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THERMODYNAMIC PROPERTIES
OF THORIA-URANIA FUELS
FOR THE ADVANCED
HEAVY WATER REACTOR

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THERMODYNAMIC PROPERTIES OF THORIA-URANIA FUELS FOR THE ADVANCED HEAVY WATER REACTOR

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Introduction

Over the last thirty years there has been increased interest in utilizing thorium as nuclear fuel, primarily because, this potential actinide is three times more abundant in the earth's crust. Many countries, particularly those rich in thorium resources, have focused on research and development on thorium-based fuels. In the last three decades the use of Th-based fuel cycles has been extensively studied in Germany, India, Japan, Russia, United Kingdom and the United States of America and significant experience has been gained on the performance of the fuel in power generation and breeding. India accounts for one-third of the world's thorium reserves and is implementing thoria utilization through the three-stage fuel cycle concept: plutonium (^{239}Pu) generation from uranium in Pressurized Heavy Water Reactors (PHWR), ^{233}U breeding from ^{232}Th in Fast Breeder Reactors (FBR), and ^{233}U burning for power production. India is also exploring the possibility of direct utilization of thorium in the Advanced Heavy Water Reactor (AHWR) configuration.

In the AHWR, thoria-based fuels will be used and the fuel will contain 2-4 % of fissile isotopes of uranium (^{233}U) or plutonium (^{239}Pu) in mixed oxide forms: $Th_{1-y}U_yO_2$ and $Th_{1-y}Pu_yO_2$. In such a reactor, while the U/Pu isotopes undergo fission by thermal neutrons, there is simultaneous burning of the abundant isotope ^{232}Th via *in-situ* generation of the daughter atom ^{233}U. About 60% of the AHWR power output is expected to be from the thorium burning process. AHWR being a new concept its technological [1] implementation needs inputs of basic data of physics and chemistry of the fuel and its fission products (fps). The data would help in understanding whether the physical and chemical evolution of the fuel during long irradiation periods is conducive to the safe operation of the reactor.

A burnup of about 50 GWD ton^{-1} would be common in the thoria-based fuels considering reprocessing difficulty. To attain an average discharge burnup of 50 GWD ton^{-1} with a typical power rating of 180-200W/cm in AHWR, the fuel will be irradiated for over 60 months. During irradiation, the fuel pin (Fig.1) generally bears the thermal profile of 1300-1500 K as the central temperature (Fig. 2) and 800-900 K as peripheral temperature and occasionally above this range in power ramp situation. At high temperatures and under a steep thermal gradient, the fps undergo transport and redistribution within the cladded pin (Fig.1) and chemically react among themselves and with the thoria matrix and the clad. Under this situation, the integrity of the fuel pin and the clad is the main issue. The integrity is governed by the physico-chemical transformation of the fuel matrix and the clad with burnup.

For the analysis and evaluation of fuel-clad integrity during long irradiation periods, the knowledge of thermodynamic and transport properties of the fuel and
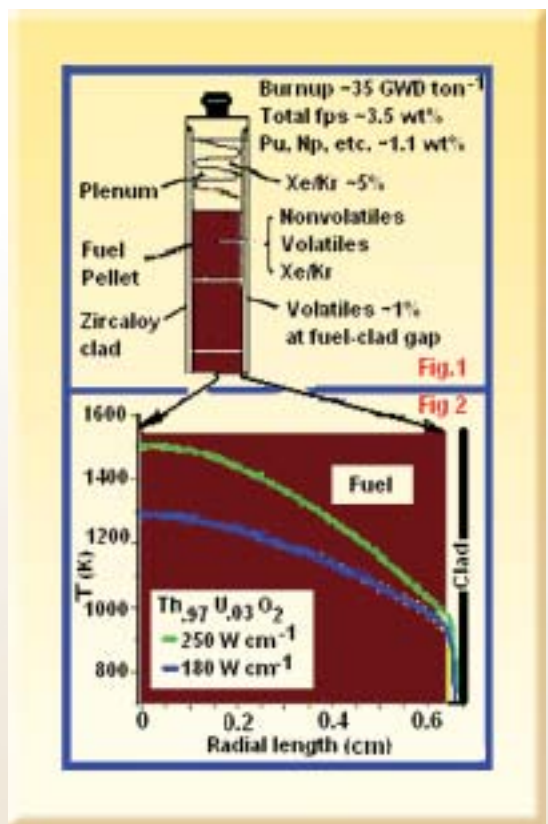
Fig. 1 : Schematic of cladded fuel pin
Fig. 2 : Typical thermal profile in the fuel

re-established for new fuel like thoria. Thoria (ThO_2) has quite a number of advantages over urania (UO_2) such as better thermophysical properties, chemical stability and radiation resistance which ensure better in-pile performance and a more stable waste form. Like the case of the conventionally used oxide fuels, the thoria based fuels do not pose any difficulty in handling and fabrication, at least in the virgin state.

Table 1: fps yields from reactor fuels

F.P. a/O	^{235}U PWR	MOX 30%PuO$_2$ PWR	^{233}U AHWR	^{239}Pu FBR
Xe+Kr	11	12	16	12
Pd+Ru Tc+Rh	11	24	7	24
Mo	10	10	10	11
Zr	16	11	17	10
Y+R.E.	28	25	27	24
Ba+Sr	10	5	9.5	6
Cs+Rb	12	11	10.5	11
Metalloids + Halogens	2	2	1.8 1.2	2

fps is necessary. Using the thermodynamic and kinetic information, the integrity analysis would require the evaluation of (i) concentration built-up of gaseous and corrosive volatile species at the fuel-clad interface and inside the fuel matrix (ii) the possible extent and pathways of chemical damage of the clad by the corrosive volatiles and (iii) the extent of fuel swelling and disintegration by gas accumulation and by different solid phase formations. The chemical picture that would emerge out of the evaluation would help in the analysis of fuel performance in normal and also off normal situations of reactor operation.

The above mentioned aspects, though well-known for the conventional urania fuels, need to be

The fuel chemistry with thoria would not be the same as with urania in case of conventional reactors, though the same set of fps with similar yields (Table1) are formed and settle down inside the respective fuel matrices made of MO_2 (M = Th^{+4}, U^{+4}) fluorite lattice, with similar crystal radii of the cations.

Distinguishable features of thoria based fuels and the general scenario of the fission products inside the thoria matrix.

The difference in chemistry of thoria originates from the rigid four valency of Th in its compounds as against the flexible valency of four to six in the case

Table 2 : Chemical states of fps in oxide fuels

Types of fps	Chemical states
Non-vo la tiles:	
Rare-earths (Nd, La, Ce etc), transition metals (Y, Zr, Nb) .	Dissolved state in fuel matrix (MO_2). Perovskite, MM^*O_3 (grey) phase.
Alkaline earths (Sr, Ba), к Zr, U, Pu, Mo, Ce .	Alloy (white) phases.
Noble metals (Pd, Ru, Rh), and Mo.	Dispersed microbubbles in fuel. Fractional release at ffiel-clad gap sc. at plenum.
Gases at volatiles:	MI, M_2Te at low-moderate burnup. Conversion of MI, M£Te to uranate/ molybdates at high burnup.
Inert gases (Xe, Kr).	In alloy phases.
Alkali metals (Cs, Rb).	As alkali metal compounds.
Cd,Te,Sb.	
Te, I, Br.	

of U. In compounds like Cs-uranates, U acquires higher valencies. Urania can oxidize to hyperstoichiometric composition UO_{2+x}, and by this it can buffer oxygen pressure to a large extent. The chemical affinity for additional oxygen being absent in thoria, the buffering action will be evidently weak in thoria-based fuels. For the same reason oxygen transport in thoria-rich matrix is expected to be predominantly by self diffusion unlike in urania where oxygen makes faster transport through the chemical affinity-driven diffusion process. These subtle features as compared to urania, can lead to faster growth of oxygen pressure in the fuels and thereby alter the thermochemistry of fps.

Fission of the actinide M, in MO_2 generates the fps and releases oxygen. The released oxygen undergoes redistribution among reactive fps, fuel and clad for their

(i) How fast and to what extent oxygen pressure inside the thoria-based fuels grows with burnup

(ii) whether the O-pressure growth could be buffered by the oxidation of reactive fission products and clad or

(iii) whether there could be oxygen transport impediment in thoria-rich matrix resulting in much higher oxygen profile than in urania? If the last point is true then :

-what is the altered thermochemistry of the fps under the higher oxygen pressures inside thoria fuel?

-can it lead to increase in free iodine concentration and formation of oxygen-rich bulky phases and from there to the pin-clad incompatibility problem?

-can the fission product Mo buffer it by its ready oxidation?

oxidations. The states of oxidized fps inside the urania matrix are fairly well established and are summarized in Table 2 for typically high burnt fuel of pressurized water reactor [2]. For thoria fuels, the distribution of fps in metallic phases, oxides and gases is expected to be similar though there can be thoria-based compounds in the oxide phases. As in the case of urania, the fluorite lattice of thoria can accommodate many of the fps. The alkaline earth based thorates $MThO_3$ can be chemical components in the grey (perovskite) phase. Additionally, there can be tetragonal/cubic phases due to alkali thorates of composition M_2ThO_3. However, considering the stated subtle features of thoria, one needs to address to a couple of specific issues for the fuel. These issues are included in the text box given on the previous page.

