SAND2022-8116C

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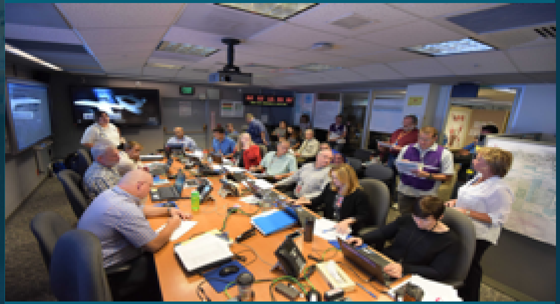
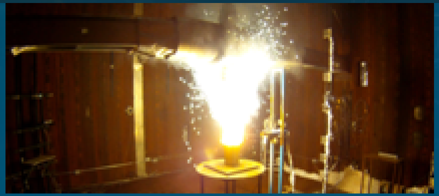
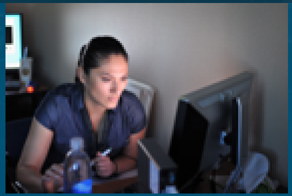
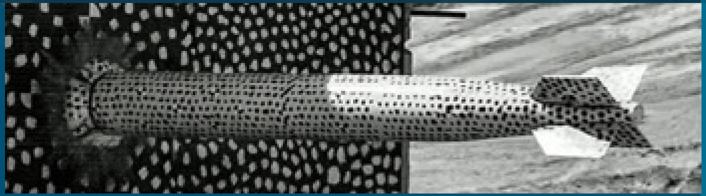
MELCOR for Molten Salt Reactor Modeling









MELCOR Workshop
June 13-17, 2022

PRESENTED BY

Brad Beeny

U.S. DEPARTMENT OF ENERGY NNSA

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Overview

MSR radionuclide transport in theory

- DCH sets class specific powers as normal
- GRTR framework
  - User defined forms and their characteristics
  - Transfer processes between user defined forms and existing built-in forms (aerosol/vapor in pool/atmosphere)
    - CF-directed, or
    - Built-in modeling
  - Provisions for form-wise class mass initialization and sourcing input structures
- GRTR run sequence and theoretical application to MSRs

MSR radionuclide transport in practice

- Input structures
  - GRTR framework (CVH)
  - Form-wise initialization and sourcing (RN1)
- Example : GRTR applied in MSR context

Conclusions

MELCOR MSR
Modeling and Development
Radionuclide Transport - Theory

Physics Package Roles

COR package (still) has no role

- No solid fuel structure to retain and/or release class mass to CVH/RN1
- RN inventories by form and class for CVs are input through RN1 initialization and sourcing (compare to RN1_FPN)

CVH/FL does form-wise class mass advection between CVs

HS present for RN deposition (including GRTR user-defined deposition form)

DCH class specific decay power applies to GRTR form-wise class masses for energy generation

- In CV pool phase for pool-associated GRTR forms
- In CV atmosphere phase for atmosphere-associated GRTR forms
- On HS surfaces for deposition-associated GRTR forms

RN1 retains its aerosol physics capabilities to include interactions with the vapor form (as normal)

GRTR Framework

Generalized Radionuclide Transport and Retention (GRTR) framework entails a capability to define arbitrarily many new radionuclide forms that are either:

- Sectionwise distributed identified with pool phase or atmosphere phase, or
- Non-sectionwise distributed identified with pool phase, atmosphere phase, or HS surface (as in deposition)

