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D. Rochman

Discussion for a decay heat benchmark description (updated slides)

SG12 online meeting, May 18th, 2022

Zertifiziertes Managementsystem STARS ISO 9001

Summary

- General observations
- Feedback
- Proposal for input and output
- Discussion
  (updated on 18/05/2022)
- Summary/wrap up
  (updated after the meeting 19/05/2022)

General observations

- Goal: compare calculated decay heat (DH) for a simple benchmark with understanding
  - Known inputs (code, library, method, constants)
  - Simple geometry & irradiation
- Define outputs: DH, nuclide concentrations, energy releases, fission rates,

Feedback from V. Vallet (CEA)

1. Pincell UO_2 3.7% enriched 235U, with different burnup steps
2. Same for a MOX pincell
3. 2D simulation, reflective boundaries
4. Calculate both UO_2 and MOX case, or only one
5. Fast calculations -> Eventually repeat for different enrichments/burnup

Feedback from S. Sato (CRIEPI)

1. Step 1: Detailed comparisons of data used in each depletion code

   (ex.) direct and cumulative fission yield, recoverable energy by fission (MeV/fission, including its definition), decay energy (alpha, beta, gamma), decay constant, etc.

2. Step 2: Depletion calculation in a simple geometry and condition

   (ex.) 2-D pin cell geometry, constant linear power density, constant void fraction (if BWR) or constant boron concentration (if PWR), etc.

3. Step 3: Detailed comparisons of calculation results

   (ex.) decay heat (alpha, beta, gamma), nuclide inventory, number of fissions of each fissile, etc. at 10, 20, 30, 40, 50, 60 GWd/t -> 0, 1, 2, 3, 5, 10, 15, 20 years cooling.

Feedback from J.F. Martin (OECD)

1. Shall we consider a case close to an assembly with measured DH ?

2. WPRS benchmark from 2006
   https://www.researchgate.net/publication/237631432_International_comparison_of_a_depletion_calculation_benchmark_devoted_to_fuel_cycle_issues_Results_from_the_Phase_1_dedicated_to_PWR-UOx_fuels
   (Takahama PWR case)

PHYSOR-2006, ANS Topical Meeting on Reactor Physics
Organized and hosted by the Canadian Nuclear Society. Vancouver, BC, Canada. 2006 September 10-14

International comparison of a depletion calculation benchmark devoted to fuel cycle issues
Results from the Phase 1 dedicated to PWR-UOx fuels

B. Roque*[1], R. Gregg[2], R. Kilger[3], F. Laugier[4], P. Marimbeau[1], A. Ranta-Aho[5], C. Riffard[1], K. Suyama[6], J.F. Thro[7], M. Yudkevich[8], K. Hesketh[2], E. Sartori[9]

Feedback from J.F. Martin (OECD)

5.3 Results of code to code comparison for calculated decay heat

Table 2 shows that a good agreement is obtained for the total decay heat calculation. However, because of the lack of measurement for this quantity, a conclusion about how accurate the calculation is cannot be drawn.

Table 2: RSD results for assembly and cell calculations of decay heat

	Discharge	5 years	50 years	100 years	300 years
Assembly calculation	3%	2%	1%	2%	2%
Cell calculation	3%	1%	1%	3%	5%

Feedback from A. Launey (ORANO)

- Shall we consider complete fuel ?
- Compensation…

Input example

- Example from SERPENT: http://serpent.vtt.fi/mediawiki/index.php/Tutorial
  – 2D PWR pin-cell, infinite lattice, UO_2, 3%wt

```
% --- Simple 2D PWR pin-cell geometry for Serpent tutorial

/************************
 * Material definitions *
 ************************/

% --- Fuel material (3.0 wt-% enriched uranium dioxide), density 10.1 g/cm3

mat fuel     -10.1
92235.03c    -0.02644492
92238.03c    -0.85505247
 8016.03c    -0.11850261

% --- Cladding material for fuel rod
%     (100 % natural zirconium)

mat clad     -6.55
40000.03c    -1.0

% --- Water at 1.0 g/cm3
%     Defined using atomic fractions for the composition.
%     Hydrogen is flagged as a bound scatterer with the "moder"-card

mat water    -1.0 moder MyThermLib 1001
 1001.03c     2.0
 8016.03c     1.0

% --- Define thermal scattering libraries associated with hydrogen in light water

therm MyThermLib lwj3.00t

/************************
 * Geometry definitions *
 ************************/

% --- Fuel pin structure

pin p1
fuel    0.4025
clad    0.4750
water

% --- Square surface with 1.5 cm side centered at (x,y) = (0,0)

surf s1 sqc 0.0 0.0 0.75

% --- Cell c1 belongs to the base universe 0, is filled with the pin p1
%     and covers everything inside surface s1

cell c1 0 fill p1   -s1

% --- Cell c2 belongs to the base universe 0, is defined as an "outside" cell
%     and covers everything outside surface s1

cell c2 0 outside    s1

/*******************
 * Run parameters *
 *******************/

% --- Neutron population: 5000 neutrons per cycle, 100 active / 20 inactive cycles

set pop 5000 100 20

% --- Boundary condition (1 = black, 2 = reflective, 3 = periodic)

set bc 2
```

Output quantities

- Energy releases
  - Q values for fission (U5, U8, Pu9, Pu1)
  - Energy distribution (E_{kin}, gamma prompt, decay…)