In order to address the questions mentioned in the text box, one makes a detailed balance of fission generated oxygen, considering its consumption according to the hierarchies of oxidation of the fps. The thermochemistry that a fp assumes with evolution of the oxygen potential is to be considered, for understanding the oxygen consumption. The detailed balance of incessantly generated oxygen, takes note of the oxygen used in oxidizing the most reactive fps, and the distribution of the leftover part in alloy oxidation and as transported component to clad. The analysis of detailed balance requires not only thermodynamic data of the oxidized fps but also kinetic data of alloy oxidation, oxygen transport inside the matrix and across fuel-clad gap and oxygen incorporation in zircaloy clad.

Detailed O-balance from thermodynamic and kinetic analyses

As already mentioned, the actinide element undergoing fission from the oxide matrix, produces two fps and two oxygen atoms. The fission released oxygen is consumed by the fps, fuel and clad according to their oxidation hierarchies. The oxygen potentials of the two-phase mixtures of the fp elements and their oxides

in the respective cases form the thermodynamic basis of oxidation -lower the oxygen potential or oxygen partial pressure (p_{O2}) of the mixture, higher the hierarchy in oxidation. The potential is related to pressure as $\Delta \overline{G}_{O2} \equiv RT \ln p_{O2}$. To understand oxygen redistribution among the fps and clad, the O potentials of the relevant metal/metal oxide systems are plotted as functions of temperature in Fig. 3a. The O-potential of the fuel, $Th_{0.97}U_{0.03}O_2$ at different temperatures is indicated in Fig.3b. The intercomparison of the potentials when made, for example, at 1473 K, indicates, that at first, yttrium and rare earths (RE) will be oxidized to their respective trivalent oxides and this will be followed by the oxidation of alkaline earths (Sr, Ba) and zirconium to their divalent and tetravalent oxides respectively. The Zr in zircaloy clad will be oxidized approximately at the Zr/ZrO_2 potential. The result of the hierarchical oxidations is given in Fig. 3c. The extent of oxidation of the other fps (Cs, Mo, etc.) less oxidizing than Zr, cannot be deduced, without considering the oxidation of fuel and clad and the thermodynamic stabilities of their ternary compounds. Oxygen uptake by clad depends on both O-transport and oxidation kinetics, and these aspects will be discussed separately. Although Cs/Cs_2O potential (Fig. 3a and 3b) is way above that of the fuel, oxidation of Cs and fuel starts almost parallely because of the formation of highly stable oxide-based compounds like alkali uranates, molybdates, zirconates and thorates. The Cs case suggests that the *prima-facie* knowledge of oxygen potential of the binary equilibria of metal/metal oxide systems of the fps is necessary but not sufficient for the oxygen consumption analysis. One needs to have complete information on the thermochemistry of the fps, which will be mentioned in the next subsection. The fuel $Th_{0.97}U_{0.03}O_2$ with typical O/M $\sim$ 2.0000 will share an insignificant part of the fission-released oxygen to raise its O/M ratio. It is apparent from Fig. 3b that the O/M ratio will hardly rise when the O-potential of the fuel attains that of Mo/MoO_2 and Mo oxidation starts buffering the potential. In urania fuels, in
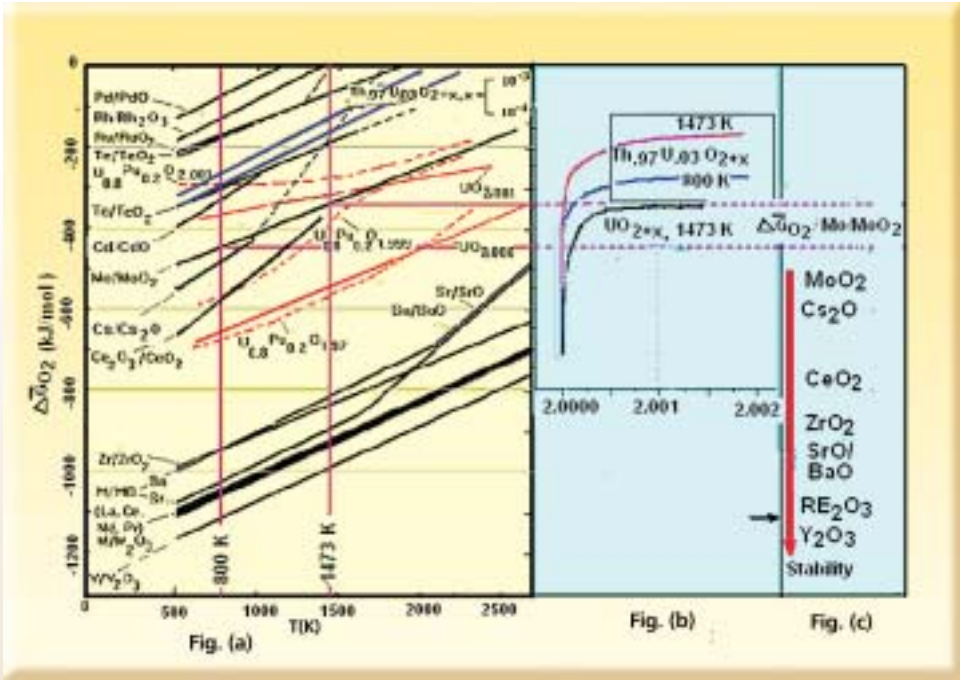
Fig. 3(a) : Oxygen potential of fp/fp-oxide systems
Fig. 3(b) : Oxygen potential of AHWR fuel
Fig. 3(c) : Fp-oxides formation hierarchies

contrast, the O/M ratio at 1473 K should rise to the value of 2.001 (Fig. 3b) before Mo gets oxidized. The extent of Mo oxidation is however subjective to the detailed balance of fission generated oxygen considering the consumption. Using the fps yields in AHWR fuel (Table1) and the oxidation hierarchies (Fig. 3a, 3c), the oxygen uptakes by the fps is given in Table 3. If all the fission generated oxygen is available for fps oxidation, the rare earths, alkaline earths, and zirconium use about 83.5 atom %O in forming their respective binary oxides RE_2O_3, Sr(Ba)O and ZrO_2. Another 3.7% is used for Ce_2O_3 oxidation to CeO_2 which gets stabilized as cerate

Table 3 : Oxygen redistribution among fps. and clad

AHWR $UO_2 \rightarrow 2Fps + 2O)$	Yields a/0	Oxide types	Oxygen Content a/0
Y + R.E.	27	M_2O_3	40.5
Ba + Sr	9	MO	9
Zr	17	MO_2	34
Ce	7.4	Ce_2O_3 ► CeO_2	3.7
Cs + Rb	10	M_2O	5
Mo	10	MO_2	20
Mo + Ru Pd + Rh	8	–	0
Xe + Kr	16	–	0
Metalloids + Halogens	1.8 1.2	–	–
Fps-yield	100	0 in fps's oxides	
Oxygen Yield (a/0)	100	(i) No MoO_2 92.2 (ii) MoO_2+MO 100	

components in the perovskite (grey) phase, (Ba,Sr)(Zr,Th, U,Ce)O_3, constituted mainly of zirconates of the alkaline earth fps. From the balance of 12.8% oxygen (Table 4) a part would be transported to clad while the rest of the O will be used for the oxidation of Cs/Rb, fuel and Mo. To understand the redistribution behavior of the 12.8% oxygen, a brief mention is now made of the thermodynamic aspect of the fps states and kinetic aspects of the O-transport and oxidation.

apparatus for these techniques are shown in Fig.5 and Fig.6. The remaining fission generated oxygen of 12.8 atom % which raises the potential above Zr/ZrO_2, will cause the formation of O-rich ternary compounds of Cs. The extent of O-uptake by the alkali metals, depends on the amount of O-partitioning among their thorates/ zirconates and uranates/molybdates.
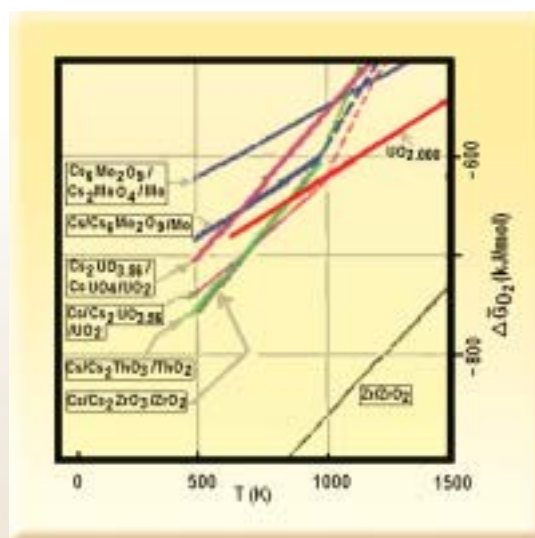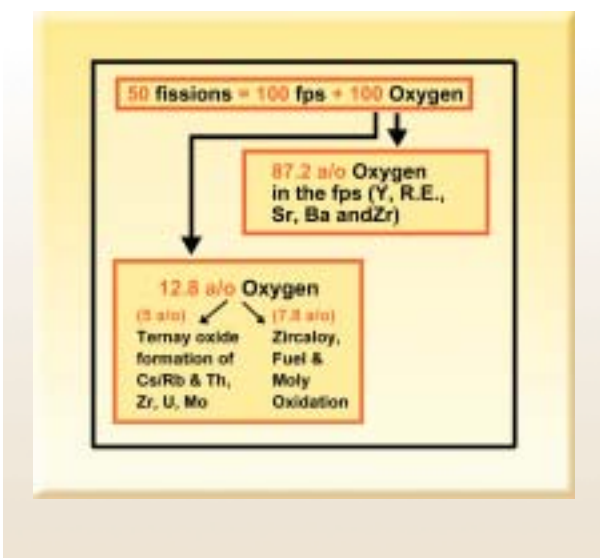

