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Fuel analysis code 'fair' and its high burnup modelling capabilities

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ABSTRACT: A computer code FAIR has been developed for analysing performance of water cooled reactor fuel pins. It is capable of analysing high burnup fuels. This code has recently been used for analysing ten high burnup fuel rods irradiated at Halden reactor. In the present paper, the code FAIR and its various high burnup models are described. The performance of code FAIR in analysing high burnup fuels and its other applications are highlighted.

1 INTRODUCTION

The importance of fuel performance analysis codes in understanding and improving the performance of nuclear reactor fuel pins is well accepted. This has been possible through continuous improvements in modelling by incorporating latest experimental evidences and by adopting efficient computational algorithms and computing platforms. These endeavours are driven by the needs to enhance the fuel performance and achieve cost effective fuel designs. In the later context, high burnup fuels have made their impact during the last few years. The analysis of high burnup fuel pins poses major challenges as many new mechanisms were found to influence the fuel behaviour, which are still under investigation. At the outset, it has been observed that, phenomena like thermal conductivity degradation of pellet, enhanced release of fission gas and pellet rim effect are some of the phenomena, which must be modelled in a fuel performance analysis code for analysing high burnup fuel pins. Of late, many existing fuel performance analysis codes have incorporated relevant models to analyse these phenomena and the new codes that are being developed are also taking a cue in this process.

In India, efforts are going on towards the utilisation of high burnup fuels. Advanced fuel cycles utilising MOX and Thorium based fuels and developmental efforts in Advanced Heavy Water Reactors which also use Thorium based fuels are significant steps in this direction. As a part of this programme, a validated fuel performance analysis code capable of analysing high burnup fuels is needed. The development of computer code FAIR (Fuel Analysis for Indian Reactors) has been done to fulfill this objective. The main thrust during the development of this code has been to incorporate latest mechanistic

models for analysing various physical and chemical phenomena occurring in the fuel pin during irradiation, and to use finite element method for thermo-mechanical structural integrity analysis. The development of this code was started in the year 1990 and this code is constantly being updated based on latest information. This code has been recently tested against ten high burnup fuel rods irradiated at Halden reactor. as a part of Coordinated Research Project (CRP) on Fuel Modelling at EXtended burnups FUMEX conducted by IAEA.

2 GENERAL FEATURES OF FAIR

The computer code FAIR (Swami Prasad et al, 1994) is a mechanistic code for analysing fuel pins of water cooled reactors. Fuel pins with both collapsible and free standing clads can be analysed using this code. The code incorporates relevant models capable of analysing various phenomena associated with high burnup fuels. The organisation of the code 'FAIR' follows the proven principles in fuel rod modelling, such as, coupling of thermal and mechanical calculations through current gap conductance value, concurrent anlysis of different sections of fuel rod to consider axial mixing of fission gas and provision for performing local analysis, such as clad ridging analysis. The thermo mechanical analysis is carried out using 2-D axisymmetric finite element method. The thermal module can handle both steady and transient states. The mechanical module can perform thermal-viscoplastic calculations. The thermal and mechanical analysis modules consider temperature and irradiation dependant material properties. The material property data base is adopted from MATPRO (Hagrman et al, 1981). The nonlinear coupling between thermal and mechanical modules through gap conductance is analysed by a proper convergent iterative scheme based on physical gap/contact pressure between pellet and sheath.

The implementation of some of the common physical and chemical phenomena related to the pellet, such as, densification, swelling and grain growth are based on MATPRO. The gap conductance calculations follow the typical Ross and Stout approach (Ross et al, 1962) with additional inputs from MATPRO for modelling the conductivity of mixture of gases and extrapolation lengths at pellet-gas and gas-clad interfaces. The effect of pellet cracking and relocation is considered by pseudo strain approach. Though these models were initially developed with no high burnup interests, these are being used in modern codes for analysing high burnup fuels also. It may be mentioned here that a host of literature is available for modelling these phenomena. Some of these models such as URGAP model for gap conductance (Lassmann et al, 1987), Assmann-Stehle's densification model (Stehle et al, 1975) etc.,are being incorporated in code FAIR as alternatives to the existing models.

Certain mechanisms such as flux redistribution across pellet radius, change in stoichiometric ratio affect the fuel performance severely at high burnups. A key feature of the code FAIR is to consider these high burnup mechanisms using relevant models. The code FAIR also addresses the pellet clad interaction mechanism since this is very important for fuel pins with collapsible clad being used in Indian reactors. This mechanism may become important for free standing clads also at high burnups. The analysis of high burnup fuels using mechanistic codes requires large computation times. Parallel processing systems can reduce computational times for such analysis

and hence code FAIR is commissioned on a parallel processing system ANUPAM developed at BARC. A description of the high burnup models and effective use of parallel processing for fuel analysis are given in the following sections.

