Nuclear Reactors

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# Physics of Thermal Reactors: Excitements and Challenges

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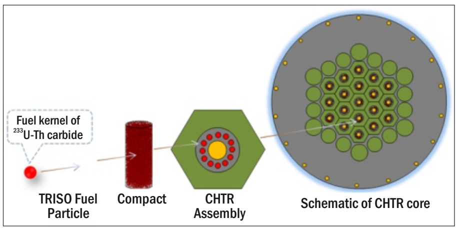


*Schematic of fuel particles and the CHTR core*

ABSTRACT

Physics of reactors is exciting and engaging due to its multi-disciplinary nature. Probing the nucleus has unleashed the potential of the atom and the role of the fascinating neutral particle-the neutron! The understanding of the complex phenomena of energy transfers within the nucleus along with the interplay of the isolated neutron, has thrown open several opportunities for energy generation. The discovery of fission chain reaction was a great Eureka moment for the world and this idea has been successfully exploited. As we look back at the 80 years since the Chicago Pile, we have come a long way and successfully designed and operated several types of nuclear reactors. Of the total power reactors in the world, more than 90% is based on thermal neutron energy spectrum. The physics characteristics of thermal reactors are governed by the complex neutron transport in a scattering medium to achieve the desired neutron spectrum. The new generation reactors usually have to cater to four major aspects i.e. sustainability, better fuel utilization, inherent safety and better economics. This article aims to run through the design challenges in these new reactor designs where advanced fuels are used to achieve the objectives listed above and the neutron spectrum is tuned to achieve higher a degree of safety. Thus, we must use newer materials and traverse through uncharted regimes. This article is kept simple to make even readers from other fields also to appreciate these features of physics of reactors.

KEYWORDS: *Thermal reactors, PHWR, Nuclear fission, Gen-IV reactors, MSBR, Thorium, IPWR*

## Introduction

Currently, there are 449 power reactors operating in the world, of which more than 350 are Light Water Reactors (LWRs) [1]. Out of these, 306 are Pressurised Water Reactors (PWR) and 56 are the boiling water type BWRs. These constitute about 81% of the total operating reactors. There are 50 reactors using heavy water and are called Pressurised Heavy Water Reactors (PHWRs). Reactors based on fast spectrum constitute about 12% The different types of reactors operating in the world are shown in Fig.1. India currently has 19 PHWRs, 2 PWRs and 2 BWRs and considerable experience has been gained in operation, design, and safety of all the thermal reactor types.

Uranium-235 is the only fissile material available in nature and has been exploited for power production. The fission of U-235 with thermal neutrons is the workhorse of most of the reactors operating in the world. The basic physics is governed by the achievable neutron spectrum and the behavior of neutron interactions in the energy and space domains of interest. The interplay of all the emitted particles with the different materials in a reactor result in more complex behavior. Thus, the modelling of the physical phenomena will have to be very realistic and as accurate as possible.

The major objectives of current generation nuclear reactors are better fuel utilization, enhanced safety and economics of power generation. The neutronics is also interlinked with heat removal and other engineering aspects such as selection of materials, irradiation behavior, radiological assessment, fuel cycle and final safe disposal [2]. This article will attempt to detail the challenges in reactor design encompassing all these multiple stages of nuclear energy production.

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## Today's Designs

In its GEN-IV forum, IAEA has focused on several types of reactors with Molten Salt Breeder Reactor (MSBR), Super Critical Water Reactor (SCWR) and Very High Temperature Reactor (VHTR) as potential thermal reactor designs [3]. Sodium and lead cooled fast reactor designs are also considered. The objectives for all these types of reactors have also been lucidly elaborated. Molten salt Breeder reactor is designed to use thorium-based fuel where the nuclear properties of the bred U-233 can be efficiently used for power production in a breeder configuration. With the engineering advances in using super critical water as coolant, the fuel

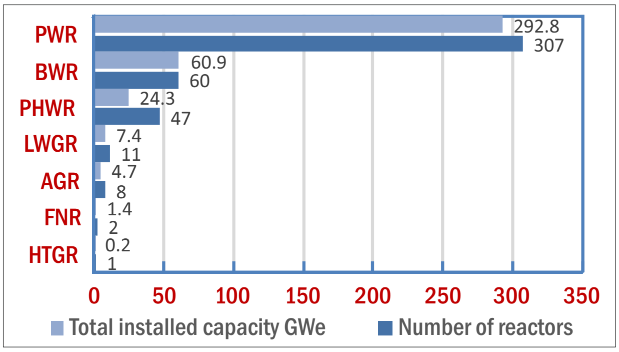



*Fig.1: Operating reactors in the world by their types. https://www.world-nuclear.org*

*Table 1: Comparison of fuel utilization of thermal reactors.*

| Reactor Type | Reactor Power Electric / Thermal / Fission (MW) | Feed enrichment in equilibrium cycle (%) | Discharge Burnup Gwd / Te | Cycle length | Equivalent mined uranium Tonne / Twhr (e) |
|---|---|---|---|---|---|
| BWR | 1330/ 3990/ 4070 | ~2.4 | 22.0 | 24 months | 25.0 |
| PWR | 1280 / 3800 /3900 | ~3.3 | 33.0 | 12 months | 23.38 |
| VVER | 1000 /3000 /3150 | ~3.92 | 43.0 | 295 days | 22.26 |
| PHWR -220 | 220/750/802 | 0.71 | 6.7 | On power fuelling | 22.67 |
| PHWR -540 | 540/1760/1830 | 0.71 | 7.0 | On power fuelling | 20.17 |

utilization can be enhanced again by exploiting the uranium and water combination to achieve an effective neutron spectrum. Very high temperatures are required to use the process heat to disassociate water. The high temperature reactors design with gas cooled or liquid metal cooled offer themselves as good candidates for hydrogen production. It is once again emphasized that the physics of these reactors are very different and the challenge is to design systems with a prudent choice of fuel and material composition to achieve the desired objectives.

BARC is engaged in design of advanced reactors based on thorium utilization such as Advanced Heavy Water Reactor (AHWR) and Molten Salt Reactors (MSR) and High Temperature Reactors (HTR) for hydrogen production [3]. An advanced light water reactor IPWR based on enriched uranium for longer operating cycle is also being developed. As mentioned earlier, the physics of these systems are challenging and mostly must balance the competing objectives. For example, the active length of fuel in AHWR and power distribution in the core had to be optimised for effective heat removal through natural circulation. In an MSR, the fuel and coolant being liquid requires a different approach for simulation of near homogenous systems and achieve effective heat removal and take care of radiological aspects throughout the core and design associated engineered systems. To achieve breeding through online refuelling requires management of constant excess reactivity throughout the burnup or operating cycle. MSRs also advocate use of advanced materials to arrest corrosive nature of these molten salt mixtures. Advanced LWR designs on the other hand are looking towards enhanced fuel utilisation or longer cycle lengths which is achieved by high strength fuel clad materials for higher burnups. Advanced CANDU reactors have addressed the undesirable feature of positive void coefficient issue with ingenious fuel design and interleaving of coolant channels.

### Comparison of fuel utilization

The parameters defined by the Gen-IV international forum are fuel utilization, margin of safety, proliferation resistance. As an important design feature, fuel utilization can be compared for all reactors by estimating the energy produced per unit mass of fuel. In Table 1, few currently operating thermal reactors are compared on an equal footing of equivalent mined uranium[a] required to produce energy of 1 Terrawatt-hr (e) [4]. The lower the mined uranium required,

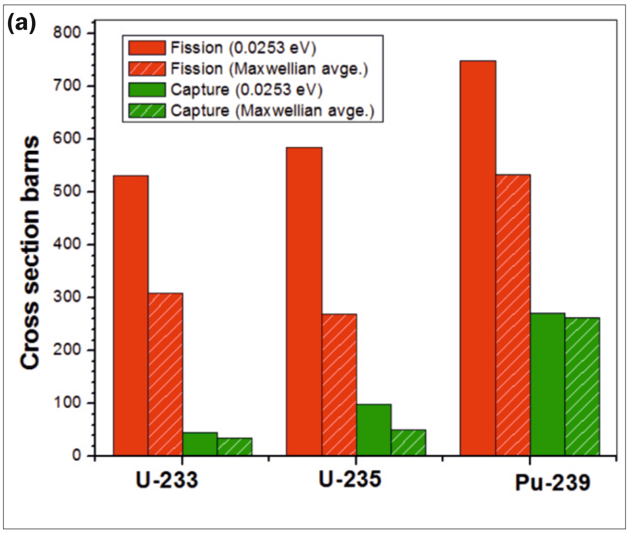



*Fig.2 (a): Comparison of fission and capture cross section of U-233, U-235 and Pu-239 at thermal energies.*

