



Blind prediction exercise on modeling of PHWR fuel at extended burnup

D.N. Sah^{a,*}, U.K. Viswanathan^a, C.S. Viswanadham^b, K. Unnikrishnan^a, B.N. Rath^a

^a Post Irradiation Examination Division, Raja Ramanna Fellow, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India

^b Materials Science Division, Bhabha Atomic Research Centre, Mumbai 400085, India

A B S T R A C T

A blind prediction exercise was organised on Indian Pressurised Heavy Water Reactor (PHWR) fuel to investigate the predictive capability of existing codes for their application at extended burnup and to identify areas of improvement. The blind problem for this exercise was based on a PHWR fuel bundle irradiated in Kakrapar Atomic Power Station-I (KAPS-I) up to about 15 000 MWd/tU and subjected to detailed post-irradiation examination (PIE) in the hot cells facility at BARC. Eleven computer codes from seven countries participated in this exercise. The participants provided blind predictions of fuel temperature, fission gas release, internal gas pressure and other performance parameters for the fuel pins. The predictions were compared with the experimental PIE data which included fuel temperature derived from fuel restructuring, fission gas release measured by fuel pin puncturing, internal gas pressure in pin, cladding oxidation and fuel microstructural data. The details of the blind problem and an analysis of the results of blind predictions by the codes vis-à-vis measured data are provided in this paper.

© 2008 Elsevier B.V. All rights reserved.

1. Introduction

The design and operating conditions of Indian Pressurised Heavy Water Reactor (PHWR) fuel differ from light water reactor (LWR) fuels in many respects [1]. The fuel pins in PHWR use thin wall collapsible cladding. They are short in length (0.5 m) and have no separate plenum. Because of collapsible cladding, the fuel and cladding come in contact shortly after the beginning of life. The PHWR fuel pins operate at considerably higher linear heat rating compared to LWR fuel pins. Higher heat rating in PHWR pins causes significant fuel restructuring, which promotes new processes of fission gas release which are not present in LWR fuels. Because of closed fuel-clad gap, the cladding creeps outwards unlike LWR fuel pins, which initially experience cladding creep down till fuel-clad gap is closed and subsequently creep out at higher burnup after the gap closure. The fuel modeling codes for PHWR have to take into account the above factors.

The current maximum discharge burnup of PHWR fuel bundle is 15 000 MWd/tU. It is proposed to be extended to 20 000–25 000 MWd/tU. The behaviour of fuel pins at extended burnup is not fully understood with respect to fission gas release, pellet clad interaction and cladding corrosion. Computer codes capable of predicting PHWR fuel performance at such high burnup are required to check the adequacy of current design to withstand the high

burnup which is almost 1.5 times the current discharge burnup, and to investigate the effect of possible design changes for achieving this burnup. For reliable prediction of PHWR fuel performance at high burnup, codes need to be validated against experimental data. Keeping this in view, a code prediction exercise was organised in connection with the IAEA Technical Meeting on PHWR Fuel Modelling held during December 5–8, 2006 at Mumbai. The approach followed in this code exercise was similar to the approach adopted earlier during D-Com Blind Problem exercise [2], IAEA Coordinated Research Program FUMEX-I [3] and IAEA Coordinated Research Program FUMEX-II [4] for LWR fuel.

In order to facilitate the validation of PHWR fuel modeling codes at extended burnup, the problem selected for code exercise was based on the data of a PHWR fuel bundle irradiated at Kakrapar Atomic Power Station-I (KAPS-I), which was irradiated to about 15 000 MWd/tU and was subjected to detailed PIE at the BARC hot cells,

2. The code exercise

In this blind prediction code exercise, the participants were provided with a data package and they were asked to simulate the irradiation of an Indian PHWR bundle/element using their codes and submit the results of their calculation by a due date. The results of actual experimental measurements on irradiated fuel bundle were provided to the participants after the submission of all the code calculations.

* Corresponding author. Tel.: +91 22 25595009; fax: +91 22 25505151.
E-mail address: dnsah@barc.gov.in (D.N. Sah).