3 HIGH BURNUP MODELS IN FAIR

The fuel performance at high burnups is typically characterised by enhanced fuel temperatures, enhanced fission gas release, formation of a porous rim at the pellet edge and change of stoichiometric ratio for pellet. The code FAIR incorporates relevant models for analysing these phenomena based on recent works in high burnup fuel modelling and here follows a description of these models.

3.1 Pellet conductivity degradation with burnup

Accurate computation of fuel temperatures is of utmost importance for a fair prediction of overall mechanistic behaviour. The fuel temperatures depend on pellet conductivity to a great extent. The thermal conductivity of UO_2 as documented in standard literature such as MATPRO, is a function of porosity and temperatures. This conductivity of UO_2 is contributed mainly by phonons and electrons. The burnup dependence of pellet conductivity has been established only in the recent years. A 17% decrease in pellet conductivity after reaching a burnup of 30 GWD/tU at 550 $^{\circ}$C has been reported by in-core Halden experiments (Kolstad et al, 1992)and out-of-core SIMFUEL experiments (Lucata et al, 1992). This degradation of pellet conductivity is attributed to the build up of fission gas bubbles and solid fission products, increase in microgaps and change in fuel stoichiometric ratio. In code FAIR, three different options are available for modelling thermal conductivity of UO_2. These are MATPRO model, Halden model and SIMFUEL model. The degradation of pellet conductivity in the later two models is incorporated by modifying the phonon contribution to UO_2 conductivity. In Halden model the burnup dependant phonon contribution to conductivity is represented by

$$\lambda = 1/(0.0375 + 2.165 \times 10^{-4} T + 0.015 \times bu) \quad (1)$$

The SIMFUEL correlation is given by

$$\lambda = 1/[0.053+(0.016\pm0.0015)b] + [2.2-(0.005\pm0.002)bu] \times 10^{-4} T \quad (2)$$

where bu is the burnup in at % units, T is temperature in Kelvin and λ is the UO_{22} conductivity. The Halden model is based on the in-reactor fuel centre line temperatures, whereas the SIMFUEL model is based on out of core fuel where the burnup is simulated by doping UO_2 with stable additives in an appropriate amount. The SIMFUEL model as implemented in FAIR at present takes care of conductivity degradation due to solid fission products only.

3.2 High burnup fission gas release model

One of the main parameters determining the success of a fuel performance analysis code is fission gas release. It is a strong function of fuel temperatures and is interdependent on thermo

mechanical behaviour of fuel. The fission gas release process in UO_2 fuels consists of two mechanisms, namely athermal mechanism and thermal mechanism. The thermal release is dictated by fuel temperatures whereas the athermal release is linearly dependant on fission rate. Booths diffusion model (Booth, 1957) has been the basis for analytical modelling of thermal release. Some of the analytical models which have found wider acceptance for modelling thermal fission gas release are physically based model, ANS 5.4 model, Halden model and URGAS model. The physically based fission gas release model is based on mechanistic principles and its roots are attributed to Hargreaves and collins (Hargreaves et al, 1976). Subsequently, it has further been improved by many others like Hastings, White and Tucker, Turnbull and Nakajima. The ANS 5.4 model is a semi mechanistic model and Halden model is an empirical model. All these three models are implemented in FAIR.

The microstructure dependant physically based model assumes that fission gas release occurs due to a combination of mechanisms, such as, fission gas diffusion to grain boundaries , grain boundary sweeping, resolution of gas atoms in to the grain matrix from grain boundaries and saturation of grain boundaries before ultimate release to fuel pin free volume. The diffusion coefficient is affected by intragranular bubbles. These bubbles are created due to fission spikes and have a tendency to trap gas atoms in them. These gas atoms cannot take part further in diffusion unless they are redissolved back into matrix. This is considered using an apparent diffusion coefficient (D') given by

$$D' = D\, b'/(b'+g) \qquad (3)$$

where, D is the single gas atom diffusion coefficient. This consists of contributions from intrinsic diffusion, vacancy assisted diffusion and irradiation enhanced athermal diffusion. The expression for D is given by

$$D = 7.6 \times 10^{-10} \times \exp(-7 \times 10^{4}/RT) + S^{2} J_v V + 2 \times 10^{-40} F \qquad (4)$$

where S is atomic jump distance, J_v is jump frequency of vacancy, F is fission rate. The factor 'g' is the probability of a gas atom in solution being captured by intragrannular gas bubbles and b' is the probability of a gas atom within intragrannular bubble being redissolved. The expressions for b' and g can be derived using bubble concentration, mean bubble radius, fission range, the range of influence and equation for Van der walls gas. Turnbull has recently suggested a modification to this expression. In this modification the second and third terms of this expression are multiplied by a factor of four (Turnbull, 1994).

