XA9744791

HIGH BURNUP MODELS IN COMPUTER CODE FAIR

B.K. DUTTA, P. SWAMI PRASAD, H.S. KUSHWAHA,
S.C. MAHAJAN, A. KAKODAR
Bhabha Atomic Research Centre,
Trombay, Mumbai,
India

Abstract

An advanced fuel analysis code FAIR has been developed for analysing the behaviour of fuel rods of water cooled reactors under severe power transients and high burnups. The code is capable of analysing fuel pins of both collapsible clad, as in PHWR and free standing clad as in LWR. The main emphasis in the development of this code is on evaluating the fuel performance at extended burnups and modelling of the fuel rods for advanced fuel cycles. For this purpose, a number of suitable models have been incorporated in FAIR. For modelling the fission gas release, three different models are implemented, namely Physically based mechanistic model, the standard ANS 5.4 model and the Halden model. Similarly the pellet thermal conductivity can be modelled by the MATPRO equation, the SIMFUEL relation or the Halden equation. The flux distribution across the pellet is modelled by using the model RADAR. For modelling pellet clad interaction (PCMI)/stress corrosion cracking (SCC) induced failure of sheath, necessary routines are provided in FAIR. The validation of the code FAIR is based on the analysis of fuel rods of EPRI project "Light water reactor fuel rod modelling code evaluation" and also the analytical simulation of threshold power ramp criteria of fuel rods of pressurized heavy water reactors. In the present work, a study is carried out by analysing three CRP-FUMEX rods to show the effect of various combinations of fission gas release models and pellet conductivity models, on the fuel analysis parameters. The satisfactory performance of FAIR may be concluded through these case studies.

1. INTRODUCTION

India has adopted Pressurized Heavy Water Reactors as the mainstay of its nuclear power programme in the current stage. Since our natural Uranium resources are limited, our power programme has placed considerable emphasis on Plutonium recycle. Further, we are endowed with large resources in terms of Thorium and we, thus, have a strong interest in exploitation of Thorium for our nuclear electricity production.

At the present time, the Indian PHWR fuel bundles are used to an average burnup of 8000 to 10000 MWD/ton and peak burnup is of the order of 15000 MWD/ton. Due to our limited resources of natural Uranium, there is a strong desire to improve the burnup significantly to utilize this resource optimally. Various alternatives through advanced fuel cycles, based on MOX fuel and Thorium are being considered for this purpose. In parallel we are in the process of developing an Advanced Heavy Water Reactor System (AHWR) to facilitate the utilization of Thorium through thermal reactor cycles. This also would need fuel capable of achieving high burnup. One of the important necessities for design of high burnup fuel is to have a validated fuel analysis code with different up to date models. The development of computer code FAIR (Fuel Analysis for Indian Reactors) [1] has been done with this objective in mind.

2. GENERAL FEATURES OF FAIR

The computer code FAIR is a mechanistic code for the fuel analysis of water cooled reactors with multiple modules for analysing different features of a fuel pin based on latest literature. The code is specially designed for analysing high burnup fuels by selecting different modules typically suited for this purpose. Special feature has been introduced for collapsible clads to make it suitable for PHWR fuel pins also. The mechanics of the pellet and clad (thermal as well as deformations) is solved by using 2-D axisymmetric finite element analysis. The thermal module can handle steady state as well as transient cases considering change in material properties with temperature. The variation in gap conductance between pellet and clad is considered by coupling the thermal module with the mechanical module to obtain convergence on physical gap for a given time instant. The mechanical module is a thermal-elastic-plastic module with the consideration of material properties as a function of temperature and creep strain. Special creep laws for UO_2 pellet and Zircaloy clads have been incorporated.

Other general features of FAIR are typical of a fuel analysis code. These are, consideration of densification, swelling, relocation, grain growth, cracking of pellets, etc. Gap conductance is calculated using Ross and Stout model with the more accurate modelling for the conductivity and extrapolation length for pellet-gas and gas-clad interfaces.

In the following sections, the four important modules of code FAIR, which are specially incorporated for the analysis of high burnup fuels, are described in detail.