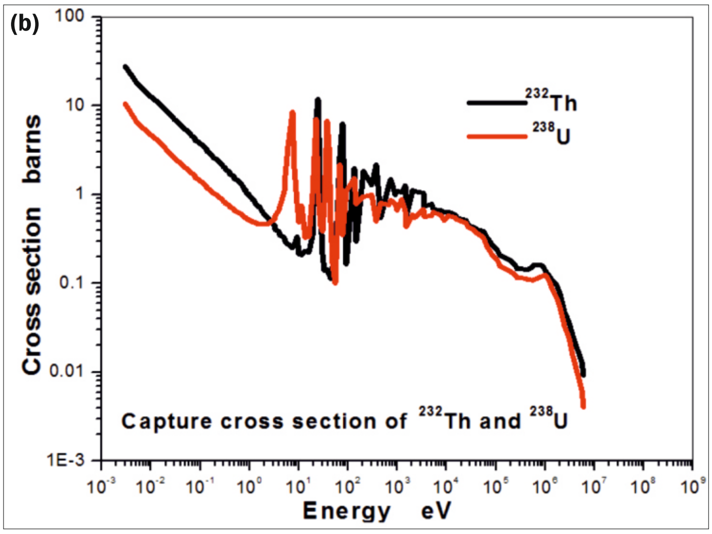



*Fig.2 (b): Energy dependence of capture cross section of Th-232 and U-238.*

[a]*Equivalent mined uranium for any reactor or fuel cycle is defined as the amount of uranium required to produce 1 TWhr (e) of electricity considering 0.2% enrichment tails.*

the better would be the fuel utilization. Another quantity, fissile inventory ratio (FIR) can also be defined which gives an idea of how the fissile content has burnt and gives a measure of remaining fissile content in the discharged fuel which also includes conversion and production of other fissile material usually Plutonium in the Uranium fuelled reactors. It is defined as the amount of fissile content in discharged fuel to that in the initial fuel. The FIR is about 0.72 for a PHWR at discharge of 7.0 GWd/Te and 0.35 for a PWR at a discharge of 45 GWd/Te [5].

It can be seen from Table 1 that PHWRs give the best fuel utilization with respect to mined uranium. In water cooled reactors, which use enriched uranium, energy is required to enrich the uranium too.

### *Fuel cycle and fuel performance*

The fissile isotope/nuclide available in nature is U-235 and constitutes 0.71 % in weight in natural uranium. Pu-239 and U-233 can be produced in reactors by neutron interactions. The basic neutronic cross section[b] of three fissile isotopes are compared in Fig.2a. Pu-239 and U-233 have higher cross section in thermal/Maxwellian spectrum and so advanced fuel cycles are based on U-Pu or Th-U233 fuel. In Fig.2b, the neutron capture cross section of the fertile species or precursor to the fissile isotope i.e. U-238 and Th-232 is compared. The Capture-to-Fission ratio is least in U-233 in thermal energies and fission contribution is larger than U-235. This means that U-233 is the best fuel in thermal spectrum reactors.

Eta (η) is the regeneration factor[c] which is measure of how many neutrons are produced in a fission reaction. The spectrum dependent eta values are compared for fissile nuclides in Table 2. In order to aid to fissile breeding, this factor should be greater than 2.0 in the reactor spectrum. Fig.3 shows the plot of eta (η) as a function of energy for the three types of fissile nuclides, namely, U-233, U-235 and Pu-239. Here again it is seen that U-233 has a flat characteristic throughout the complete energy range. In thermal spectrum U-233 has the highest eta (η) and this should be exploited for in-situ conversion or breeding [4]. It also goes to say that Pu-239 is the best option for fast reactors.

The fuel and spectrum are chosen based on these physical properties and used to design reactors for better fuel utilization. A few thermal reactor designs are compared in Table 3 with respect to the fissile requirement and average U-235 contents in the core. It is seen that a 600 MW (e) PHWR usually uses 85 Te of natural $UO_2$ fuel. The spent fuel from a PHWR will have 0.25% (2.5 g/kg) U-235 and about 0.3% (3 g/kg) of plutonium. On the other hand, discharged fuel from PWR has about 0.8% U-235 and 0.6% plutonium [5,6]. It would be prudent to reuse these fissile contents remaining in the discharge fuel by reprocessing and enhance the fuel utilization by recycling into these reactors.

With respect to the discharged fuel, it is important to estimate the radiotoxicity so that the fuel can be safely disposed. In Fig.4 the radiotoxicity of discharged fuel of a

*Table 2: Fissile requirement in thermal reactors.*

| Reactor Type | BWR* (1330 MWe) | PWR* (1300 MWe) | PHWR* (600 MWe) |
|---|---|---|---|
| **Fuel** | Enriched $UO_2$ | Enriched $UO_2$ | Natural $UO_2$ |
| **Fuel loading (Heavy Metal) Te** | ~148 | ~101 | ~85.5 |
| **Average core enrichment %** | 1.9 | 2.8 | 0.71 |
| **Feed fissile content %** | 2.6 | 3.3 | 0.71 |
| **Fissile content in the core Te** | 2.81 (U-235) | 2.82 (U-235) | 0.61 (U-235) |

**Source Glasstone and Sesonske*

*Table 3: Comparison of eta in thermal and fast spectrum for fissile = nuclides.*

| Isotope | Thermal spectrum Maxwellian average | Fast spectrum Fission spectrum average |
|---|---|---|
| $^{233}U$ | 2.3 | 2.41 |
| $^{235}U$ | 2.077 | 2.32 |
| $^{239}Pu$ | 2.109 | 2.834 |

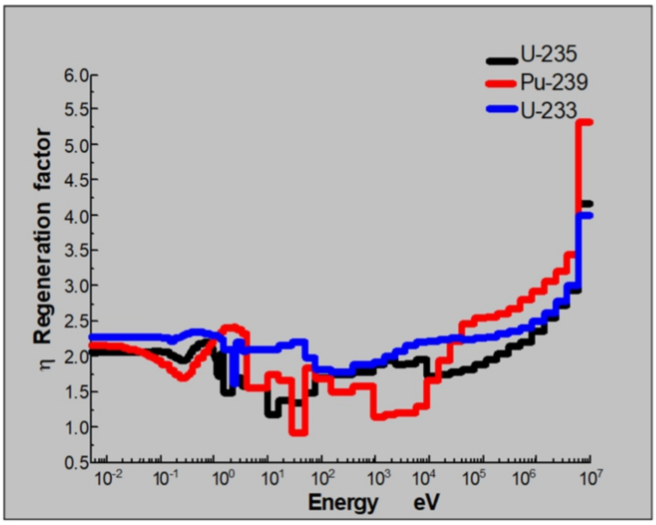



*Fig.3: Variation of with energy for fissile isotopes.*

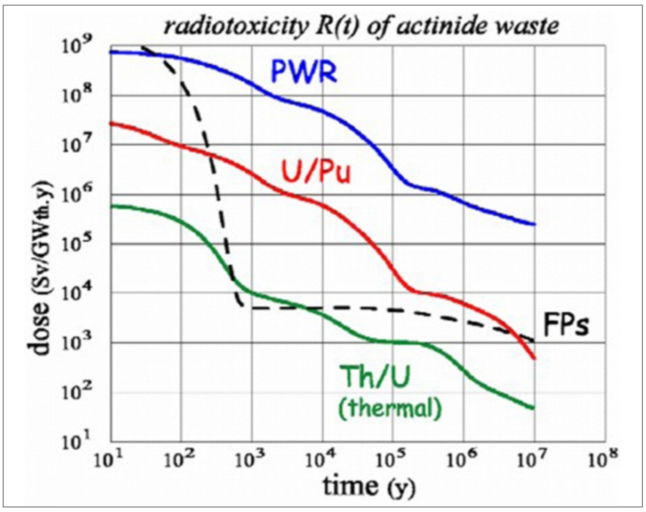



*Fig.4: Radiotoxicity of actinide wastes in Uranium and Thorium fuel cycle.*

[b] *Reaction cross section is measured in barns which is $10^{-24}$ $cm^2$. Physically this can be understood as the effective area offered by a nucleus for any type of reaction.*

[c] *Regeneration factor is defined as the number of neutrons produced per neutron absorbed.*

typical PWR is compared with that of (U,Pu) and (Th,U) cycle. When thorium is used as the initial fuel, the radio toxicity of the spent fuel is much less than in the discharged fuel of uranium cycle, which is clearly seen in Fig.4. Thorium being lower in the periodic table, the concentration of higher actinides produced in the thorium-based fuel during its residence time in a reactor and subsequent cooling is lesser than that of the uranium fuel of the same burnup.

