Russian Academy of Sciences (IBRAE)

Future MELCOR 2.x Code Features

Presented by N. Mosunova
Nuclear Safety Institute of Russian Academy of Sciences (IBRAE RAS)

European MELCOR User Group
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Outline

- MELCOR overview
- New MELCOR code features to be implemented in future 2.x code versions
  - CF-TF from restart;
  - Activity calculations;
  - Simplified accumulator model.

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Background

- MELCOR has been developed at Sandia National Laboratories for the US Nuclear Regulatory Commission
  - Project began in 1982;
  - Development of new capabilities still underway;
  - IBRAE has been involved in MELCOR code development and validation since 1992.

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MELCOR Development

- U.S. NRC and SNL provide directions for code activities at IBRAE
  - Coordination meetings;
  - Regular conference-calls;
  - Review of new models design reports.
- MELCOR activities in IBRAE
  - Code conversion from FORTRAN 77 to FORTRAN 95 – MELCOR 2.0 version;
  - Input CONVERTER (1.8.6 inputs to 2.0 format) and GUI;
  - Code validation and assessment;
  - New models.

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CF-TF from restart

- Currently MELCOR code has the ability to stop a calculation at any time, modify the input file and to continue the calculation using the restart file.
- Currently MELCOR has a very limited capability of modifying a control function using a restart file (can only change min and max values).
- For user flexibility the following capabilities have been added:
  - the user is allowed to change any CF parameters from the restart;
  - new CFs and TFs can be set from the restart.

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

WWWWWWWWWWWWWWWWWWWWWWWWWWWWW

Diagnostics during MELCOR input processing CF package:

ATTENTION: Control function name MyTestCF

was added from the restart

NO Errors during MELCOR input processing CF package

WWWWWWWWWWWWWWWWWWWWWWWWWWWWW

Diagnostics during MELCOR input processing TF package:

ATTENTION: Tabular function name AppliedPower

was added from the restart

NO Errors during MELCOR input processing TF package

WWWWWWWWWWWWWWWWWWWWWWWWWWWWW

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.

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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.**

Additional data in MELCOR

- The isotopes database (half-life times, decay energies, etc.). Since it contains physical properties of the isotopes the changing of this database is not allowed for the user.
- The initial isotopes inventory – data on relative mass of each isotope at the reactor shutdown (in kg/tU). If user wants to change initial inventory, he is allowed to change the corresponding file.

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: $A_{ZA}(t) = A_{CL}(t) a_{CL,ZA}(t).$

Two options for activity calculations

Option 1. The use of the old MELCOR inputs. The initial data for $a_{CL,ZA}$ are chosen to correspond to some standard reactor campaign (e.g. stationary three-year irradiation). Then $a_{CL,ZA}$ values are calculated at each time instant and the activity of the class is calculated as:

$$A_{CL}(t) = \frac{H_{CL}^{MELCOR}(t)}{\sum_{Z \in CL} \sum_{A} E_{ZA} a_{CL,ZA}(t)} = \frac{h_{CL}^{MELCOR}(t) M_{CL}(t)}{\sum_{Z \in CL} \sum_{A} E_{ZA} a_{CL,ZA}(t)}.$$

Option 2. User chooses the variant of irradiation regime from the above mentioned library. Then the calculations are performed by special code component both for decay heats and activities.

Example of the input

```
DCH_INPUT ! DCH package start record
!
DCH_ACT   ON   NEW  ! Activity calculations will be
                    ! performed, the new format of
                    ! input be used, that is decay heats
                    ! will and activities will be
                     ! calculated inside the code
! File containing initial inventory
DCH_INV  “MyInventory.txt”
DCH_CL    'XE'    USER   1   !     N    Element name
                                  1      'XE'  ‘ON’
```

Example of the output

CLASSES ACTIVITIES IN BQ

CLASS	CORE	GAP	CAVITY	CVTYPE01
XE	8.326E+02	4.382E+01	0.000E+00	0.000E+00
CS	0.000E+00	2.352E+01	0.000E+00	0.000E+00
BA	3.682E+02	3.720E+00	0.000E+00	0.000E+00
I2	0.000E+00	0.000E+00	0.000E+00	0.000E+00
TE	7.744E+01	4.076E+00	0.000E+00	0.000E+00
RU	7.744E+01	4.076E+00	0.000E+00	0.000E+00

