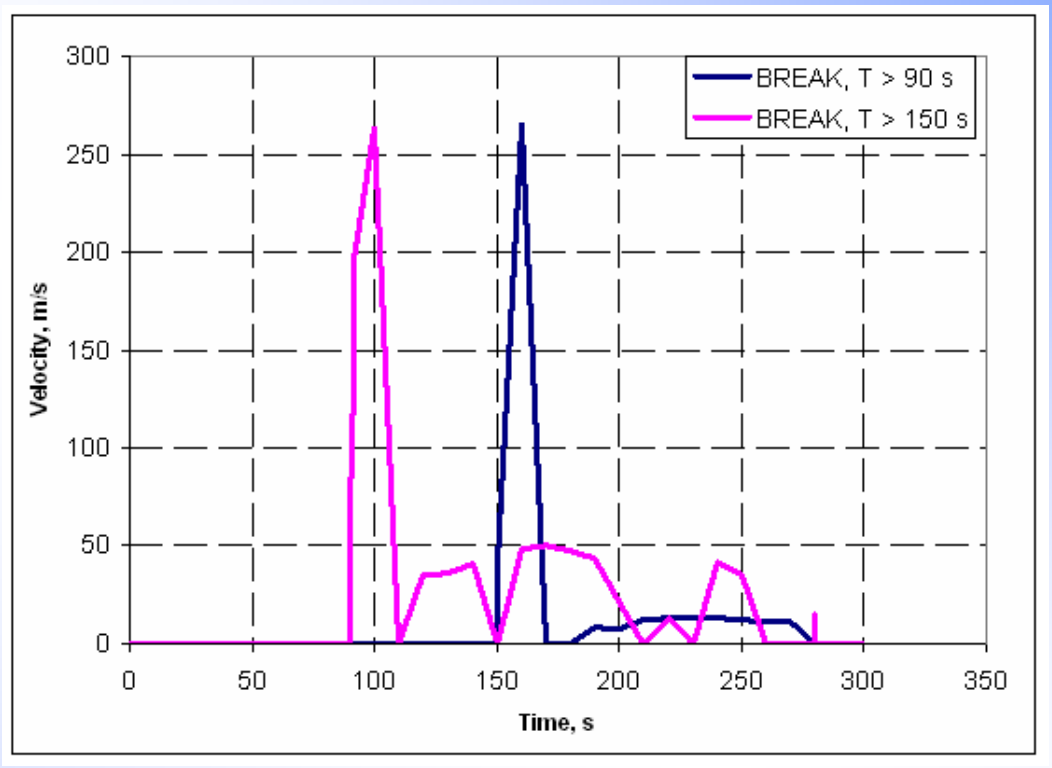
```
Program MELCOR
!* Block: TF data ****************
TF_INPUT ! TF package start record
!*     1 - Number of Tabular Functions********
!*     1 - Next TF data ****************
TF_ID 'AppliedPower'  2.0    3.0
TF_TAB 5 ! NTFPAR  X                  Y
                 1       0.0                0.0
                 2     12.65306         10000.0
                 3     941.3265         19259.26
                 4     2732.143         19629.63
                 5     182398.0         31111.11
END Program MELCOR data
```

Diagnostics

```
WWWWWWWWWWWWWWWWWWWWWWWWWWWW
Diagnostics during MELCOR input processing CF package:
ATTENTION: Control function name MyTestCF
                          is added from the restart
WARNING: Some parameters for control function name CF1
                 are changed  from the restart
NO Errors during MELCOR input processing CF package
WWWWWWWWWWWWWWWWWWWWWWWWWWWW
Diagnostics during MELCOR input processing TF package:
ATTENTION: Tabular function name AppliedPower
                       is added from the restart
NO Errors during MELCOR input processing TF package
WWWWWWWWWWWWWWWWWWWWWWWWWWWW
```

Testing

- One PWR loop input deck.
- Break in the hot leg is modeled.
- In original input break occurs at TIME = 90 s.
- Using new capability to change any CF and TF parameters from restart, time of break has been changed to TIME = 150 s.