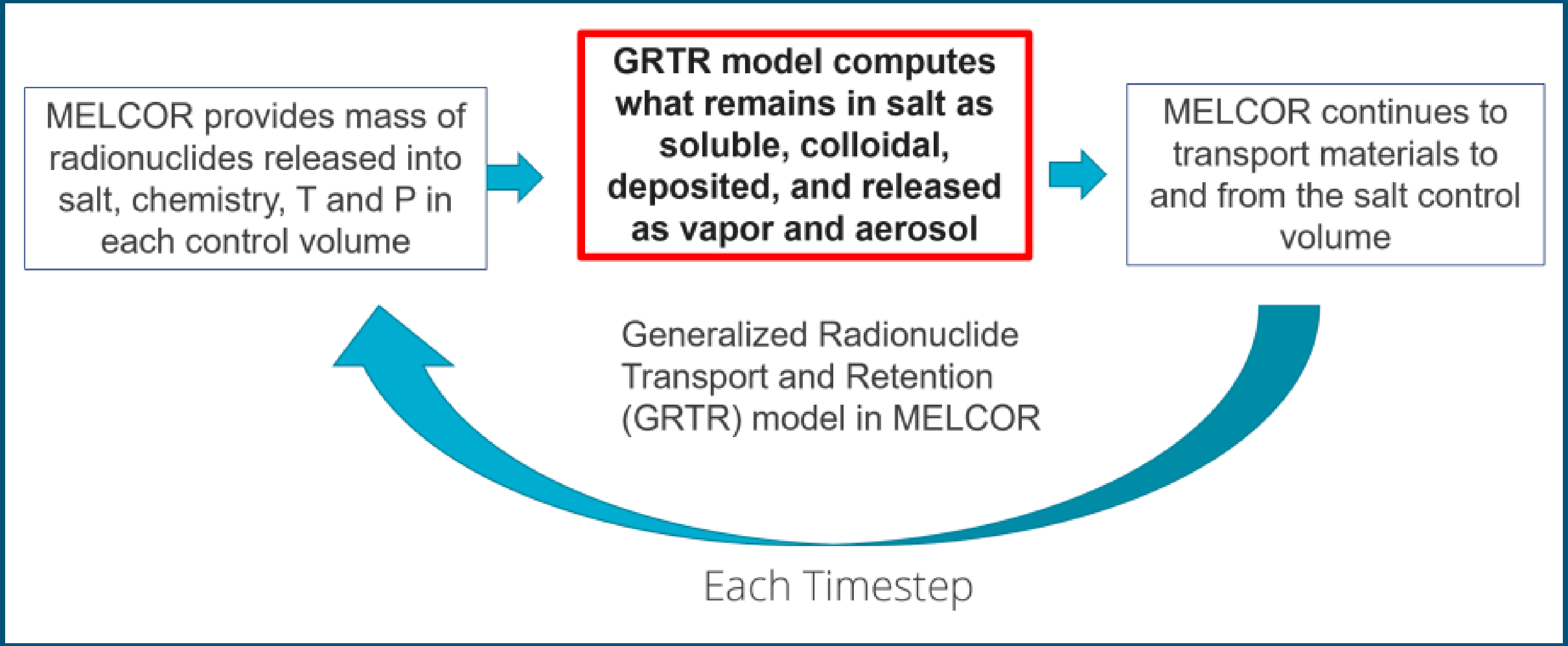
Built-in forms are preserved (vapor and aerosol in the pool or atmosphere phase) as is the HS deposition capability for the built-in forms

Define transfer processes that apply within like RN classes and:

- Between GRTR forms, or
- From GRTR forms to built-in forms, or
- From built-in forms to GRTR forms, but
- NOT from built-in forms to built-in forms…this is beyond the scope of GRTR

Transfer process pairs generally have a unique rule for each RN class, and the rule is either CF-specified or a built-in model (Thermochimica, pure substance vaporization, etc.)

