Application of the Zirconium-Steam Reaction Model to the CFX Code

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1. Introduction

As a part of a CFX simulation of the CS28-2 high temperature experiment, we have been developing the zirconium-steam reaction model to complete the transient calculation of this experiment. Since this CFX analysis will be used to support the verification work of the CATHENA code for the post-blowdown event, the zirconium-steam reaction model of the CATHENA code is reviewed. Then this reaction model is implemented to a User Fortran for its application to the CFX-10 code.

2. Review of the Zirconium-Steam Reaction Model in the CATHENA Code

2.1 Urbanic and Heidrick Model

The decay energy in the fuel rods during a post-blowdown period of a CANDU reactor heats up the zirconium of the fuel rods and pressure tubes. It also ignites a chemical reaction between zirconium (Zr) and steam (H_2O). This is an exothermic reaction, i.e., it results in production of heat as well as a hydrogen gas (H_2) as follows:

$$Zr + 2H_2O = ZrO_2 + 2H_2 + 586 \text{ kJ.} \qquad (1)$$
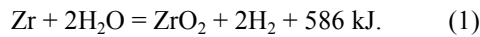
It is generally accepted that the mechanism which governs this reaction is the diffusion of oxygen anions through the anion-deficient ZrO_2 lattice [1]. The reaction rate can be described by a parabolic expression of the form

$$\omega^2 = K_p t, \qquad (2)$$

where ω is a measure of the extent of reaction (i.e., weight of zirconium reacted per unit area), t is the reaction time, and K_p is the parabolic reaction rate constant. The K_p is related to temperature by an expression of the form

$$K_p = A \exp\left(-\frac{E}{RT}\right). \qquad (3)$$

where A is a constant, E is the reaction activity energy, R is the ideal gas constant, and T is the temperature of the oxidization layer (K).

Several investigations have been made to determine K_p as a function of temperature. One of these works, the oxidation model by Urbanic et al. [1] is used for the default model of the CATHENA code [2]. The resulting K_p is given by the following correlations:

$$K_p = 29.6 \exp\left(-\frac{16820}{T}\right) \text{ for } T \leq 1850 \text{ K} \quad (4)$$

$$K_p = 87.9 \exp\left(-\frac{16610}{T}\right) \text{ for } T > 1850 \text{ K} \quad (5)$$

Substituting $\rho_z \times \delta$ for ω in the Eq. (2) and differentiating with respect to time [3], we can obtain:

$$\frac{d\delta}{dt} = \frac{K_p}{2\rho_z^2 \delta}, \qquad (6)$$

where δ is the thickness of the zirconium consumed during oxidation and ρ_z is the density of the zirconium.

2.2 CATHENA Model

For the CATHENA code, the rate of heat generation (Q) as a result of the zirconium-steam reaction at high temperatures is expressed as:

$$Q = CA_s \frac{d\delta}{dt}. \qquad (7)$$

where C is the heat generation per unit volume of Zr (4.22×10^{10}) and A_s is the surface area of the reaction. This reaction requires that there be a Zr and a ZrO_2 region. The Zr-steam oxidation model starts to be applied when solid component temperatures reach 827°C.
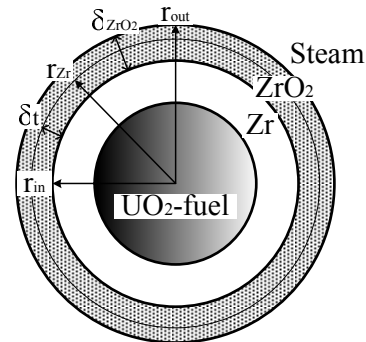

Figure 1. Configuration of the growth of the ZrO_2 layer in a fuel pin.