Summary

- The capability to add or change CFs and TFs from restart has been added to MELCOR code.
- For long-running calculation there is no need for the user to start it from beginning if it is necessary to change only some parameters that are defined through TF or CF. The user can change them from any restart file time point without repeating preceding computations.

Activity calculations

- For radiological impact estimation it's necessary to have activity values.
- Current MELCOR version outputs masses of RN classes.
- User should perform additional calculations to obtain activities.
- Activity calculations inside MELCOR code would significantly simplify users' work.

ИБРАЭ

BONUS code

- In the perfectly designed integral code all its components should be of near the same level of accuracy.
- BONUS code has been elaborated in IBRAE that can be considered as a simplified version of ORIGEN.
- The full version of BONUS allows express-evaluation of temporal evolution of the nuclide composition of the fuel, decay heat and activity of FPs or their classes in thermal reactors both during regular reactor campaign and after the reactor shutdown.
- The BONUS component that provides calculations of FP evolution after reactor shutdown has been implemented in MELCOR 2.1.

ИБРАЭ

Model for activity calculations

The activity A_{ZA} (Bq) of isotope (Z, A) in the volume under interest is calculated as: $$A_{ZA}(t) = \lambda_{ZA} N_{ZA}(t),$$

where N_{ZA} is the total number of isotopes (Z, A) in the volume and λ_{ZA} is the decay constant (s^{-1}).

The variable $a_{CL,ZA}$ measures the relative contribution of isotope (Z, A) to the total activity A_{CL} of the class CL:

$$a_{CL,ZA}(t) \equiv \frac{A_{ZA}(t)}{A_{CL}(t)} = \frac{A_{ZA}(t)}{\sum_{Z \in CL} \sum_{A} A_{ZA}(t)} = \frac{\lambda_{ZA} N_{ZA}(t)}{\sum_{Z \in CL} \sum_{A} \lambda_{ZA} N_{ZA}(t)}.$$

The total class activity A_{CL} (Bq) is calculated as

$$A_{CL}(t) = \frac{H_{CL}(t)}{\sum_{Z \in CL} \sum_{A} E_{ZA} a_{CL,ZA}(t)} = \frac{M_{CL}(t)}{m_n \sum_{Z \in CL} \sum_{A} \lambda_{ZA}^{-1} A a_{CL,ZA}(t)} = \frac{h_{CL}(t) M_{CL}(t)}{\sum_{Z \in CL} \sum_{A} E_{ZA} a_{CL,ZA}(t)},$$

where m_n is the mass of nucleon (kg), A is a mass number, h_{CL} - the total specific decay heat of the class (J/kg/s), E_{ZA} - the decay energy of isotope (Z, A) (J) .

The activity of each isotope in the class: $A_{ZA}(t) = A_{CL}(t) a_{CL,ZA}(t).$

Initial data

- For activity calculations it's necessary to have isotopic composition by the moment of reactor shutdown.
- MELCOR does not explicitly treat isotopes. It works in terms of "elements" that are summed into RN classes.
- It seems to be reasonable to prepare beforehand a special library for a number of typical reactor campaigns and then use it in practical calculations in combination with the total decay heats of elements.
- If the user utilizes the old MELCOR input file without providing any information about initial inventory, some default library variant is to be chosen.

Properties of fission products

- The isotopes database (half-life times, decay energies, etc.).

  File 'FissProd.in' (properties of fission products)

  Default values are prepared based on tables T.R.England, B.F.Rider. Evaluation and Compilation of Fission Yields, ENDF-349, LA-UR-94-3106.