GRTR Run Sequence

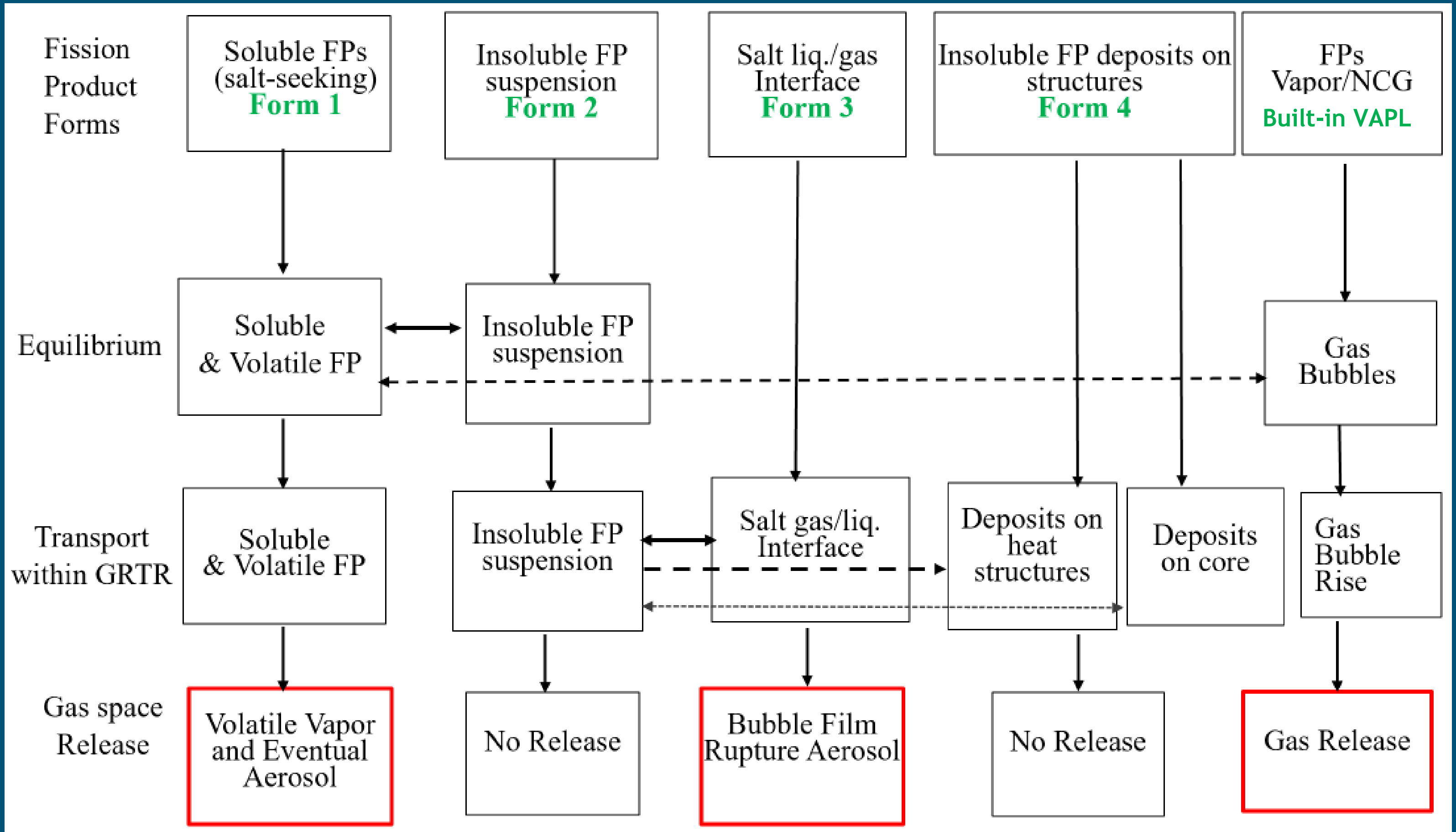


Thermal hydraulic conditions are frozen in a given time-step

GRTR in RN1 computes transfers due to user-specified rules by class

MELCOR continues on to advect form-wise mass and update thermal hydraulic conditions

GRTR Applied to MSRs in Theory



Form 1 – Soluble
- Non-sectionwise distributed
- Identified with pool phase

Form 2 – Insoluble/colloid
- Sectionwise distributed
- Identified with pool phase

Form 3 – Surface insoluble/colloid
- Sectionwise distributed
- Identified with pool phase

Form 4 – Insoluble/colloid HS deposition
- Sectionwise distributed
- Associated with HS deposition surfaces

MELCOR MSR
Modeling and Development
Radionuclide Transport – Practice

Input Structures – CVH GRTR

CV_GRTR – Tabular input declaring each form in turn

- Object name for each form
- Declaration of “type”
  - Sectionwise distributed
  - Non-sectionwise distributed
  - HS deposition
- Phase association (pool or atmosphere)

CV_GRTR – GRTR Form Definitions

Optional.

User defined RN1 forms – section wise distributed, non-section wise distributed, and HS deposition – are characterized in this tabular input.