Fig.4 : Relevant chemical states of Cs

Thermodynamic aspects

Fig.4 shows the oxygen potentials of relevant chemical equilibria involving the alkali metal fp Cs. The metal oxide phases have O-potentials of roughly 200 kJ mol^{-1} above that of Zr/ZrO_2 and almost the same amount below that of Mo/MoO_2. In the figure, the potential values for different oxide systems are obtained from our experimental results and the reported information as summarized in Table 5. The thermodynamic stabilities of oxide compounds such as BaThO$_3$, SrThO$_3$, Cs$_2$ThO$_3$, Cs$_2$ZrO$_3$ and Rb$_2$ThO$_3$ were measured using Knudsen effusion and transpiration techniques. The indigenously developed

Fig. 5 : Knudsen effusion assembly

Table 5 : Summary of thermodynamic data of relevant ternary compounds of the fission products

Ternary compounds (molar volume w.r.t. ThO2 at ambient)	$\Delta_f G^\circ$ KJ mol-1 800≤T≤1500 K	Ternary compounds (molar volume w.r.t. ThO2 at ambient)	$\Delta_f G^\circ$ KJ mol-1 800≤T≤1500 K	Ternary compounds (molar volume w.r.t. ThO2 at ambient)	$\Delta_f G^\circ$ KJ mol-1 800≤T≤1500 K
BaThO3 (orthorhombic; 1.31)	-1802+ .279T	BaZrO3 (cubic: 1.6)	-1787+0.2954T	Cs2MoO4 (orthorhombic:2.28) Hexagonal Cs2MoO4(liq)	-1514+0.3605T, T<952 K; - 1649.6+0.5209T, T>952K -1611.3+0.4897T, T>1229.5 K
SrThO3 (monoclinic; 1.47) (orthorhombic; 1.41)	-1825+0.29T	Cs2ThO3 (cubic; 1.57)	-1780+0.44T	SrMoO4 (tetragonal; 2.12)	-1540.6+0.3576T
BaUO3 (orthorhombic; 1.32)	-1687+0.2705T	Rb2ThO3 (cubic 1.65)	-1822+ .45T	BaMoO4 (tetragonal;2.02)	-1555.5+ 0.387T
BaMoO3 (cubic; 1.41)	-1229+0.2615T	Cs2ZrO3 (orthorhombic 1.93)	-1672+0.44T	SrUO4 (tetragonal;1.27)	-1980.2 + 0.34T
SrMoO3 (cubic; 1.53)	-1289+0.2702T	Cs2UO4 (tetragonal; 1.51)	-1926+0.4108T, T<952 K; - 2062+0.5532T, T>952 K	BaUO4 (orthorhombic; 1.32)	-1988.8+0.3597T

Fig. 6 : Transpiration assembly

The alkali thorates formation would be favorable to zirconates, as Zr in the fps preferentially forms the more stable alkaline earth zirconates. The data of the thorates, zirconates, uranates and molybdates of alkali and alkaline earth fps are given in Table 5. As seen in Fig. 4 the oxygen potential rise will result in formation of cesium thorate and cesium uranate depending upon the temperature. Thermo-dynamically, Cs_2UO_4 conversion from the thorate is favored by the following reaction $Cs_2ThO_3(s) + [UO_2] + 1/2O_2(g) = ThO_2(s) + Cs_2UO_4(s)$. For similar reason, the interconversion of thorate to molybdate is also possible as $Cs_2ThO_3(s) + [Mo]_{alloy} + 3/2\ O_2(g) = ThO_2(s) + Cs_2MoO_4(s)$. Out of the two possibilities the former one is preferred. In the conventional urania-based fuels Cs is preferentially fixed in the uranate form. At 5 atom% burnup, alkali metals when consumed as their uranates, will take about half percent of the total uranium content of the fuel. Because of U-233 isotope production, the initial urania content of 3 mol% will hardly be lowered at a burnup of 50 GWD ton[-1]. Cesium uranate formation will consume ten atoms of oxygen leaving thereby 2.8 % out of the 12.8%. It is to be noted here that one atom of oxygen is consumed per alkali atom in uranate formation. Thorate ($M_2ThO_3(s)$) and molybdate (M_2MoO_4) formations would have consumed 0.5 and 2.0 O atoms respectively. However, for evaluating oxygen consumption

by the alkali metals, one should consider the thermodynamic as well as kinetic aspects. The latter aspect comes into play due to the restricted accessibility of Cs by the competing reactants, thoria, urania and Mo-alloy. The restriction arises from very low diffusion of the alkali metal atom. The diffusion coefficient of Cs in the fuel is lower than even that of the oxygen in the fuel matrix. With low urania content in AHWR fuel and the presence of a small quantity of the evenly dispersed alloy phase, the Cs and oxygen uptake by thoria matrix, is expected to be predominant. All Cs and Rb preferentially converted to cesium and rubidium thorates, the oxygen balance will be set to 7.8 atom% instead of 2.8 obtained from purely thermodynamic considerations. The actual value of oxygen balance will lie somewhere in between. Any augmented consumption of oxygen by the alkaline earth molybdates/uranates formation is not possible, as their formation requires BaO/SrO components to be displaced from the more stable perovskite phase. In the absence of detailed information of cesium transport and alloy phase distribution in the matrix, kinetic considerations are difficult to quantify. Rest of the presentation is thus based on the redistribution of the residual oxygen of 2.8 % obtained from thermodynamic considerations. This will give a lower limit of oxygen potential rise in the fuel. The 2.8 a/o of the fission generated oxygen, constantly available from 12.5 mm dia. fuel pellet at 180 W cm^{-1} power rating, will have the O-flux of 4.5 x10^{-8} g.atom d^{-1} cm^{-1}. Subsequent analysis considers these aspects.

Kinetic aspects of residual flux of fission-released oxygen

The residual flux of the fission released oxygen, will be consumed by molybdenum and parallely transported out to clad. The molybdenum oxidation kinetics is considered, taking

the reported result studied on metal surface. The oxidation rate of Mo surface expressed as $dN_{Mo}/dt = A \exp[-E/RT]$, $A = 5.3 \times 10^{-3}$ g.atom cm^{-2}s^{-1}, and $E = 82.4$ kJ mol^{-1}, suggests that the rate is as high as 91x10^{-4} g.atom cm^{-2} d^{-1} even at the lowest temperature of 800 K prevalent at the fuel surface. This value being several orders of magnitude higher than the residual O-flux of 4.5 x10^{-8} g.atom d^{-1} cm^{-1}, one may conclude that finely divided state of Mo can easily buffer the oxygen potential. Kinetically, freshly generated Mo is expected to oxidize faster, rather than forming alloy with the noble metals.

The parallel kinetic path of overall O-transport to clad will be governed by the slowest of the three processes: a) transport through matrix b) transport across fuel clad gap and c) oxidative incorporation in clad, which are briefly described below :

a) The reported data of the chemical diffusion of oxygen in thoria-urania matrix given in Fig.7 at 1000K shows that, the diffusion coefficient falls sharply to a low value when the urania content is less. Our study of AHWR SIMFUEL of 20 GWD
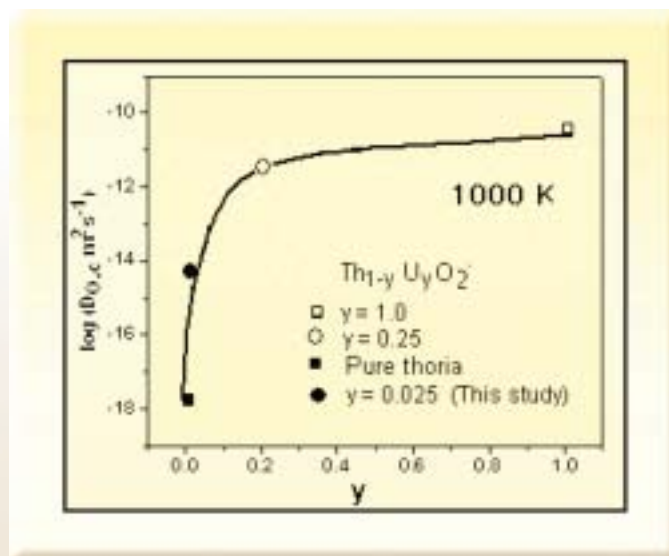

Fig.7 : Trend of oxygen transport in Th$_{1-y}$U$_y$O$_2$

ton^{-1} burnup has shown, that the oxygen transport coefficient in the fuel is orders of magnitude lower than that of pure urania. The temperature dependence of the transport (chemical diffusion) coefficient for the thoria SIMFUEL and pure urania are given respectively by log $D_{o,c}$ (± 0.25 m^{2}s^{-1}) = -5383/T –8.82, and log($D_{O,c}$/m^{2}s^{-1}) = -4680/T-5.74.