The grain boundary saturation limit is found out by using the expression for density of gas atoms over the grain boundaries at saturation. This is given by

$$N^{max} = \frac{4\, r\, f(\theta)}{3\, k\, T \sin^{2}\theta}\, f_b \left[\frac{2\,\gamma}{r} + P_{ext}\right] \qquad (5)$$

Where $r\phi$ is the radius of grain face bubble, θ is the semi dihedral angle, k is the Boltzmann constant, γ is the free surface energy and P_{ext} is the external force.

The Halden fission gas release model (Vitanza et al, 1978) suggests the presence of a threshold burnup (buh) before appreciable fission gas release can take place at any temperature (T). In this model, the incubation period, which corresponds to duration for 1 % fission gas release is calculated by

$$buh = 5 \times \exp(9800/T) \quad (6)$$

The fractional release is calculated using the following relations:

$$fgr = 0 \quad \text{if bu} < buh \quad (7a)$$
$$= (T/1800)^5 \quad \text{if bu} > buh \text{ and } T < 1800^{\circ}C \quad (7b)$$
$$= 1 \quad \text{if bu} > buh \text{ and } T > 1800^{\circ}C \quad (7c)$$

The standard ANS 5.4 model implemented in code FAIR is based on (NUREG/CR-2507, 1982). At high burnups, there is an increase in both thermal and athermal releases. It is established that at a constant power level, the fuel temperatures increase at high burnup. These increases in fuel temperatures lead to enhanced thermal release. The experimental results of third RISO fission gas project established the shifting of the threshold temperature location for thermal release towards the pellet rim at high burnups. This increases the volume of pellet where fission release occurs. This is also attributed to radial redistribution of power profile because of Plutonium formation and also change in fuel stoichiometric ratio. For modelling high releases associated with high burnups, some analytical models multiply the diffusion coefficient by a burnup dependant term.

The athermal release, which represents gas release by recoil and knockout mechanisms, is a linear function of fission rate up to moderate burnups. This release will be significantly affected at high burnups because of the Rim effect. The modelling of this particular high burnup phenomenon in code FAIR is presently in progress.

The prediction of Iodine release is very important for calculating the damage to the sheath of the fuel pin because of stress corrosion cracking. The iodine release calculations are performed in the code FAIR based on MATPRO.

3.3 Radial flux distribution at high burnup

The radial power density profile across the pellet radius is a function of burnup. At low burnups, the fissile concentration is uniform across the pellet radius and only small variation in power profile is observed across the pellet. But as fuel burnup increases, there is an increase in Plutonium concentration and at pellet edge this concentration is still high because of resonance absorption of epithermal neutrons. This leads to a formation of porous region at pellet edges of 100-200 μm thickness which is depleted of Xenon. Modelling of this mechanism is very important for analysing high burnup fuels as explained in the section 3.2. In computer code FAIR, the well known RADAR (Rating Depression Analysis Routine) model has been implemented for modelling this phenomenon (Palmer et al, 1983). This model is later on improved by K.Lassmann and his group as TUBRNP model (Lassman et al,1994) which was reported to yield good results for both UO_2 and MOX based fuels. This model will form the basis for further improvements in radial power profile modelling in code FAIR.

3.4 Stress corrosion cracking of sheath due to PCMI

The prediction of stress corrosion cracking in the sheath due to pellet clad mechanical interaction (PCMI) is important to improve the performance of fuel bundles. This can occur for free standing clad fuel pins at high burnups due to pellet swelling. This is far more important for collapsible clad fuel rods used in PHWRs where the sheath has to follow the pellet during the entire operation of reactor. A special purpose module has been implemented in the code FAIR to predict the stress corrosion cracking (SCC) induced sheath failure during the history of fuel rod operation based on the work of Yaung, 1983.

