

Decay Heat (DCH) Package Reference Manual

The MELCOR decay heat (DCH) package models the decay heat power resulting from the radioactive decay of fission products. Decay heat is evaluated for core materials in the reactor vessel and cavity and for suspended or deposited aerosols and gases. MELCOR couples thermal-hydraulic processes and fission product behavior during the calculation.

Both the radionuclides present in the reactor at the time of the accident and the radionuclide daughter products contribute to the decay heat. In the calculation of decay heat, MELCOR does not explicitly treat each decay chain, since detailed tracking of radionuclide decay chains would be too costly. When the RadioNuclide package is active, the decay heat is calculated for each radionuclide class by using pre-calculated tables from ORIGEN calculations. If the RadioNuclide package is not active, the whole-core decay heat is computed from one of several possible user-specified calculations.

This Reference Manual describes the various models and options available in the DCH package. User input for these models and options is described in the DCH Package Users' Guide.

DCH Package Reference Manual

Contents

1. Introduction5

2. Elemental and Radionuclide Class Decay Heat5

 2.1 SANDIA-ORIGEN Calculations5

 2.2 Radionuclide Classes.....7

3. Whole Core Decay Heat Calculation8

 3.1 Summation of ORIGEN Data9

 3.2 ANS Standard Calculation9

 3.3 User-Defined Functions14

References15

List of Tables

Table 2.1. Default Radionuclide Classes and Member Elements8

Table 3.1. Tabular Values from ANS Standard [3] Used in MELCOR.....10

Table 3.2. DCH Package Input Variables for ANS Decay Heat Power14

DCH Package Reference Manual

1. Introduction

The MELCOR Decay Heat Power (DCH) package models the heating from the radioactive decay of fission products. Decay heat power is evaluated for the fission products assumed to reside in reactor core materials, cavity materials, and in suspended or deposited aerosols and vapors. Decay heat power levels as a function of time are supplied as a utility function within MELCOR that may be called by other phenomenological packages. The DCH package is not involved in the calculation of fission product transport or chemical interactions. These processes are calculated by the RadioNuclide (RN) package (see the RN Package Reference Manual).

Both the radionuclides present in the reactor core and/or cavity from the time of reactor shutdown and the radionuclide daughters from decay contribute to the total decay heat power. In the calculation of decay heat power, the DCH package does not explicitly treat decay chains. Detailed tracking of radionuclide decay chains was seen as computationally costly and too detailed for MELCOR. Instead, when the RN package is active, elemental decay heat power information based on ORIGEN calculations[1,2] is summed into the RN class structure, as described in Section 2.

There are also several options for calculating decay heat power when the RN package is not active (that is, when tracking of fission products is not desired). These are called *whole-core calculations* in the DCH package, although they may be applied to cavity inventories of melt debris as well, and are described in Section 3.

2. Elemental and Radionuclide Class Decay Heat

The DCH package models the decay heat power as a function of time and the total initial inventories of individual *elements*. The default decay heat curves and inventories were obtained from ORIGEN calculations [1], as described in Section 2.1. The grouping of elements into classes for use by the RadioNuclide package is described in Section 2.2.

2.1 SANDIA-ORIGEN Calculations

Calculations were made for prototypical BWR and PWR reactors using the Sandia National Laboratories version of the ORIGEN computer code, and tables of the associated fission product initial inventories and their decay heat powers out to ten days were generated [1,2]. In these tables, all isotopes of an element were summed, and daughters were assumed to remain with the parents. This resulted in 29 elemental groups accounting for over 99% of the decay heat power out to at least two days after reactor shutdown.