3. HIGH BURNUP MODELS IN FAIR

3.1 CONSIDERATION OF CONDUCTIVITY DEGRADATION WITH BURNUP

Accurate computation of pellet temperature is of utmost importance for a fair prediction of overall mechanistic behaviour. One of the important inputs to temperature computation module is the pellet conductivity. The expression characterizing variation of UO_2 conductivity as a function of porosity and temperature is generally well established and is available in standard documents, such as, MATPRO [2], etc. However, understanding of degradation of conductivity with burnup, is still evolving. Besides having burnup independent conductivity expression from MATPRO, the computer code FAIR has two burnup dependent conductivity expressions. The first expression is based on the experimental results available from Halden [3]. In this model the burnup dependent phonon contribution to conductivity is represented by

$$\lambda_{UO2}^{phonon} = 1/(A + B.T + C \times \text{burnup}) \qquad (1)$$

where A, B and C are tuning coefficients to match experimental data. The second expression for conductivity is based on the findings with simulated high burnup fuel, SIMFUEL [4]. The correlation is given by

$$\lambda = [0.053 + (0.016 \pm 0.0015)b] + [2.2 - (0.005 \pm 0.002(b) \times 10^{-4}\, T \qquad (2)$$

where b is the burnup (at%), T is the temperature in K and λ is the UO_2 conductivity.

3.2 HIGH BURNUP FISSION GAS RELEASE MODEL

The fission gas release model is an important routine for any fuel analysis code. The accurate determination of fission gas release is important to calculate fission gas pressure and dilution of filler gases. This in turn affects the gap conductance and pellet temperature. The computer code FAIR has got three independent fission gas release models, specially suited for high burnup fuels. These are as follows.

The first model is the physically based model considering diffusion, sweeping, resolution of gas atoms in the grain matrix and saturation of grain boundaries for ultimate release [5]. The apparent diffusion coefficient (D′) is given by

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

where, D is the single gas atom diffusion coefficient given by

$$D = 7.6 \times 10^{-10} \times \exp(-7 \times 10^{4}/RT) + S^2 J_v V + 2 \times 10^{-40} F \quad (3b)$$

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 Wallis gas.

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

$$N_f^{max} = \frac{2 r_f \, f_r(\theta)}{3 \, k \, T \sin^2\theta} \, f_b \left(\frac{2\gamma}{r_f} + P_{ext} \right) \quad (4)$$

Where r_f 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 physically based model of code FAIR has been tested against experimental results for isothermal pellets up to high burnups quoted in the literature.

Besides the physically based mechanistic model, the code FAIR has got two more fission gas release models based on empirical relations. These are the standard ANS 5.4 model [6] and the Halden fission gas release model [7]. In the Halden model, the incubation period, up to which the fission gas release is less than 1%, is calculated by

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

The fractional fission gas release is calculated using the following relations:

fgr	=	0	if bu < buh	(6a)
	=	$(T/1800)^5$	if bu > buh and T < 1800 °C	(6b)
	=	1	if bu > buh and T > 1800 °C	(6c)

The athermal release of fission gas is computed using the ANS 5.4 model. 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 [2].

3.3 MODEL FOR RADIAL FLUX DISTRIBUTION AT HIGH BURNUP

The radial power density profile across the pellet of fuel rods operating in a thermal reactor exhibits flux depression, which changes with the burnup due to build up of plutonium in a thin later near the pellet surface. In computer code FAIR, the well known RADAR (Rating Depression Analysis Routine) model [8] has been implemented for this purpose.

3.4 MODEL FOR STRESS CORROSION CRACKING OF SHEATH DUE TO PCMI

The prediction of stress corrosion cracking in the sheath due to PCMI at high burnup and high temperature is an important information to improve the performance of fuel bundles. This is 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 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. This model is based on the work of reference [9]. The important inputs for this module are the sheath strains, the material properties, especially the decrease in ductility. The first step in this methodology is to check whether sheath strain is more than the threshold to initiate a crack. This is given by

$$\Sigma = exp\left[\frac{1}{K6} \times log[\frac{-K_5}{\log\ (I/I_2)}]\right] \qquad (7)$$

where I is the threshold Iodine required for intragrannular failure, I_2 is the effective Iodine available and K_5, K_6 are constants.

Once this strain is exceeded, the next step is to calculate the rate of iodine penetration to the crack tip by using the expression

$$\frac{dI}{dt} = \frac{h}{w}\left[\ exp\ (-Q/KT)\ \left[I_{eff}\ \ exp\ (-K_5/\varepsilon^{K_6})\ -\ I\right]\right] \qquad (8)$$

If the Iodine concentration at the crack tip exceeds the threshold for intergrannular stress corrosion cracking or transgrannular stress corrosion cracking, the crack propagates further. In this case a redistribution of the stress and strain 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 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.