2.1. Data package

The data package provided to the participants consisted of

(a) Description of PHWR fuel bundle/fuel pins

The nineteen pin fuel bundles used in 220 MWe Indian PHWRs consist of short (about 0.5 m long) fuel pins, containing natural uranium dioxide pellets within collapsible Zircaloy cladding. A typical fuel bundle design is schematically shown in Fig. 1. Each bundle contains 12 outer pins, 6 middle pins and 1 central pin.

(b) The following data on fuel, cladding, fuel pin and irradiation details:

Fuel pellet data: Composition, O/M ratio, pellet dimensions, pellet end geometry (dished/flat), dish depth, dish diameter, fuel density, grain diameter, fuel surface roughness, UO_2 powder route, enrichment (Pu fraction), sintering temperature and time.

Cladding data: Cladding radii and thickness, surface roughness, material, metallurgical condition, mechanical properties (YS, UTS, %elongation, burst strength, total circumferential elongation), hydrogen content.

Fuel pin data: Active fuel stack length, axial gap in fuel pin, fuel-clad gap, total void volume inside pin, filling gas composition and pressure, assembly geometry.

Irradiation details: Coolant temperature vs. time/burnup at bundle location, coolant pressure, fast neutron flux, pin linear heat rating (LHR) vs. time/burnup.

Bundle average power and time data was converted into the LHR vs. time/burnup data for the three types of fuel pins. The linear power ratings of the fuel pin in the outer ring, in the middle ring and in the central pin were derived from the bundle power using radial power factors. The variation of radial power profile in the bundle with burnup was ignored.

The irradiation histories of the three types of fuel pins provided to the participants histories are plotted in Fig. 2. Bundle averaged coolant temperature and fast neutron flux (>0.8 MeV) were also provided.

2.2. Parameters required to be calculated

The participants were required to provide the following calculations as plots and data sheets, for outer ring fuel pins, middle ring fuel pins and central pin.

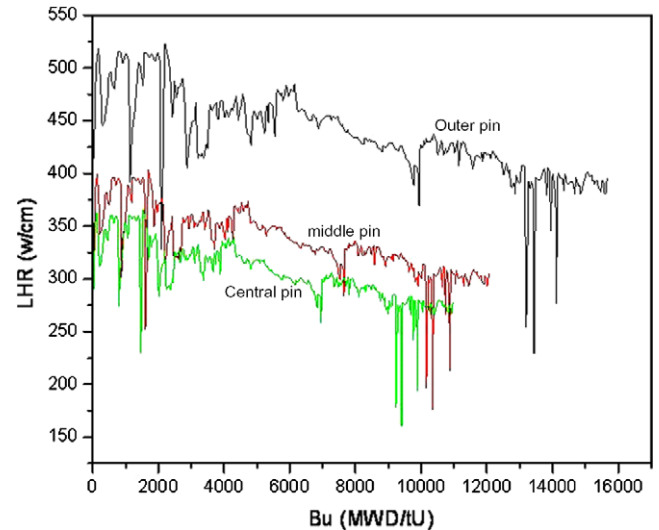


Fig. 2. The irradiation histories of the three types of fuel pin in the bundle.

Fuel centre temperature ($^{\circ}\text{C}$) vs. Burnup MWd/KgU (Mandatory)

Internal gas pressure (MPa) vs. Burnup (Mandatory)

% Fission gas release (FGR) vs. Burnup (Mandatory)

Volume gas release vs. Burnup (Mandatory)

Fuel-clad cold gap at the end of life (EOL) (Optional)

Fuel grain size at centre vs. Burnup (Optional)

Retained gas profile in pellet at EOL (Optional)

Radial porosity profile: EOL (Optional)

Cladding oxidation on external surface: EOL (Optional)

2.3. PIE data for comparison

The experimental results generated through PIE, for comparison with calculation consisted of the following data for outer, middle and central pins.