The important inputs for this module are the sheath strains, the amount of free iodine available to attack the sheath and sheath material properties , especially its decrease in ductility. The first step in this methodology is to check whether sheath strain is more than the threshold to initiate a crack based on the Iodine concentration. Once this strain is exceeded, the next step is to calculate the rate of iodine penetration to the crack tip. If the Iodine concentration at the crack tip exceeds the threshold for intragrannular or transgrannular stress corrosion cracking, the crack propagates further. In this case a redistribution of the stresses and strains in the clad is to be carried out for the new length of the crack, which is done analytically based on the hoop stress and moment equilibrium. The ultimate rupture of the sheath occurs, when the strain in the remaining ligament of the sheath exceeds the ductile rupture strength of the material. This ductile rupture strength of the sheath material decreases due to irradiation and triaxiality at the crack tip. This model has been found to be very effective for analytical simulation of threshold power ramp criteria. The mathematical expressions governing this model are not described here for brevity. They are explained in Swami Prasad, 1993.

A semi mechanistic approach has been put forward (Tayal et al, 1994) for finding out the probability of fuel failures due to stress corrosion cracking. This approach has emanated from an analytical simulation of threshold power ramp criteria based on in reactor fuel failure data. These are generally expressed as empirical relations between power ramp and burnup, and, ramped power and burnup. In this semi mechanistic approach a damage factor and probability of fuel failure are evaluated based on work density at failure prone region of sheath, corrodant concentration and sheath susceptibility to stress corrosion cracking at given fluence. These parameters are determined as a function of fuel material characteristics and geometry, power ramp conditions and burnup. The empirical constants used in this approach are based on reactor data and are not available in open literature.

4 PARALLELISATION OF FAIR FOR CONSIDERING AXIAL MIXING OF FISSION GAS

A mechanistic fuel performance analysis code such as FAIR, which consists of finite element based thermo mechanical module and mechanistic models for modelling physical fuel behaviour requires significant computation time. During fuel pin analysis similar calculations have to be performed at various axial locations depending on the axial power variation. Since these calculations at each section are independent of other sections, but for fission gas mixing, parallel processing features can be exploited for this purpose. The

data and algorithm structure of fuel codes is highly suitable for exploiting the parallel processing systems. The code FAIR is implemented on ANUPAM parallel processing system developed at Bhabha Atomic Research Centre. It is a loosely coupled Multiple Instruction Multiple Data (MIMD) type of computer system that makes use of Reduced Instruction Set Computer (RISC) based CPUs. Each processor analyses a particular section of the fuel pin. Corresponding to a given time step, the analysis steps include gap conductance convergence loop over thermal and mechanical routines and fission gas release calculations at each axial location. Then fission gas mixing calculations are performed after obtaining the releases from all the processors and the process is repeated till the whole history of fuel pin is analysed. The details of implementation are reported in Swami Prasad, 1995.

5 CURRENT TRENDS IN FUEL MODELLING

Considerable efforts are still being pursued for improving the performance of fuel analysis codes for analysing high burnup fuels, MOX fuels and Thorium based fuels. These efforts are of diverse nature ranging from understanding of fuel chemistry at microstructure level to using stochastic approach to explain deviations from experimental results due to uncertainties in various models. Models for treating oxide redistribution in pellets under thermal gradients, high burnup effects on grain growth and gas swelling and micro gap closure due to rim effect have recently been published. Though, understanding of different models has gone in depth, it is still a matter of concern for fuel analysts to explain the differences in computed and experimental results. Probabilistic methods such as Monte-Carlo technique, Numerical noise method are being applied to explain the discrepancies. The incorporation of these latest developments should help to improve the performance of fuel analysis codes.

6 VALIDATION AND APPLICATIONS OF FAIR

The individual models of the code FAIR were tested against the standard bench mark cases quoted in the literature. The performance evaluation of FAIR as an integral fuel analysis code was done against two case studies. The first study was based on an earlier project on fuel rod modelling code evaluation by Electric Power Research Institute (EPRI-NP-369, 1977). The COMETHE-III J code was adjudged most versatile among all the codes which had participated in this project. All the cases of this report were analysed to evaluate the code FAIR. The results for case-C of this project computed by code FAIR are shown in Fig.1 along with the results of the other participated codes in this project and experimental values. The results of the code FAIR can be seen to be more in agreement with those of COMETHE-III J, which incidentally deviated from the experimental results. The end of life fission gas release was calculated as 5.83 % by FAIR, as against 5.6% reported by the code COMETHE-III J.

The second study was carried out for simulating analytically the threshold power ramp criteria (P_{cc}, ΔP_{cc} curves) for a PHWR fuel rod. The Iodine release module, thermo mechanical module and the PCMI model were successfully used for generating these curves. The simulated

threshold peak power results are plotted in Fig.1 along with the experimental results from Penn, 1977. A good comparison between the two can be noted.

