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FTR POWER-TO-MELT STUDY PHASE I
EVALUATION OF DETERMINISTIC MODELS

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FTR POWER-TO-MELT STUDY PHASE I
EVALUATION OF DETERMINISTIC MODELS

EVALUATION OF SIEX DETERMINISTIC MODEL

EVALUATION OF PEFT DETERMINISTIC MODEL

I. EVALUATION OF SIEX DETERMINISTIC MODEL

INTRODUCTION

SIEX is a HEDL fuel thermal performance code. It is designed to be a fast running code for steady state thermal performance analysis of coolant, cladding and fuel temperatures throughout the history of a fuel element.

The need to have a good predictive model coupled with short running time in the probabilistic analysis has made SIEX one of the potential deterministic models to be adopted.

The probabilistic code to be developed will be a general thermal performance code acceptable on a national basis. It is, therefore, necessary to ensure that the physical model meets the requirements of an analytical tool. Since SIEX incorporates some physically-based correlated models, its general validity and limitations should be evaluated before being adopted.

PREDICTION OF EXPERIMENTAL RESULTS

The SIEX code includes correlated models that have been calibrated against P-19 data. However, other data now exists, namely those of the P20 and the F20. It is therefore logical to check the code against some of these data to determine its predictive capability. The representative pins chosen are the P20-33, F20-S1, F20-S3 and F20-S4.

Some preliminary preparation is needed for using SIEX in the prediction of the results. This is because the SIEX code does not have an option for directly reading in cladding outside surface temperature profile nor does it have an option for analyzing encapsulated pins. The F20 and P20 pins are encapsulated pins and therefore cannot be analyzed straight forward using SIEX.

Inputting the cladding outside surface temperature profile was tried first and did not come out fully satisfactory. This is because SIEX does not read in the power history at each time step. It is difficult to input the correct cladding outside temperature profile corresponding to the power of the pin at each time step unless some modifications of the code are carried out.

The more satisfactory approach is to introduce an equivalent film heat transfer coefficient. This is done by using a film heat transfer coefficient value such that the predicted cladding temperature profile in the absence of a capsule is equal to or very close to that of an encapsulated pin. The idea of using an equivalent film heat transfer coefficient works only under the steady state condition and the value is an average over the whole pin.

Figures 1 to 4 show the SIEX prediction of boundary locations and those observed. All except F20-S4 pin show good agreement. Table 1 shows the predicted and observed fission gas release values. Here, again, all except F20-S4 pin show good agreement.

Figure 5 shows the prediction of correlated cold gap model. Except for the F20-S1 pin, for which the prediction is in the right trend, all other pin gaps are predicted too small and in the reversed trend. From a heat transfer

point of view, the under predicted gap would mean an under prediction of fuel temperature field. For a conductive model using melting temperature as a criterion for power-to-melt prediction, a more accurate estimate of the fuel temperature is essential.

COMPARISON WITH LIFE4 ANALYSIS

The SIEX analysis of the selected F20 and P20 fuel pins shows that it generally predicts the experimental results with good agreement except for the high power pin F20-S4. As a predictive tool it should be able to extend the analysis to fuel pins of different design - for example those that will be used in the commercial fast reactor. It is, therefore, necessary to determine the general validity of the code which has incorporated correlated models derived from specific experiments.

The SIEX code can be evaluated by comparing its prediction with that of the LIFE detailed code. The choice of the latter as a reference is based upon its more comprehensive and fundamental formulations in the description of the evolution of the fuel element throughout the operating history. In addition, the LIFE code has been calibrated and checked out against the P19, P20 and F20 experimental pin data.

The FTR fuel pins with operating conditions shown in Table 2 are used in the comparison of performance predictions. An operating time of about 9000 hours was analyzed with the LIFE4 code. It was expected that the SIEX code would be valid for the start of life and/or early life predictions because of its reliance upon the P19 data in the correlated models.

Figure 6 shows the LIFE4 and SIEX predictions of the inner surface temperatures of the mid sections of three FTR fuel pins over a long period of time. The general temperature profiles of both predictions are quite similar for an extended period. For the hot and peak pins, SIEX predicted

lower temperatures in early life and for the average pin, higher temperature. However, no melting was predicted by either codes for the FTR pins.