Internal gas pressure in the fuel pins

Volume of fission gas release measured in fuel pins

% Fission gas release in fuel pins

Void volume in fuel pins

Centre temperature of pellets estimated from fuel restructuring

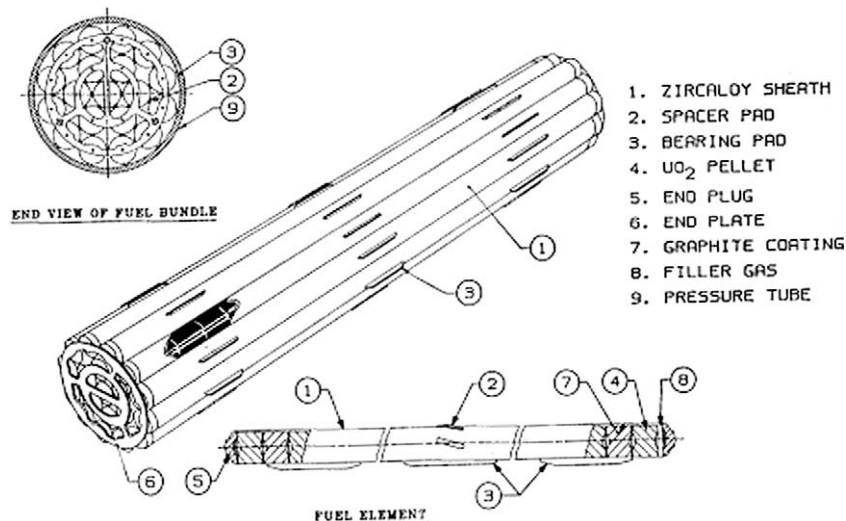


Fig. 1. A schematic drawing of a PHWR fuel bundle.

Table 1
Codes which participated in the blind prediction exercise

S. no	Name of code	Organisation	Country
1.	PROFESS	BARC	India
2.	ELESTRES 2.0	AECL	Canada
3.	FEMAXI- V	NRI Rez plc	Czech Republic
4.	DIONISIO	CNEA	Argentina
5.	GAPCON	BARC	India
6.	BaCo	CNEA	Argentina
7.	TRANSURANUS	INR	Romania
8.	FUELSIM	INR	Romania
9.	SATURN-FS1	IGCAR	India
10.	ELESTRES	KAERI	Korea
11.	–	CIAE	China

Radial porosity profile in fuel pellet
Grain size at centre of pellet

3. Codes which participated in the blind prediction exercise

A total of eleven codes from seven countries including India participated in the exercise. The names of the codes and participating organizations are listed in Table 1. Details of some of these codes are available in Refs. [5–10].

4. PIE results on the bundle used in the blind prediction exercise

The blind prediction exercise was based on PHWR fuel bundle 56504 from KAPS-I irradiated to a burnup of 15000 MWd/tU. Post-irradiation examination of this bundle was carried out in the Hot Cell Facility at BARC. The detailed results of PIE of this bundle are given in Ref. 11. A summary of these results is presented in Table 2. The radial porosity profiles in the fuel pellets of outer, middle and central fuel pins are shown in Fig. 3.

5. Code predictions and comparison with experimental results

5.1. Fuel centre temperature and fission gas release

5.1.1. Outer fuel pin

Fig. 4 shows the fuel centre temperature predicted by the codes for the outer fuel pin as function of fuel burnup. The wide variation in the temperature predicted by the codes is obvious. The trend of the predicted temperature variation during irradiation appears to follow the fuel pin power history for most codes except one which showed higher temperature towards higher burnup. Fig. 5 shows the comparison of the predicted fission gas release volume with end-of-life fission gas release volume measured in the outer fuel pin during PIE. Only four codes have predicted significant fission gas release in the fuel pin. The volume of fission gas release pre-