The code FAIR is recently used for analysing high burnup fuel rods as a part of coordinated research project FUMEX (FUel Modelling at EXtended burnups) conducted by IAEA (IAEA/IND/7348) . Nineteen agencies participated in this blind code comparison exercise. The computed results of these agencies are compared with experimental observations in Halden reactor for various fuel performance parameters. A set of ten high burnup fuel rods grouped into six cases are to be analysed under this project. These distinctly dissimilar cases are formulated to analyse a range of varying inputs. The average rod burnups varied from 30 to 50 MWD/KgUO2. Some rods were ramped at the middle of life, some were ramped at end of life. Fuel enrichment varied from 3.5 to 13%. Fuel diameters range from 5.92 to 10.75 mm. The diametral gaps varied from 50 to 260 μm. The rods are filled with either Helium, Xenon or Helium/Xenon mixture under different pressures.

All the cases under this CRP are analysed by FAIR. The results of Fumex 3.2 are presented here as a representative case. This rod is filled with Xenon at a pressure of 1 bar and subjected to a ramp of 45 KW/m at end of life (30 MWd/KgUO2). The salient details of this rod are : Fuel diameter - 10.7 mm ; Diametral gap - 100 μm ; Stack length - 140 mm ;Enrichment - 10% ; Fuel density - 95% TD and Grain size - 20 μm. The results for this case are shown in Fig.2. The variation of centre line temperature with burnup is shown in Fig.2a. for the entire history of fuel pin. The maximum temperature corresponding to the peak power is 1750 °C. The variation of centre line temperature with burnup at different constant power levels is shown in Fig.2b. It is of interest to note that after initial densification, the temperatures continue to drop with burnup even at high burnups. This is attributed to the Xenon filler gas. For such rods, the release of fission gas improves the gap conductance value, which is not the case with Helium filled rods. Hence centre line temperature continues to decrease with burnup. The fission gas release and internal rod pressure as a function of burnup are shown in Fig.2c. The end of life fission gas release is 10.8% and the fission gas pressure at the peak of ramp is 8 bars.

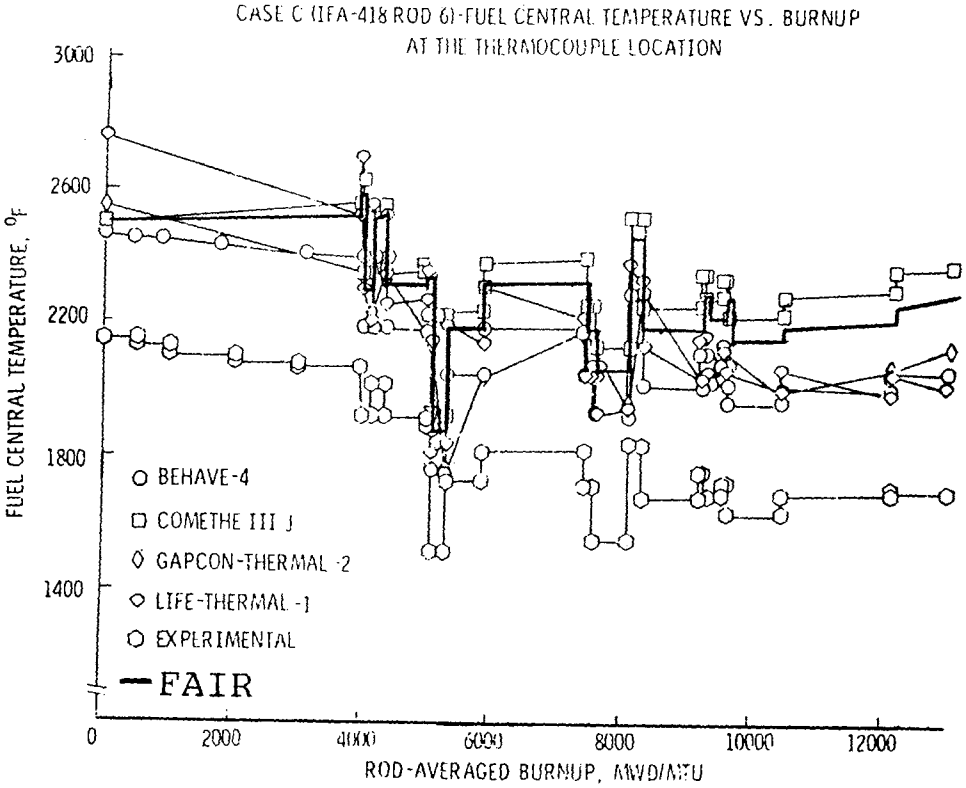
The IAEA later on provided the experimental results for all the cases and compiled the results of all the participating agencies along with experimental results. Results for Temperatures, fission gas release and rod internal pressure are compiled at burnups corresponding to the end of initial densification, start and end of power ramps of interest. The results computed by FAIR are compared with the experimental results provided by IAEA and are plotted in Fig.3. The temperature comparison is shown in Fig.3a and the fission gas release / rod internal pressure comparison are shown in Fig.3b. The code FAIR has been able to predict fuel behaviour at high burnups with good accuracy.