### *How thermal is a thermal reactor?*

It is interesting to investigate the average neutron energies in thermal reactors. The moderator-to-fuel ratio plays an important role in defining the effective collisions with neutrons and thus has a bearing on fuel utilization and safety parameters. Most of the safety parameters such as temperature coefficient of reactivity, coolant void reactivity depends on the spectrum. In order to exploit the neutronic properties to designer's advantage, it is important to tune the neutron spectrum. For example, in AHWR, a harder neutron spectrum is achieved by reducing the lattice pitch and the void coefficient is made negative by neutron captures in Th-232 and Pu-239. The average neutron energy in AHWR is about 0.45 eV as compared to that in PHWR which is about 0.08 eV [7]. Physics design aims at optimizing the fuel performance w.r.t net reaction rates, i.e. maximize the fissile production and fertile captures for breeding. In thermal reactors the objective is to maximize thermal fission reaction rates. Table 4 presents the epithermal-to-thermal neutron flux ratio and it is highest in a PWR which is obvious because in a light water environment, the separation between the pins is adjusted so as to minimize neutron absorption.

*Table 4: Spectral indices in thermal spectrum reactors.*

| | PHWR | AHWR | PWR | BWR |
|---|---|---|---|---|
| Average neutron energy eV | 0.08 | 0.45 | 5.5 | 2.44 |
| Epithermal-to-Thermal ratio | 0.52 | 1.82 | 7.5 | 5.2 |
| Fissions below 0.625 eV (%) | 96 | 80 | 73 | 83 |
| Average thermal flux n/cm$^2$/s | $2.1 \times 10^{14}$ | $7.3 \times 10^{13}$ | $6.1 \times 10^{13}$ | $2.5 \times 10^{13}$ |

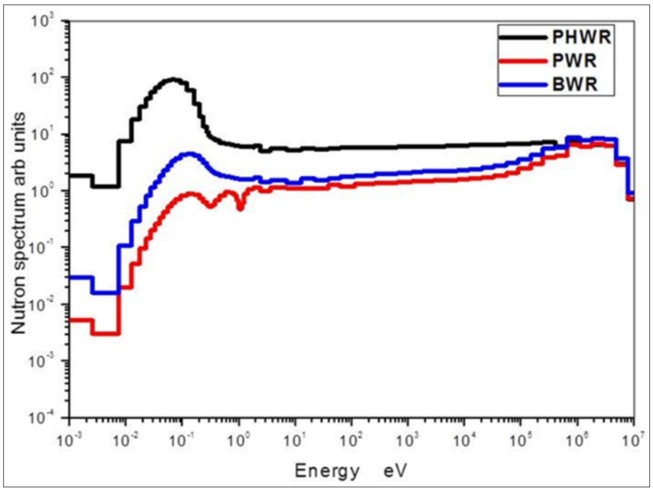



*Fig.5: Comparison of neutron spectrum in PHWR, PWR and BWR.*

The neutron spectrum has been compared for PHWR, BWR and PWR in Fig.5. The normalization is that the total flux is unity. The effect of 0.3 eV fission resonance of Pu-239 is more prominent in the PWR due to the fact the plutonium build-up rate is faster in PWR than other thermal reactors.

### Neutron Transport and Neutron Life Cycle

The aim of reactor physics simulation is to determine two most fundamental quantities that are the neutron flux and the k-effective[d] which is measure of neutron multiplication in the core. The neutron transport in any medium is defined by the inter collision distance or relaxation length. It may be noted that collision with fuel atoms could result in fissions and thereby production of more neutrons. In reactor physics terms this is seen as a measure of distance travelled by uncollided neutron and translates to migration length[e] when neutrons of all energies are considered. This factor coupled with the physical dimensions of the reactor determine the neutronic stability of the core. The neutron cycle in a thermal reactor may be perceived as a neutron born as a fission neutron undergoing successive collisions, and finally absorbed by a fissile atom. The different processes that happen with neutrons can be estimated in a probabilistic simulation by accounting of different probable reactions and estimating the neutron

*Table 5: Neutron induced cross section of some actinides at thermal energies.*

| | | $^{232}$Th | $^{233}$U | $^{234}$U | $^{235}$U | $^{236}$U | $^{238}$U | $^{239}$Pu |
|---|---|---|---|---|---|---|---|---|
| Cross sections at (0.0253 eV) 2200 m/s | $\sigma_c$ barns | 7.336 | 45.24 | 100.89 | 98.69 | 5.1319 | 2.6826 | 270.33 |
| | $\sigma_f$ barns | 0.00 | 531.21 | 0.067 | 585.09 | .0471 | 1.68E-05 | 747.40 |
| | $\alpha$ | - | 0.085 | - | .169 | - | - | 0.36 |
| | $\nu$ | - | 2.49 | 2.36 | 2.437 | 2.37 | 2.493 | 2.88 |
| | $\eta$ | - | 2.30 | - | 2.077 | - | - | 2.114 |
| Maxwellian averaged (1.0E-05-0.1 eV) | $\sigma_c$ barns | 6.88 | 43.21 | 94.39 | 92.266 | 4.84 | 2.529 | 273.56 |
| | $\sigma_f$ barns | 0.00 | 497.84 | 0.063 | 539.63 | 0.044 | 1.58E-05 | 721.32 |
| Maxwellian averaged (1.0E-05-10 eV) | $\sigma_c$ barns | 3.45 | 35.18 | 115.88 | 50.60 | 39.14 | 18.019 | 262.70 |
| | $\sigma_f$ barns | | 308.67 | 0.0730 | 269.14 | 0.0457 | 1.57E-05 | 532.63 |

[d] *K-effective is the multiplication factor in a medium where neutron fission chain reaction occurs and is a measure of the processes of production and destruction of neutrons.*

[e] *Migration length is the distance over which a neutron travels without getting absorbed.*

density. The various governing processes are fission, capture and scattering reactions. Each of these processes would create a change in the neutron population with respect to space, energy and time. Deterministically, the neutron balance equation is set up and the different production and loss mechanisms of neutrons are quantified. The life time of the neutron is characterized by the slowing down of neutron in a medium. The prompt neutron lifetime[f] for an infinite medium is defined as the inverse product of velocity and the macroscopic absorption cross section which is a material property of the medium. In an LWR, the average prompt neutron life time is about 0.2 ms and in a heavy water reactor this is one order higher about 2.5 ms.

### *Nuclear cross section sets for nuclear reactor design*

Neutron-induced cross section for all the types of reactions occurring in a reactor is a major input required for reactor design. Although the measured cross sections are available at discrete energies and fitted into continuous energy data using both theory and experiments, the data required for deterministic simulation will be reactor specific energy weighted neutron reaction cross sections. The weighting is carefully performed so as to conserve the reaction rate over the energy bins considered [8]. A summary of the various neutron interaction cross section both at specific energies and spectrum averaged values for major actinides are presented in Table 5 just to understand the interplay of cross section and the ambient neutron spectrum.

It is also to be noted that with a different thermal spectrum as seen in different thermal reactors, these cross sections would be different. The energy dependent cross section for some fissile isotopes is in relation with a typical neutron spectrum of AHWR as an example is given in Fig.6.

Availability of validated nuclear data for different nuclides and at all energies of interest is a challenging task. Mega facilities like CERN neutron time-of-flight (n_TOF) are required to experimentally determine the reaction cross section. The experimental data is required to be qualified and undergoes rigorous evaluation through best estimate approach before it becomes usable by reactor designers [8].

However, Monte Carlo codes use continuous energy cross section set which reduces one level of uncertainty of spectrum averaging.