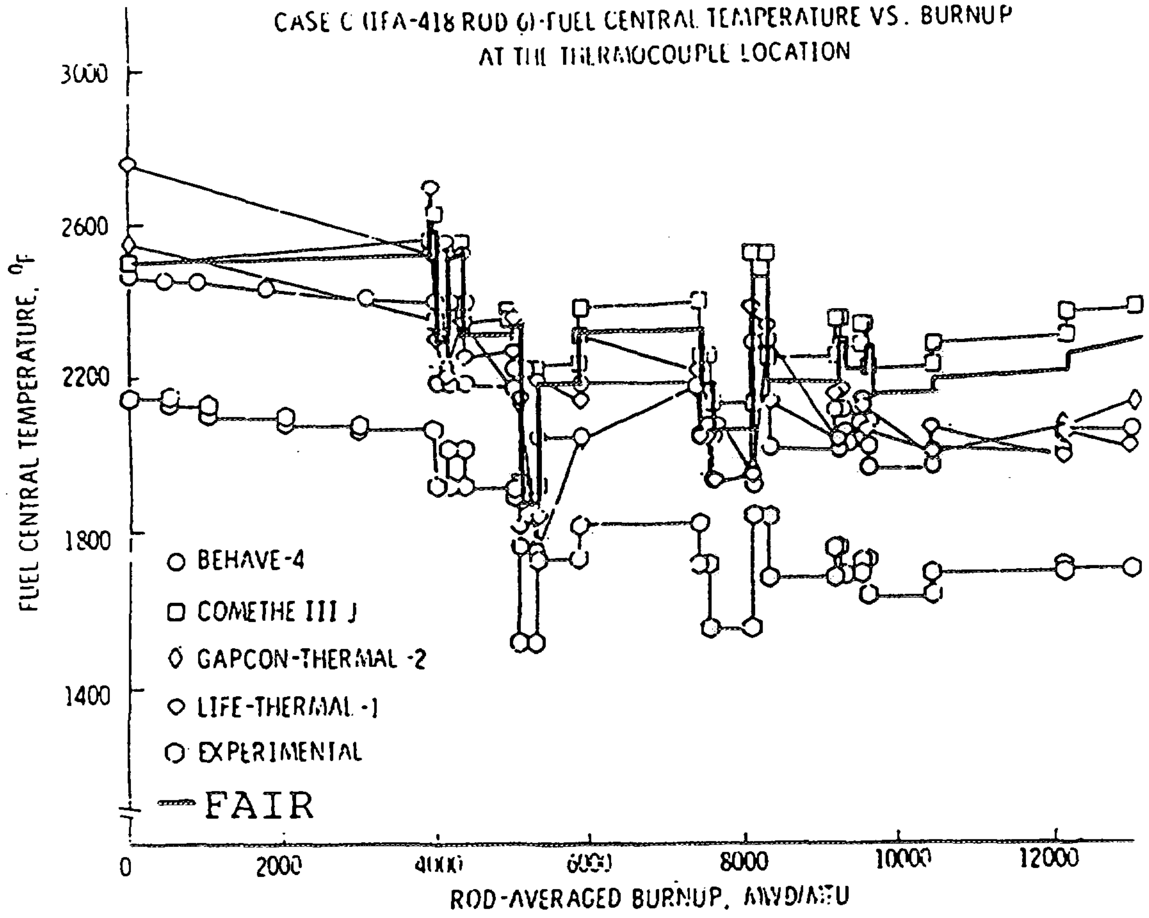
4. EXERCISES

The performance evaluation of a fuel analysis code is a difficult task due to limited availability of experimental data in the open literature. The individual models of the code FAIR have been tested against the standard bench mark cases quoted in the literature. However, the performance evaluation of this code as an integral fuel analysis code was done against the following case studies.

The Electric Power Research Institute (EPRI) sponsored a research project (397-1) to evaluate six fuel rod modelling codes as a step towards a more effective utilization of these codes by the electric utility industry. The findings of this project were reported in an EPRI report [10]. The major conclusion of this research project was that the COMETHE-III J code was the most versatile code among all the participating codes. All the cases reported in that report were used as bench mark cases to evaluate the computer code FAIR. The results for case-C of this report as computed by code FAIR have been shown in Fig. 1 along with the results quoted by the other participating codes 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 values. The end of life fission gas release was calculated as 5.83% by FAIR, as against the value of 5.6% reported by the code COMETHE-III J.