  http://ie.lbl.gov/toi.html, http://ie.lbl.gov/fission.html

A	Name	t1/2	E_gamma	E_beta	E_alpha	sig_c_b	Ind-235%	Cum-235%	Ind-239%	Cum-239%	Ind-241%	Cum-241%
66	Mn						7.200E-10	7.220E-10	3.690E-10	3.700E-10	3.260E-10	3.260E-13
66	Fe						3.760E-08	3.830E-08	3.630E-08	3.670E-08	2.860E-08	2.890E-08
66	Co	0.23s					2.810E-08	6.640E-08	1.150E-07	1.520E-07	9.910E-08	1.280E-07
66	Ni	54.6 h		6.720E-02			5.780E-09	7.210E-08	6.780E-08	2.190E-07	3.850E-08	1.670E-07
66	Cu	5.10 m	8.470E-02	1.070E+00			1.430E-11	7.220E-08	1.380E-09	2.210E-07	6.150E-10	1.670E-07
67	Mn						5.380E-10	5.380E-10	7.580E-11	7.580E-11	9.060E-11	9.060E-11
67	Fe						6.870E-08	6.920E-08	1.820E-08	1.830E-08	2.460E-08	2.470E-08
67	Co						2.000E-07	2.700E-07	1.860E-07	2.040E-07	2.330E-07	2.580E-07
67	Ni	21 s					9.040E-08	3.600E-07	2.290E-07	4.330E-07	2.360E-07	4.940E-07
67	Cu	2.580d	1.150E-01	1.550E-01			9.680E-10	3.610E-07	1.560E-08	4.480E-07	1.100E-08	5.050E-07

Isobaric chains

File 'FPChains.in' (structure of isobaric chains)

The β- and γ-decays of FPs are taken into account in BONUS, which do not change the mass number so that the FP decay sequence represents the isobaric chain. It is supposed that the β-decay results in one or two daughter nuclides (in the ground and isomeric states). The thermal neutron capture also is taken into account, which also produces one or two daughter nuclides with the increased by 1 mass number and therefore results in coupling of the current chain with the next one(s).

```
|  beta-decay    n-gamma   Branch_ratios
    1-st 2-nd  1-st 2-nd beta       neutron
-------------------------------------------
80
Se
-------------------------------------------
81
Se   Br
Br
-------------------------------------------
82
Se
-------------------------------------------
83
Se   Br
Se*  Br
Br   Kr*  Kr             .999754
Kr*  Kr
Kr
-------------------------------------------
```

Initial inventories

File ' InitInventory.in' by default

(file name can be changed by the user in input)

Contains masses of isotopes by the moment of reactor shutdown. The data can be set for different reactor campaigns, then each block should start with REACTOR_XYZ line, where XYZ… is user-defined characters defining the campaign name (for example, REACTOR_PWR1Y, REACTOR_BWR_2Y). The block name used in particular calculations is set on DCH_RCT record.

```
REACTOR_PWR
Se-80    4.06405E-01
Se-81    1.31432E-05
Br-81    6.81138E-01
Se-82    1.04052E+00
Se-83    1.77636E-05
Se*-83   7.74357E-07
Br-83    2.20323E-04
Kr*-83   1.67048E-04
Kr-83    1.63820E+00
Se-84    8.22949E-06
```

Two options for activity calculations

Option 1. This variant implies the use of the old MELCOR inputs, in particular time-decay heat table. The initial data for $a_{CL,ZA}$ are chosen to correspond to some standard reactor campaign (these values are calculated using isotope masses from the initial inventory file for standard campaigns). Then, the BONUS modules calculate isotope activity values.

Option 2. In this case the MELCOR input file chooses the variant of irradiation regime from the above mentioned library. Then the calculations are performed by BONUS both for decay heats and activities.

Modifications of input (1)

DCH_ACT – Activity calculation options

Optional

This record specifies the switches that allow user to enable or disable activity calculations and set the format of input. If RN package is not active, activity calculations can not be enabled.

Examples

!	Key	Input format
DCH_ACT	ON	NEW
DCH_ACT	ON	OLD
DCH_ACT	OFF	

Modifications of input (2)

DCH_SUR – Output activity data

Optional. Allowed if IACTIV = ON on DCH_ACT record

Specifies the control volumes or heat structures sides for which isotope activities data will be printed to the output. If control volume is set, the data on isotopes activities will be summarized for control volume and heat structures associated with the corresponding control volume. By default isotopes activities will be printed for flow paths set on FL_MACCS record and different control volume types.