(1) NFRM
Total number of user-defined forms for GRTR execution
(type = integer, default = none, units = -)

The following data are input as a table with length NFRM:

(1) NGRTR
Table row index
(type = integer, default = none)

(2) FRMNAME
Object name of user-defined form
(type = character, default = none, units = -)

(3) FRMTYPFLG
Flag indicating the type of user-defined form:
(a) 0 - Non-section wise distributed form
(b) 1 - Section wise distributed form
(c) 2 - HS deposition form
(type = integer, default = none, units = -)

(4) PHSFLG
Flag indicating the phase associated with user-defined form:
(a) P - Pool phase
(b) A - Atmosphere phase
(type = character, default = none, units = -)

Example

```
CV_GRTR   1   !  N   FRMNAME     FRMTYPFLG  PHSFLG
                 1   'SOLUBLE'   0          P ! Form named 'Soluble', no sections, pool phase
```

Input Structures – CVH GRTR

CV_GRXFRnn – Tabular input declaring transfer rules fro

- One tabular record per user defined form plus an extra four
- CV_GRTR 1st tabular record corresponds to nn = 1
- CV_GRTR last tabular record corresponds to nn = N
- CV_GRXFR[(N+1)…(N+4)] available for “from” built-in forms
- One or more “to” forms for each given “from” form nn
- Per from/to form-wise pair, either:
  - Give one universally applicable rule to all RN classes, or
  - Give one rule for each RN class in turn
- XFRRULE options are under development and expanding

Example

```
CV_GRXFR01 'Soluble' 11
    1  VAPG        'CS'  'XFR01_FRAC'
    2  'Colloid'  ALL   'XFR02_FRAC'
    4  VAPL        'CS'  'XFR03_FRAC1'
    5  VAPL        'BA'  'XFR03_FRAC2'
    6  VAPL        'I2'  'XFR03_FRAC3'
    7  VAPL        'CE'  'XFR03_FRAC4'
    8  VAPL        'LA'  'XFR03_FRAC5'
    9  VAPL        'UO2' 'XFR03_FRAC6'
    10 VAPL        'CSI' 'XFR03_FRAC7'
    11 AERG        ALL   'XFR03_FRAC1'
```

CV_GRXFRnn – GRTR Formwise Transfer definitions

Optional.

User defined RN1 forms can transform/transfer to other user defined RN1 forms or to conventional RN1 forms like vapor and aerosol (in pool or atmosphere). This tabular input specifies the rules by which such transfers occur. One instance of tabular input (CV_GRXFRnn) is allowed per user defined RN1 form. Four extra instances of tabular input account for transfers from vapor in atmosphere (VAPG), vapor in pool (VAPL), aerosol in atmosphere (AERG), and aerosol in pool (AERL) to user defined forms if necessary. The value of nn should increment from 01 (…02, 03, 04…).

(1) FRMNAME
Object name of user defined RN1 form
(type = character, default = none, units = -)

(2) NFRMXFR
Number of transfers from FRMNAME defined in this tabular input
(type = character, default = none, units = -)

The following data are input as a table with length NFRMXFR:

(1) NGRXFR
Table row index
(type = integer, default = none)

(2) TOFRMNAME
Object name of a form to which FRMNAME transfers, either a user defined form from CV_GRTR or one of the conventional forms (VAPG, VAPL, AERL, AERG)
(type = character, default = none, units = -)

(3) RNCLSNAM
DCH/RN1 class name for which the transfer rule applies. A keyword ‘ALL’ indicates that one rule applies for all DCH/RN1 classes with respect to the given formwise transfer:
(type = character, default = none, units = -)

(4) XFRRULE
Transfer rule definition (CF is the only allowed option for now)
(a) CFNAME - Name of CF that governs transfer from form FRMNAME to form TOFRMNAME with respect to RNCLSNAM
(type = character, default = none, units = -)

Input Structures – RN1 Form-wise Initialization and Sourcing

RN1 initialization

- Sectionwise distributed form (RN1_GRXS like RN1_AG)
- Nonsectionwise distributed form (RN1_GRXN like RN1_V

RN1 sources (under development)

- Sectionwise distributed form (RN1_GRSSS, RN1_GRSS
  - Like RN1_AS and RN1_AS01
  - Limited options for specifying size distribution
  - No need for phasic identification as this is implied by form object name
- Nonsectionwise distributed form (RN1_GRNSS)
  - Like RN1_VS
  - No need for phasic identification as this is implied by form object name

RN1_GRXN – GRTR Formwise Mass Initialization for Non-section Wise Distributed Forms

Optional.

Non-section wise distributed GRTR user defined forms can be initialized in terms of class mass content by control volume in this tabular record.