### *Material challenges for advanced reactors*

Newer reactors such as Gen-IV reactors, AHWR, Metal fuelled fast reactors or MSRs use advanced fuel such as (U,Pu)MOX, (Th,Pu)MOX, U-Pu-Zr alloys or molten fluoride salts for features such as higher fuel utilization, irradiation stability and high temperature performance. These compounds are challenging to model as their physical and chemical properties themselves are not well known and material testing reactors using cutting edge technology are not available today. BeO is used a as a reflector in many thermal reactors, the scattering properties and irradiation behavior of BeO as a compound is not well understood even today. Both deterministic simulations and experiments are required to generate data for such materials. When designers target high burnups, the fuel clad material is also required to withstand the fission gas pressures and larger residence time. New alloys are being studied and

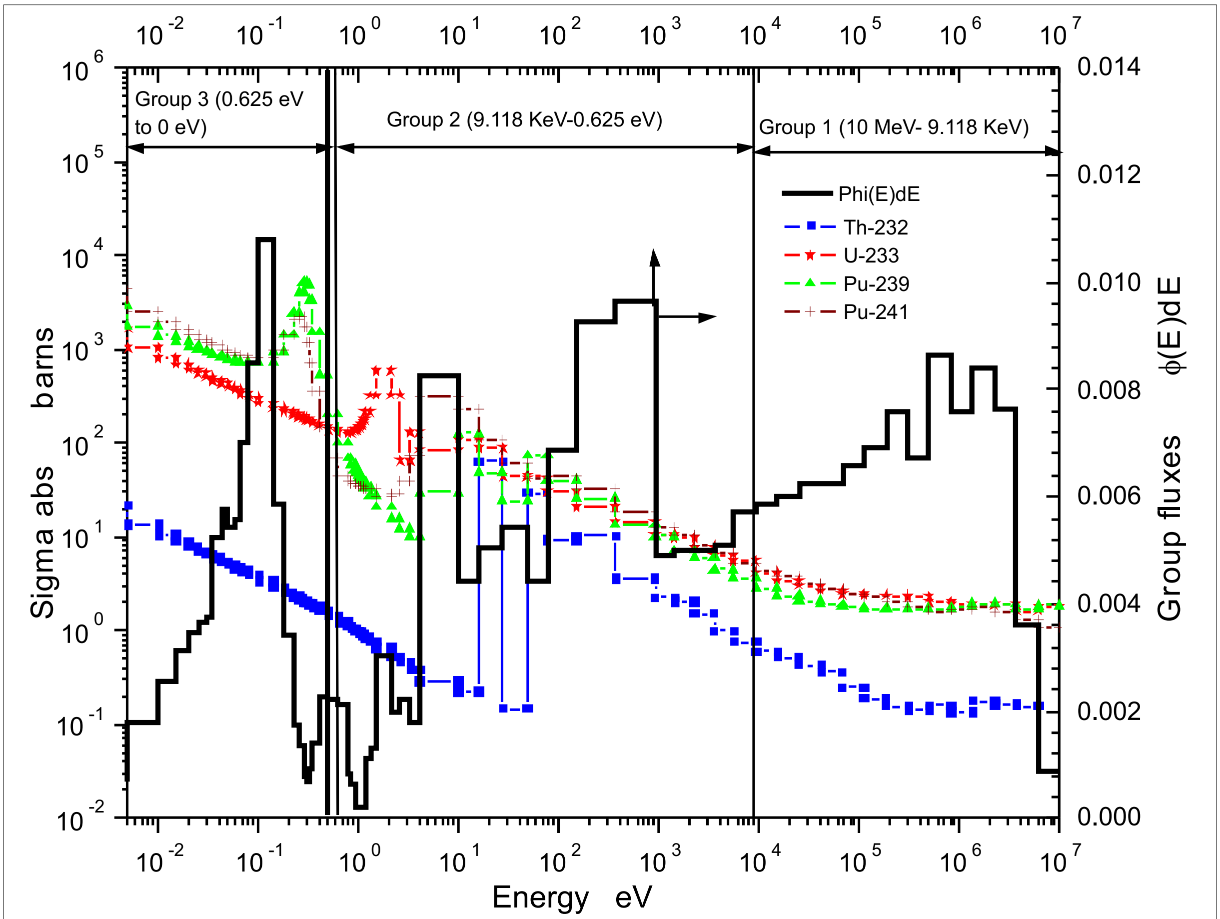



*Fig.6: Energy dependent absorption cross section of $^{232}$Th, $^{233}$U, $^{239}$Pu and $^{241}$Pu in relation to the neutron spectrum in AHWR.*

[f] *Prompt neutron life time is a measure of life of a neutron in a medium which is characterised by scattering, multiplication and captures. For finite medium, the quantity is derived from moderation or slowing down and can be measured.*

experiments are performed in accelerated environment to study radiation damage. M5, an alloy of Zr has been used a clad material in PWRs. An innovative idea of using pyrocarbon as moderating material in AHWR was suggested to reduce the effective moderation and to tune the neutron spectrum to achieve better safety performance [9]. In MSR, the candidate material for the vessel is Hastelloy and some high temperature reactors use Niobium. The choice of these structural material is dictated by the competing effect of neutron absorption and mechanical strength for the design pressure and temperature conditions.

With respect to enhanced safety, accident tolerant fuels are being designed where both better fuel matrix to withstand internal gas pressures and better clad to retain fission products are used.

### Advanced Reactor Designs

BARC is engaged in design of advanced reactors catering to different objectives of power generation. All the basic concepts of neutron physics discussed above have been prudently used in design of advanced reactors such as Advanced Heavy Water Reactor (AHWR), Indian Pressurised Water Reactor (IPWR), High Temperature (HTR), Molten Salt Reactors (MSR) etc. In this article some of these designs and their physics challenges are discussed.

### *AHWR challenges*

The AHWR is a 920 MWth, vertical pressure tube type thorium-based reactor cooled by boiling light water and moderated by heavy water designed to maximize power production from thorium [10, 11]. This is a unique reactor designed for large scale commercial utilization of thorium and integrated technological demonstration [12]. The objective has been to design an advanced reactor system utilizing thorium with several passive safety features incorporated. The aims of the design are to achieve relatively higher fraction of power from Th-$^{233}$U, self-sustenance in $^{233}$U, a high discharge burnup with minimum makeup fuel and the inherent safety feature of negative void reactivity coefficient [13]. Plutonium is used as makeup fuel to achieve high discharge burn up and self-sustaining characteristics of Th-$^{233}$U fuel cycle [11].

Light water coolant in a pressure tube system makes the void reactivity positive. The cluster design is mainly dictated by the objective of achieving negative void reactivity. The cluster design has undergone several levels of iteration. Also, from the heat removal considerations the cluster has been designed to have two axial enrichments in the outermost pins to obtain minimum critical heat flux ratio(MCHFR) with adequate margins [12]. The optimized equilibrium core cluster designed from all these competing objectives is presented in Fig.7a. The core layout is shown in Fig.7b. The breeding of U-233 in the cluster is clearly shown in Fig.7c.