b) The O-flux flow from fuel to clad has to travel across a thin gap (typically 50 microns) filled with helium gas at high pressure ($\sim$25 bar). The transport coefficient D_g of oxygen according to the kinetic theory is of the order of $u_{av}/(3\pi N \sigma^2)$, where u_{av} is the average speed of O_2 molecules at the gap temperature of $\sim$800 K, N is the total gas density and σ is the mean collision diameter of He+O_2 gas mixture. D_g value works out to be 0.054 cm^{2}s^{-1}. With this value, one thus addresses the question as to whether the residual O-flux load of 4.5 x10^{-8} g.atom d^{-1} cm^{-1} from the fuel can be transported radially outwards across the thin annular gap of 50 micron. This transport process through gas diffusion needs an O_2 concentration drop of 6x10^{-15} g.mol cm^{-3}, or, pressure drop of 3.5x10^{-10} bar across the gap. It needs too high oxygen pressure gradient, than could be met by the low p_{O2} ($<$10^{-25}bar), on the fuel surface decided by the O/M ratio. The oxygen transport across the gap, can however be enhanced, by the presence of augmented concentration of oxygen bearing gaseous species like $H_2O(g)$, $Cs_2O(g)$ and CsOH(g), formed via the involvement of various chemical equilibria between reactive species like H_2 or Cs(g) with the oxide fuel (for example, $MO_{2+x} + \delta H_2(g) = MO_{2+x-d} + \delta H_2O(g)$). The H_2/H_2O reductive equilibrium, effectively converts all hydrogen in contact with the fuel to moisture. Sources of hydrogen are in fact, the moisture impurity in the fuel and also that resulting out of nuclear reaction. Cs(g) is the product of volatilization process of Cs bearing condensed and vapor phases present in the fuel. Thus oxygen can undergo chemical vapor transport, to reach the clad and oxidize it as

$2H_2O(g) + [Zr] = ZrO_2 (s) + 2H_2(g)$,
$2CsOH(g) + [Zr] = ZrO_2 (s) + 2Cs(g) + H_2(g)$.
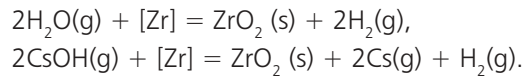
The products, hydrogen and cesium vapor return back to react with the oxide fuel forming the oxygenbearing species once again. Considering that the fuel reduction and zircaloy oxidation are nearly quantitative with least kinetic hindrances in them and noting that the transporting species ($H_2O(g)$ or CsOH(g)) prevail at significantly higher partial pressures than the required values ($\sim$3.5x10^{-10} bar) for the diffusion flow of 4.5 x10^{-8} g.atom d^{-1} cm^{-1}, one sees the effectiveness of chemical vapor transport mechanism for oxygen across the fuel-clad gap.

c) The clad oxidation takes place in steps. The oxide layer grows initially with cubic rate law and after a certain thickness is attained, it follows a comparatively slow growth linearly. The reported linear growth rate of 0.83x10^{-6} μm ZrO_2/d (equivalently, 5.70x10^{-7} g.atom d^{-1} cm^{-1}) is again an order of magnitude higher than the available O-flux.

The significance of oxidation of Mo as compared to that of clad, for the removal of the residual oxygen flux in thoria fuel, follows from the fact that the transport out process becomes competitive, only when the oxygen pressures inside the fuel develops much above the Mo/MoO_2 potential. Fig. 8 shows the steady state oxygen profile (right axis), inside the thoria SIMFUEL, to be established for transporting out the residual O-flux of 4.5 x10^{-8} g.atom d^{-1} cm^{-1}, in the absence of Mo oxidation. The profile is calculated using the mentioned transport coefficient and under a given temperature distribution (left axis). The result
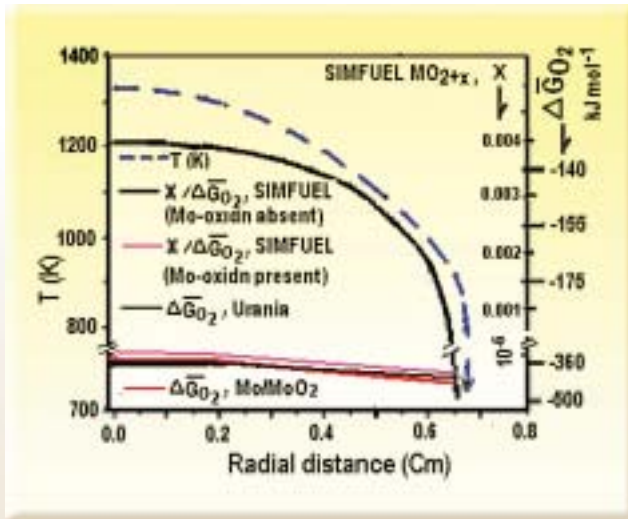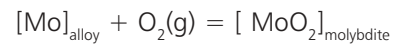
Fig. 8 : Profiles of oxygen and O/M ratio under a given temperature distribution and O-flux (4.5 x10^{-8} g.atom d^{-1}).

may remain as pure MoO_2 or as molybdite component or get further oxidized to molybdate. The oxygen potential is governed by the following equilibria:

$$[Mo]_{alloy} + O_2(g) = [\ MoO_2]_{molybdite}$$

At 50 GWD ton^{-1}, the molybdenum content in the hexagonal phase of metallic inclusions (Mo-Ru-Rh-Pd quaternary) is about 34 atom%. Mo activity in the phase considering reported data of Mo-Ru-Pd ternary (Fig. 9) is assumed to be within 0.25-0.3 over the temperture range of 800 to 1500K. The molybdites will be formed out of alkaline earths, Sr and Ba, that are normally present as zirconates in the perovskite phase. Considering however, higher stability of $BaZrO_3$, the molybdite component

of such calculation suggests that the O-transport inside the fuel is the slowest of the kinetic steps and also proves the important role of Mo in buffering the oxygen potential in thoria-based fuel. Urania case shown in the figure is distinctly different.

Oxygen potential at high burnup situation

The Mo oxidation playing a decisive role of controlling oxygen pressure in the burning process of the fuel, the chemical states of oxygen-rich phases that can be formed in the neighborhood of $[Mo]_{alloy}$/ MoO_2 potential will be considered in the subsequent analysis of high burnup situation. Depending on the oxygen potential the oxidized molybdenum
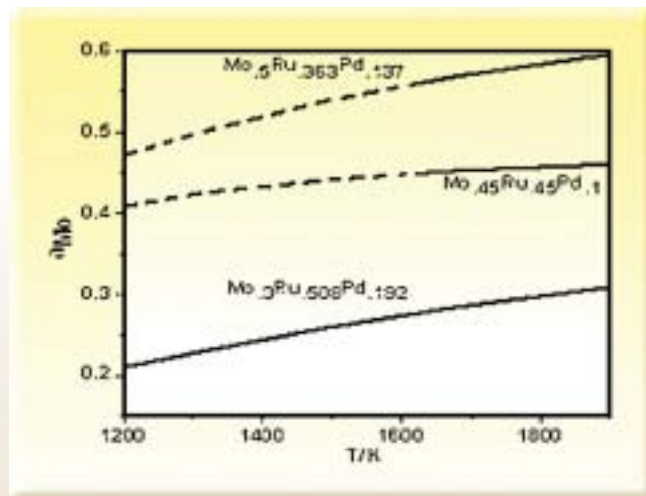

Fig. 9 : Mo activity in hexagonal phase of Mo-Ru-Pd ternary

will be mainly as $SrMoO_3$. Considering the residual part of oxygen as well as barium yield per fission and also the fact that practically all barium is present as

zirconate, the molybdite, to zirconate ratio is expected to be 0.44. In other words, the strontium molybdite mol fraction of the perovskite phase is 0.22. The oxygen potential is thus worked out considering the equilibrium

$$[SrO] + [Mo] + O_2(g) = [SrMoO_3] \qquad (1)$$
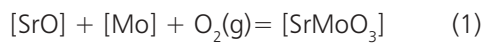
in which the SrO activity is governed by

$$[ZrO_2] + [SrO] = [SrZrO_3] \qquad (2).$$
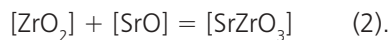
The ZrO_2 activity in (2) can be expressed by noting the dissolved part of ZrO_2 in thoria and the solution behavior of ZrO_2-ThO_2 pseudo-binary. The dissolved part is essentially the total Zr yield minus Zr present as $Ba(Sr)ZrO_3$. The $SrZrO_3$ activity in the perovskite phase, is iteratively worked out from an initially assumed value of 0.5, using equilibrium reaction (2) and the observation that the neodymium oxide component of the fuel phase does not displace the ZrO_2 from $SrZrO_3$ to form Nd-pyrochlore. With the iterated value of $SrZrO_3$ activity as 0.25 together with the ZrO_2 activity, the equilibrium reaction (2) leads to the SrO activity as $RTlna_{SrO} = -115.7+(0.047-0.0083lnB)T$. Use of this result in (1) and taking the Mo activity as 0.3 and $SrMoO_3$ activity as 0.22 yields the oxygen potential as $\Delta\overline{G}_{O2} = -559.4+(0.117+0.0083lnB)T$ kJ mol^{-1}. At 5 atom% burnup, the oxygen potential obtained is shown in Fig.10.

The actual pressure under the constant flux of 2.8% oxygen will be higher because of the impediment of transport of the reactants participating in equation (1). The calculated oxygen potential under the kinetic impediment will be governed by local equilibrium.