The code FAIR is also used to study the effect of chamfered end pellets on reducing the failure due to circumferential cracking of welds at the clad end-cap junction of a fuel rod. It is possible to reduce this failure by generating compressive stresses at this junction. Based on the typical micrographs of actual weld profiles in this zone, an average weld profile is chosen to model the clad end-cap junction. These profiles are shown in Fig.4a. It is found from this analysis that interference free lengths beyond 5 mm generate

compressive stresses at this junction for all the values of radial interference as shown in Fig.4b. The studies carried out to check the effect of these chamfered end pellets on temperature distribution indicated an increase in fuel temperatures as shown in Fig.4c due to decrease in effective heat transfer area. However, the net increase in volumetric average of these temperatures is not much and hence overall fuel behaviour may not be affected significantly.

REFERENCES

Swami Prasad, P. et al, 1994. BARC report no:BARC/1994/E/013.
Hagrman, D.L. et al, 1981. MATPRO-Version 11 (Rev.2), NUREG/CR-0497, TREE-1280 .
Ross, A.M. & Stout, R.L. 1962. CRFD-1075.
Lassman, K & Hohlefeld, F. 1987. Nucl Engrg. Des. Vol 103, pp.215-221.
Stehle H. et al, 1975. Nucl Engrg. Des. Vol.33, pp.230-260.
Kolstad, E. & Vitanza, C. J.Nucl.Mater. Vol 188, pp.104-112.
Lucata, P.G.,et al 1993. IAEA-TECDOC-697, pp.165-171.
Nordstrow, L.A., & Ott, C. 1993. IAEA-TECDOC-697, pp 219-224.
Booth, A.H. 1957. AECL-496.
Hargreaves, R. & Collins, D.A. 1976. J.of.Brit.Nucl.Soc. Vol.15, pp.311-316.
Turnbull,J.A, 1994. Personal communication with B.K.Dutta.
NUREG/CR-2507, 1982. BAckground and derivation of ANS 5.4 standard fission gas release model.
Palmer, I.D. et al 1983. Light Water Reactor Fuel rod Computer Modelling, (Gittus, J.H. Ed) pp.321-335.
Lassmann, K. et al, 1994. J.Nucl.Mater Vol.208, PP.223-231.
James Yu-Chen Yaung 1983. A model of pellet cladding interaction to simulate operational ramp failure of water reactor fuel, University of California, Los Angeles, Ph.D thesis..
Swami Peasad, P. et al, 1993. SMiRT-12 , C03/4.
Tayal, M. et al, 1994. Paper #3.4, TCM on Water reactor fuel element modelling at high burnup and its experimental support.
Swami Prasad, P. et al, 1995 . Current SMiRT Vol.F, Paper No.420.
EPRI-NP-369 1977. an EPRI report on Light water reactor fuel rod modelling code evaluation.
Penn, W.J et al 1977. Nuclear Techology Vol.34, pp.249-268.
IAEA/IND/7348 1993. Agreement on FUMEX cases between IAEA and India



