# Sensitivity analysis on the zirconium ignition in a postulated SFP loss of coolant accident

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# 1. Introduction

In a postulated complete loss of coolant accident (LOCA) in spent fuel pool (SFP), zirconium alloy cladding could be directly exposed by air [1]. Unlike the cladding oxidation in steam, air oxidation results in rapid accident progression due to its higher exothermic reaction than in steam and the active role of nitrogen on the cladding degradation [2].

Recently the experimental program to investigate consequences of complete LOCA in the SFP (PWR spent fuel assembly configuration) 17x17 was conducted in the frame of OECD/NEA Sandia Fuel Project (SFP project; hereinafter) [3-6]. In addition, BWR 9x9 spent fuel assembly tests were performed in a postulated complete loss of coolant accident [7]. From both SFP complete LOCA experiments, it was observed that zirconium alloy cladding temperature was abruptly increased at a certain point and the cladding was almost fully oxidized. This phenomenon was called as a 'Zirconium ignition'. To capture this phenomenon, the concept of air oxidation breakaway model was adopted in MELCOR code. This paper examines this air oxidation breakaway model by comparing the SFP project test data and MELCOR code calculation results by using this model. The air oxidation model parameters are slightly altered to see their sensitivities on the occurrence of the zirconium ignition. Through such sensitivity analysis, limitations of the air oxidation breakaway model are revealed in comparison to the actual zirconium ignition phenomenon during air ingress scenarios. In addition, ways to overcome the identified limitations of the air oxidation model are recommended to estimate better the zirconium ignition phenomenon in SFP sequences.

Firstly, SFP project benchmark (17x17 PWR spent fuel assembly configuration) by using MELCOR code is performed in chapter 2, and the air oxidation breakaway model which captures the zirconium ignition is also described in chapter 2. In addition, a systematic sensitivity analysis on the air oxidation breakaway model is conducted and its results are given in chapter 3. Lastly, the identified limitations of the model and its possible way of improvement is proposed in chapter 4.

## 2. SFP experiments and model in MELCOR code

Zirconium ignition phenomenon in the SFP experiments is presented in chapter 2.1, and the model that captures this phenomenon in the MELCOR code is described in chapter 2.2. Lastly, the MELCOR code input development to represent the SFP project test data are provided in chapter 2.3.

### 2.1 Zirconium ignition in the SFP experiments

As shown in Fig. 1, the zirconium ignition was observed during the SFP complete LOCA [6].



Fig. 1 SFP experiment experiments (excerpted from [6])

The post-test spent fuel assemblies were almost fully oxidized and degraded after the zirconium ignition. In addition, its dramatic temperature escalation and simultaneous oxygen depletion were reported as shown in Fig. 2.



Fig. 2 Peak Cladding Temperature of SFP experiments (excerpted from [4] and [6], respectively)

As show in Fig. 2, it seems that  $O_2$  was abruptly consumed and the zirconium alloy cladding was immediately and intensively oxidized with a highly exothermic heat release. This released heat might trigger the zirconium ignition.

#### 2.2 Air oxidation breakaway model in MELCOR

In order to capture this observed a very sudden zirconium heat-up and the simultaneous dramatic oxygen consumption, air oxidation breakaway model was developed [4-6]. The breakaway phenomenon refers to the kinetic transition from parabolic kinetic rate law (pre-breakaway kinetics) to linear kinetic rate raw (post-breakaway kinetics). The kinetic transition is initiated when the value of "lifetime" becomes more than 1.2 (i.e. 1 is the default value for reactor and 1.2 is for SFP). The lifetime function (LF) is given in the following.

$$LF(T) = \frac{\int_0^t dt'}{\tau(T)} \text{ (eqn.1)}$$
$$\tau(T) = 10^{-12.528\log_{10}T + 42.038} \text{ (eqn.2)}$$

where T is the cladding temperature in K and  $\tau$ (T) is the breakaway transition time in seconds. As shown in (eqn.1) and (eqn.2), the breakaway transition is only dependent on the cladding temperature. At certain cladding temperature the transition time is given by (eqn.2) and the breakaway is initiated at this transition time. The model parameters (-12.528, 42.038) in (eqn.2) were determined by the fitting of the Argonne National Laboratory (ANL) Zry-4 air oxidation tests at 500-900°C [7] with only 8 data points.



Fig. 3. Air oxidation breakaway model parameter fitting (excerpted from [7])

As shown in Fig. 3, the breakaway timing data at 500-900°C (time of the kinetic transition) were plotted with temperature in log-linear scale. However, the fitting of these data was performed in log-log scale. For this reason, the function of breakaway time is given as seen in (eqn.2). In this formula of the function of breakaway time, there seems several limitations as follows:

• ANL air oxidation tests data [7] showed no "zirconium ignition phenomenon" during the air oxidation tests at 500-900°C.

• Air oxidation breakaway does not trigger the zirconium ignition. It seems a very ambitious assumption that the air oxidation breakaway is the cause of the zirconium ignition.

• The relationship between air oxidation breakaway time and temperature was considered as linearly correlated in log-log scale. However, no sound physical meaning was supported in this consideration.

• Only 8 data were fitted and each data was scattered to some extent.