Further, in view of the fact that we have used the lower limit of the residual oxygen flux for evaluating the oxygen potential, the actual extent of Mo oxidation and accordingly the O-potential will be somewhat higher, had we considered the local equilibrium with a residual O-flux of 7.8%. It may be recalled, that in actual situations, the residual flux will be somewhere between 2.8 to 7.8 %, depending on the extent of global equilibrium.
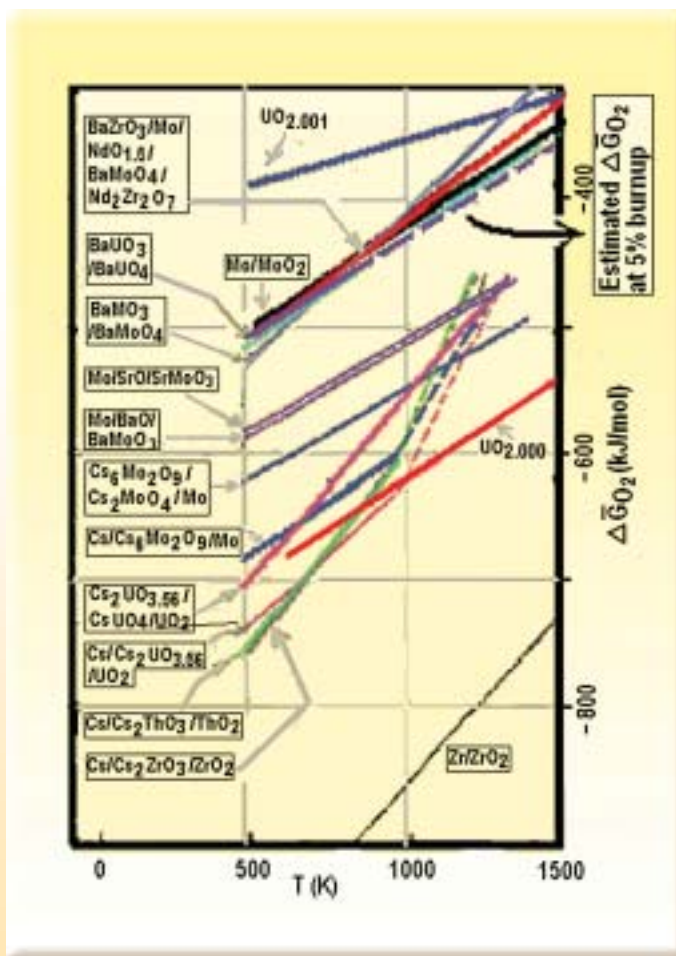
Chemical Scenario at high burnup

One can examine whether the phase equilibria involving oxygen-rich compounds other than molybdite have significance at the high burnup. The free energy considerations of the reaction, $2[SrMoO_3]+O_2(g) = 2SrMoO_4(s)$ shows that Sr-molybdite oxidation is not feasible at the high burnup. If the corresponding Ba compound had been present, similar reaction was possible at least in the peripheral region of the fuel pin (Fig 10). Since molydite oxidation to molybdate is not possible for the Sr case, the disproportionation forming the molybdate and Mo as $3[SrMoO_3]+ [ZrO_2] = [Mo] +2SrMoO_4(s) +[SrZrO_3]$ cannot occur. With the oxygen potential, one can examine whether there can be BaO partitioning from zirconate phase to result in the formations of the bulky phases like pyrochlore and molybdates, as $2[BaZrO_3]+ 2[NdO_{1.5}]+ 2[Mo]+3O_2(g) = Nd_2Zr_2O_7(s) + 2BaMoO_4(s)$. Considering the activities of the chemical components and the available thermodynamic data of the reactants and products it can be shown that even at high burnup like 10%, the pyrochlore and molybdate formations are feasible below 540 K. So for all practical purpose the forward reaction is absent within the fuel. If at all it occurs, it will be in the peripheral region (Fig.10). Under the prevailing oxygen potential, one further shows that the UO_2 oxidation, such as $2[UO_2]+O_2(g) +2[SrO] =2SrUO_4(s)$, leading to the formation of alkaline earth uranates is not feasible due to low activities of the alkaline earth oxides as well as urania in the fuel.

The uranate formation via reduction of SrO component in the fuel phase as $[UO_2]+2[SrO] = Sr(g)+ SrUO_4(s)$, depends on Sr atom transport from the reaction site. The reduction can also result in only gaseous products as $[SrO] +[MO_2] = Sr(g) + MO_3(g)$, $(M = U, Mo)$. Considerations of standard free energy changes of the reactions and the activities of the chemical components, it can be shown that, the above reduction will cause $SrMoO_3$ volatilization from the central part of the fuel and this will lead to the transport of the vapor products

and formation of $SrMoO_4(s)$ phase, in the peripheral part of the fuel pin.

The above mentioned findings about the oxygen potential and the resultant chemistry are based on the fact that residual flux of oxygen are easily consumed in molybdenum oxidations. However in high burn-up situations, the fuel matrix incorporating significant fractions of the fission gas in microdispersed states, oxygen accessibility to molybdenum alloy will be highly impeded. In this case, the oxygen potential can locally surpass the molybdenum/molybdite-control and lead to the formation of a number of oxygen-rich phases like: tellurites, tellurates and molybdates of the fps and clad materials. Thermodynamic data and volatilization characteristics of such O-rich phases have been generated in our laboratory. In the conventional oxide fuels, these phases are relevant only for the analysis of failed pin. Fuel pin failure occurs when the thin clad wall ($\sim$0.5 mm thickness) develops defects, providing permeation path of the coolant fluid with a higher oxygen potential to come in contact with hot fuel.

The thoria-based fuels will develop internal stress from the formation of the bulky oxygen-rich phase. As discussed before, the outer part of the fuel pin will be enriched with the molybdate precipitates as well as gas bubbles migrating out from the centre. Generally, all the nonvolatiles and the volatiles to a large extent ($\sim$99%), and a major fraction (90-95%) of the gaseous fps remain within the matrix (Fig 1), [2]. The dispersed bubbles as well as the undissolved solid phases formed by other fps impart internal stress to the matrix, under which the fuel pin swells, develops radial microcracks and voids and as the result, thermal conductivity of the fuel-matrix deteriorates. The gap conductivity also deteriorates progressively due to released gas that dilutes the helium column filling the gap at several tens of barspressures. As compared to the case reported for the conventional urania-based fuels, the extent of the fuel swelling from the dissolved and undissolved components of the fps will be more in thoria.

The volatile fps like I and Te, though produced in small amounts, can put stake on the fuel containment because of their corrosion and fatigue actions to the clad. Like the gases, these species undergo transport to reach the clad's surface. Chemical interaction of I and Te with the

Fig. 11 : Trend of diffusivity of volatile species with temperature

clad, results in degradation of its mechanical property and in extreme situation, leads to its brittle fracturing and, stress corrosion cracking. The availability of free I and Te depends on two factors: their transport properties and relative stabilities of their cesium compounds as compared to the ternary oxide phases of cesium. The stability of Te-intermetallics is an additional factor in Te partitioning. The measured transport properties of I, Te, Cs, Xe etc. show that, these are significantly lower in thoria-based fuels than in urania. The transport data is presented in Fig.11.

Conclusions

Thoria-based fuel is shown to have poor transport property of oxygen. The present analysis suggests that the fuel will generally bear higher oxygen potential right from the early stage of burnup. Mo plays vital role in buffering the potential in thoria fuel. This is unlike the case in urania, where the oxygen potential is controlled by fuel oxidation and easy transport to clad for its oxidation. Mo oxidation starts at a much later stage when the urania matrix attains high O/M ratio and is morphologically degenerated with dispersed gas bubbles. The higher potential in the thoria fuel, results in formation of oxidized products like $SrMoO_3$. In the cooler part of the fuel pin, there is a likelihood of the formation of more oxidized products like $SrMO_4$ (M= Mo, U). The transport properties of the volatile reactive fps like I, Te, Cs are significantly low in thoria based fuels as compared to those in urania. The fuel containment problem from clad corrosion though less in the fuel, matrix swelling will be more due to the large retention of gaseous fps and formation of oxygen-rich phases.
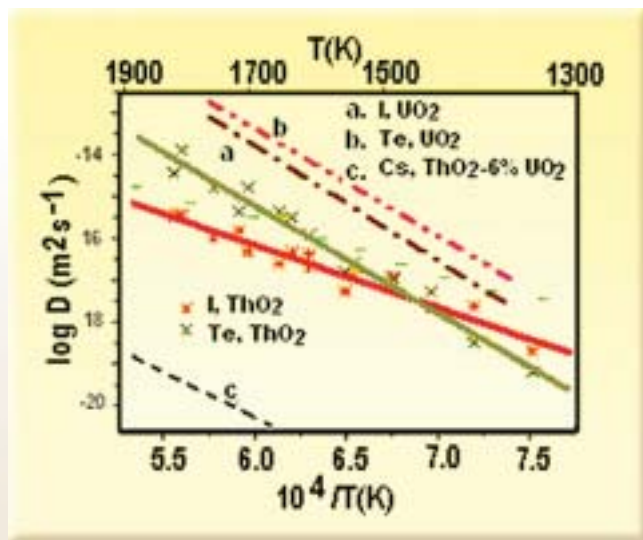
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INSA-AGM DELEGATES VISIT BARC

A visit of the Indian National Science Academy-Annual General Meeting (INSA-AGM) delegates to the Bhabha Atomic Research Centre was organized at the invitation of Dr S. Banerjee, Director, BARC, on the 23rd of December 2006. About 105 delegates, including INSA Council Members, INSA Fellows and their spouses, INSA Young Scientist Medal Awardees and INSA officials visited BARC. The visit began with a briefing by the Director, BARC, on the wide spectrum of R&D activities carried out at BARC, aimed at national development, security and societal benefits. This was followed by INSA Council Meeting, presided over by Dr R. A. Mashelkar, President-INSA, while other delegates visited BARC facilities including the Dhruva Reactor, New

INSA Council Meeting at BARC

INSA delegates at the Dhruva Reactor

Computer Centre, Food Irradiation and Processing Laboratory, Gallium/Arsenic Purification Facility, Crystal Laboratory and Waste Immobilization Plant. The visit ended with a lunch, hosted by Director, BARC. Dr S. K. Apte, Convener-INSA, Mumbai Chapter and Associate Director, Biomedical Group (B), Dr S. K. Ghosh, Head, Theoretical Chemistry Section and their colleagues coordinated the visit. In the concluding session of INSA-AGM, President-INSA, thanked Director, BARC, for hosting the event and for providing an exposition of the excellence and relevance of R&D at BARC.