ISOTOPES ACTIVITIES IN BQ

ISOTOPE	FL51	FL55	'HS12201-UPPER HE'	CV530-rx bldg'
CS-136	8.326E+02	4.382E+01	0.000E+00	0.000E+00
CS-137	0.000E+00	2.352E+01	0.000E+00	0.000E+00
CS-139	3.682E+02	3.720E+00	0.000E+00	0.000E+00

Simplified accumulator model

- **In MELCOR accumulator can be modeled using a set of control functions, because the extreme expansion of the accumulator gas can lead to the temperature drop below 273.15 K, that is a fatal problem for MELCOR model. That's why the accumulator is usually set as a source of mass and enthalpy in the control volume.**
- **The separate "accumulator" object has been developed with all necessary data for accumulator modeling in ESF package.**
- **This object is used as a source of liquid in the control volume.**
- **The simplified model to calculate liquid injection is implemented in the code.**

Calculation scheme (1)

1. Put $V_{del} = 0$, where V_{del} - the delivered volume
2. Calculate P_{acc}: a) adiabatic approximation for diatomic gas

$$P_{acc} = P_{N_2} + P_{H_2O},$$

$$P_{H_2O} << P_{N_2} \Rightarrow P_{acc} = P_{N_2} = PAC \cdot \left(\frac{V_{del}}{VN2} + 1 \right)^{-7/5}.$$

b) isothermal approximation

$$P_{acc} = P_{N_2} + P_{H_2O}$$

$$P_{H_2O} << P_{N_2} \Rightarrow P_{acc} = P_{N_2} = PAC \cdot \left(\frac{V_{del}}{VN2} + 1 \right)$$

c) user defined approximation (user sets γ value in the input)

$$P_{acc} = P_{N_2} + P_{H_2O}$$

$$P_{H_2O} << P_{N_2} \Rightarrow P_{acc} = P_{N_2} = PAC \cdot \left(\frac{V_{del}}{VN2} + 1 \right)^{\gamma}$$

Calculation scheme (2)

3. Calculate pressure drop $\Delta P = P_{acc} - P_{CVH}$.

4. If $\Delta P > 0$ calculate the velocity and amount of water transferred to the connected control volume.

$$u = \sqrt{\frac{2\Delta P}{k_{eff}\rho}},\ k_{eff} = k + \frac{4fL}{D},$$

where ρ is the water density at the temperature TH2O.

On this step the calculations of the friction coefficient is to be performed in accordance with the Colebrook-White equation or constant friction coefficient set by user is used.

5. Calculate the mass and enthalpy of delivered water

a) If no lag is set by the user:

$$\Delta m = \rho \cdot S \cdot \upsilon \cdot \Delta t.$$

$$\Delta H = H_{specific} \cdot \Delta m.$$

b) If lag is set by the user: $\Delta m = \rho \cdot S \cdot Y \cdot \Delta t,$

$$\Delta H = H_{specific} \cdot \Delta m.$$

Example of the input

```
!*   1 - Next Accumulator data **********
          ! Accumulator   Control volume name
          !    name       accumulator connected to
ACC_ID 'ACC1'  'CV240-CLA ACCUM‘
          !   Surge line   Surge line   Fraction of     Constant friction   Loss coefficient is
          !    diameter      length     open area       coefficient value       set by CF
ACC_SLP  0.17        32.0    CF 'TEST1' CONST 0.05 CF 'TEST2‘
          !       Initial N2  Initial H2O   Initial       Water          Expansion coefficient
          !       volume      volume        pressure      temperature        option
ACC_PAR  14.8664  26.193  4.2403E6 322.04            ADIAB
!*   2 - Next Accumulator data **********
          ! Accumulator   Control volume name
          !    name       accumulator connected to
ACC_ID 'ACC2' 'CV340-CLB ACCUM‘
          !   Surge line   Surge line   Fraction of     Constant friction   Loss coefficient is
          !    diameter      length     open area       coefficient value       set by CF
ACC_SLP  0.26662 32.0 CONST 1.0 CONST 0.05 CONST 5.65
!       Initial N2  Initial H2O   Initial       Water          Expansion coefficient
          !       volume      volume        pressure      temperature        option
ACC_PAR  14.8664  26.193  4.2403E6 322.04 ADIAB
```

Example of the MELCOR output

****

* ACCUMULATOR EDIT *

****

ACCUMULATORS

ACCUMULATOR	CONTROL VOLUME	INJECTED MASS KG	INJECTED ENTHALPY J
ACC1	CV240-CLA ACCUM	0.68055E+03	0.14170E+09
ACC2	CV340-CLB ACCUM	0.41869E+03	0.87198E+08
ACC3	CV440-CLC ACCUM	0.41835E+03	0.87126E+08

Control function arguments and plot variables

ESF-ACC-RAT(ACCNAM) Liquid mass flow rate for accumulator name ACCNAM.

