KW Consulting Fission Gas Release Model

Programmer's Guide

The KW Consulting fission gas release model has been coded as a Fortran subroutine. It is expected that this subroutine will be called from a driver routine which will be the input and output interface between the KW Consulting model calculations and the fuel rod performance code that uses the KW Consulting model.

The KW Consulting model subroutine is intended to be called in a loop over the axial segment indices for the fuel rod geometry. The format of the call is

```
      call KWfgr(ifirststep,iter,j,ngapfrac,nradial,bubos,bueos,
     &    gasprodrt,pressMPa,eostime,dtime,tkring,gfiss,
     &    grainradbos,grainradeos,dtaumax,fringstbl,fringrad,
     &    Ntotrad,vbubble)
```

where the subroutine input arguments are

```
ifirststep   - flag for the first time step, for array initialization
iter         - gas release calculation iteration counter
j            - fuel axial section index
ngapfrac     - switch to activate calculation of radioactive isotope
               gap fractions (= 0: gap fractions not calculated;
               = 1: gap fractions calculated)
nradial      - number of fuel radial rings in the fuel rod geometry
bubos        - beginning-of-time-step local burnup (MWd/MTU)
bueos        - end-of-time-step local burnup (MWd/MTU)
gasprodrt    - stable fission gas production rate in the current
               time step (mols/sec-m**3)
pressMPA     - rod internal pressure (MPa)
eostime      - end-of-time-step time (sec)
dtime        - time step time increment (sec)
tkring       - fuel ring temperature (K)
gfiss        - fission gas mole fraction in the gas in the rod void
               volume (-)
grainradbos  - beginning-of-time-step grain radius (m)
grainradeos  - end-of-time-step grain radius (m)
dtaumax      - maximum time substep size (-)
```

and the subroutine output arguments are

```
fringstbl    - stable fission gas fractional release in each radial ring
fringrad     - radioactive isotope fractional release in each radial
               ring
Ntotrad      - total radioactive isotope concentration in each radial
               ring (mols/m**3) (output to facilitate calculation of the
               whole rod gap fractions)
vbubble      - grain boundary bubble volume fraction in each radial ring
               (-)
```

Currently the KWfgr subroutine is dimensioned for a maximum of 50 radial rings in each axial segment, but this can be changed to meet customer code requirements. The input arguments `bubos`, `bueos`, `gasprodrt`, `tkring`, `grainradbos` and `grainradeos` are 1 dimensional arrays for the values of these variables in each radial ring in the current axial segment. The output arguments `fringstbl` and `vbubble` are also 1 dimensional arrays for the values of these variables in each radial ring in the current axial segment. The output arguments `fringrad` and `Ntotrad` are 2 dimensional arrays, with the first index the radial ring index and the second index the radioactive isotope species index. `Ntotrad` is a real variable. Currently `KWfgr` calculates the radioactive isotope fractional release for 10 isotopes: Kr-85, Kr-87, Kr-88, Xe-133, Xe-135, Cs-134, Cs-137, I-131, I-133 and I-135, in that order, but this can also be changed to meet customer code and licensing calculation requirements.

In addition, a common block, KWfgrcal, is used to transfer the model calibration constants from the interface driver routine to the KWfgr subroutine. The variables in the KWfgrcal common block are

```
 common / KWfgrcal / Aalpha1, Aalpha2, Aalpha3, Aalpha4, Adiff,
& Aarad, ANsat, AQdiff1, AQdiff2, AQdiff3, Asovd, Aadir, Aaredldir,
& Aaredlres, fmicro, fsweep, Akor, Ahibu1, Ahibu2
```

where

```
Aalpha1      - calibration factor for the resolution constant
Aalpha2-4    - constants determining the resolution constant burnup
               dependence
Aarad        - calibration factor for post-interlinkage radioactive
               isotope grain boundary bubble gas release
Adiff        - calibration factor for diffusion constant
Ahibu1       - calibration factor for the knockout/recoil release high
               burnup correction
Ahibu2       - calibration factor for the burnup dependence of the
               knockout/recoil high burnup correction (Mwd/MtU)
Akor         - calibration factor for knock-out/recoil release
               proportional to burnup
ANsat        - calibration factor for grain bubble gas concentration at
               saturation
AQdiff1      - calibration factor for the activation energy of the
               first term in the diffusion coefficient
AQdiff2      - calibration factor for the activation energy of the
               second term in the diffusion coefficient
AQdiff3      - calibration factor for the activation energy of the
               third term in the diffusion coefficient
Asovd        - direct diffusion model surface-to-volume ratio (1/cm);
Aadir        - grain radius multiplier for the direct diffusion model
               effective grain radius (-); alternative to Asovd; direct
               diffusion model surface-to-volume ratio =
               3/(Aadir*grainrad)
Aaredldir    - coefficient of [decay constant]**1/2 term in the
               direct diffusion model effective grain radius
               reduction factor
Aaredlres    - coefficient of [decay constant]**1/2 term in the
               resolution model effective grain radius reduction
               factor
fmicro       - "microcracking" instanteous release fraction (-)
fsweep       - grain boundary sweeping release fraction (-)
```

In the calibration of the KW Consulting model with the FRAPCON 3.4 code, the calibration constants Adiff, ANsat, AQdiff1, AQdiff2 and AQdiff3 are set at their nominal values, Adiff = ANsat = AQdiff1 = AQdiff2 = AQdiff3 = 1, but the flexibility to adjust these calibration constants has been retained. In addition, it is possible that the need to model a resolution constant burnup dependence is an artifact of the FRAPCON3.4 stable fission gas release database, and that the effects modeled by the Aalpha2, Aalpha3 and Aalpha4 calibration constants will not be required in implementation of the model in other fuel rod performance codes or with other stable fission gas release databases.

The KW Consulting model calculations are done in double precision accuracy, obtained either by using a Fortran compiler option to use 8 byte real words, or by explicit double precision source coding.