CONCLUSIONS

- The SIEX prediction is found to be in good agreement with most of the observed values for the representative test pins chosen in the study.
- Comparison with the LIFE4 code indicates that similar predictive trend exists for an extended period in early life.
- The SIEX prediction of the three FTR pin temperatures, namely, the hot, the peak and the average, is lower for the former two pins but higher for the last pin when compared to that of the LIFE4 for BOL and early life.
- The SIEX correlated cold gap model appears to predict gap closure very rapidly with the increase in power. This could lead to early gap closure leading to an under prediction in fuel temperature.

TABLE 1. PERCENT GAS RELEASED

PIN I.D.	OBSERVED (%)	PREDICTED (%)
F20-S1	26.2	22.24
F20-S3	31.2	23.37
F20-S4	46.1	12.41
P20-33	27.0*	23.51

*EXTRAPOLATED FROM FIG. C-7 REFERENCE (1)**.

** Reference (1). R. B. Baker, "Integral Heat Rate-To-Incipient Melting In UO_2 - PuO_2 Fast Reactor Fuel," HEDL-TME 77-23, May 1978.

TABLE 2. FTR PIN OPERATING CONDITIONS

X/L =	<u>0.1</u>	<u>0.3</u>	<u>0.5</u>	<u>0.7</u>	<u>0.9</u>
<u>HOT PIN</u>					
BOL POWER	10.58	13.22	13.35	10.94	7.52
BOL FLUX	2.77	4.01	4.01	3.32	2.14
BOL CLAD OD	670	783	909	1030	1125
EOL POWER	7.88	9.14	9.20	8.06	6.10
EOL ϕt	9.13	13.24	13.24	10.96	7.05
EOL BURNUP	6.42	7.75	7.81	6.61	4.76
<u>PEAK PIN</u>					
BOL POWER	9.33	11.65	11.76	9.66	6.63
BOL FLUX	2.44	3.54	3.54	2.93	1.88
BOL CLAD OD	651	745	858	965	1046
EOL POWER	7.19	8.42	8.48	7.38	5.51
EOL ϕt	8.05	11.66	11.67	9.65	6.21
EOL BURNUP	5.75	6.97	7.03	5.93	4.24
<u>AVERAGE PIN</u>					
BOL POWER	5.34	6.67	6.73	5.52	3.80
BOL FLUX	1.40	2.02	2.02	1.67	1.08
BOL CLAD OD	635	696	767	837	891
EOL POWER	4.60	5.54	5.58	4.73	3.42
EOL ϕt	4.58	6.65	6.65	5.50	3.54
EOL BURNUP	3.46	4.25	4.28	3.57	2.51

FIG. 1 SIEP PREDICTION OF F20-S1 PIN

FIG. 2 SIEX PREDICTION OF F20-S3 PIN

FIG. 3 SIEX PREDICTION OF F20-S4 PIN

FIG. 4 SIEX PREDICTION OF P20-33 PIN

FIG. 5 SIEX PREDICTION OF POST IRRADIATED RADIAL COLD GAP.

FIG. 5 LIFE4 AND SIEX PREDICTIONS OF FTR FUEL PIN

II. EVALUATION OF PEFT DETERMINISTIC MODEL

INTRODUCTION

The PEFT deterministic thermal performance model has been designed to be fast running in order to be incorporated into the Monte Carlo simulation routine. The model has been in existence for several years, and over the past, the entire code - PEFT probabilistic analysis of fuel temperature - has been modified and enlarged mainly in the addition of probabilistic capability; the thermal performance model, however, has been left relatively untouched.

The need to apply the code as a vehicle for the prediction of fuel temperature in an FTR fuel has prompted the validation of the model. A comparison of the results of PEFT deterministic model and LIFE using F20-S4 fuel pin data was carried out previously. Several options of the PEFT model were run. It was concluded that the PEFT results need improvement. The major discrepancy was the temperature drop across the fuel cladding gap suggesting requirement for re-examination of the gap conductance model, especially the gap size correlation.

Since the previous finding was based on the comparison of (the LIFE and PEFT) code results only, basic deficiencies in the model formulations cannot be readily pin-pointed. It is believed that a more thorough study of the model including its analytical formulation and correlations - empirical or semi-empirical, should be undertaken in order to systematically uncover the sources of errors. This report aims at presenting the findings and recommendations for modification of the model. Numerical values and results are included as far as possible to substantiate the arguments.

THE PEFT THERMAL PERFORMANCE MODEL

The PEFT model is the three-region model, i.e., the fuel is divided into three distinct regions, namely, the as-fabricated, the equi-axed and the columnar grain regions. Each region is defined by a temperature and a density. Within the region the fuel properties are assumed uniform. If the fuel melts, a melting zone is created and it is defined by a melting temperature depending on which the melting boundary is located.