TRAINING PROGRAMME ON SAMPLES, SAMPLING AND FORENSIC TRACE ANALYSIS

"A three day training programme "Samples, Sampling and Forensic Trace Analysis" was organised by the NAA Unit of CFSL, Hyderabad, Analytical Chemistry Division, (BARC) at BARC, Mumbai, from February 5-7, 2007. The course was designed with the objective of exposing forensic scientists/document examiners primarily to highlight samples and sampling procedures for trace analysis, as an aid to crime detection. The course covered lectures and familarization with equipment facilities on various nuclear, non-nuclear analytical techniques such as: importance of quality management for Forensic Science laboratories, quality assurance of analytical data,

critical assessments of uncertainties of measurement, metallurgical failure investigations/ Non-Destructive Testing (NDT) etc. A visit to 'Apsara' nuclear research reactor at BARC was also arranged. In depth discussions on use of different methods as R&D studies in forensic science applications were also covered .

The programme was inaugurated by Dr S. Banerjee, Director, BARC, on February 5, 2007 in the 'C' Block Auditorium, Modular Laboratories, BARC. Delivering the inaugural address, he stressed on the potential of nuclear and allied technologies in helping to solve criminal cases. Dr Banerjee also elaborated on the sophistication of

Dr S. Banerjee, Director, BARC releasing compiled lecture notes in the form of a book during the inaugural function. Seen in the photograph from left to right are:
Dr. N. Chattopadhyay, Deputy Director, NAA Unit of CFSL (H), ACD, BARC, Dr B. Venkataramani, Head, Analytical Chemistry Division, BARC, Dr. S. K. Shukla, Director, Central Forensic Science Laboratory, Hyderabad, Dr S. Banerjee, Director, BARC, Dr. T. Mukherjee, Director, Chemistry Group, BARC, Dr(Mrs) R. Krishnamurthy, Director, Forensic Science Laboratory, Maharashtra State, Mumbai and Dr A. K. Basu, Assistant Director, NAA Unit of CFSL (H), ACD, BARC.

Dr T. Mukherjee, Director, Chemistry Group, BARC with participants, organisers and some of the faculty members of the training programme on "Samples, Sampling and Forensic trace Analysis", organised by the NAA Unit of CFSL, Hyderabad, Analytical Chemistry Division, BARC, Mumbai.

analytical methods with modern developments in science and technology. He also suggested taking up of challenges and opportunities in R&D work related to preventive forensics. He gave a typical example of metallurgical failure analysis and its role in forensic investigation. Director, BARC also made a point to provide support and facilities from BARC to the unique forensic programme on-going at ACD, for more than three decades. Compiled lecture notes in the form of a book were released by Director, BARC, before the inaugural address.

Dr S.K. Shukla, Director, CFSL, Hyderabad, formally welcomed the participants to the course. He reiterated the importance of the NAA Unit functioning at BARC, Mumbai, giving a brief overview of how the Unit became functional at BARC, Mumbai, more than thirty years ago. He also pointed out that extreme care was necessary in performing low level analysis, on important specimens of evidence in the forensic context. Dr Shukla sincerely thanked BARC/DAE functionaries for co-operation, support and facilities provided to NAA Unit personnel

stationed at ACD, BARC, Mumbai. Dr N. Chattopadhyay, Deputy Director, NAA Unit of CFSL, Hyderabad (at ACD, BARC) who was the Course Director, briefed about the design of the training course. He also thanked all BARC/DAE functionaries for providing facilities, extending scientific expertise and above all extending special support to their efforts and work programmes which are an ongoing collaboration between CFSL (DFS,MHA) and BARC (DAE).

Dr T. Mukherjee, Director, Chemistry Group, BARC, in his presidential address, stressed the need for updating knowledge and information in the pursuit of truth. He mentioned that there was a constant increase in organised crimes in the country. In this context, he clearly pointed out the need to adopt proper sampling methods particularly for the collection of crucial evidence and subsequently the need to preserve the integrity of the samples for analysis and interpretation in the forensic context. Dr B. Venkataramani, Head, ACD, BARC, Mumbai, gave the introductory address. He mentioned about the unique on-going collaborative work

programme of the forensic Unit situated at ACD,BARC. He gave a brief account of the background for conducting such a training course in BARC. Dr (Ms) R. Krishnamurthy, Director, Forensic Science Laboratory, Mumbai spoke on the latest techniques in forensic analysis. She cited the potential role of brain finger printing, narco- analysis, psycho tests etc. in helping crime investigation. In this context, she also advised the participants to take advantage of the opportunity of exposure to the multi-disciplinary facilities existing in BARC. Dr A. K. Basu, Asstt. Director, NAA Unit of CFSL, Hyderabad (at ACD, BARC) co-ordinated the inaugural function and also proposed a vote of thanks. Dr A. B. R. Tripathi and Mr C. A. Bhadkambekar of the NAA Unit were actively associated with the training course.

Dr M. S. Rao , Director – cum- Chief Forensic Scientist, DFS, MHA, New Delhi through a message, conveyed that the course "Samples, sampling and trace analysis" was significant from the point of view of forensic analysis. He indicated that the nature of forensic exhibits received in the laboratories was very different from normal routine laboratory analysis. The examination of varied forensic exhibits requires application of appropriate technical skills by forensic experts and forensic trace analysis was an important issue. He expressed that mutual exchange of views during the training programme would certainly strengthen the scope of the programme. Dr Rao extended his good wishes for successful deliberations and fruitful interaction between the participants and the organizers. He conveyed his thanks to all the functionaries of BARC for their kind cooperation and help to the officials of NAA Unit. Dr S. K. Shukla, Director, CFSL, Hyderabad rendered full administrative and financial support towards conducting the course. A total of 21 participants from different FSL(s), CFSL(s), GEQD, Bank Note Press(s), GSI and BARC attended the course. A special lecture by Dr S.K. Shukla, on "Importance of Quality Management for Forensic Science laboratories" and a brief technical talk by Dr (Ms) R. Krishnamurthy, Director, Forensic

Science Laboratory, Mumbai were held in the "C" block auditorium, Mod. Labs. after the inaugural function. Guest faculty members/resource persons delivered lectures. Topics on a wide range of sophisticated analytical techniques like NAA, ICPAES, ICP-MS, AAS, FTIR, XRF, TXRF, TIMS, LIBS and other NDT methods were highlighted in the presentations. Chromatographic techniques like HPTLC, GC-MS, HPLC etc. and thermal analysis techniques like TG, DTA, DSC, Pyrolysis GC-MS etc. focusing on basics and forensic application aspects were also included in the lectures. Demonstration for and exposure to various analytical equipment in ACD, BARC was also arranged.

On the final day, in an informal valediction, some of the participants expressed their views on the usefulness of the course. Dr N. Chattopadhyay, Course Director expressed his observations. Dr T. Mukherjee, Director, Chemistry Group, BARC reviewed the feedback received from the participants and presented certificates to the participants. He also mentioned that the impact of interactive deliberations would be fruitful to the participants in developing awareness about the potential applications of analytical methods, in forensic studies. He wished them success in their respective endeavors.

DAE - BRNS SYMPOSIUM ON "POWER BEAMS FOR CLEAN ENVIRONMENT AND PROCESSES " (PBAMP-2006): A REPORT

The Beam Technology Development Group, in association with the Power Beam Society of India, organized the DAE-BRNS symposium on "Power Beams for Clean Environment and Processes" (PBAMP-2006) at the Multipurpose Hall of the BARC training school hostel, Anushaktinagar, during September 20 – 21, 2006. The symposium was inaugurated by Dr R. K. Garg, Former Director, Chemical Engineering Group, BARC and retired CMD, Indian Rare Earths Limited. In his inaugural address, Dr Garg reviewed the sources of pollution and the techniques for pollution control. He said that the need of the hour was to implement innovative ideas to monitor pollution and effectively control it using beam technology processes. In his opening remarks Dr A. K. Ray, Director, Beam Technology Development Group, BARC and Chairman, National Advisory Committee mentioned about the rapid growth being made in the application of power beams for clean environment by BARC and other institutes in the country and also their impact on industry, especially, in the context of waste management and disinfection processes. Dr A. K. Das, Secretary, Power Beam Society of India, welcomed the participants, dignitaries and invitees to the symposium. Dr N. K. Joshi, Convener, Organizing Committee, proposed the vote of thanks.

The inaugural session was followed by three review talks by experts working in area of lasers and plasma and electron beam technology. The talks covered included 'Laser-based Technologies for Detection of Environmental Pollution' by Mr T. P. S. Nathan, Univ. of Hyderabad, 'High Power Plasma Torches and

Dr A. K. Ray, Director, Beam Technology Development Group, BARC, giving opening remarks about the symposium. Sitting on the dais from left to right are: Dr N. K. Joshi, Convener, Mr R. K. Garg, Former Director, Chemical Engineering Group, BARC and ex-CMD Indian Rare Earths Limited, Dr A. K. Das, Secretary, Power Beam Society of India and Dr Archana Sharma, Co-Convener.

systems for Waste Treatment' by Mr P. S. S. Murty, ex-Scientist, BARC and 'Power Beams for Clean Environment and Processes and Applications in Aerospace Hardware' by Mr P. Raghuthama Rao, Retired GM, Liquid Propulsion System Center, Bangalore. All the three speakers were felicitated by PSI, President, Dr N. Venkatramani for their outstanding contributions in the field of beam technology and applications. An entrepreneur, Mr. Janardhan Nair, CMD, M/s Ion Arc Technologies Pvt. Ltd. was also felicitated, for his outstanding contribution related to the developmental work in the area of thermal plasma reactors and torches.