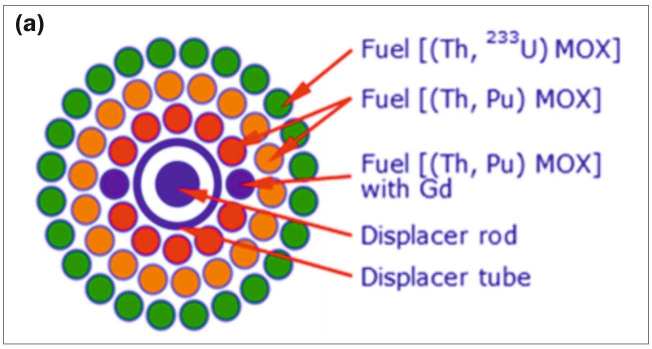



*Fig.7(a): Optimized AHWR equilibrium core fuel cluster.*

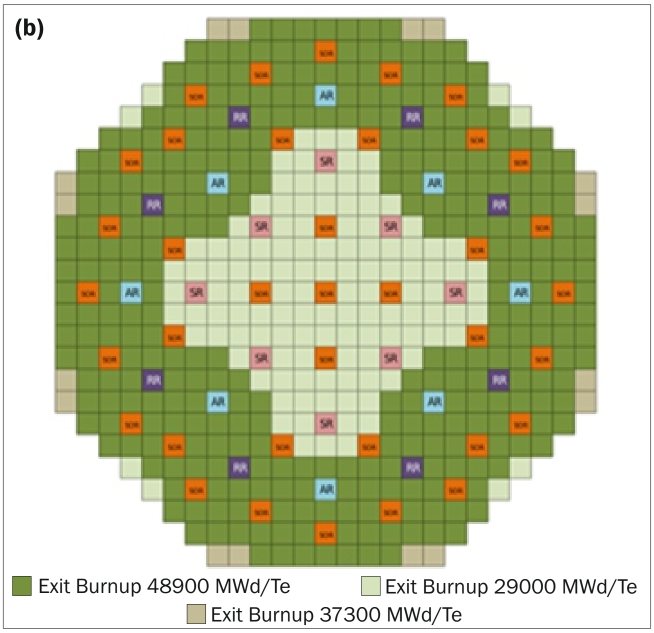



*Fig.7 (b): . Equilibrium core layout of AHWR .*

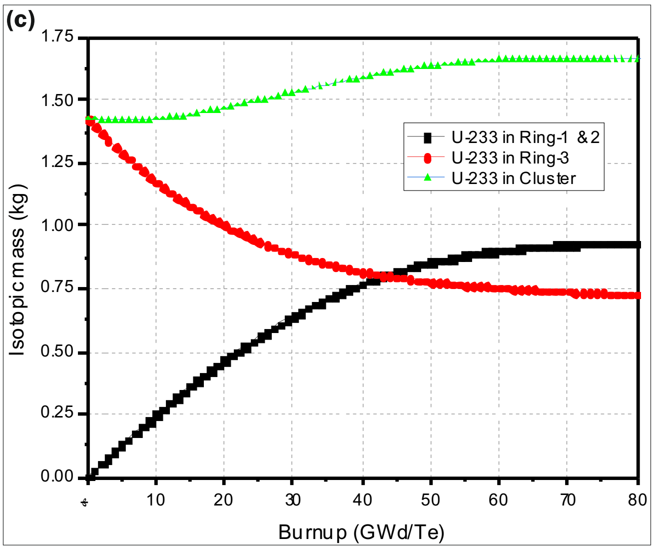



*Fig.7 (c): U-233 breeding in the equilibrium fuel cluster of AHWR.*

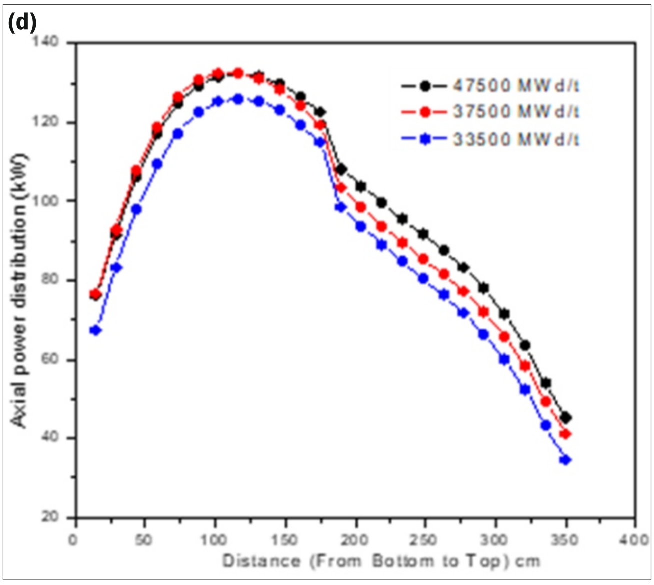



*Fig.7(d): Axial power distribution in the three burnup zones in AHWR equilibrium core.*

Table 6: Design features of AHWR core.

| | |
|---|---|
| Power to the coolant, MWth | 920 |
| Power from $^{233}U$, % | 75 |
| Total number of channels | 513 |
| No. of Fuel channels | 452 |
| Lattice type, pitch, mm | Square, 225 |
| Average discharge burnup, MWd/Te | 40000 |
| Active fuel length, mm | 3500 |
| ***Fuel material***<br>(For Pu topped variant)<br>(For U235 topped variant) | <br>(Th,U233)MOX and (Th,Pu)MOX<br>(Th,LEU)MOX |
| Fuelling scheme | On power fuelling or Mini-batch |
| Fuelling rate | 73 channels/ year |
| ***Pressure tube***<br>Material<br>Inner Diameter/ Wall Thickness (mm) | <br>Zr-2.5%Nb<br>120/ 4 |
| ***Calandria tube***<br>Material<br>Outer Diameter/ Wall Thickness (mm) | <br>Zircaloy-4<br>168/ 2 |
| ***Heat removal aspects***<br>Average heat rating, kW/m<br>MCHFR at 20% over power | <br>10.8<br>1.7 |
| ***Control and safety devices***<br>Control rods (CRs), Nos.<br>Shut Down System-1<br>Shut Down System-2 | <br>24 (8 ARs, 8 RRs, 8 SRs)<br>Mechanical Shut-off rods ($B_4C$) 37 Nos.<br>Liquid poison injection (Gadolinium Nitrate solution) |

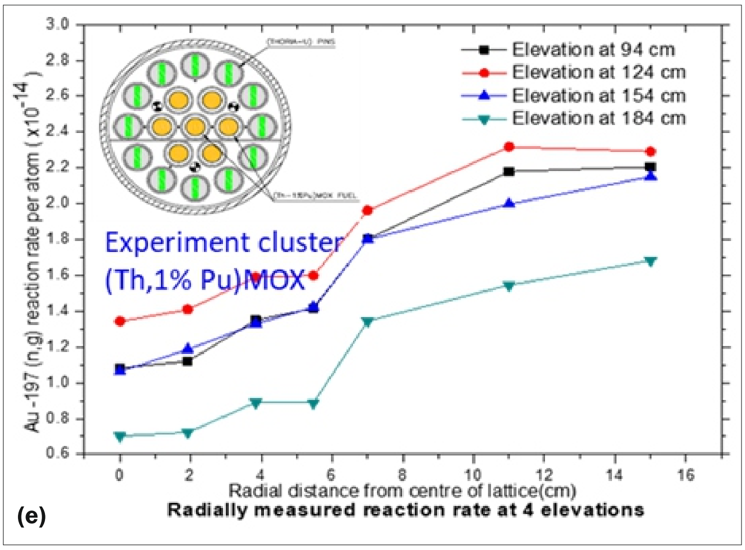



Fig.7(e): Radial power distribution across experimental cluster at different elevations.


Fig.7(f): Arrangement of HDP blocks for measurement of coolant void worth for different void fractions in experimental (Th,Pu)MOX cluster.

A uniform radial core power distribution that is preferred from natural convection standpoint is obtained by multi-zone fuelling. The number of fuel channels is large at 452 due to low core height of 3.5 m [14]. This increases the core or calandria radius as compared to a typical PHWR of similar thermal power. In order to achieve power distribution conducive for heat removal through natural circulation and achieve better thermal margins, a bottom peaked power distribution is desirable. This has been achieved by using differential enrichment in top and bottom of the fuel cluster and it is illustrated in Fig.7d. The basic design features of AHWR is presented in Table 6.

Several experiments have been performed in the AHWR critical facility to qualify thorium-based fuel and validate the neutronic codes and nuclear data used for design [15]. Integral parameters such as critical heights, level coefficient of reactivity, reactivity worths etc. were measured in Thoria, (Th, Pu) MOX and (Th, LEU) MOX fuel clusters and compared with theoretical estimates. Experiments for measurement of safety parameters such as coolant void worth, flux profile across the cluster were designed and performed. Axial and radial neutron fluxes were measured in the experimental thoria based cluster and coolant void worth in the (Th, Pu) MOX experimental cluster also was measured recently [16]. The experimental measurements were in good comparison with calculated parameters and these were used to validate the design codes used for AHWR. Some results are shown in Fig.7e. The experimental arrangement for measurement of fractional coolant voids is shown in Fig.7f. The AHWR physics design has been indigenously evolved and the inherent safety has been demonstrated through several experimental programs.

### *Physics design of IPWR and its challenges*

The Indian Pressurised water Reactor (IPWR) is being designed with enriched uranium fuel and light water as coolant in a hexagonal lattice arrangement. The core design has been achieved by optimising the U-235 content with an objective to achieve a target discharge burnup of about 45 GWD/T in a multi-cycle batch fuelling mode [17]. The rated power was aimed at 900 MW(e) or 2700 MWth. The burnup reactivity control during the cycle is achieved by soluble boron. IPWR has been designed as per current safety standards where all the reactivity coefficients are negative. Another important objective of IPWR was to have neutron monitorability at all phases of operation in the core, namely cold, hot conditions, xenon free, transient conditions and over the complete operating cycle from beginning to end of cycle of fuel residence time.