The movement of the molten fuel is described either by the slumping or the void filling model. The former is based on the assumption that once the fuel is melted, the molten portion is slumped away, thus reducing the local power generation. The correct fuel centerline temperature has to be evaluated iteratively. The latter (void filling) option requires that the molten fuel will fill up the void. The correct fuel temperature is again iteratively determined.

There are provisions for fuel melting, oxygen redistributions, restructuring kinetics etc., but these are all currently not operational in the model calculation.

From the thermal performance point of view, the multi-region conduction model formulation is relatively simple. The temperature field is described by a one-dimensional steady state heat conduction equation in cylindrical coordinates with a zero heat transfer boundary condition at the fuel center (or inner surface), and a temperature boundary at the cladding outside surface. The additional requirements are the continuity in temperatures and fluxes at the region boundaries.

It is at once apparent that, any inaccuracies in the predictive capability of the model do not lie in the basic formulation of the energy equation. The sources of inaccuracies derive from the inability of the model to provide accurate information on the fuel melting, restructuring, thermal conductivity and gap conductance.

The fuel melting is the main current interest. It is the capability to accurately predict the fuel melting that is being developed. For the conductive model, the fuel melting is defined by its melting temperature. Since the mixed oxide fuel is not a pure element, its melting is not fixed by a simple temperature. The current melting point is a single value of 2760°C. The solidus temperature correlation in terms of plutonium content and/or burnup should be used.

The columnar and equi-axed densities and boundary temperatures need to be examined. Higher boundary temperatures will lead to higher predicted center line fuel temperature - but higher densities will give lower value. In addition, the inner surface radius will be larger.

The fuel thermal conductivity is a function of porosity (or density), temperature and O/M ratio. The temperature dependent effect makes the energy equation non-linear and an iterative solution is needed. The W-ARD conductivity correlation has been adopted in the code that is somehow different from that used in LIFE. The problem encountered related to the conductivity integral is that raised by O'Reilly of AI concerning the convergent criterion used in integrating the equation. Within the practical range it is believed that the convergent problem is not the main concern.

The gap conductance can be the major contributor to the error of prediction in the PEFT thermal model. The gap conductance model is the widely used Ross-Stout version. But unfortunately, the model needs the correct hot gap size, plenum pressure, fuel cladding interface pressure, and fission gas mixture composition to predict the gap conductance. The PEFT model has to input the pressures and gas mixture composition. The hot gap size is assumed to be given by the HEDL post-irradiation cold gap correlation. The inability of the code to generate the correct inputs for the conductance model can make the prediction unreliable.

COMPARISON WITH LIFE DETAILED MODEL

The LIFE code considers in detail the evolution of the fuel. Thus, unlike the three-region model, the LIFE model determines the grain boundary temperatures from the grain growth behavior (equi-axed region) or the densification of the fuel (porosity consideration in columnar region). The boundary locations are determined from the fuel movement due to thermomechanical as well as irradiation effects. All the basic input for the gap conductance model are self-generated through more fundamental consideration. The code has been checked and calibrated against experimental data such as F20. It is therefore suitable to be taken as a bench mark for PEFT deterministic model evaluation.

The results from the previous study would have been a more valuable parametric study of the PEFT deterministic model if the input parameters for determining the gap conductance are consistent with those from LIFE. These are: plenum gas pressure, fuel cladding interface pressure, power cycle (defined in PEFT as reactor cycle - which is confusing for the user) and fission mixture composition (code default value). These values were not taken from the LIFE output. Further, for an open gap, the constant associated with the surface roughness is a function of gas pressure according to the Ross Stoute model. It was found that the LIFE code was coded incorrectly using the total interface pressure. Since the coding in PEFT is technically identical to that of LIFE, this error is carried over. But in the LIFE code, the total interface pressure becomes equal to the gas pressure when no contact is assumed and the result remains correct. In the case of PEFT, the interface pressure is independently input, the result is therefore incorrect in general.

In as much as PEFT deterministic model is one of the potential choices for the application to fuel thermal performance study, its exact current status should first be known. Without any modification, the model was run again.

with equivalent input as that of LIFE. The input conditions and the results can be seen in Tables 1 and 2. In Table 1, the set of inputs from the previous study is the only set which is similar to the operating conditions chosen in the study except the plenum and interface pressures. The present study used the LIFE values in order to be consistent. In Table 2, the PEFT and LIFE results obtained from the previous and the present studies are shown. Both the results show no melting, but their center temperature predictions are different, with the value obtained in the former being higher. This difference apparently is due to the different input in the pressures. (The detail will be explained later). It is also noted that the LIFE results obtained in the two cases are not identical, but the differences are not critical. This is probably due to the different input in property correlations.