Examples

```
DCH_SUR 4  ! N TYPE      NAME          IKEY
           1  CVH    CORE-INLET       ALL
           2  LHS    INLET-FLOOR    ISOTOPE  'Cs-137' 'I-131'
           3  CVH    'CONTAINMENT'    ALL
           4  LHS    'CORWALL6'     ISOTOPE  'Cs-137' 'I-131'

DCH_SUR 1  ! N TYPE      NAME        IKEY
           1  CVH       CV110-CORE    ALL
```

Modifications of input (3)

DCH_RCT – Reactor type for initial mass inventories calculation

Optional

This record enables the user to specify the type of reactor or filename and data block with initial inventories.

If IACTIV = OFF or 0, the old format of DCH_RCT record must be used.

Examples

```
!        Reactor type File name          Block name
DCH_RCT   PWR "initInventory.in"  "REACTOR_PWR"

DCH_RCT "initInventory.in"   "REACTOR_BWR"
```

Example of input

```
DCH_INPUT ! DCH package start record
DCH_ACT ON NEW
DCH_RCT 'InitInventory.in' REACTOR_PWR
DCH_SUR 1  ! N TYPE       NAME       IKEY
                1  CVH     CV110-CORE    ALL
```

Modifications of output (1)

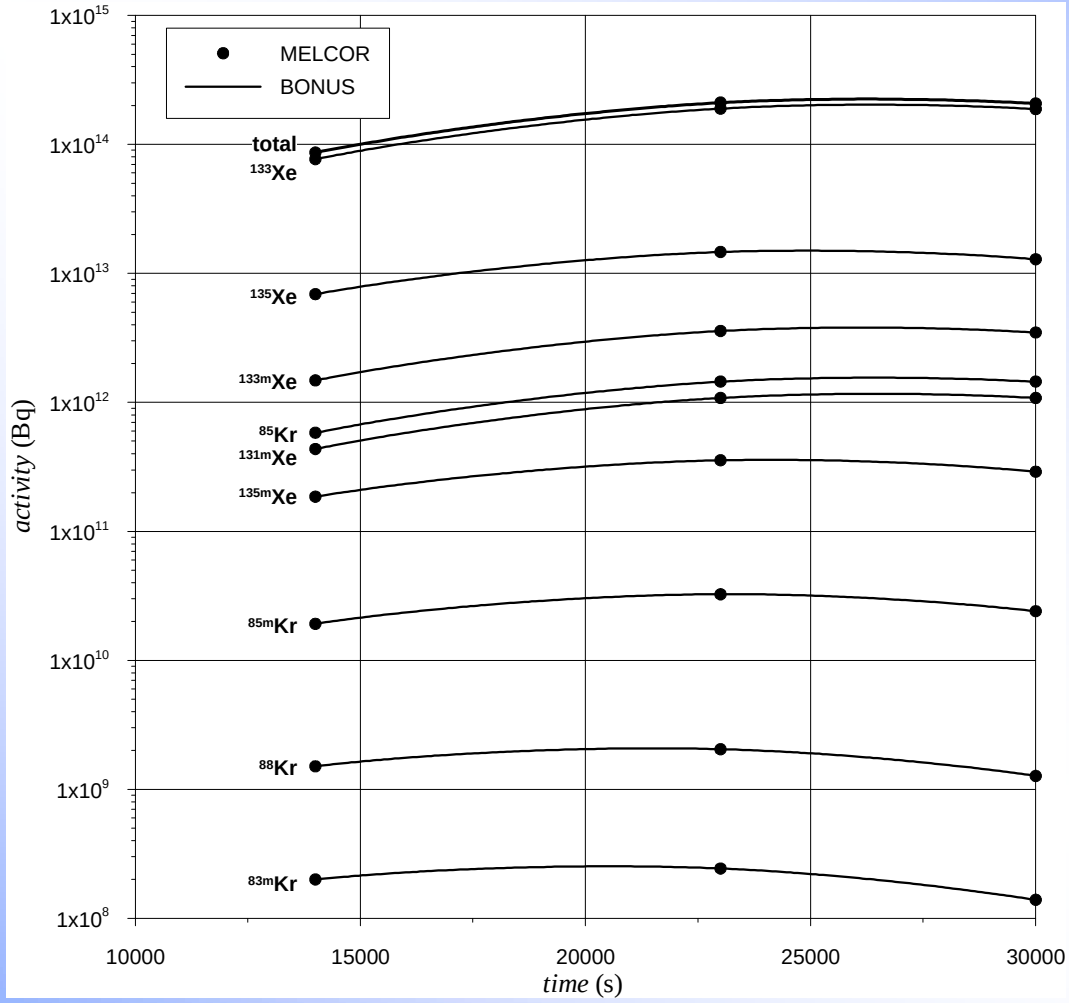
```
      ****************************************
      *                                      *
      *            ACTIVITY    EDIT          *
      *                                      *
      ****************************************


ACTIVITY (BQ) FOR CONTROL VOLUMES AND HEAT STRUCTURE SIDES DEFINED BY THE USER

                        CVH
                     CV110-CORE
          Se-80      0.000000E+00
          Se-81      0.159909E+17
          Br-81      0.000000E+00
          Se-82      0.804288E-03
          Se-83      0.206375E+17
         Se*-83      0.136319E+11
          Br-83      0.818937E+17
```