There were in all, eight technical sessions including the inaugural and the concluding session. The scientific program comprised seventeen invited talks and thirty one contributed papers. The symposium covered a wide spectrum of topics and plasma waste treatment schemes at Australia, China and India; electron accelerators for treatment of industrial water and flue gases in Korea and Russia; laser-assisted decontamination of radioactive waste and laser-aided diagnostics for determination of trace level toxic pollutants etc. The contributory papers reflected the research being carried out at universities and institutes in India in this newly emerging important technology area. It was particularly interesting to see papers on plasma-assisted synthesis of nanomaterials and their role in environmental cleaning. For many environmental problems, a combination of different technologies may be necessary to achieve a cost effective solution. During the symposium all the contributory papers were rapporteured by Dr N. K. Joshi, L&PTD, BARC. All the contributory papers were peer-reviewed and displayed in the poster session, a few were selected for oral presentation and three students (Mr. Dinesh Mantri, IIT, Mumbai, Mr. P. Navaneetha, Bharthiar University, Coimbatore and Ms. Harshada Nagar, Pune University) were awarded certificates for "Best paper with student participation" and a cash prize of Rs.1000/- each.

The proceedings of the symposium were distributed to all the delegates.

The symposium provided a forum for exchange of ideas and information on various basic and engineering issues related to power beam-assisted processing, effluent/emission management and production and recycling technologies for sustainable development. There were about 225 registered participants from various National Institutions/Universities/Colleges and industrial houses. The response to this symposium from India and abroad was overwhelming. It was technically very beneficial for the participants to have Prof. N. K. Kuksanov from Budekar Institute of Nuclear Physics, Russia and Prof. A. B. Murphy, CSIRO Industrial Physics from Australia. In India, apart from various divisions of BARC, contributions had come from RRCAT Indore, LPSC-ISRO Bangalore, IPR Gandhinagar, IISc., Bangalore, IITs of Mumbai, Delhi and Kharagpur, NEERI, Nagpur, RRL, Bhubaneshwar BHEL, Ranipet, IITM, Pune, Univ. of Hyderabad, Univ. of Pune, Bharathiar Univ., Coimbatore, CMET, Pune, NIT, Rourkela, MIUCT, Mumbai, RRL, Thiruvanantapuram, CPP, Guwahati and PIIT, New Panvel. It was also very heartening to note the enthusiastic response from the student community. The industry response to the symposium was also encouraging. In view of the industrial significance of the power beam technology and applications, an exhibition of beam technology related equipment, accessories, products etc. was organized at the venue of the symposium hall. Ten exhibitors participated in the exhibition.

In the concluding session, Dr A. K. Ray thanked all the delegates for the lively discussions during the two days and hoped that the symposium would generate several collaborative programs between the Department of Atomic Energy and other institutions.

DAE-BRNS TOPICAL SYMPOSIUM ON "THE ROLE OF ANALYTICAL CHEMISTRY IN NUCLEAR TECHNOLOGY" (RACNT) : A REPORT

Analytical Chemistry is an integral part of the nuclear energy programme and plays a crucial role in materials characterization and quality assurance. In fact, one of the first chemistry activities in the saga of the Indian atomic energy programme, was the analysis of minerals for the exploration and estimation of uranium. Since then, analytical chemistry has become an integral part of the Indian nuclear energy programme.

Analysis of various materials is an essential aspect of all nuclear power plants, industrial units such as NFC, HWB, UCIL, IRE, AMD, fuel reprocessing, waste management facilities, production of isotopes for societal needs, etc.

Apart from these analytical chemistry plays an important role in the development of new and advanced materials for various applications in the nuclear industry.

With the Indian nuclear energy programme poised to make greater strides in terms of enhanced power production and adopting diverse advanced reactor concepts, analytical chemists will be called upon to play even greater roles. Keeping this in view and on the occasion of the Golden Jubilee Year of BARC, the DAE-BRNS Topical Symposium on *Role of Analytical Chemistry in Nuclear Technology (RACNT)* was organized by the Analytical Chemistry Division (ACD),
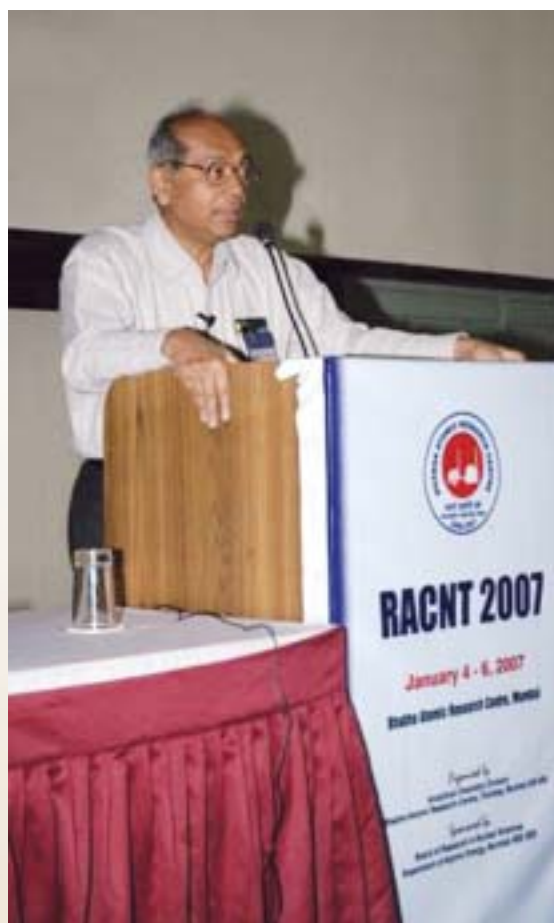

The Inaugural function

BARC. It was held at the Multipurpose Hall, Training School Hostel, Anushaktinagar, Mumbai during January 4-6, 2007. The objective of the Symposium was to provide a forum for the analytical chemists in DAE to interact and chalk out a roadmap for meeting the future needs of the Department.

The topics covered in the Symposium were on the role of analytical chemistry in areas that constitute the future mandate of BARC and DAE. They included: Nuclear materials, Reactor systems, Thorium technology, Alternate energy sources, Biology, Agriculture and environment, Water technology, Isotope, radiation and laser technology, Materials development and processes, Development of analytical instruments, Reference materials and inter-comparison exercises. Twenty one invited talks were delivered by experts from BARC and other DAE units, who are actively engaged in these areas. There were 95 contributed papers from various units of DAE, Universities and National Institutes. These were displayed as posters during all the three days of the Symposium. Five young scientists from ACD, BARC, presented summaries of the contributed papers presented during the rapporteuring sessions. Two separate sessions were allotted for viewing the posters. The proceedings of the symposium, containing the text of the invited talks and the contributed papers, were published in the form of a book. Nearly 250 delegates attended the Symposium.

Dr S. Banerjee, Director, BARC, inaugurated the Symposium. He emphasised the important role of analytical chemistry in nuclear energy programmme, by citing examples such as hydrogen pick-up by zircaloy during reactor operation and the need to control the hydrogen content right from the fabrication stage. Prior to this, Dr B. Venkataramani, Convenor of the Symposium and Head, ACD, BARC, welcomed the delegates. Dr K.K. Swain, Joint Secretary of the Symposium briefed about the Symposium and its content. Dr T. Mukherjee, Chairman of the National Organising Committee of the Symposium and Director,

Chemistry Group, BARC presided over the inaugural function. He said that the Symposium was unique in the sense that the whole DAE community had come together to discuss the importance of analytical chemistry in the nuclear energy programme. He also complimented the organisers for the invited talks delivered by senior scientists from different fields. Dr Rakesh Verma, Secretary of the Symposium proposed a vote of thanks.

On the last day of the Symposium, a feedback session was arranged where participants gave their views about the Symposium and which was followed by a panel

Dr S. Banerjee, Director, BARC, delivering the inaugural address

Valedictory function

discussion and the valedictory function. Dr P. R. Vasudeva Rao, Director, Chemistry Group, IGCAR, chaired the session. Dr B. Venkataramani, Convener, RACNT and Head, ACD, BARC; Dr K. L. Ramakumar, Chairman, RACNT Technical Committee and Head, Radioanalytical Chemistry Section, BARC and Dr P. P. Chandrachoodan, Programme Officer, BRNS were present during the panel discussion. Dr. Chandrachoodan pointed out that it was essential to start a collaborative project, which would be of relevance to DAE and to the environment. The following points emerged from the discussions during the sessions :

- Periodic meetings be held to meet new challenges in analytical chemistry in DAE.

- Efforts be made to maintain sophisticated instruments. It was emphasized that efforts also be made to develop instruments of international quality indigenously.

- An agency be constituted for maintaining sophisticated instruments across the country and for reuse / redistribution of the instruments among DAE units.

- Need to prepare reference materials, relevant to the DAE programme and the need to participate in inter-comparison exercises.