To correctly simulate oxidation and the thermal response of the oxidizing layer, the growth of the ZrO_2 layer must be traced. For a fuel pin as shown in Fig. 1, let r_{out} and r_{in} be the instantaneous radii of the ZrO_2-steam interface and the ZrO_2-Zr interface, respectively. The original (no-oxidation: $\delta = 0$) outer radius of the fuel element is r_{Zr}. When zirconium is consumed by oxidation, r_{in} moves inward. At the same time, r_{out} moves outward as a result of the volume expansion caused by converting Zr to ZrO_2. The thickness of zirconium consumed up to time t is obtained by integration of Eq. (7) to give:

$$\delta_t = \left(\delta_{t-\Delta t}^2 + \Delta t \cdot \frac{K_p}{\rho_z^2} \right)^{1/2}. \qquad (8)$$

where $\delta_{t-\Delta t}$ is the thickness of zirconium consumed up to time $t - \Delta t$ and Δt is the current time step size.

Then the hydrogen generation rate, H_{out} (mole/s) is

$$H_{out} = C A_s \left(\delta_t - \delta_{t-\Delta t} \right), \qquad (9)$$

where, C is a constant (1.436×10^5).

3. Implementation of the Oxidation Model to a User Fortran of the CFX code

3.1 CFX Expression Language (CEL) in ANSYS CFX-Post

The oxidation model described in the previous section is implemented to the CFX-10 [4] code. For this purpose, a User CEL Function which uses a user subroutine for the oxidation model of the CFX-10 is created. Then this subroutine is compiled and the library file required by the CFX-10 solver is created.

When creating a User CEL Function, we need some variables available for use in CEL expressions.

Table 1 CEL variables used in a User CEL Function

Name	Units	Meaning
ctstep	-	Current time step
dtstep	s	Time step interval
mf	-	Mass fraction
T	K	Temperature

3.2 A CFX User Fortran for the Oxidation Model

A part of the CFX-10 user subroutine for the oxidation model is shown in Fig. 2. Finally this subroutine is tested to confirm that the CATHENA oxidation model is well implemented to it.


```
C----------------------------------------
C    URBANIC & HEIDRICH REACTION RATES
C----------------------------------------
     IF ( TT.LT.1850.D0 ) THEN
        XK=3.447D-7*EXP(-16820.D0/TT)
     ELSE IF ( TT.LT.2123.D0 ) THEN
        XK=1.024D-6*EXP(-16610.D0/TT)
     ELSE
        XK=8.1452D-10
     END IF

     d_t=sqrt(d_t0**2+DT*2.0d0*XK)
     ddt=d_t-d_t0

!    Amount of Zr consumed is so small, it presents roundoff problems
     if ( ABS(ddt/d_t0).LT.1.D-6 ) then
        hflux=0.0d0
        h2out=0.0d0
        goto 888
     endif

     rin=rzr-d_t0
     CHKZR=ABS(rin-rgap)-XRTOL2   ! Reaction limited by Zr thickness
     IF ( ddt .LT. CHKZR ) THEN
        d_tDT=XK/d_t0
     ELSE
        d_tDT=CHKZR/DT
        ddt=CHKZR
     END IF
!----------------------------------------
     hflux=4.22d10*d_tDT    ! Heat generation rate (W/m2)
     h2out=1.436088d5*ddt   ! Hydrozen production (mole/m2)

! prepare to save the values at current time step
     temp(ILOC,face)=d_t
!----------------------------------------
888  if (ILOC .eq. 1) h2sum(face)=0.0d0  ! Reset before summation
     h2sum(face)=h2sum(face)+h2out       ! accumulated hydrogen (kg/s)

     if (source .eq. 1) then
        RET(ILOC,1)=hflux
     else
        RET(ILOC,1)=2.016d-3*h2out  ! 2.016 g/mole
     endif
```

Figure 2. A user subroutine for the oxidation model of the CFX-10.

4. Conclusion

The CATHENA oxidation model was reviewed for the feasibility study of its CFX-10 application. The Urbanic and Heidrick model was analyzed for this purpose. Then the relevant subroutine of the CATHENA code is implemented to a user subroutine of the CFX-10. This user subroutine was well tested to be used for the transient calculation of a CS28-2 experiment in the future work.

REFERENCES

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