

Benchmark Test of the Zircaloy/Steam Oxidation by CFX-10

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1. Introduction

As a preliminary work of Computational Fluid Dynamics (CFD) simulation of the CS28-2 high temperature experiment [1,2] for this accident analysis, a Zircaloy/steam reaction models based on the parabolic rate law are implemented in a commercial CFD code (CFX-10) [3] through a user FORTRAN. The oxidation model for CFX-10 application is validated by the benchmark tests. These benchmark tests well represent the conditions for validity of the parabolic reaction model such as constant temperature and unlimited steam. Over various range of temperatures the CFX-10 with the oxidation model is shown to reproduce the results by the oxidation correlation.

2. Overview of the Zircaloy/Steam Oxidation Models

2.1 Oxidation Model

The reaction rate can be described by a parabolic expression [4] of the form

$$\omega^2 = K_p t, \quad (1)$$

where ω is a weight (kg) of Zircaloy reacted per unit area (m^2), t is the reaction time (sec), and K_p is the parabolic reaction rate constant ($kg^2/m^4 \cdot s$). The K_p is related to temperature by an expression of the form

$$K_p = A \exp\left(-\frac{E}{RT}\right). \quad (2)$$

where A is a pre-exponential factor ($kg^2/m^4 \cdot s$), E is the reaction activity energy (J/mole), R is the ideal gas constant (8.31 J/K-mole), and T is the temperature (K) of the oxidization layer.

2.2 Comparison of Reaction Constants

The reaction constants reviewed in the present work are listed in Table 1 and plotted in Fig. 1.

Table 1 Parabolic reaction constants

Reference	Reaction constant, K_p ($kg^2/m^4 \cdot sec$)
Urbanic-Heidrick [4]	$29.6 \times \exp(-16820 / T)$ $87.9 \times \exp(-16610 / T)$
Baker-Just [5]	$3330 \times \exp(-22896 / T)$
Cathcart-Pawel [6]	$294.2 \times \exp(-20100 / T)$
Leistikow-Schanz [7]	$425.8 \times \exp(-20962 / T)$
Prater-Courtright [8]	$26763.6 \times \exp(-26440 / T)$

The comparison of the reaction constants in Fig. 1 shows that the reaction correlation by Baker-Just [5] overestimates the reaction rate, although it is proper to use Baker-Just correlation in safety analysis for obtaining conservative results. The correlation values by Cathcart-Pawel [6] and Leistikow-Schanz [7] are similar to that by Urbanic-Heidrick, but the temperature range of their applicability is restricted to low temperature ($T < 1773$ K). The Prater-Courtright [8] correlation is similar to that by Baker-Just, but its applicable range is only within the range of high temperature ($T > 1783$ K).

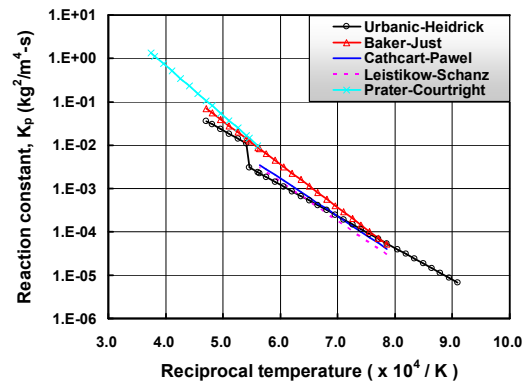


Figure 1 Oxidation reaction constant (K_p) of the Zircaloy with the temperatures

3. Benchmark Test

3.1 Set up of the Benchmark Problem

In the benchmark problem, a constant steam flow is introduced in the annulus between the cylinder of the Zircaloy (outer radius: 0.00765 m) and the surrounding tube (inner radius: 0.0215 m). The initial and boundary conditions for the benchmark test are shown in Table 2. The benchmark problems with a total of 6 cases are calculated for 30 sec of simulation time.