(1) FRMNAME
Object name of user defined RN1 form
(type = character, default = none, units = -)

(2) NFRMXFR
Number of transfers from FRMNAME defined in this tabular input
(type = character, default = none, units = -)

The following data are input as a table with length NFRMXFR:

(1) NGRXFR
Table row index
(type = integer, default = none)

(2) TOFRMNAME
Object name of a form to which FRMNAME transfers, either a user defined form from CV_GRTR or one of the conventional forms (VAPG, VAPL, AERL, AERG)
(type = character, default = none, units = -)

Example

```
RN1_GRXN 'Soluble' 2 ! User defined GRTR form 'Soluble'
  1 "cvl" CS 1.0 0.002384 ! Put 0.002384 kg of 'Soluble' CS in volume 'cvl', all radioactive
```

Input Example : GRTR Applied to MSR

```
CV_GRTR 4 ! 4 UDEF RN1 forms
    1 'Soluble'   0 P   ! nonsectionwise dist, associated with pool, named Soluble
    2 'Colloid'   1 P   ! sectionwise dist, associated with pool, named Colloid
    3 'FloatCol'  1 P   ! sectionwise dist, associated with pool, named FloatCol
    4 'HsColl'    2 P   ! HS deposition type, associated with pool, named HsColl

CV_GRXFR01 'Soluble' 9 ! Table defining transfer processes from Soluble form
    1  VAPG      'CS'   CF 'XFR01_FRAC'   ! Transfer Soluble to VAPG, rule for CS class only, CF
    2  'Colloid' 'MO'   CF 'XFR02_FRAC'   ! Transfer Soluble to Colloid, rule for MO class only, CF
    3  VAPL      'CS'   CF 'XFR03_FRAC1'  ! Transfer Soluble to VAPL, different class rules to row 9…
     4  VAPL     'BA'   CF 'XFR03_FRAC2'  ! …
    5  VAPL      'I2'   CF 'XFR03_FRAC3'  ! …
    6  VAPL      'CE'   CF 'XFR03_FRAC4'  ! …
    7  VAPL      'LA'   CF 'XFR03_FRAC5'  ! …
    8  VAPL      'UO2'  CF 'XFR03_FRAC6'  ! …
    9  VAPL      'CSI'  CF 'XFR03_FRAC7'  ! …

CV_GRXFR02 'Colloid' 3 ! Table defining transfer processes from Colloid form
    1  'Soluble'   'CE'  CF  'XFR04_FRAC'
    2  'FloatCol'  ALL   CF  'XFR05_FRAC'
    3  'HsColl'    'MO'  CF  'XFR06_FRAC'

CV_GRXFR03 'FloatCol' 2 ! Table defining transfer processes from FloatCol form
    1 'Colloid'  ALL  CF  'XFR09_FRAC'
    2 AERG       ALL  CF  'XFR10_FRAC'
```

```
RN1_GRXN 'Soluble' 2 ! Soluble form initialization
  1 "cv1" CS 1.0 0.002384 ! start with dissolved molten salt
  2 "cv1" MO 1.0 0.0005   ! start with dissolved molten salt

RN1_GRXS collCE "cv1"  MO 1.0 'Colloid' ! colloid form initialization
  1  0.0e-3
  2  0.0e-3
  3  0.0e-3
  4  0.1e-3  ! Nonzero mass begins in section 4
  5  0.0e-3
  6  0.0e-3
  7  0.0e-3
  8  0.0e-3
  9  0.0e-3
  10 0.0e-3
```

Input Example : GRTR Applied to MSR

Existing plot variables expanded when GRTR invoked as appropriate:

- RN1-TOTMAS
- RN1-TYCLAIR, RN1-TYCLLIQ, and RN1-TYCLDEP
- Under development with more to come

New plot variables added that pertain uniquely to GRTR:

- RN1-GRXNONSWMASS (sums TOTAL mass in all non-sectionwise distributed forms for a given RN class)
- RN1-GRXSWMASS (sums TOTAL mass in all sectionwise distributed forms for a given RN class)
- RN1-GRXRADNONSWMASS (sums RAD mass in all non-sectionwise distributed forms for given RN class)
- RN1-GRXRADSWMASS (sums RAD mass in all sectionwise distributed forms for a given RN class)
- Under development with more to come

Under development and future work

- CF arguments
- Text outputs and HTML outputs

Conclusions

Radionuclide transport aspects of MSR modeling in MELCOR were discussed

New input structures were reviewed

Input example on application of GRTR framework to MSR was reviewed