Since the data used are from the F20-S4 test, the prediction accuracies of the results can be readily checked. The LIFE gives good reproduction of the fuel center line condition but not the columnar and equiaxed locations. The PEFT prediction needs considerable improvement. A systematic investigation of the model is therefore undertaken in the following sections.

THE GAP CONDUCTANCE AND THE GAP SIZE

The gap conductance is so important in the accurate determination of the fuel center line temperature that the effects of PEFT input parameters in determining the gap conductance warrant more detail consideration.

The PEFT gap size is determined by the GASIZ subroutine that uses an older version of HEDL post-irradiation cold gap correlation. This is shown in Fig. (1). Figure (2) is the version adopted by SIEX. The code assumes that the cold gap correlation should approximate hot gap. This approximation is found to be highly unsatisfactory. For early life operation, the thermo-mechanical effect is predominant. The hot gap is dependent upon the fuel-cladding differential thermal expansion. The following shows a comparison of the PEFT and the LIFE results under similar operating conditions.

Cladding Inside Temp. = 561°C
 Initial Gap Size = 5.7 mils
 Power = 17.6 kw/ft
 Plenum Pressure = 25.1 psi

<u>Code</u>	<u>Hot Gap Size (mils)</u>	<u>Conductance</u>	<u>Center Line Temp. Drop</u>
	Gap = Press. Loading + Irrad. SW + Th. Effects	Btu/in ² sec. °F	(C°)
PEFT 1.77 =	0 + 1.77 + 0	5.1×10^{-3}	2001
LIFE 0.73 =	(0.14) + 0.59	2.5×10^{-3}	2221

It is seen that the PEFT gap size besides being too high is fundamentally incorrect. The conductance is also seen to depend on parameters other than the gap size alone. Figure (3) is a plot of PEFT gap conductance versus gap size with plenum pressure as parameter. The error can be significant if consistent input parameters cannot be used. Figure (4) shows the variation of non-dimensional fuel center line temperature rise with the non-dimensional gap conductance for open gap.

THE RESTRUCTURED TEMPERATURES AND DENSITIES

In the three-region model the grain boundary temperatures and densities are the necessary input parameters for the determination of the fuel inner surface temperature. The accuracy of prediction therefore depends much on these values which, in turn, depend on the accuracy of experimental deduction. In a relative sense, the fuel temperature prediction is more sensitive to the input values of the columnar grain temperature and density than to those of the equi-axed grain. A higher columnar temperature will give a higher fuel inside temperature. A higher columnar density on the other hand, will give a lower temperature prediction because of better conductivity. In addition, the inner surface radius will be larger as a result of the conservation of mass. A PEFT run with adjusted gap conductance, a LIFE run and the F20-S4 data are shown in Figure (5) and Figure (6).

THE FUEL MELTING TEMPERATURE

The fuel melting temperature is the parameter for determining the melting condition of the fuel. For the mixed oxide fuel, the melting temperature

is not unique. Its value depends upon the fuel composition and burnup at the time of operation. A correlation in terms of the fuel composition and burnup is therefore required for a more accurate estimate of the melting temperature. Also, it is to be noted that there are two temperatures, namely, the solidus and the liquidus, associated with the fuel melting. The solidus temperature should be used for a conservative estimate. The current PEFT melting temperature is a simple value of 2760°C (5000°F). It has to be replaced with a melting temperature correlation for better prediction.

Of interest for consideration in fuel melting is the fraction of melt. Accurate information on this value may not be essential for a later estimate of the probability of the number of pellets melted in the core under a given operating condition. However, if a limited fraction of the fuel is allowed to melt, this fraction has to be accurately determined so as not to exceed the allowable limit. In that case, more detailed information on the solidus and liquidus densities, temperature, latent heat of fusion and thermal conductivities will be required.

The Fuel Thermal Conductivity

The fuel thermal conductivity is the major parameter that renders the thermal analysis of the mixed oxide fuel uncertain. However, with the correlations calibrated against experimental data, the form of the expression is relatively well established.