Table 2 Initial and boundary conditions for benchmark tests

Type	Parameter	Group1	Group2
Initial condition	Oxidation thickness, δ_t (m)	1.0×10^{-6}	1.0×10^{-4}
	Steam inlet flow (mole/ $m^2 \cdot s$)*	1.7318	
Boundary condition	Zircaloy surface temperature (K)	1273	1873
		1373	1973
		1473	2073

* for the Zircaloy surface area: $9.6130 \times 10^{-3} m^2$

3.2 Benchmark Test Results

Since the simulation of an oxidation phenomenon is to calculate the amount of the exothermal heat and hydrogen production on the Zircaloy/steam interface, CFX-10 predictions for these parameters are compared with the results of the Urbanic-Heidrick correlation [4].

Fig. 2 shows the distribution of H₂ mole fraction which is circumferentially symmetric, because the composition of steam/hydrogen mixture and the Zircaloy surface temperature are uniform along the circumferential direction.

The predictions of H₂ mole fraction and oxidation heat flux are shown in Figs. 3 and 4, respectively. These parameters are well agreement with the calculation results by the oxidation correlation, which shows that the oxidation model is well implemented in the CFX-10.

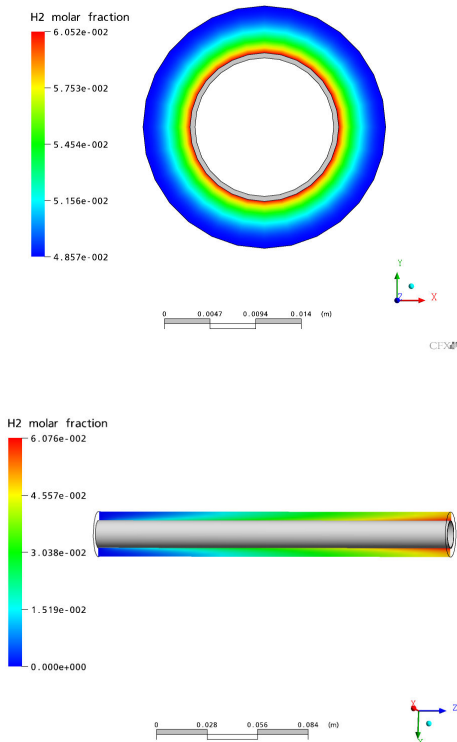


Figure 2. Distribution of the H₂ mole fraction

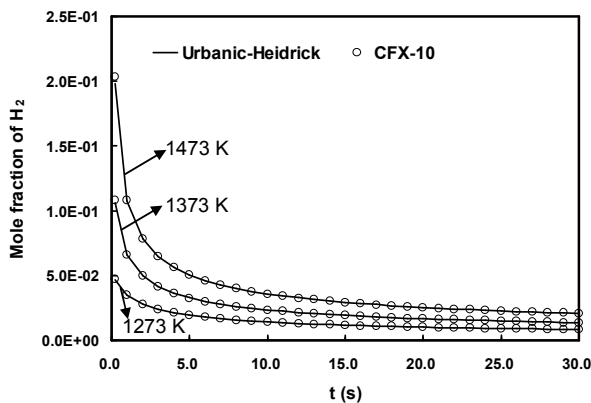


Figure 3. Comparison of H₂ mole fraction

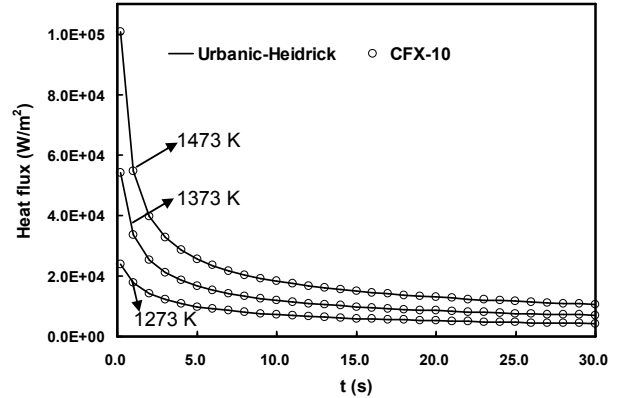


Figure 4. Comparison of oxidation heat flux

4. Conclusion

The benchmark tests well represent the conditions for validity of the parabolic reaction model such as constant temperature and unlimited steam. Over various range of temperatures the CFX-10 with the oxidation model is shown to reproduce the results by the oxidation correlation.

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