The challenge was to achieve longer cycle length and use of neutron absorber Gadolinium as integral fuel burnable absorber. Fuel assembly has been profiled with different U-235 content and Gadolinium to achieve better local peaking factor and fuel burnup. The IPWR fuel assembly is presented in Fig.8a. The short-term and long-term reactivity control requirement in IPWR is achieved by control rods having neutron poison and chemical shim in the form of soluble boron respectively. With respect to the core design, soluble boron content at beginning-of-cycle has been minimized to achieve negative feedback coefficients through the heating phase and over the cycle. The fuel management patterns are being developed using both traditional schemes and heuristic approach. The optimized loading pattern of the equilibrium cycle of IPWR is shown in Fig.8b. The experience in designing IPWR has been effectively used to design an LWR core for lower power to be used in Small Modular Reactor (SMR). Table 7 shows certain salient features of the equilibrium cycle of IPWR. The IPWR design conforms to the current PWR standards of long cycle length and improved safety.

*Table 7: Design features of IPWR core.*

| | |
|---|---|
| Rated Power MW(e)/MW(th) | 900/2700 |
| No. of fuel assemblies (FA) | 151 |
| FA lattice arrangement | Hex |
| Fuel type/Enrichment | Enriched Uranium ~4.24% |
| Discharge burnup MWd/Te | 46000 |
| Average Linear Heat Generation Rate w/cm | 159.6 |
| Power density Mw/m$^3$ | 87.4 |
| Core periphery diameter mm | 3306 |
| Core baffle diameter mm | 3455 |
| Material of the core baffle | SS + water |
| Core barrel ID/OD mm | 3455/3600 |
| Material of the core barrel | SS |
| Thermal shield ID/OD mm | 3630/3780 |
| Reactor Pressure vessel ID/OD mm | 4170/4670 |
| System pressure MPa | 15.7 |
| Active core height mm | 3600 |
| Coolant inlet/Outlet temperature °C | 291/325 |
| Fuel management | Three batch fuelling |
| Reactivity control | Soluble boron ($H_3BO_3$ in water) |
| Shutdown and Control | Rod clusters in fuel assembly |
| Control rod material | $B_4C$ and $Dy_2TiO_3$ |

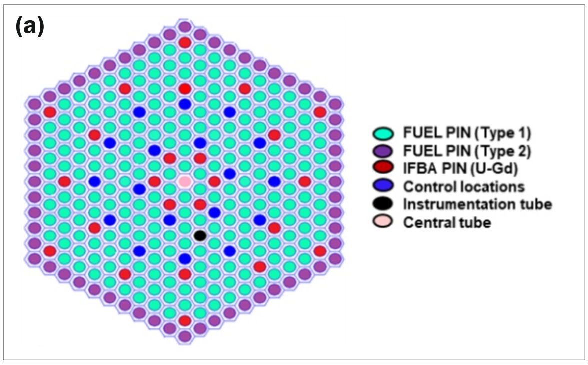



*Fig.8(a): Profiled fuel assembly of IPWR.*

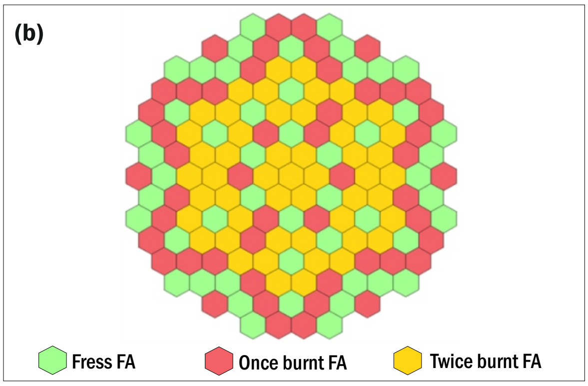



*Fig.8(b): Equilibrium core loading of 900 MWe of IPWR.*

### *Molten Salt Breeder Reactor (MSBR)*

In keeping with the mandate of designing an efficient thorium breeder system for the third stage of the Indian Nuclear Program, MSR is considered as a promising candidate. The fluid in an MSR is under circulation. By temporarily storing the irradiated thorium based molten salt in dedicated tanks, Pa-233 which has a 27-day decay half-life can be easily converted to fissile U-233 and pumped back into the reactor. By adjusting the feed and bleed of the molten salt, effective breeding can be achieved. The challenge is the physics simulation of liquid systems and managing the reactivity of the core. Studies of refueling rates and its effect on core reactivity have been done. Refueling study for a typical molten fluoride salt is shown in Fig.9a. The movement of liquid fuel results in a distributed delayed neutron source and hence the flow induced reactivity must be estimated more accurately (Fig.9b). Several core configurations have been designed with fluoride salts and fuel performance has been optimized. The current focus is on design of a thermal spectrum based 5 MWth demonstration reactor. Both Th-U233 and LEU based cores have been

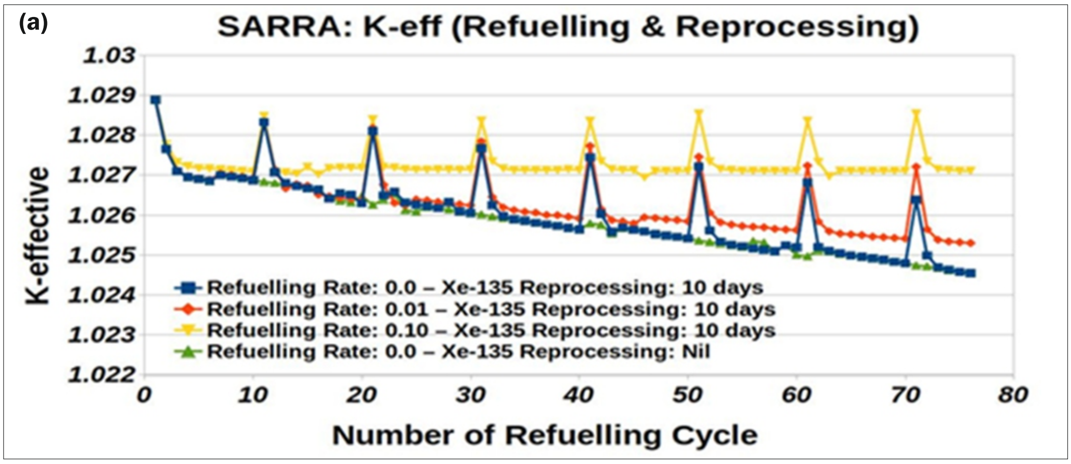



*Fig.9(a): Optimising of refueling cycle in MSR.*

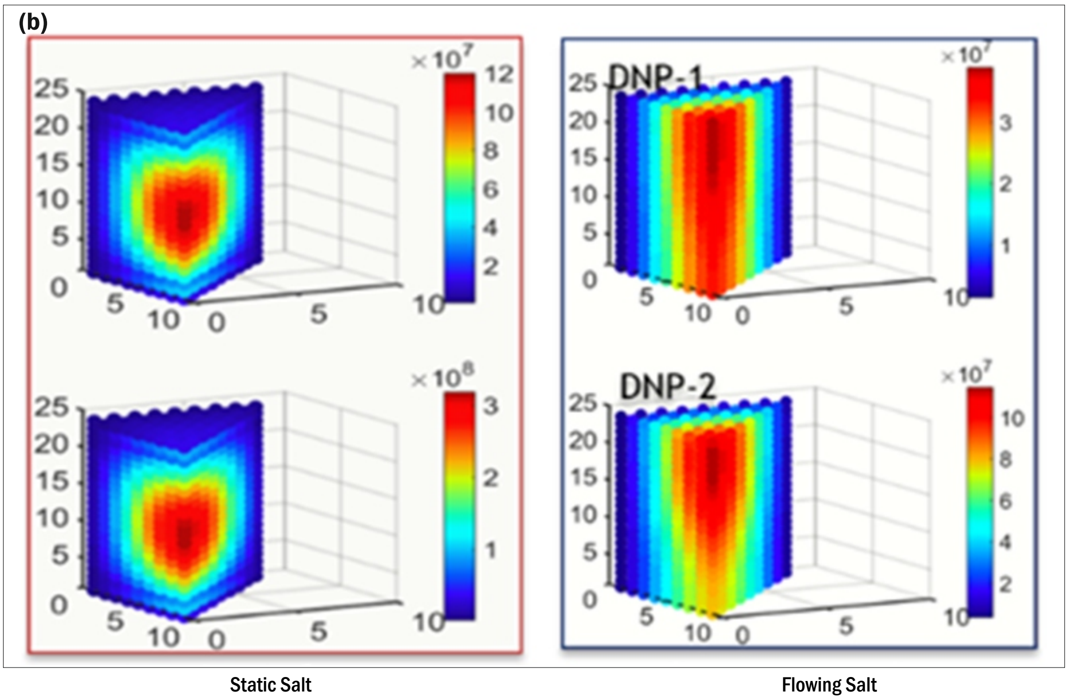



*Fig.9(b): Simulation for dynamics of molten salt - Movement of delayed neutron precursor.*

designed [18,19]. A typical core design of Th-U233 based 5 MWth MSR is shown in Table 8.