• The fitted breakaway time is given in function of temperature with a very coefficient as follows:

Time to breakaway (T) =  $T^{-12.528} \cdot 10^{42.038}$ 

If model parameters are slightly altered, the breakaway timing will be significantly shifted. Let the one model parameter (-12.528) calls  $A_0$  and the other (42.038) calls B<sub>0</sub>. For example, at the fixed temperature of 1100K with the A<sub>0</sub> and B<sub>0</sub>, time to breakaway is 8619 sec. If  $A_0$  becomes altered from -1 to 1% with the fixed  $B_0$  at the fixed temperature of 1100K, the time to breakaway changes from 3591 to 20683 sec. The variation in the breakaway time is -58 to 140% when the model parameter A<sub>0</sub> varies from -1 to 1%. The model parameter A<sub>0</sub> was from the fitting of the experimental data, and this fitted value had its own error by the curve fitting. In this view, the concept of model (i.e. curve fitting model) includes its high uncertainty to predict the target value. Another example is the variation of the other parameter  $B_0$  from -1 to 1% with the fixed  $A_0$  at the fixed temperature of 1100K. In this case, the variation of the breakaway time is 3277 to 22669 sec and its percentage is -62 to 163%. From these simple sensitivity calculations to see the effect of a very small variation of model parameters on the breakaway time, the air oxidation model predictions were tremendously varied. This model seems not reliable against any errors that evolved from the data fitting. In this chapter, only simple sensitivity calculations were performed at the fixed temperature of cladding. However, the actual cladding temperature in a postulated SFP complete LOCA is not fixed but varied with the accident progression. The sensitivity analysis in the postulated SFP complete LOCA is performed in chapter 3. Before performing this sensitivity analysis the MELCOR code input deck to simulate the SFP complete LOCA was prepared in the following chapter and it is validated with the SFP project experimental data (17x17 PWR SFP configuration).

## 2.3 MELCOR code input development

MELCOR input model of SFP was developed to simulate a single fuel assembly (FA). A single FA contained a 17x17 PWR fuel bundle with ca. 4 m of height, and its nodalization is shown in Fig. 4.



Fig. 4 SFP MELCOR input nodalization

The peak cladding temperature from MELCOR code calculations and the results of experimental data are given in Fig. 5.



As shown in Fig. 5, the time of the abrupt zirconium ignition (i.e. the time immediately after the breakaway) of developed MELCOR model input is very comparable with the experimental data. The calculated time to ignition is 12.52 hour and the experimental value is 12.66 hour. Based on the developed MELCOR input, various calculations are performed to see the sensitivity of model parameters on the time to ignition in the postulated SFP complete LOCA.

#### 4. Sensitivity analysis on zirconium ignition

In this chapter, a systematic sensitivity calculation is performed by varying the model parameters  $A_0$  and  $B_0$  from -3 to 3% with an increment of 1%. The simulation matrix is given in Table. 1.

Case	A		Bo	
S1	0%	-12.528	0%	42.038
S2	0%	-12.528	+1%	42.458
S3	0%	-12.528	-1%	41.618
S4	0%	-12.528	+2%	42.879
S5	0%	-12.528	-2%	41.197
S6	0%	-12.528	+3%	43.299
S7	0%	-12.528	-3%	40.777
<b>S</b> 8	+1%	-12.403	0%	42.038
S9	-1%	-12.653	0%	42.038
S10	+2%	-12.277	0%	42.038
S11	-2%	-12.779	0%	42.038
S12	+3%	-12.152	0%	42.038
S13	-3%	-12.904	0%	42.038

 $\begin{array}{|c|c|c|c|c|c|c|c|c|} \hline S12 & +3\% & -12.152 & 0\% & 42.038 \\ \hline S13 & -3\% & -12.904 & 0\% & 42.038 \\ \hline \end{array}$  In order to see the time to ignition variation with the

In order to see the time to ignition variation with the change of  $A_0$  from -3 to 3% at the fixed  $B_0$ , the calculated peak cladding temperatures are plotted in Fig. 6.



Fig. 6 Peak cladding temperatures (variation of A<sub>0</sub>)

As shown in Fig. 6, the time to ignition is varied with the variation of model parameter  $A_0$ . Likewise the variation of time to ignition by the model parameter  $A_0$ , the variation by the model parameter  $B_0$  is also plotted from its -3 to 3% range at the fixed  $A_0$  as shown in Fig. 7.



Fig. 7 Peak cladding temperatures (variation of B<sub>0</sub>)

Table 1. Simulation matrix of sensitivity calculation

As shown in Fig. 7, variation of the time to ignition by the change of  $B_0$  looks similar with that by the change of  $A_0$ . The time to ignition according to the variation of  $A_0$  and  $B_0$  in the sensitivity calculations is plotted to see its variation by each change of model parameter.



Fig. 8 Variation of time to ignition

As shown in Fig. 8, the time to ignition is significantly varied with the variation of  $A_0$  and  $B_0$  from -3 to 0%. Its variation in comparison to the experimental value is ca. -20 to 2% in percentage. This variation is not high as expected by the simple calculation in chapter 2.2. However, the time variation is more than 2 hours in some cases, and this time variation may lead to an uncertainty in the analysis of the spent fuel pool accident sequences.

#### 4. Conclusion

In this paper, the zirconium ignition phenomenon was reviewed and the model to capture this phenomenon was investigated. The model is the air oxidation breakaway model in MELCOR code, and its sensitivity of the model parameters on the time to ignition was studied. From the sensitivity analysis, the slight change of model parameters induce the large variation of the time to ignition. The model itself includes its weakness to fully represent both the air oxidation breakaway phenomenon and the followed zirconium ignition behavior. Furthermore, this model considers no effect of  $N_2$  on the cladding degradation and its promoted exothermic heat release. From this study, it is recommended that the current air oxidation breakaway model should be improved by adopting the new formula of the model (rather than log-log curve fitting model) and considering the active role of  $N_2$  on the kinetics.

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