The code FAIR was used for analytical simulation of the threshold power ramp criteria (P_c, ΔP_c curves) for a PHWR fuel rod. These curves have been originally generated based on the experimental results. For generating these curves, it is necessary to reach a particular burnup before subjecting the fuel rod to a ramp. The fuel rod can reach a given burnup through many combinations of power maneuvering. Hence in analytical simulations, different routes are assumed to reach a given burnup by specifying different constant initial power ratings. After reaching a particular burnup, the fuel pin is subjected to power ramps of varying magnitude. The fuel pin is assumed to reside at this power for a time long enough to consider the dwell period to be more than 2.5 hours. By using the PCMI model of the code FAIR, the maximum ramped power was computed which did not cause the sheath failure. This threshold peak power as a function of burnup and different initial power ratings is plotted in Fig. 1. along with the experimentally generated points quoted in reference [11].

The code FAIR recently participated in a co-ordinated research project FUMEX conducted by IAEA [12]. The project consisted of the blind code comparisons of different fuel performance parameters computed by different participating agencies, with the experimental results obtained in the Halden reactor.



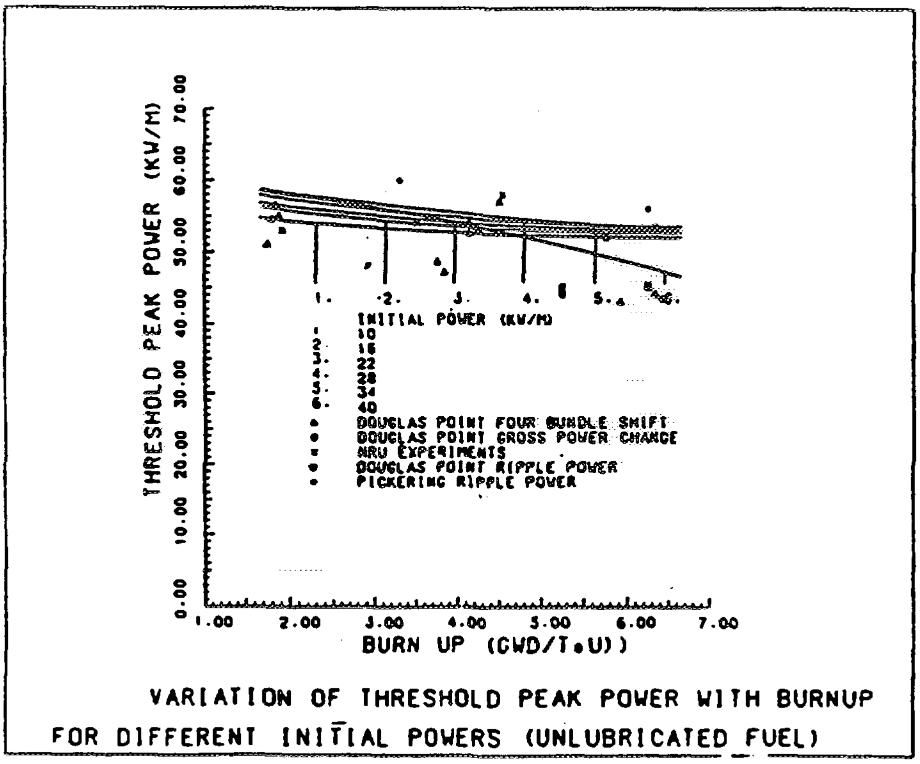


FIG. 1. Results of the case studies to evaluate code FAIR.