(units = kg/s)

ESF-ACC-MAS(ACCNAM) Total liquid mass injected from accumulator name ACCNAM.

(units = kg)

ESF-ACC-PRS(ACCNAM) Accumulator name ACCNAM pressure.

(units = Pa)

ESF-ACC-REM(ACCNAM) Total liquid mass remaining in the accumulator name ACCNAM.

(units = kg)

ESF-ACC-ENG(ACCNAM) Integral of energy flow out for the accumulator name ACCNAM.

(units = J)

Comparison of results for different models

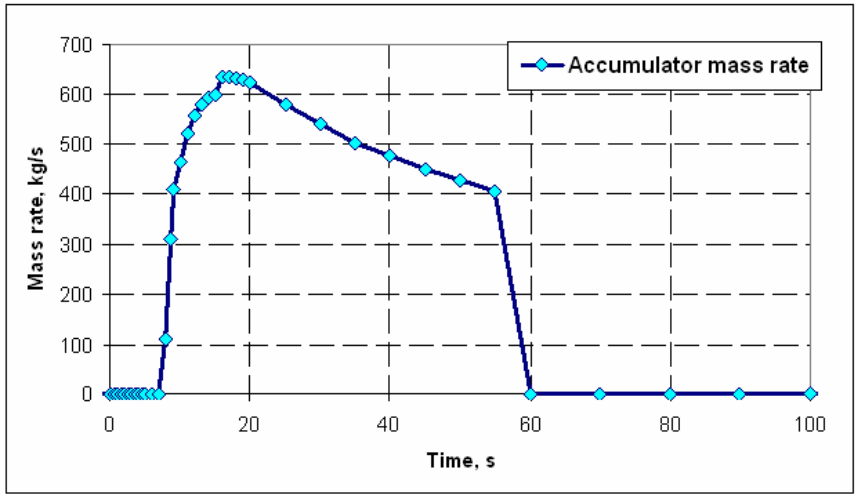

Figure 1. The accumulator mass rate

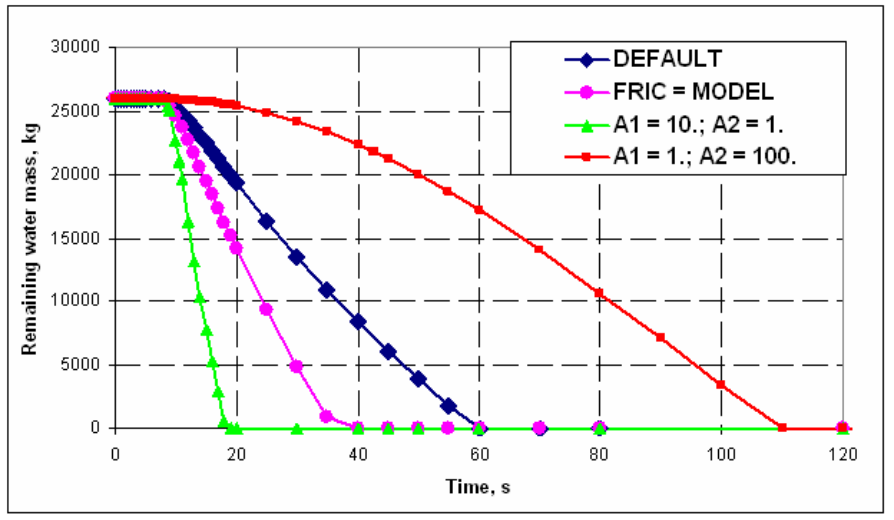

Figure 2. The accumulator remaining water mass

Summary

- The review of new MELCOR features has been presented that will be available in future MELCOR 2.x versions:
  - CF-TF adding and parameters changing from the restart (completed);
  - Activity calculations inside MELCOR code (under development);
  - Simplified accumulator model (completed).

THE END

Thank you for attention

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