Modifications of output (2)

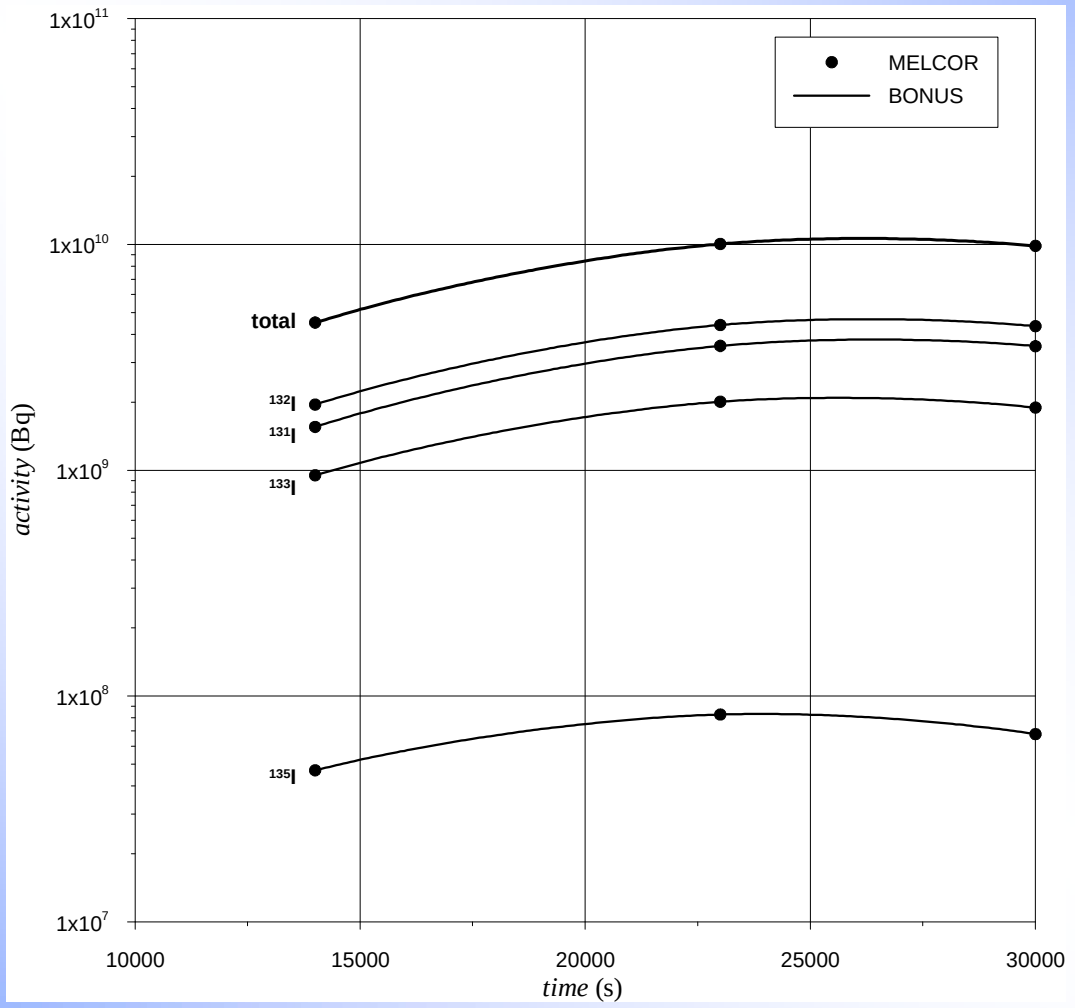
ACTIVITY (BQ) FOR CONTROL VOLUMES OF THE SAME TYPE