The correlation used in PEFT is:

$$K = 1.33 \left(\frac{1 - P}{1 + P + 10 P^2} \right) \left(\frac{1}{A + BT} + CT^3 \right)$$

Where P = porosity

A = 4.022

B = 2.6088 x 10⁻²

C = 4.3835 x 10⁻¹³

The LIFE correlation (for NOK $\neq$ 5) is:

$$K = DTK \left(\frac{1 - PORI}{1 + 0.5 PORI + 4.62 POR^2} \right) \left(\frac{1}{ATK + BTK * T} + CTK * T^3 \right)$$

Where

DTK	=	QQ(1)	=	0.196×10^3
ATK	=	QQ(2)	=	0.832×10^1
BTK	=	QQ(3)	=	0.271×10^{-1}
CTK	=	QQ(4)	=	0.116×10^{-11}
POR	=	porosity		
PORI	=	porosity + fission gas swelling porosity		

The comparison of the two correlations was carried out in the previous study. The LIFE correlation has a higher conductivity at temperatures above $\sim 1650^\circ K$. Both correlations reflect the effect of O/M ratio. However, the LIFE correlation has been calibrated. Since the form of the correlation is similar, it is easy to calibrate. Further, at present, the PEFT model inaccuracy is stemmed from sources other than the conductivity itself, the latter is therefore not considered as the main focus of improvement in the model.

PROPOSED MODIFICATIONS

- The gap conductance has to be more accurately determined. This can be improved by internally generating the necessary parameters for inputting to the gap conductance model. These are the gap size, the plenum pressure, the interface pressure and the fission gas mixture composition. Depending on the user's input values will render the prediction uncertain.
- The 3-region model requires a more accurate input of the grain boundary temperatures and densities. The PEFT values have to be updated.
- The simple melting temperature used in PEFT should be replaced by a solidus temperature correlation.
- The molten fuel movement models should be left out or by-passed to avoid error in fuel temperature prediction.

TABLE 1

INPUT CONDITIONS FOR PEFT ANALYSIS

- Fuel restructuring takes place at current steady state
- Operating power is at current steady state
- Data: F20-S4 (RODS File) Corresponds to Fuel Section #1 of LIFE4

<u>STUDY</u>	<u>PREVIOUS</u>	<u>PRESENT</u>
Fuel Thermal Conductivity	PEFT Value*	PEFT Value
Equi-axed Region Temp.	1600°C	1600°C
Columnar Region Temp.	1800°C	1800°C
Porosity @ Equi-axed Region	0.05	0.05
Porosity @ Columnar Region	0.02	0.02
Number of Power Cycle	1	1
Plenum Gas Pressure	40.0 psi	25.1 psi
Interface Pressure	40.0 psi	0.0/25.1 psi**

$$* \quad K = 1.33 \left(\frac{1 - p}{1 + p + 10p^2} \right) \left(\frac{1}{A + BT} + CT^3 \right)$$

p = porosity

A = 4.022; B = 2.608 x 10⁻²; C = 4.3835 x 10⁻¹³

** The correct input for open gap is zero; coding error in gap conductance routine requires 25.1 psi (= gas press) to account for the mistake.

TABLE 2

COMPARISON OF PEFT AND LIFE RESULTS

- Time from beginning of Life (hrs.) 7.68
- Linear power on hot condition (kw/ft) 17.63
- Burnup (Mwd/MT) 45.32

<u>STUDY</u>	<u>PEFT</u>		<u>LIFE</u>	
	<u>(PREVIOUS)</u>	<u>(PRESENT)</u>	<u>(PREVIOUS)</u>	<u>(PRESENT)</u>
Fuel cladding gap temp. drop (F)	555	408	730	809
Fuel outside temp. (F)	1597	1450	1773	1852
Temp. at the equi-axed region (F)	2912	2912	3456	3467
Temp. at the columnar region (F)	3272	3272	3754	3761
Fuel center line temp. (F)	4797	4674	4982	5040
Equi-axed grain growth radii (mils)	86.6	83.39	83.06	83.11
Columnar grain growth radii (mils)	80.2	76.69	77.27	77.52
Central void radii (mils)	23.1	22.16	18.03	17.12
Fuel cladding gap size (mils)	1.77	1.77	1.04	0.73
Fuel cladding gap conductance Btu/hr-ft ² -F	1934	2628	1416.5	1281.2

Fig 1 CURRENT PEFT GAP MODEL

Fig 2. SIEX COLD GAP CORRELATION

Fig. 3. PEFT Fuel Cladding Gap Conductance vs. Gap Size

Fig. 4 - Fuel Temperature Rise vs. Gap Conductance

Fig. 5 Fuel Temp. Profile Predicted by LIFE - PEFT with Melting

Fig. 6 Fuel Temp Predicted by LIFE and PEFT without Melting