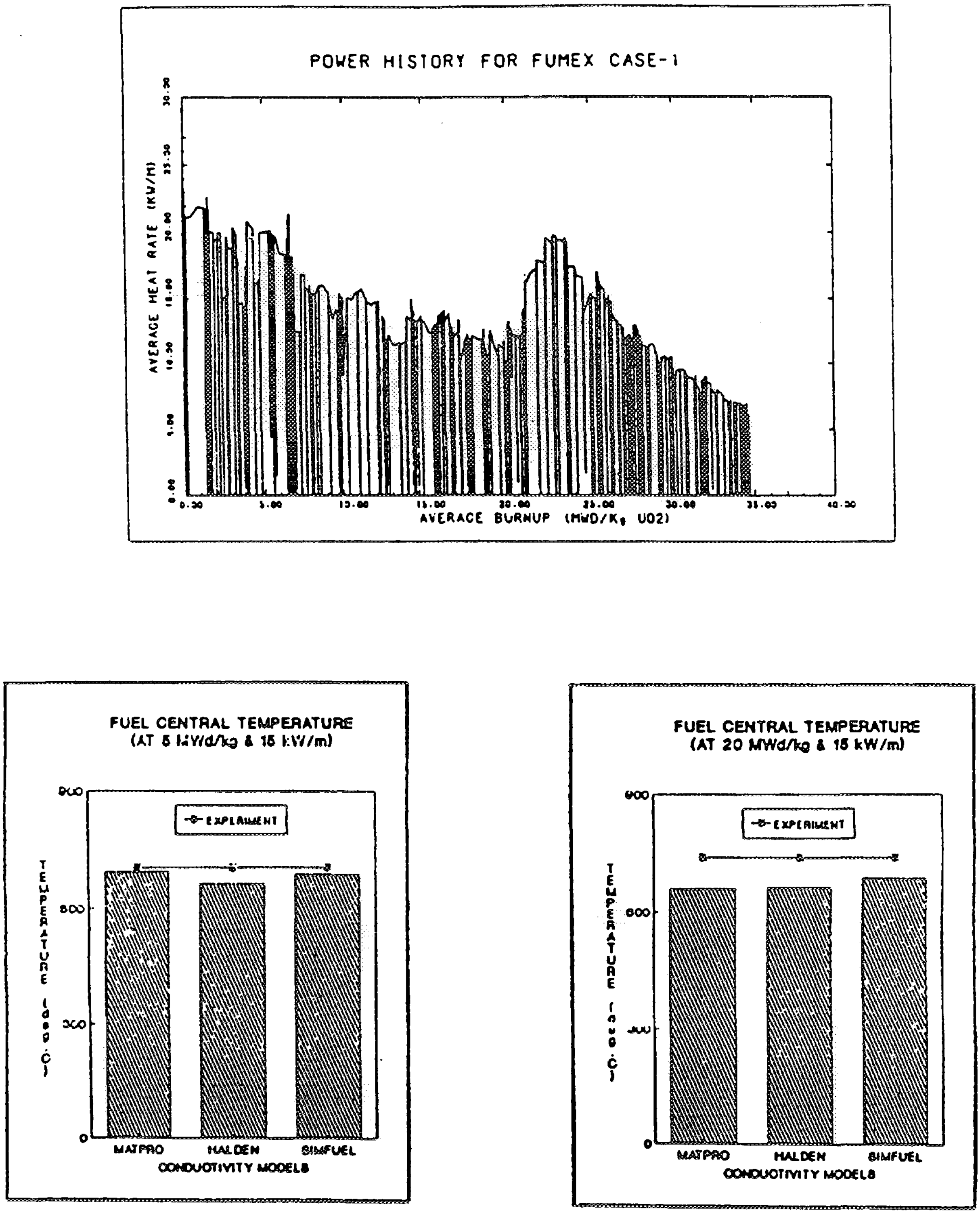
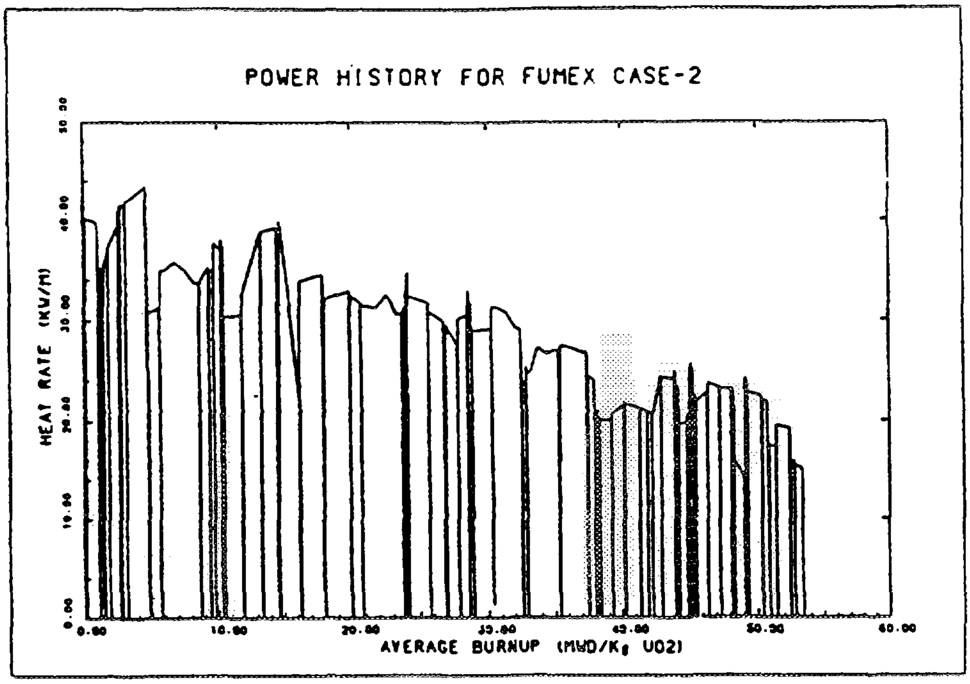