भा. प. अ. केंद्र के वैज्ञानिकों को सम्मान
BARC SCIENTISTS HONOURED

Dr S.K. Apte

डॉ एस. के. आप्टे, सह निदेशक, जैवआयुर्विज्ञान वर्ग (बी) एवं अध्यक्ष, आण्विक जीव विज्ञान प्रभाग, भाभा परमाणु अनुसंधान केंद्र को अप्रैल 1, 2007 से मार्च 31, 2009 तक कोशिका जीव विज्ञान की भारतीय संस्था का अध्यक्ष निर्वाचित किया गया है। डॉ आप्टे की अनुसंधान रुचियों में आयनाइज़िंग विकिरण का बैक्टीरिया एवं पौधों पर कोशकीय एवं आण्विक आधारित प्रतिक्रिया, कृषि-संबंधी प्रभावशाली बल जैसे खारापन, सूखा, तापमान, पोषक भुखमरी एवं कीटनाशक, भी शामिल है। ये भारतीय राष्ट्रीय कृषि वैज्ञानिक अकादमी एवं महाराष्ट्र वैज्ञानिक अकादमी के सदस्य हैं।

Dr S.K. Apte, Associate Director, Biomedical Group (B) and Head, Molecular Biology Division, BARC, was elected President of the Indian Society of Cell Biology from April 1, 2007 to March 31, 2009. Dr Apte's research interests encompass cellular and molecular basis of responses of bacteria and plants to ionising radiation and agriculturally important stresses, such as salinity, drought, temperature, nutrient starvation and pesticides. He is a fellow of the Indian National Academy of Agriculural Sciences and Maharashra Academy of Sciences.

Dr Mainak Roy

डॉ मैनक रॉय, ठोस अवस्था रसायनिकी अनुभाग, रसायनिकी प्रभाग, भाभा परमाणु अनुसंधान केंद्र, को फरवरी 12-14, 2007 के दौरान नैशनल फिज़िकल लैबोरेटरी (राष्ट्रीय भैतिकी प्रयोगशाला), नई दिल्ली में आयोजित वार्षिक आम सभा के दौरान उनके कार्बन थिन फिल्म्ज़ पर "करेक्टरैज़ेशन ऑफ डायमंड एन्ड सिलिकॉन कार्बाइड थिन फिल्मज़

ग्रोन बाई केमिक्ल वेपर डिपोज़िशन एन्ड एलाइड टेक्नीक्स" नामक शोध-पत्र पर "मेटीरियल रिसर्च सोसाइटी ऑफ इन्डिया" के द्वारा संस्थापित प्रतिष्ठापूर्ण "जी सी जैन मेमोरियल प्राइज़ फॉर दि बेस्ट पीएच.डी थीसिज़ इन मेटीरियल साइंस (2005-06)" पुरस्कार प्रदान किया गया। डॉ रॉय के श्रेय में 25 पत्रिकाओं एवं 32 परिचर्चाओं के प्रकाशन हैं। इसके अतिरिक्त इन्होंने पदार्थ रसायनिकी (आइ एस एम सी-2006/ ISMC-2006) पर अंतर्राष्ट्रीय परिचर्चा की कार्यवाही का सह-संपादन भी किया है।

Dr Mainak Roy of Solid State Chemistry Section, Chemistry Division, BARC has been conferred the prestigious "G C Jain Memorial Prize for the Best Ph.D Thesis in Materials Science (2005-06)" instituted by the "Material Research Society of India" during their Annual General Meeting held at the National Physical Laboratory, New Delhi between February 12-14, 2007 for his thesis on carbon thin films entitled "Characterisation of diamond and silicon carbide thin films grown by chemical vapour deposition and allied techniques." Dr. Roy has to his credit 25 journal publications and 32 symposium publications. Besides this, he also co-edited the proceedings of the International Symposium on Materials Chemistry (ISMC-2006).

Dr Virendra Kumar

डॉ वीरेंद्र कुमार, विकिरण तकनीकी विकास अनुभाग, रेडियो रसायनिकी एवं आइसोटोप वर्ग, भाभा परमाणु अनुसंधान केंद्र को जनवरी 29-31, 2007 के दौरान नैशनल सेंटर फॉर अल्ट्रा फास्ट प्रोसेसिज़, मद्रास विश्वविद्यालय, चिन्नई, में आयोजित एन एस आर पी 2007 में इन्डियन सोसाइटी फॉर रेडियेशन एन्ड फोटोकेमिक्ल साइंस," इन्डिया के द्वारा डॉ पी.के.भट्टाचार्या मेमोरियल अवॉर्ड फॉर यंग सांइटिस्टस फॉर

ईयर 2006" पुरस्कार प्रदान किया गया। यह पुरस्कार इन्हें बहुलकों की विकिरण प्रक्रिया का मूल एवं प्रायोगिक पहलू, जिनमें बहुलकों का विकिरण एवं प्रतिरोपण के द्वारा संशोधन, उच्च उपलब्धि बहुलक नेनो संयोजित विलेपन का ई बी चिकित्सा एवं विकास, जल समाधेय बहुलकों के पॉलिइलेक्ट्रोलाइट, पॉलिएमफोलाइट एवं उत्तेजक अनुक्रिया हाइड्रोजल प्रणाली एवं रेडियोलायसिज़ परीक्षण, पर महत्वपूर्ण योगदान के लिए प्रदान किया गया।

Dr Virendra Kumar of Radiation Technology Development Section, Radiochemistry & Isotope Group, BARC, was conferred the " Dr. P. K. Bhattacharya Memorial Award for Young Scientist for Year 2006" by the "Indian Society for Radiation and Photochemical Science", during NSRP-2007 held at the National Centre for Ultra-fast Processes, University of Madras, Chennai, January 29-31, 2007. He was conferred this award for his significant contribution in basic and applied aspects of radiation processing of polymers, which includes modification of polymers by radiation grafting, EB curing and development of high performance polymer nanocomposite coatings, synthesis and characterization of polyelectrolyte, polyampholyte and stimuli-responsive hydrogel systems and pulse radiolysis studies of water soluble polymers.

Mr. N. K. Goel

श्री एन.के.गोयल, विकिरण तकनीकी विकास अनुभाग, रेडियो रसायनिकी एवं आइसोटोप वर्ग, भाभा परमाणु अनुसंधान केंद्र, को फरवरी 8-11, 2007 के दौरान स्कूल ऑफ केमिकल साइन्सिज़, महात्मा गांधी यूनिवर्सिटी कोटायम, केरल, इन्डिया के द्वारा आयोजित, एन.के.गोयल, विरेंद्र कुमार, वाइ.के भारद्वाज, के.ए.दुबे, सी.वी. चौधरी, एस.सभरवाल द्वारा लिखित ऐन इंटरनैशनल कॉन्फ्रेन्स ऑन फ्रन्टियर्स ऑफ रेडियेशन एन्ड फोटोकेमिस्ट्री (फोटोरॉडकेम 2007) नामक सम्मेलन मे श्रेष्ठ पोस्टर प्रस्तुति पुरस्कार प्रदान किया गया। इस शोध-पत्र में प्रति-जीवाणु सूती वस्त्र के विकास एवं चरित्र-चित्रन हेतु विकिरण उत्प्रेरित प्रतिरोपण प्रणालीके प्रयोग का वर्णन है।

Mr. N. K. Goel of Radiation Technology Development Section, Radiochemistry & Isotope Group, BARC, received the best poster presentation award for the paper entitled "Antibacterial cotton fabric prepared by radiation grafting technique" authored by N. K. Goel, Virendra Kumar, Y. K. Bhardwaj, K. A. Dubey, C. V. Chaudhari and S. Sabharwal presented at the "International Conference on Frontiers of Radiation and Photochemistry (PhotoRadChem 2007)" held during February 8-11, 2007 organized by the School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala. The paper describes the application of radiation-induced grafting process for development and characterization of antibacterial cotton fabric.

Ms Mala Mukherjee

श्रीमती माला मुखर्जी (सीएसआइआर-एसआरएफ) , नाभिकीय कृषि एवं जैव-प्रौद्योगिकी प्रभाग ने फरवरी 15-17, 2007, के दौरान पुणे में आयोजित "बीवाइएफएफ-2007: इन्टरनैशनल कॉन्फ्रेन्स ऑन दि बायोलोजी ऑफ यीस्टस एन्ड फिलामेन्टस फन्गी" सम्मेलन में सर्वश्रेष्ठ पोस्टर पुरस्कार प्राप्त किया। इन्होंने एक स्मारिका एवं एक प्रमाण-पत्र प्राप्त किया। इन्हें समापन समारोह में अपने "रोल आफ सीएएमपी सिग्नलिंग इन ग्रोथ, जरमिनेशन एन्ड बयोकंट्रोल प्रोपरटीज़ आफ ट्रिकोडरमा वाइरन्ज़-क्लोनिंग एन्ड फंक्शनल एनालिसिज़ ऑफ दि एडेनिलेट सैक्लेज जीन" नामक पोस्टर की मौखिक प्रस्तुति के लिए भी आमंत्रित किया गया था।

Ms Mala Mukherjee, CSIR-SRF of Nuclear Agriculture and Biotechnology Division received the Best Poster Award at the "BYFF-2007 : International Conference on the Biology of Yeasts and Filamentous Fungi", held at Pune from February 15-17, 2007. She received a memento, a certificate and cash award. She was also invited to present her poster entitled "Role of cAMP signalling in growth, germination and biocontrol properties of Trichoderma virens – cloning and functional analysis of the adenylate cyclase gene" as oral presentation at the valedictory function.