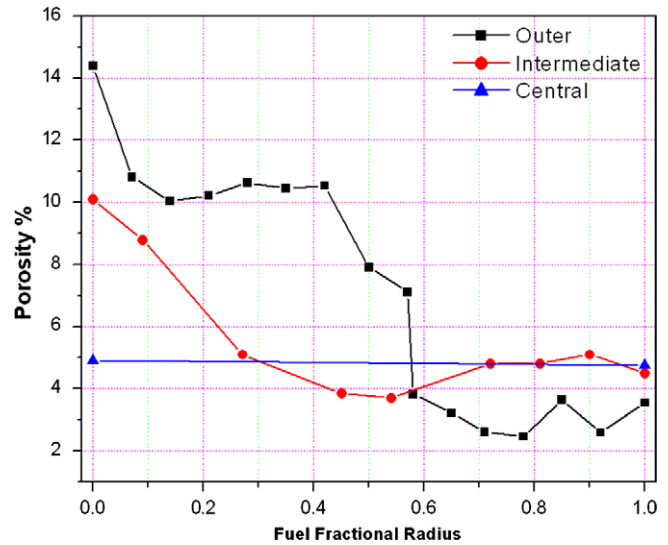


Fig. 3. Radial porosity profile measured during PIE.

dicted by all the other codes is very low compared to the experimental value.

Fig. 6 shows the maximum fuel centre temperature achieved during irradiation, predicted by the codes for the outer pin along with the PIE estimated value for comparison. Predictions of most codes were within $\pm 10\%$ of experimentally estimated temperature. It may be noted that the fuel centre temperature was estimated from fuel restructuring and some uncertainty in the estimated temperature may not be ruled out (see Section 5.4).

The fission gas release percentage in the outer pin predicted by the codes is compared with the experimental result in Fig. 7. There is a wide variation in the values predicted by the codes, all the codes under-predicting the gas release with varying extent of under prediction. It was found that codes which predicted very low release had also predicted low temperature of fuel.

5.1.2. Middle pins and central pin

The predicted fuel centre temperature in these pins by most codes fell within $\pm 10\%$ of experimental value. Most codes predicted low fission gas release in these fuel pins. Measured fission gas release was also low. However, some codes over-predicted the gas release in these fuel pins.

5.2. Internal pin pressure

The measured end-of-life internal gas pressure (at room temperature) in the fuel pins is compared in Table 3 with the pressures predicted by the codes. It is found that several codes predicted

Table 2
PIE results

Parameter	Measured/estimated values		
	Outer fuel pin	Middle fuel pin	Central fuel pin
Internal pressure at room temperature (bar)	21.4–27.6 (Average 24.5)	4.2–4.4 (Average 4.3)	3.2
Volume of FGR (cc STP) including He	70.1–80.8 (Average 74.3)	12–12.6 (Average 12.3)	9.3
% Fission gas release	22.5–26 (Average 24.1)	1.7–2.1 (Average 1.9)	0.64
Void volume in fuel pin (cc)	3.1–3.7 (Average 3.36)	3.0–3.3 (Average 3.15)	3.2
Maximum fuel centre temperature ($^{\circ}\text{C}$)	1724	1250	1174
Fuel grain size at pellet centre (μm)	33	19	15
Maximum outer oxide layer thickness (μm)	3.7	3	3.3
Average fuel-clad cold gap – radial (μm)	26	24	16
Radial porosity profile	Shown in Fig. 3		