Neutronic tools have been developed for fuel management and treatment of dynamics of the molten salt [20,21]. The analysis studies include state-of-the-art studies on the advanced MSR fuel dynamics, benchmarking and validation, coupled neutronics-thermodynamics analysis; fission product, tritium transport; and effective thorium utilization and breeding. A molten salt fuel experiment is being designed and will be performed in critical facility to assess the integral parameters. The experimental results of the declassified MSRE experiments were analyzed with ARCH code and the results were found matching very well [22]. Other irradiation experiments for simulation of flow is being planned in research reactors.

### *Physics challenges of High Temperature Reactor (HTR)*

BARC is engaged in development of High-Temperature Reactors. The objective is to use the process heat for production of green hydrogen as an energy carrier of the future. A 100 kW Compact High Temperature Reactor (CHTR) was designed using the thorium. The physics design of CHTR has

*Table 8: Physics design features of 5MWth MSR of AHWR.*

| | |
|---|---|
| Power | 5 MWth |
| Fuel Salt inventory | 1.57 Tonne |
| U-235 inventory | 172 Kg |
| Graphite inventory (moderator) | ~6 Tonne |
| Number of Fuel Channels | 1176 |
| Fuel salt/Composition | LiF-CaF2-ThF4-UF4 : 70%-8%-0%-22% |
| Enrichment (U-235, Li-7) | 19.75%, 99.9% |
| Control and Shutdown material | B4C |
| Fuel Temperature Coefficient (Doppler) | - 4.0 pcm/°C |
| Loss of Delayed Neutron Precursor(DNP) due to salt flow | 272 pcm |

*Table 9: Physics design features of 5MWth MSR of AHWR.*

| | |
|---|---|
| Reactor Power | 100 kW (thermal) |
| Fuel | TRISO particles of ($^{233}$U-Th)$C_2$ or (Th,LEU)$C_2$ |
| Core fuel cycle | 15 effective FPYs |
| Coolant | Lead-Bismuth Eutectic |
| Core inlet/outlet | 900/1000$^0$C |
| Moderator/Reflector | BeO/BeO and Graphite |
| Height & diameter | 100 cm & 127 cm |

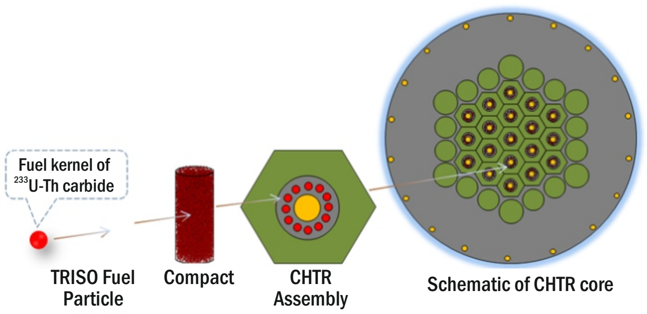



*Fig.10: Schematic of fuel particles and the CHTR core.*

advanced features like thorium-based TRISO coated fuel, long core life cycle, negative temperature reactivity coefficients, core heat removal by natural circulation, and decay heat transfer to the surroundings passively during severe accidents [23]. The physics challenge here is to design long life core spanning 10 to 15 years with sufficient burnable absorber to sustain reactivity throughout the core life. The compact nature poses issues of locating the reactivity mechanisms and optimizing the fuel performance. The optimized core characteristics of CHTR core is presented in Table 9. The simulation of heterogeneous CHTR core with graphite bores containing TRISO particles is illustrated in Fig.10.

The natural circulation cooled and TRISO particles fueled CHTR design necessitates multi-physics investigations of the high-temperature core under normal operations and anticipated transients. An indigenous capability, code ARCH-TH, for simulations of full core neutronics coupled with thermal-hydraulics has been developed and extensively validated for viability. Subsequently, the anticipated transients in CHTR were investigated in detail. The analyses of CHTR transients demonstrate the designed passive features of the core.

It is also worth mentioning that these types of core design can be successfully used for district heating or as power packs for remote areas. In another version of HTR, a pebble bed core was simulated which has potential for hydrogen generation [20]. In a pebble, several thousand of TRISO fuel particles are embedded in a graphite matrix. The core design envisaged movement of these pebbles from bottom to top, thereby facilitating online refueling. The physics challenge was the treatment of double heterogeneity. A code PebMC was developed to solve for the flux/power distribution in the core [24].

## New Energy Systems

In order to exploit the physics properties of different materials, many new concepts have been developed both in India and elsewhere in the world. For example, if super critical water is used, the moderating properties can be tuned to achieve breeding in thermal reactor systems. Use of lead and lead bismuth eutectic as coolants has been explored in order to go to high temperatures and improve the heat removal [25]. Inert matrix fuel has superior metallurgical properties and can be used to retain the fission gases inside the fuel matrix. Few systems that are being designed are briefly explained here.

### *Advanced LWRs*

In order to increase the fuel utilization, LWRs are being designed with longer cycle lengths. This would require higher fissile content or enrichment. Longer burnups are limited by degraded fuel behavior, fission product release and degradation of clad. Different reactors are being proposed with elegant solutions for each of these issues. Studies on the use of low neutron absorbing clads have been done to aid the use of higher enrichment in fuel. Plutonium recycle is another option to improve the burnup in thermal reactor systems. High burnup fuel would also require the use of neutron poison like Gadolinium or Erbium to be mixed with fuel. Several fuel cycle options in thermal reactor systems with thorium as a carrier either with weapons grade or reactor grade Plutonium have been extensively studied [6].

### *Small modular reactors (SMRs)*

It is seen from the operating experience of LWRs, that small reactors are easy to operate and have enhanced safety features. SMRs are smaller than traditional nuclear reactors, and can be used to provide a reliable source of energy in a variety of settings. They are designed to be factory-built and transported to the site for installation, allowing for faster and more efficient construction. The current designs envisage that all reactor components are placed inside the pressure boundary and can be treated as an integrated module. The power rating of these modules typically ranges from 20 to 200 MW(e). Such units can be combined in a reactor site to increase the power output. SMRs are ideal to replace the aging coal fired plants. However, the key to success of SMRs in this application will be to design systems with more passive safety features leading to a much lower risk of accidents or malfunctions.

Design of these compact integrated modules is challenging. The power density is designed to be higher and will require enriched fuel in a better matrix so that fission products and fission gasses can be contained. The reactor core being considered is a hexagonal core with enriched uranium fuel in a once through mode. The U-235 content is adjusted to achieve large cycle lengths.

### *HTRs - Gas cooled and Liquid Metal cooled*

Gas-cooled reactors (GCRs) have been used since the earliest days of nuclear power using graphite as moderator and helium or $CO_2$ as the coolant. In early history, GCRs used natural uranium as fuel in thermal spectrum and competed with LWRs without relying on the enriched uranium fuel. Both UK and France developed Magnox-type gas cooled reactors, with France building nine reactors and the UK building 24 reactors. This was followed by development of Advanced Gas Cooled Reactors (AGRs) which were built in UK and are classified as generation-II gas cooled reactors. Unlike the first-generation Magnox reactors, which were optimized for plutonium, AGRs were made to economically produce power similar to the coal fired plant and thus required higher operating temperatures. The AGR designs, therefore, are developed with stainless steel cladding and enriched uranium fuel leading to higher burn-ups of about 18GWD/T. The AGR's oxide fuel, with higher operating temperature compared to the metallic Magnox fuel, also resulted in improved power conversion efficiency of about 42%, compared to around 28% in a Magnox.