DCH Package Reference Manual

The base case ORIGEN run for a PWR used the following assumptions:

| | |
|----|--|
| 1. | 3412 MWt Westinghouse PWR |
| 2. | end-of-cycle equilibrium core |
| 3. | three region core, each initially loaded with fuel enriched to 3.3% U-235 |
| 4. | constant specific power density of 38.3 MW per metric ton of U |
| 5. | three-year refueling cycle |
| 6. | 80% capacity factor |
| 7. | three regions having burnups of 11,000, 22,000, and 33,000 MWd per metric ton of uranium |

The base case ORIGEN run for a BWR used the following assumptions:

| | |
|----|---|
| 1. | 3578 MWt General Electric BWR |
| 2. | five types of assembly groups |
| 3. | initial enrichment for assemblies, either 2.83% or 2.66% U-235, depending on assembly group |
| 4. | assemblies in core for either 3 or 4 years, depending on assembly group |
| 5. | refueled annually |
| 6. | 80% capacity factor |

Within the RN package, daughter isotopes are assumed to be transported along with the parents. Thus, the daughter products are assumed to retain the physical characteristics of their parents. This assumption may not be appropriate in some cases, but the ORIGEN analyses showed that the decay heat from the parent elements is generally much greater than that of the daughter products. Because of these considerations, the decay heat of an element's daughter products is included in the decay heat tabulation for the parent element.

The ORIGEN decay heat data are represented in the DCH package in normalized form as decay heat power per unit of reactor operating power at 28 time values after reactor shutdown for each of the 29 elements treated. The ORIGEN results for the PWR were nearly the same as those for the BWR during the first few days after reactor shutdown (within 4%). This similarity results because (1) both reactors use thermal fission of U-235 and Pu-239 as the power source, and (2) decay power during the first few days after shutdown results principally from short-lived radionuclides. Inventories of short-lived radionuclides are proportional to reactor operating power and are relatively insensitive to reactor design and fuel management. Therefore, a single table of normalized decay powers out to 10 days after shutdown is used in the DCH package as representative of both PWRs and BWRs. However, the user may redefine the decay heat power for a given

element (or create one for a “new” element) using the DCHNEMnn00 and DCHNEMnnmm input records, or the user may apply multipliers to the default curves with sensitivity coefficients 3210 and 3211, as described in the DCH Package Users’ Guide.

In general, mass inventories of elements are sensitive to fuel burnup and reactor design. Therefore, two default mass inventories are included in the DCH package for the representative BWR and PWR used in the ORIGEN calculations. The inventory masses of the elements, normalized to grams per unit of reactor operating power (for the PWR and for the BWR), were given by ORIGEN at four times in the equilibrium fuel cycle: start-of-cycle, one-third point, two-thirds point, and end-of-cycle. By default, end-of-cycle values are used, but the user may specify a different fraction of the equilibrium cycle (through sensitivity coefficient 3212), in which case linear interpolation is used to determine the elemental masses at shutdown. For analyses of specific reactors, for which fission product inventories are known (perhaps through separate ORIGEN calculations), the MELCOR user can directly input the element masses using the DCHNEMnn00 input record (see the DCH Package Users’ Guide).

The decay heat power and mass for each element were summed over only core fission products and actinides. Thus, the total mass of zirconium in the core at the time of shutdown does not include the mass of the Zr in core structural materials.

The decay heat power for a given element at a certain time is estimated by logarithmic interpolation in time of the normalized decay heat powers and dividing by the normalized mass of the particular element in the reactor at the time of shutdown (which includes the masses of its daughter products and is therefore constant) to get a decay heat power per unit mass of the element.

2.2 Radionuclide Classes

The 29 radioactive elements treated by the DCH package are further grouped into chemical classes for tracking by the RN package. Table 2.1 lists the default classes treated by the RN and DCH packages. The remaining elements that do not contribute significant decay heat (< 1%) are enclosed in parentheses. More discussion on classes and their properties is given in the RN Package Reference Manual.

The decay heat power is computed for each class by weighting the elemental decay heats by the relative mass of each element in the class given by the ORIGEN calculations described in Section 2.1. The user may redefine the default class element compositions or define the composition of new classes through input (see input records DCHCLSnnn0 and DCHCLSnnnm in the DCH Package Users’ Guide).

All packages that require decay heat power (i.e., COR, CAV, and RN) access a utility provided by the RN package to calculate the total power for the RN class masses residing at a particular location. When the RN package requests a class decay heat power from the

DCH Package Reference Manual

DCH package for any problem time within the range of the present timestep, the returned answer is the average of the class decay heat at the current problem time and the class decay heat at the end of the timestep. Thus, the energy balance calculation is done consistently in the DCH package and the other MELCOR packages distributing the decay heat power. The DCH package edits also reflect this averaging. However, since the first timestep size is not known during the MELGEN setup phase, the MELGEN edit does not show exactly the same decay heat powers as those shown in the first MELCOR edit.