ISOTOPE NAME	CORE	DRYWELL	WETWELL	CONTAINMENT	ENVIRONMENT	FILTERS
Se-80	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
Se-81	0.499953E+15	0.228914E+13	0.728978E+16	0.308654E+16	0.758805E+10	0.758044E+13
Br-81	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
Se-82	0.641286E-04	0.293627E-06	0.935055E-03	0.395908E-03	0.973314E-09	0.972339E-06
Se-83	0.756828E+15	0.346530E+13	0.110353E+17	0.467240E+16	0.114868E+11	0.114753E+14
Se*-83	0.404858E+03	0.185373E+01	0.590321E+04	0.249946E+04	0.614475E-02	0.613859E+01
Br-83	0.609599E+16	0.622116E+12	0.109876E+18	0.586421E+17	0.865953E+15	0.000000E+00
Kr*-83	0.758137E+16	0.133008E+11	0.138959E+18	0.746423E+17	0.110320E+16	0.000000E+00
Kr-83	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
Se-84	0.303587E+12	0.139004E+10	0.442658E+13	0.187424E+13	0.460770E+07	0.460308E+10
Br-84	0.448464E+16	0.457672E+12	0.808321E+17	0.431413E+17	0.637056E+15	0.000000E+00
Br*-84	0.192596E+13	0.196550E+09	0.347139E+14	0.185273E+14	0.273587E+12	0.000000E+00
Kr-84	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
Br-85	0.898410E+11	0.916858E+07	0.161932E+13	0.864252E+12	0.127622E+11	0.000000E+00
Kr*-85	0.137162E+17	0.240640E+11	0.251406E+18	0.135043E+18	0.199591E+16	0.000000E+00
Kr-85	0.949924E+15	0.166656E+10	0.174112E+17	0.935247E+16	0.138228E+15	0.000000E+00
Rb-85	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
Br-86	0.932174E+00	0.951314E-04	0.168017E+02	0.896732E+01	0.132418E+00	0.000000E+00

Testing (1)


MELCOR
BONUS
total
133Xe
135Xe
133mXe
85Kr
131mXe
135mXe
85mKr
88Kr
83mKr
1x10^15
1x10^14
1x10^13
1x10^12
1x10^11
1x10^10
1x10^9
1x10^8
activity (Bq)
10000
15000
20000
25000
30000
time (s)

Testing (2)


MELCOR
BONUS
total
132I
131I
133I
135I
1x10^11
1x10^10
1x10^9
1x10^8
1x10^7
activity (Bq)
10000
15000
20000
25000
30000
time (s)

Summary

- Activity calculation model for implementation in MELCOR code has been developed.
- The model has been implemented in the code including necessary changes in the input and output.
- Testing demonstrates workability and good results agreement of activity values obtained in MELCOR in comparison with other codes including high-precision one.

ИБРАЭ

THE END

Thank you for attention

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