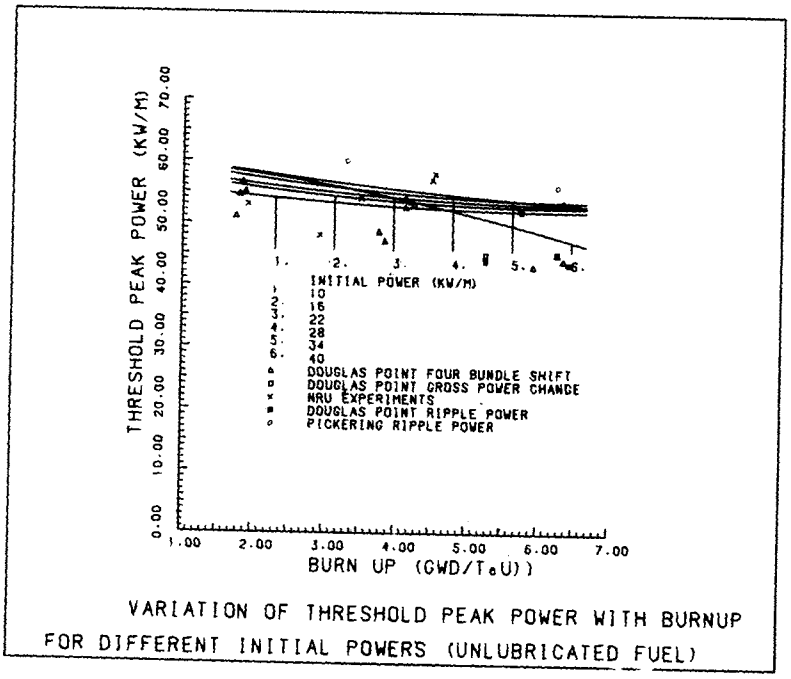


FIG.1 RESULTS OF THE CASE STUDIES TO EVALUATE FAIR

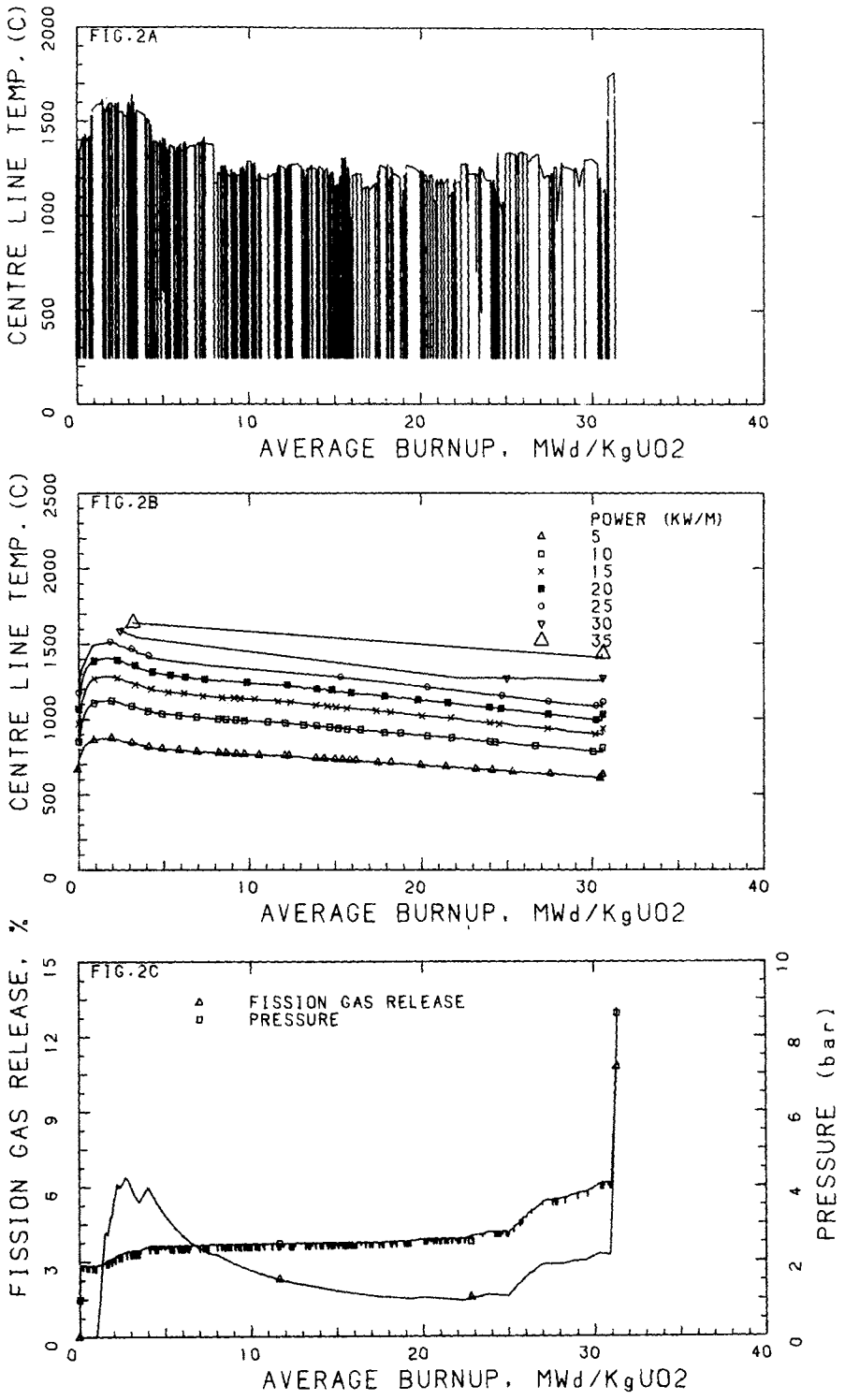


FIG.2 RESULTS COMPUTED BY FAIR FOR CASE 3.2 OF IAEA CRP ON FUMEX

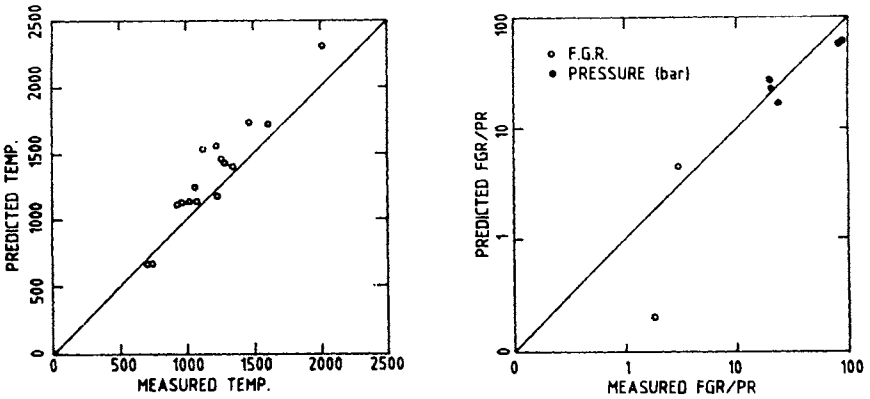


FIG.3 COMPARISON OF BLIND PREDICTIONS OF CODE FAIR WITH EXPERIMENTAL RESULTS