Table 2.1. Default Radionuclide Classes and Member Elements

| Class Number and Name | Member Elements |
|-------------------------------------|---|
| 1. Noble gases | Xe, Kr, (Rn), (He), (Ne), (Ar), (H), (N) |
| 2. Alkali Metals | Cs, Rb, (Li), (Na), (K), (Fr), (Cu) |
| 3. Alkaline Earths | Ba, Sr, (Be), (Mg), (Ca), (Ra), (Es), (Fm) |
| 4. Halogens | I, Br, (F), (Cl), (At) |
| 5. Chalcogens | Te, Se, (S), (O), (Po) |
| 6. Platinoids | Ru, Pd, Rh, (Ni), (Re), (Os), (Ir), (Pt), (Au) |
| 7. Transition Metals | Mo, Tc, Nb, (Fe), (Cr), (Mn), (V), (Co), (Ta), (W) |
| 8. Tetravalents | Ce, Zr, (Th), Np, (Ti), (Hf), (Pa), (Pu), (C) |
| 9. Trivalent | La, Pm, (Sm), Y, Pr, Nd, (Al), (Sc), (Ac), (Eu), (Gd), (Tb), (Dy), (Ho), (Er), (Tm), (Yb), (Lu), (Am), (Cm), (Bk), (Cf) |
| 10. Uranium | U |
| 11. More Volatile Main Group Metals | (Cd), (Hg), (Pb), (Zn), As, Sb, (Tl), (Bi) |
| 12. Less Volatile Main Group Metals | Sn, Ag, (In), (Ga), (Ge) |
| 13. Boron | (B), (Si), (P) |
| 14. Water | (Wt) |
| 15. Concrete | (Cc) |

3. Whole Core Decay Heat Calculation

If the RN package is not active in MELCOR, the decay heat power is calculated for the entire core. The user may specify one of four possible options on input record DCHDECPOW for this calculation:

- (1) a summation of decay heat data from the ORIGEN-based fission product inventories for representative BWRs and PWRs [1,2], scaled if necessary,
- (2) the 1979 ANS standard for decay heat power [3],

- (3) a user-specified tabular function of whole-core decay as a function of time, or
- (4) a user-specified control function to define decay heat.

Each option is described in the following subsections.

3.1 Summation of ORIGEN Data

As discussed in Section 2, a Sandia version of ORIGEN [2] has been used to perform decay heat calculations for prototypical PWR and BWR systems [1]. For the whole-core calculation, the tabulated results of the ORIGEN calculation are summed to produce a total reactor decay heat power, P_{WC} . No elemental or class information is retained; a single decay power value is returned when called by other packages. This is the default whole-core calculation and is the same for PWRs and BWRs.

3.2 ANS Standard Calculation

MELCOR can compute the total decay heat power from the American Nuclear Society's National Standard for light water reactors [3]. This standard prescribes fission product decay heat power for reactor operating histories. Currently, the DCH package uses a user-specified operating time (input on record DCHOPRTIME) with a constant reactor power, and it also assumes an instantaneous shutdown. The standard prescribes the recoverable energy release rates from fission product decay, but it does not specify the spatial distribution of the deposition of the energy in the reactor materials. This aspect of the problem is reactor specific and must be dealt with by the MELCOR Core package.

The decay heat power is related to the operating power of the reactor via the fission rate and the recoverable energy per fission during operation. The ANS standard assumes that the energy release per fission is independent of time and depends upon the energy spectrum of the neutron flux in the operating reactor and the composition of the reactor core. The energies per fission for U-235, Pu-239, and U-238 are defined in sensitivity coefficient array 3201.

Decay heat power from activation products in reactor structural materials is not specified in the standard, but decay heat powers from U-239 and Np-239 as prescribed by the standard are implemented in the DCH package. The effect of neutron capture in fission products is accounted for by using a formula from the ANS standard for the correction out to a time-since-shutdown of 10^4 s. The DCH package then uses Table 10 from the standard that sets an upper bound on the effect of neutron capture and provides a conservative estimate of the decay heat power. The values from this table are reproduced here in Table 3.1. Because of the conservatism of this table, the ANS standard decay heat power actually contains a discontinuity manifested by a small increase at 10^4 seconds.