FIG. 2. *Inter comparison of conductivity models for FUMEX case-1.*



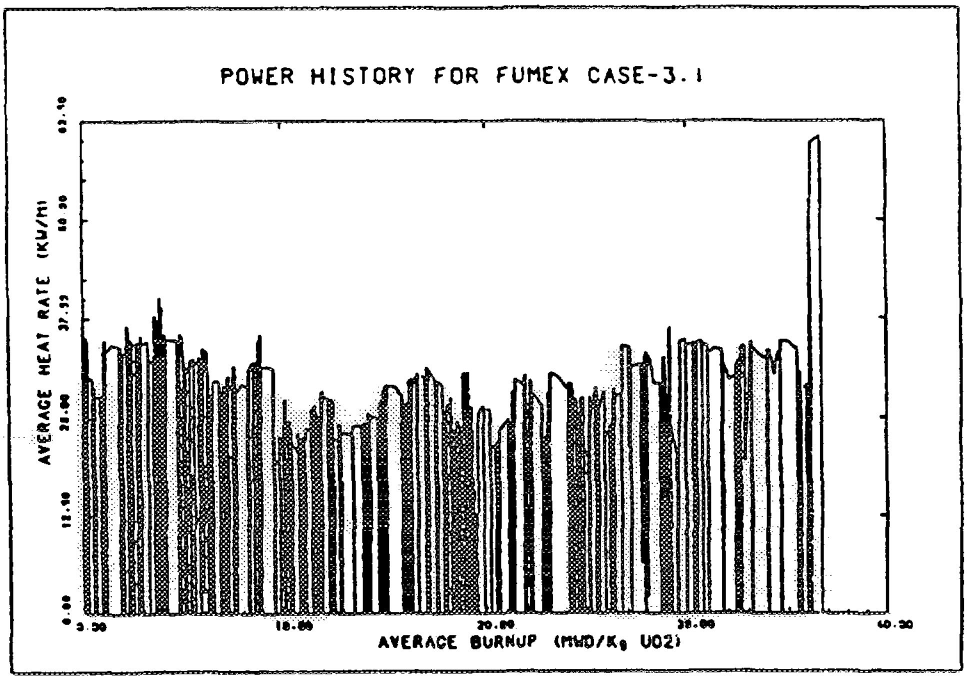


FIG. 3. Power histories for FUMEX case-2 and FUMEX case-3.1 [12]