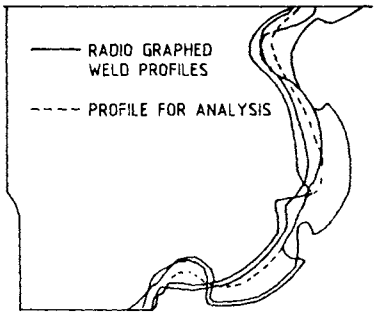


FIG. 4a WELD PROFILES NEAR CLAD END CAP JUNCTION

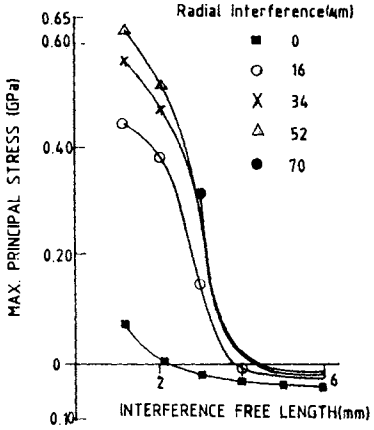


FIG. 4b EFFECT OF INTERFERENCE FREE LENGTH ON PRINCIPAL STRESSES AT WELD JUNCTION.

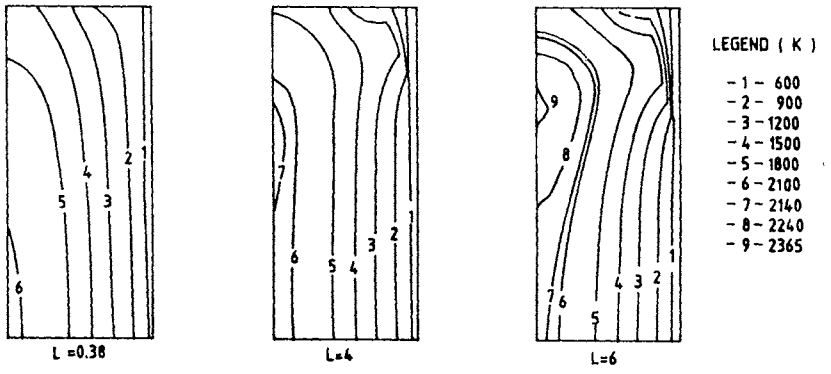


FIG. 4c TEMPERATURE CONTOURS IN END PELLET FOR VARIOUS INTERFERENCE FREE LENGTHS (L)