DCH Package Reference Manual

MELCOR uses the tables from the ANS standard that prescribe decay heat power from products resulting from the fission of the major fissionable nuclides present in LWRs, specifically thermal fission of U-235 and Pu-239, and fast fission of U-238. These values (from ANS standard Tables 4, 5, and 6) are also reproduced in Table 3.1. The values at the time of shutdown ($t = 0.0$) were calculated from Tables 7, 8, and 9 of the standard.

Table 3.1. Tabular Values from ANS Standard [3] Used in MELCOR

| Time After Shutdown, (sec) | Neutron Capture Correction Factor $G_{\max}(t)$ | Decay Heat Power $F(T, \infty)$ | | |
|----------------------------|---|---------------------------------|-------------------|------------------|
| | | ^{235}U | ^{239}Pu | ^{238}U |
| 1.0 | 1.020 | 1.231E+1 | 1.027E+1 | 1.419E+1 |
| 1.5 | 1.020 | 1.198E+1 | 1.003E+1 | 1.361E+1 |
| 2.0 | 1.020 | 1.169E+1 | 9.816 | 1.316E+1 |
| 4.0 | 1.021 | 1.083E+1 | 9.206 | 1.196E+1 |
| 6.0 | 1.022 | 1.026E+1 | 8.795 | 1.123E+1 |
| 8.0 | 1.022 | 9.830 | 8.488 | 1.070E+1 |
| 1.0E+1 | 1.022 | 9.494 | 8.243 | 1.029E+1 |
| 1.5E+1 | 1.022 | 8.882 | 7.794 | 9.546 |
| 2.0E+1 | 1.022 | 8.455 | 7.476 | 9.012 |
| 4.0E+1 | 1.022 | 7.459 | 6.707 | 7.755 |
| 6.0E+1 | 1.022 | 6.888 | 6.251 | 7.052 |
| 8.0E+1 | 1.022 | 6.493 | 5.929 | 6.572 |
| 1.0E+2 | 1.023 | 6.198 | 5.685 | 6.217 |
| 1.5E+2 | 1.023 | 5.696 | 5.262 | 5.621 |
| 2.0E+2 | 1.025 | 5.369 | 4.982 | 5.241 |
| 4.0E+2 | 1.028 | 4.667 | 4.357 | 4.464 |
| 6.0E+2 | 1.030 | 4.282 | 3.993 | 4.072 |
| 8.0E+2 | 1.032 | 4.009 | 3.726 | 3.804 |
| 1.0E+3 | 1.033 | 3.796 | 3.516 | 3.598 |
| 1.5E+3 | 1.037 | 3.408 | 3.128 | 3.220 |
| 2.0E+3 | 1.039 | 3.137 | 2.857 | 2.954 |
| 4.0E+3 | 1.048 | 2.534 | 2.276 | 2.366 |
| 6.0E+3 | 1.054 | 2.234 | 2.002 | 2.078 |
| 8.0E+3 | 1.060 | 2.044 | 1.839 | 1.901 |