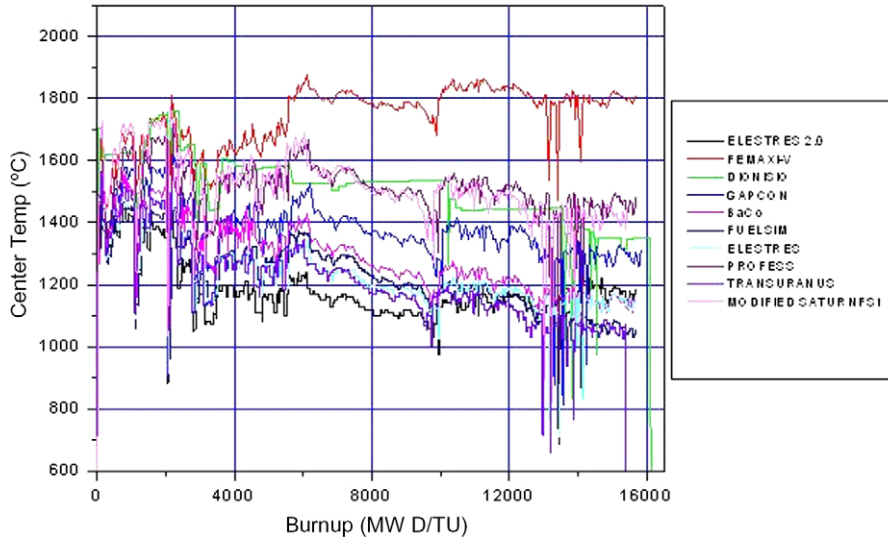


Fig. 4. Fuel centre temperature in the outer pin predicted by the codes.

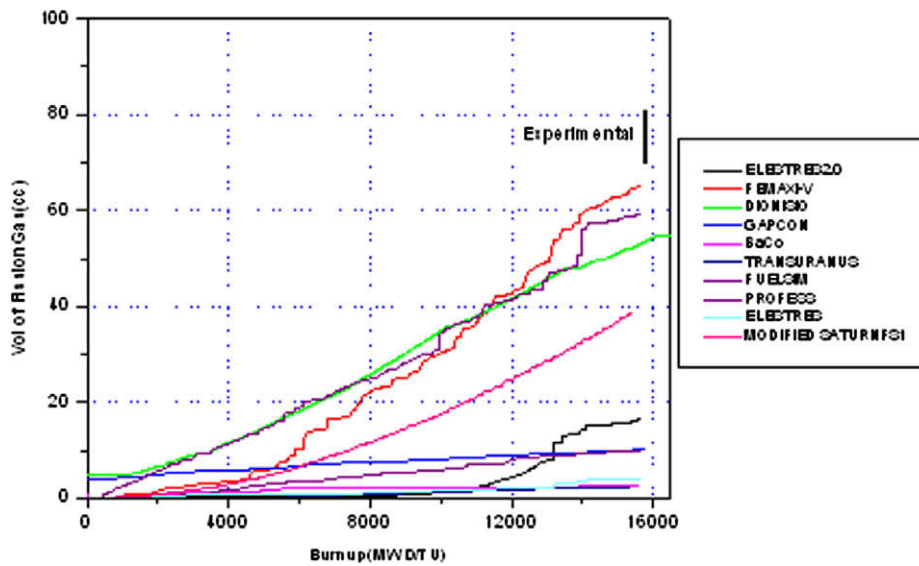


Fig. 5. Fission gas release volume in the outer pin predicted by the codes.

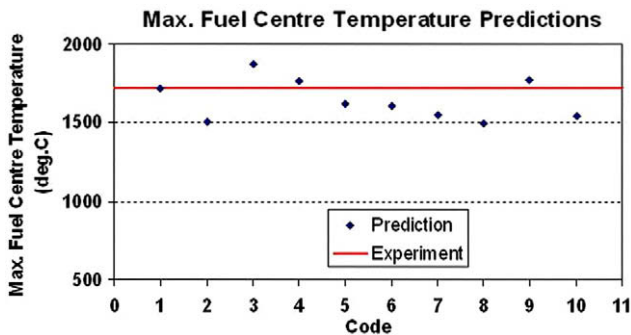


Fig. 6. Maximum fuel centre temperature predictions for the outer pin compared with the experimental measurement.

internal pressure in the outer fuel pin close to or higher than the measured values. Other codes under-predicted the internal pressure in this pin.

In the case of the middle and central fuel pins the measured pressure was low. Most codes predicted low pressure in these fuel pins, but one code tended to grossly over-predict the pressure in these fuel pins.