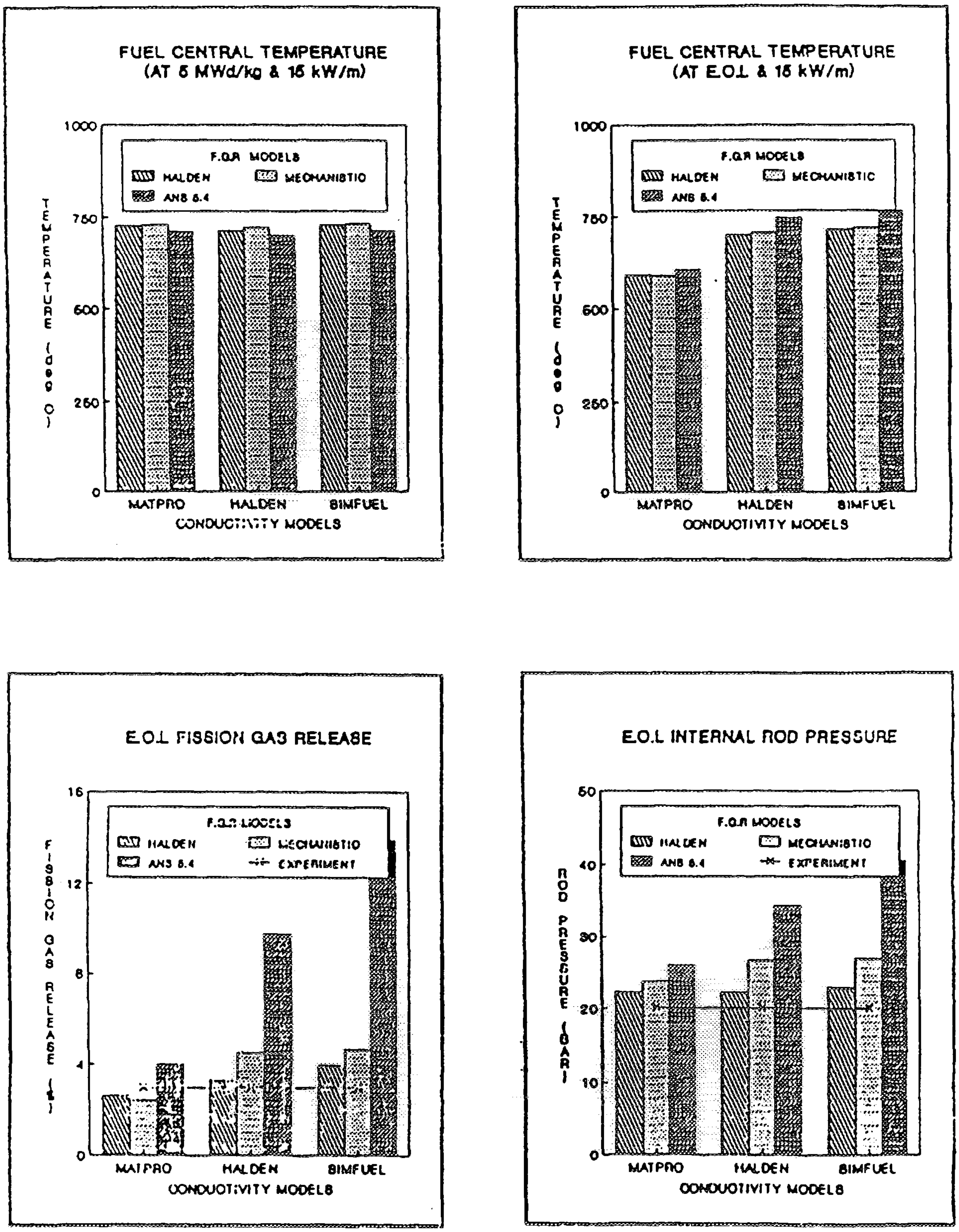


FIG. 4. Inter comparison of conductivity and F.G.R. models for FUMEX case-2.