Table 3.1. Tabular Values from ANS Standard [3] Used in MELCOR

| Time After Shutdown, (sec) | Neutron Capture Correction Factor | Decay Heat Power $F(T, \infty)$ | | |
|-------------------------------|-----------------------------------|---------------------------------|-------------------|------------------|
| | $G_{\max}(t)$ | ^{235}U | ^{239}Pu | ^{238}U |
| 1.0E+4 | 1.064 | 1.908 | 1.727 | 1.777 |
| 1.5E+4 | 1.074 | 1.685 | 1.548 | 1.578 |
| 2.0E+4 | 1.081 | 1.545 | 1.437 | 1.455 |
| 4.0E+4 | 1.098 | 1.258 | 1.204 | 1.204 |
| 6.0E+4 | 1.111 | 1.117 | 1.081 | 1.077 |
| 8.0E+4 | 1.119 | 1.030 | 1.000 | 9.955E-1 |
| 1.0E+5 | 1.124 | 9.691E-1 | 9.421E-1 | 9.383E-1 |
| 1.5E+5 | 1.130 | 8.734E-1 | 8.480E-1 | 8.459E-1 |
| 2.0E+5 | 1.131 | 8.154E-1 | 7.890E-1 | 7.884E-1 |
| 4.0E+5 | 1.126 | 6.975E-1 | 6.634E-1 | 6.673E-1 |
| 6.0E+5 | 1.124 | 6.331E-1 | 5.944E-1 | 6.002E-1 |
| 8.0E+5 | 1.123 | 5.868E-1 | 5.462E-1 | 5.530E-1 |
| 1.0E+6 | 1.124 | 5.509E-1 | 5.097E-1 | 5.171E-1 |
| 1.5E+6 | 1.125 | 4.866E-1 | 4.464E-1 | 4.544E-1 |
| 2.0E+6 | 1.127 | 4.425E-1 | 4.046E-1 | 4.125E-1 |
| 4.0E+6 | 1.134 | 3.457E-1 | 3.163E-1 | 3.224E-1 |
| 6.0E+6 | 1.146 | 2.983E-1 | 2.741E-1 | 2.784E-1 |
| 8.0E+6 | 1.162 | 2.680E-1 | 2.477E-1 | 2.503E-1 |
| 1.0E+7 | 1.181 | 2.457E-1 | 2.282E-1 | 2.296E-1 |
| 1.5E+7 | 1.233 | 2.078E-1 | 1.945E-1 | 1.941E-1 |
| 2.0E+7 | 1.284 | 1.846E-1 | 1.728E-1 | 1.717E-1 |
| 4.0E+7 | 1.444 | 1.457E-1 | 1.302E-1 | 1.299E-1 |
| 6.0E+7 | 1.535 | 1.308E-1 | 1.099E-1 | 1.113E-1 |
| 8.0E+7 | 1.586 | 1.222E-1 | 9.741E-2 | 1.001E-1 |
| 1.0E+8 | 1.598 | 1.165E-1 | 8.931E-2 | 9.280E-2 |
| 1.5E+8 | 1.498 | 1.082E-1 | 7.859E-2 | 8.307E-2 |
| 2.0E+8 | 1.343 | 1.032E-1 | 7.344E-2 | 7.810E-2 |
| 4.0E+8 | 1.065 | 8.836E-2 | 6.269E-2 | 6.647E-2 |

Table 3.1. Tabular Values from ANS Standard [3] Used in MELCOR

| Time After Shutdown, (sec) | Neutron Capture Correction Factor | Decay Heat Power $F(T, \infty)$ | | |
|----------------------------|-----------------------------------|---------------------------------|-------------------|------------------|
| | $G_{\max}(t)$ | ^{235}U | ^{239}Pu | ^{238}U |
| 6.0E+8 | 1.021 | 7.613E-2 | 5.466E-2 | 5.746E-2 |
| 8.0E+8 | 1.012 | 6.570E-2 | 4.783E-2 | 4.979E-2 |
| 1.0E+9 | 1.007 | 5.678E-2 | 4.195E-2 | 4.321E-2 |

For the ANS standard option, the whole-core power (wc), $P_{wc}(t)$, is given by:

$$P_{wc}(t) = M_{user} G(t) \sum_{i=1}^3 \frac{P_i F_i(t, T)}{Q_i} + P_{dHE}(t, T) \quad (3.1)$$

where

- M_{user} = user-input multiplier (default = 1.0)
- $G(t)$ = neutron capture correction factor
- t = time since reactor shutdown(s)
- i = index for fissioning nuclides: U-235, Pu-239, U-238
- T = reactor operating time(s)
- P_i = power from fissioning of nuclide i (W)
- $F_i(t, T)$ = decay power due to nuclide i (MeV/fission)
- Q_i = energy per fission of nuclide i (MeV/fission)