- Specific burnup points
  - k_{inf}
  - Fission rates/initial fissile atoms (total and contributions from U5, U8, Pu9, Pu1)
  - Nuclide concentrations
  - …
- Cooling time fixed: 0, 10, …
  - Decay heat
  - Nuclide concentrations
  - Neutron/gamma emission
  - Delayed fission rates

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The following slides were written during the meeting

Discussion (notes during the discussions)

- Define inputs and outputs
- Run in parallel pincell and assembly (2D)
- Select an assembly with measurement. Define the input quantities for all
- Use a SKB-2006 case (PWR, BWR)
- Recommend to release the MERCI measured data ? (Oystein to ask, edf/cea/??) + draft a letter from SG12
- Was the MERCI pincell critical ? Complexity of the modeling
- PWR easier case ? 47 MWd/kgU, 17x17, 3.4 %
- Sent a table to fill “a cross” for pincell, PWR or BWR cases

Discussion (notes during the discussions)

- Outputs

- Kinf, nuclide concentrations, fission rates (separate between 4 main actinides)
- DH, neutron/gamma, activities (contributions from different isotopes)
- Make a list of isotopes (+provide top 20 for DH by different codes with %, as a function of cooling time)
- Delayed fission
- Time scale
- Sensitivity analysis

- Define specific inputs

- Libraries, codes, decay data,…

- Existing gaps ? Nuclear data ?

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The following slides were written after the meeting

Discussion (notes after the discussion)

Brief summary from the discussion part, using the notes from J.F. Martin and D. Rochman

- 34 Participants:

A. Algora	F. Alvarez Velarde	O. Buss	O. Bremnes	O. Cabellos	S. Caruso
R. Dagan	D. Foligno	F. Fernandez Lopez	L. Giot	F. Gomez Salcedo	K. Govers
S. Hakkinen	V. Hannstein	A. Hoefer	G. Ilas	P. Juutilainen	S. Lahaye
V. Leger	J.F. Martin	A. Koning	M. Kromar	A. Launey	L. McManniman
D. Rochman	S. Sato	M. Seidl	P. Schillebeeckx	A. Shama	T. Simeonov
A. Sjoland	S. Tittlebach	A. Tsilanizara	E. Vlassopoulos		

Discussion (notes after the discussion)

Relevant remarks/discussion chronologically ordered:

- K. Govers: supported the idea to start with a pincell
- J.F. Martin: pincell, possibly followed by a real case assembly
- A. Sjoland: supported the idea of a pincell too
- L. Giot: Remark on the previous work from B. Roque (Takahama sample): not really suited for our benchmark
- G. Ilas:
  - notes importance of calculating assemblies since this is what being stored and that's the application case
  - Calculate cell pins, ok, they're different, but the conclusions are still the same in the end
  - Importance to calculate fuel assemblies as a whole!
- A. Launay:
  - Agrees with G. Ilas
  - also notes compensation effects that may contribute to the calculation. Hence the importance to calculate full assemblies
- O. Bremnes:
  - recommends to study a simple situation
  - Code validation focused. Simplest possible approach. Although final aim is to understand decay heat of assemblies. Recommend to start with pin cell and then move towards more complete modelling
- S. Hakkinen: Start with pin cell to start simple and in the future move to 3d effects esp. for VVER (BWR?) - void fraction effects vs elevation
- M. Seidl:
  - need to take into account the calculations based on “standards” (e.g. DIN)
  - Suggest to start with a simple case, and move to a more complex one

Discussion (notes after the discussion)

- A. Sjoland:
  - notes that calorimetry was performed at pellet level.
  - Timeline for this exercise would help to define the strategy
  - whether we go bottom up (pellet / cell / assembly), if we have enough resources for this
  - Also, what do we expect to learn in terms of transposition / representativity between cell and assembly
- M. Kromar:
  - Pincell is useful, but not representative,
  - avoid 3D (too complex for now)
  - Compare codes/libraries/methods for a particular problem
- O. Cabellos: proposed to provide a nuclide inventory, and to perform decay calculations (no depletion)
- F. Alvarez Velarde: Agrees with Oscar, and recall the importance of nuclear data and uncertainty propagation
- J.F. Martin:
  - Link with WPNCS SG10 for ND & inventory calculations including after cooling time.
  - Enhance cross collaboration between both groups. Coordinators not able to join today.
- A. Koning
  - Output of the group to provide the needs in terms of nuclear data and their uncertainties
  - Uncertainty: simple approach is to switch from one library to the other

Summary/Wrap up

The following recommendations were supported by the group:

1. Perform in parallel 2D calculations for an assembly and one of its pincell
2. Select a PWR assembly from the SKB 2006 campaign for comparison with measured decay heat
3. Provide to participants all relevant geometry/irradiation information (*e.g.* irradiation steps, cooling steps)
4. Ask participants the "maximum" information about their simulations: inputs (*e.g.* libraries, energy releases…)

5. Provide the following output
   - K_{inf}, nuclide concentrations, fission rates (separate between 4 main actinides)
   - Decay heat, neutron/gamma, activities (contributions from different isotopes)
   - Make a list of isotopes (+provide top 20 for DH by different codes with %, as a function of cooling time)
   - Delayed fission
   - Possibly sensitivity analysis
6. Assessing gaps, for instance in nuclear data
7. Provide a letter of interest from the SG12 for the availability of the MERCI experiment

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