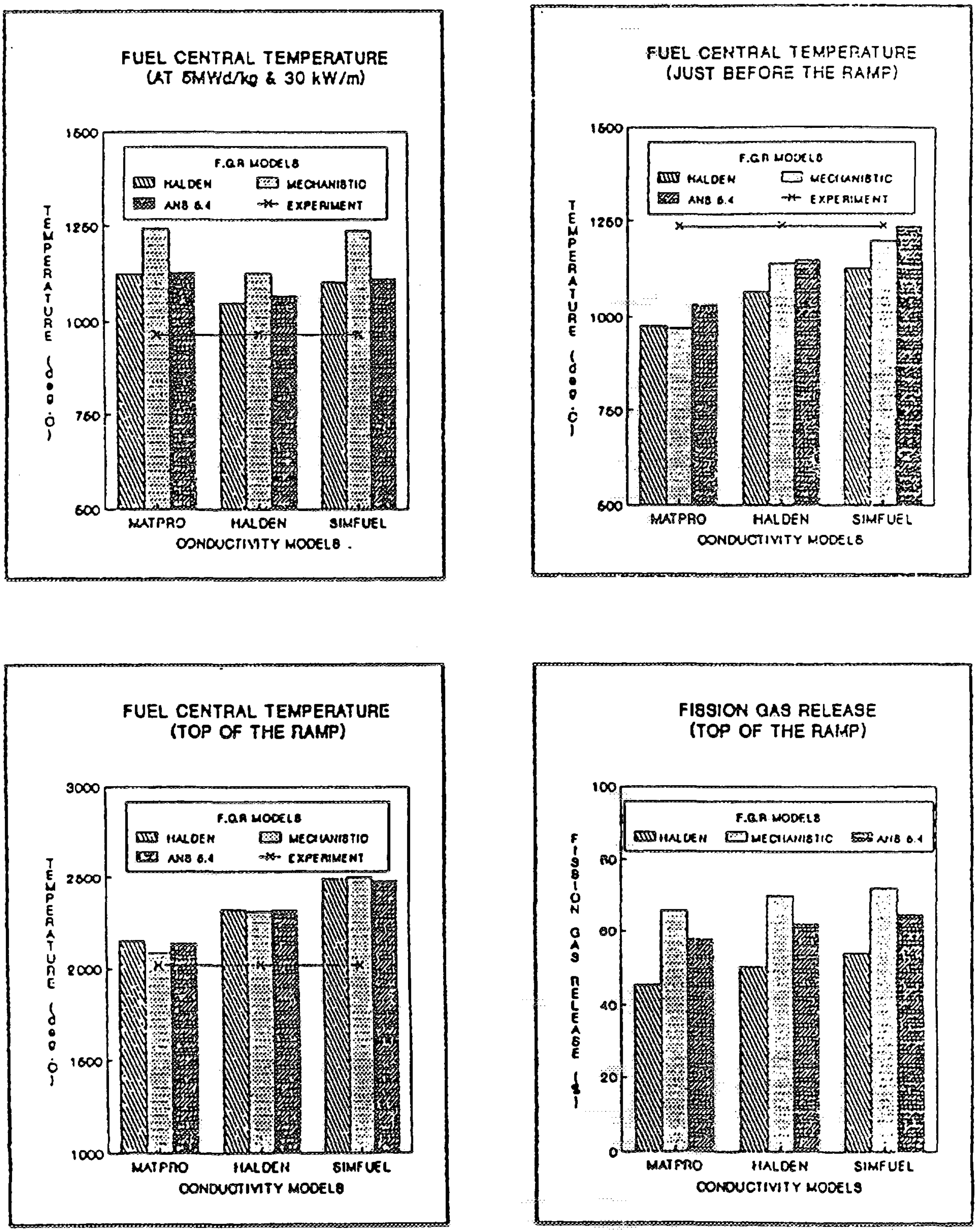


FIG. 5. Inter comparison of conductivity and F.G.R. models for FUMEX case-3.1.

The results computed by the participating codes and the experimental results are being published in an IAEA document to be presented in the present conference.

We have used three cases of this CRP for further study. These are FUMEX-1, FUMEX-2 and FUMEX-3 Rod 1. The study consists of computation of results by three burnup dependant conductivity models and the three fission gas release models implemented in the code FAIR. The conductivity models are based on MATPRO (burnup independent), HALDEN and SIMFUEL models. The fission gas release models are Halden model, ANS 5.4 model and mechanistic model of code FAIR. Each of the above three FUMEX cases is run for nine different combinations and the results obtained along with the power histories [12] are shown in Figs. 2-5.

5. CONCLUSIONS

From the performance analysis of various fuel rods using FAIR, the following conclusions can be drawn.

i) The code FAIR computed consistent results for all the cases analysed.

ii) The results computed by FAIR for the case-C of EPRI project show close match with the results quoted by using COMETHE-III J, for both temperature and fission gas release values.

iii) The threshold peak power curves simulated analytically using FAIR, have a good match with the experimentally generated data of PHWRs.

iv) The performance of various conductivity models implemented in the code FAIR, with respect to the cases analysed show the following:
   a) SIMFUEL model computes temperatures higher than the Halden model at high burnups.
   b) As MATPRO model does not consider the degradation of pellet conductivity with respect to burnup, the temperatures computed by MATPRO model are the lowest among the temperatures computed by all the three models of code FAIR.

v) The performance of various fission gas release models implemented in the code FAIR, suggest the following:
   a) The Halden model computed the lowest fractional fission gas releases among all the three models.
   b) For power histories devoid of severe power transients, the ANS 5.4 model computed the highest releases among all the three models.
   c) During severe power transients, the increase in the fractional release computed by using the mechanistic model of FAIR is the highest compared to the other two models.

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