The additive term $P_{dHE}(t, T)$ is the decay power from U-239 and Np-239, prescribed by the ANS standard as:

$$P_{dHE}(t, T) = \sum_{i=1}^3 \frac{P_i}{Q_i} [F_{^{239}\text{U}}(t, T) + F_{^{239}\text{Np}}(t, T)] \quad (3.2)$$

where

$$F_{239U}(t, T) = E_{239U} R [1 - \exp(-\lambda_1 T)] \exp(-\lambda_1 t) \quad (3.3)$$

$$F_{239Np}(t, T) = E_{239Np} R \left\{ \lambda_1 [1 - \exp(-\lambda_2 T)] \right\} \exp(-\lambda_2 t) / (\lambda_1 - \lambda_2) \\ - \lambda_2 [(1 - \exp(-\lambda_1 T)) \exp(-\lambda_1 t) / (\lambda_1 - \lambda_2)] \quad (3.4)$$

E_{239U} = average energy from decay of one U-239 atom (MeV/atom)

E_{239Np} = average energy from decay of one Np-239 atom (MeV/atom)

R = number of atoms of U-239 produced per second per fission per second at shutdown

λ_1 = decay constant for U-239

λ_2 = decay constant for Np-239

For shutdown times less than 10^4 s, the neutron capture correction factor $G(t)$ is given by the ANS standard as:

$$G(t) = 1.0 + (3.24 \times 10^{-6} + 5.23 \times 10^{-10} t) T^{0.4} \psi \quad (3.5)$$

where ψ is the number of fissions per initial fissile atom (user input). For times greater than 10^4 s, $G(t)$ is given in tabular form by $G_{\max}(t)$, which may be input as sensitivity coefficients or allowed to default to the values given by the ANS standard.

$F_i(t, T)$ is used in tabular form as given in the ANS standard. The values at each time t are found by logarithmic interpolation between successive points in the ANS tables. This form of evaluation does not have significant accuracy loss and is much faster when compared with the primary ANS formulation expressed as a sum of exponentials.

Table 3.2 lists the MELCOR input variables and sensitivity coefficients that are used to implement the ANS decay heat power calculation.

3.3 User-Defined Functions

The whole-core decay heat power, P_{wc} , can be defined by a user-input tabular function of time after shutdown. Alternatively, P_{wc} can be defined as a user-specified control function of other MELCOR system variables. Either option may be specified on input record DCHDECPOW.

Table 3.2. DCH Package Input Variables for ANS Decay Heat Power

| ANS Parameter | MELCOR Variable | Input Record |
|----------------------------------|-------------------------------------|----------------------------------|
| $P_i, i = 1, 2, 3$ | U235P, PU239P, U238P | DCHFPOW |
| T | OPRTIM | DCHOPRTIME |
| ψ | PSINC | DCHNCPSI |
| $Q_i, i = 1, 2, 3$ | FEU235, FEP239, FEU238 | SC3201(I), I=1,2,3 |
| t , time in tabular functions | TIMDCH(I), I=1,...,56 | SC3202(I), I=1,...,56 |
| $F_i(t, \infty), i = 1, 2, 3$ | DCHPOW(I,J), I=1,...,56, J=1,2,3 | SC3203(I), I=1,...,56 J=1,2,3 |
| $G_{MAX}(t) \{10^4 < t < 10^9\}$ | CAPNEU(I), I=1,...,56 | SC3204(I), I=1,...,56 |
| R | R | SC3205(1) |
| E_{239U} | E239U | SC3205(2) |
| E_{239Np} | E239NP | SC3205(3) |
| λ_1 | DCU | SC3205(4) |
| λ_2 | DCNP | SC3205(5) |
| M_{user} | ANSMUL | SC3200(1) |

References

1. R. M. Ostmeyer, An Approach to Treating Radionuclide Decay Heating for Use in the MELCOR Code System, NUREG/CR-4169, SAND84-1404, Sandia National Laboratories, Albuquerque, NM (May 1985).
2. D. E. Bennett, SANDIA-ORIGEN User's Manual, NUREG/CR-0987, SAND79-0299, Sandia National Laboratories, Albuquerque, NM (October 1979).
3. American Nuclear Society Standards Committee Working Group ANS-5.1, American National Standard for Decay Heat Power in Light Water Reactors, ANSI/ANS-5.1-1979, American Nuclear Society, La Grange Park, IL (1979).