5.3. Fuel-clad gap, oxide thickness, fuel grain size and porosity

Table 4 gives the comparison of the end-of life values of fuel-clad cold gap, cladding oxide layer thickness and fuel grain size at the pellet centre, predicted by some of the codes, with the experimental results. It is found that the predictions have better agreement with experiments in the middle fuel pin and central pin than in the outer fuel pin. The radial porosity profile in the fuel

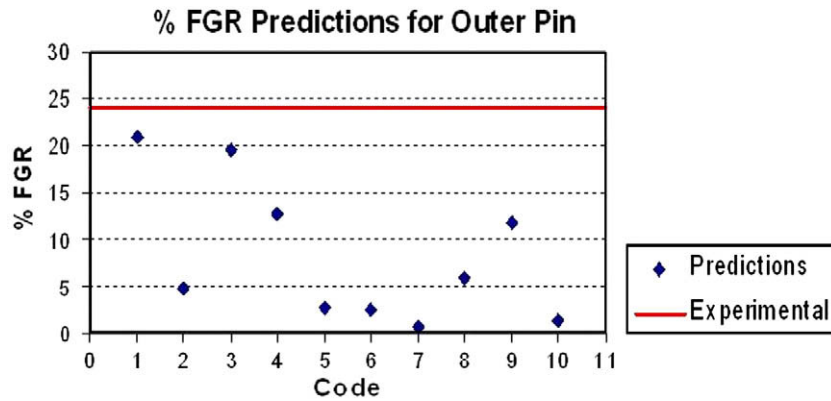


Fig. 7. Percentage FGR predictions for the outer pin by the codes compared with the experimental measurement.

Table 3
Comparison of predicted and measured internal gas pressure in the fuel pins

Code no.	Internal gas pressure (bar)					
	Outer pin		Middle pin		Central pin	
	Predicted	Measured	Predicted	Measured	Predicted	Measured
1	29.6	21.4–27.6	2.9	4.2–4.4	1.2	3.2
2	8.6		1.2		1.0	
3	20.7		1.2		1.2	
4	18		6.3		3	
5	5.1		3.1		2.9	
9	14.2		10.3		8.7	
10	3		1.3		1.3	

pellets was predicted only by two codes. The radial profile predicted by code DIONISIO in the outer fuel pin and central pin was somewhat similar to the experimentally measured profile.

5.4. Recommendation for further work

Since the present exercise was based on a PHWR bundle from a commercial reactor, there was no instrumentation to get directly measured values of test data like pin power and fuel temperature. The irradiation power history used in the present exercise was obtained by using a computer code. There could be some uncertainty in these values. Similarly fuel centre temperatures were estimated from fuel restructuring during PIE. Hence fuel centre temperatures used in this exercise are expected to have some uncertainties. For example, the estimated fuel centre temperature for the outer pin was higher than the temperature above which columnar grain

growth is believed to occur, but columnar grain growth was not observed in the fuel pellet microstructure.

The measured fission gas release in the outer fuel pin was indicated [12] to be higher than that observed in typical CANDU fuel irradiated at similar power/burnup condition. Post irradiation examination (PIE) of fuel pins from more fuel bundles and investigation of as-fabricated fuel microstructure and microchemistry will be needed to understand the fission gas release behaviour observed in the outer fuel pin.

Following recommendations are made for further actions with regard to validation of codes for PHWR fuel:

- (i) Recalculation of all the cases taking into account the uncertainties in the various data used for calculation e.g., fuel thermal conductivity, fuel pin power rating, fission gas diffusion coefficient, etc.
- (ii) In-pile irradiation of well documented fuel pins with in-pile instrumentation for power, fuel temperature, fission gas pressure etc followed by detailed PIE.
- (iii) PIE of more irradiated high burnup fuel bundles from operating PHWRs.

6. Summary

1. A blind prediction exercise on Indian PHWR fuel was organised for the first time for investigating the predictive capability of codes at extended fuel burnup. 11 codes from 7 countries participated in this exercise.
2. The maximum fuel centre temperature predicted by most codes was within $\pm 10\%$ of the fuel centre temperature estimated from fuel restructuring.

Table 4
Grain size, oxide layer thickness and fuel-clad gap comparison

Code name	Outer pin			Middle Pin			Central Pin		
	Cold gap radial (μm)	Oxide thickness (μm)	Grain size (μm)	Cold gap radial (μm)	Oxide thickness (μm)	Grain size (μm)	Cold gap radial (μm)	Oxide thickness (μm)	Grain size (μm)
ELESTRES 2.0	41.68 (PMP)* 58.23 (PPI)**	–	16.46	32.08 (PMP) 49.36 (PPI)	–	10.04	37.73 (PMP) 51.25 (PPI)	–	10.01
DIONISIO	32.00	11.52	53	21.50	7.44	27	18.50	5.87	11
PROFESS	–	–	48.19	–	–	12.35	–	–	10.00
Code from CHINA	60.75	1.55	–	23.61	1.46	–	24.60	1.42	–
EXPERIMENTAL	26	3.7	33	24	3	19	16	3.3	15

* PMP : Pellet midplane.

** PPI: Pellet pellet interface.

3. Fission gas release in the outer pin which operated at high power rating, was under-predicted by the codes. However, the end-of-life internal pressure in the pin was predicted close to the measured values, by some codes.
4. For the middle and central pins, some codes over-predicted the fission gas release and internal pin pressure.

Acknowledgements

The authors express their gratitude to Mr John Killeen, Scientific Secretary, IAEA, Dr S. Banerjee, Director, BARC and Mr S. A. Bhardwaj, Director (Technical), Nuclear Power Corporation of India Ltd for their valuable help and support in this work.

References

- [1] S.S. Bajaj, A.R. Gore, Nucl. Eng. Des. 236 (April) (2006) 701.
- [2] I. Misfeldt, OECD-NEA-CSNI/IAEA Specialists' Meeting on Water Reactor Fuel Safety and Fission Product Release Under off Normal and Accident Conditions, Riso National Laboratory, Denmark, 1983 (May 16–20).
- [3] IAEA TECDOC – 998, Fuel Modelling at Extended Burnup, A Report of the Co-Ordinated Research Program FUMEX, IAEA Publication, January 1998.
- [4] John Killeen, V. Inozemtsev, J.A. Turnbull, Paper presented at the IAEA Technical Meeting on PHWR Fuel Modelling held at Mumbai, vols. 5–8, 2006.
- [5] D.N. Sah, Bull. Mater. Sci. 8 (1985).
- [6] G.G. Chassie, K.-S. Sim, B. Wong, G. Papayiannis, in: Proceedings of the Ninth International CNS Conference on CANDU Fuel, Belleville, Ontario, 2005 (September 17–21).
- [7] K.-S. Sim, G.G. Chassie, Z. Xu, M. Tayal, C. Westbye, Progress in Qualifying ELESTRES-IST 1.0 Code: Verification and Interim Results of Validation, in: Proceedings of the Seventh International CNS Conference on CANDU Fuel, Kingston, Ontario, 2001 (September 23–27).
- [8] Armando C. Marino, Eduardo J. Savino, Santiago Harriague, J. Nucl. Mater. 229 (2) (1996) 155–168.
- [9] Armando C. Marino, Strategy for the development of BaCo: a fuel rod behaviour simulation code, in: International Conference on Advances in Nuclear Materials: Processing, Performance and Phenomena (ANM 2006), December 12–14, 2006, & Conference on "Materials Behaviour: Far from Equilibrium" (MBFE), Mumbai, India, December 15–16 2006.
- [10] Alejandro Soba, Alicia Denis, Simulation with DIONISIO 1.0 of thermal and mechanical pellet clad interaction in nuclear fuel rods, J. Nucl. Mater. 374 (1–2) (2008) 32–43.
- [11] D.N. Sah, U.K. Viswanathan, K. Unnikrishnan, Prerna Mishra, R.S. Shrivastaw, S. Anantharaman, Post Irradiation Examination of High Burnup PHWR Fuel Bundle 56504 from KAPS-I, Report No. BARC/2007/E/002, Bhabha Atomic Research Centre, Mumbai, 2007.
- [12] Ki-Seob Sim, AECL, Canada, Personal Communication.