BARC is looking at the feasibility of developing gas cooled reactors for hydrogen generation. GCRs have several advantages over LWRs, such as use of natural uranium fuel and use of gas coolant but are bulky and have lower power densities. The High Temperature Reactors (HTRs) are also categorized as GCRs which are designed with specialized TRISO coated fuel and with inert helium gas coolant. A preliminary physics study has been recently initiated.

### *Accelerator driven sub-critical system (ADSS)*

In an ADSS, particles or ions are accelerated to high energies and made to bombard on heavy elements which then produce a large number of neutrons. High energy protons, on colliding with a target of high-density element (such as lead, tungsten, and uranium cause the detachment of a large number of neutrons from these nuclides in a process known as "spallation." The ADSS consist of three components namely, the accelerator, the target and the blanket in addition to heat removal and electrical generating equipment. The blanket can be fertile or fissile, or irradiated fuel having fission products. Copious number of neutrons could be produced if the energetic beams are incident on the high-Z target material.

Typically, an accelerator producing intense high energy proton beams of 1GeV energy and current of 10mA is used. These protons are made to be incident upon a heavy metal target such as Lead to produce neutrons by the spallation reaction. The number of neutrons per proton depends upon the target material, its size and the proton energy. For example, for when a 1GeV proton is incident on Pb target, about 20–30 neutrons may be produced. A typical schematic of ADSS is shown in Fig.11.

Energy amplification can be demonstrated from first principles in an ADSS. A 1 GeV proton beam mentioned above requires about 40 MeV to produce one neutron and the electrical energy required will be about 100 MeV. The subcritical multiplication resulting from this spallation can provide additional neutron population in the subcritical blanket. Considering a multiplication factor of 0.98 the net fission neutrons generated by one spallation neutron will be about 20 and the fission energy converted to electrical energy released will be about 1.3 GeV [26]. Therefore, this system is also called an "energy amplifier."

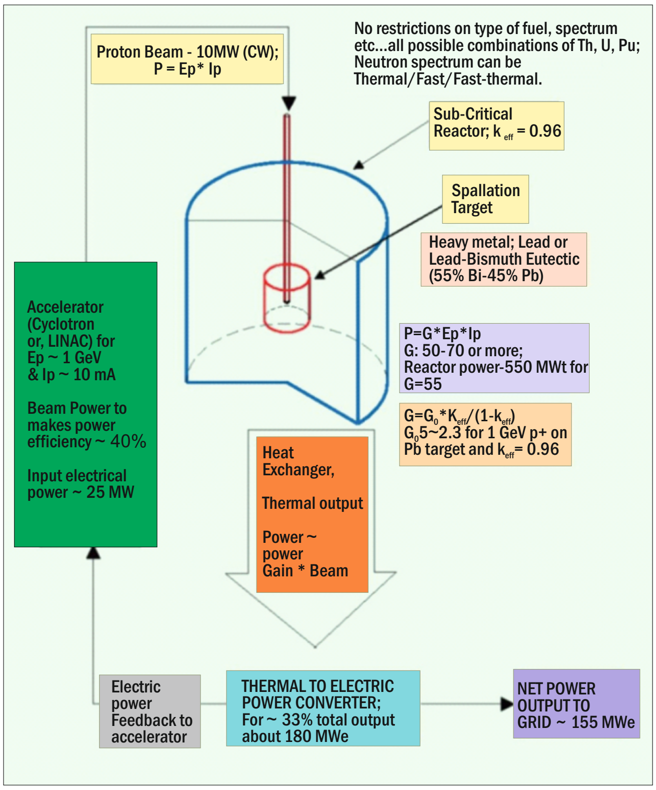



*Fig.11: Components of Accelerator Driven Sub-critical core (ADSS).*

### Hybrid Reactors

Fission-Fusion hybrid reactor systems have a good potential to breed fissile content. The inner fusion core is a good source of neutrons and if it is surrounded by a fertile or fissile blanket region, breeding or transmutation can be achieved. The fusion core is usually based on the efficient D-T reactions. The core design is governed by the balance between use of the neutrons from fusion core to breed fissile species and to breed tritium. The temperature in the inner fusion core will be about a few keV and the neutrons emitted usually have energies of 3-5MeV. These high energy neutrons can be made to cause either fissions or captures in the surrounding blanket. Transuranic elements have significant fission cross sections for high energy neutrons and if the blanket is fueled with these elements, they can be converted to other actinides and reduce the waste volume.

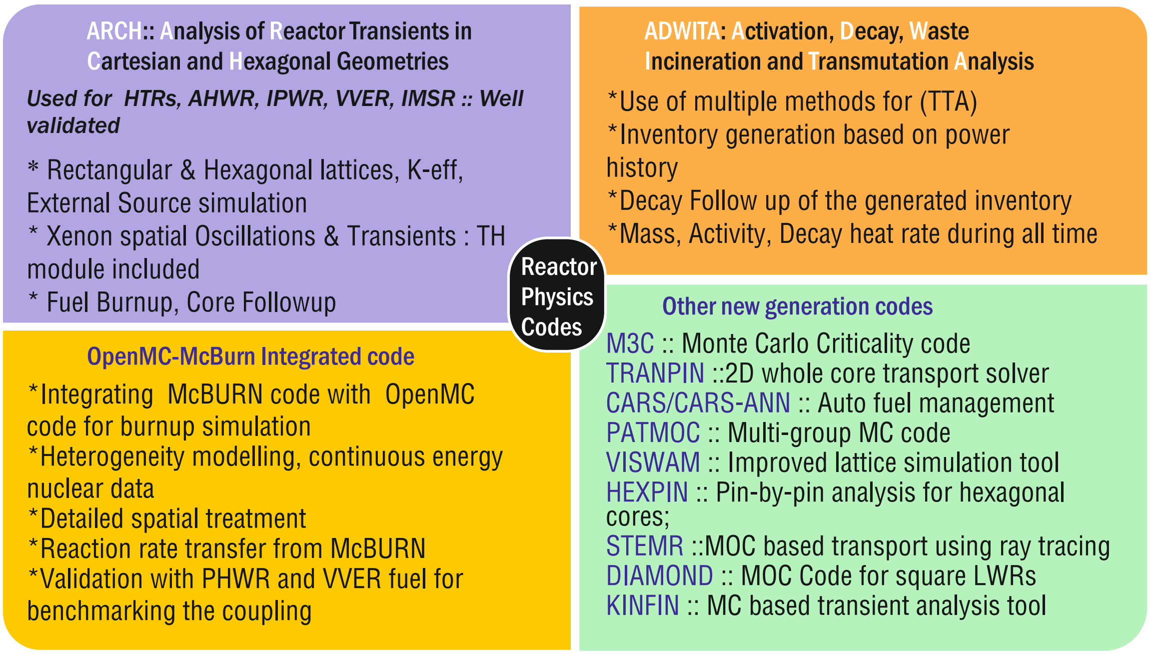
### Simulation Techniques and Methods

The fundamental quantity to be calculated are the neutron flux distribution and the effective multiplication factor. Advanced reactors have several design objectives to cater to and are phenomenologically more intensive to simulate. More heterogeneities are introduced for enhanced safety and to improve fuel utilization. Thus, these advanced energy systems are characterized by multi-physics phenomena and are required to be modeled exactly.

On the deterministic front, the discretization in space and energy are being taken to higher levels. The reactor core is being analyzed over larger number of both regular and irregular nodes or meshes and the flux can be determined more accurately using advanced numerical techniques. The parameters are required at pin section, pin level, fuel assembly level and global core level. The energy domain is being discretized to finer bins to span nine orders of neutron energies from MeV to meV range [27]. The time domain to be dealt with in reactor physics simulations must also cover a huge range. The reaction mechanisms are to be understood in the femtosecond scale. The reactivity feedbacks are modeled in micro second range. The transients are modeled in steps of milliseconds to estimate the power rise phenomenon over time intervals of a few seconds to minutes. Fuel management in reactors are performed over a few days or months. The isotopic concentrations of fuel out of the core are governed by natural decay and could vary from milliseconds to millions of years. Thus, it is obvious that a single code or single technique cannot cater to these varied simulations required and that too with good accuracy [27]. A brief on some codes and methods developed are detailed here.

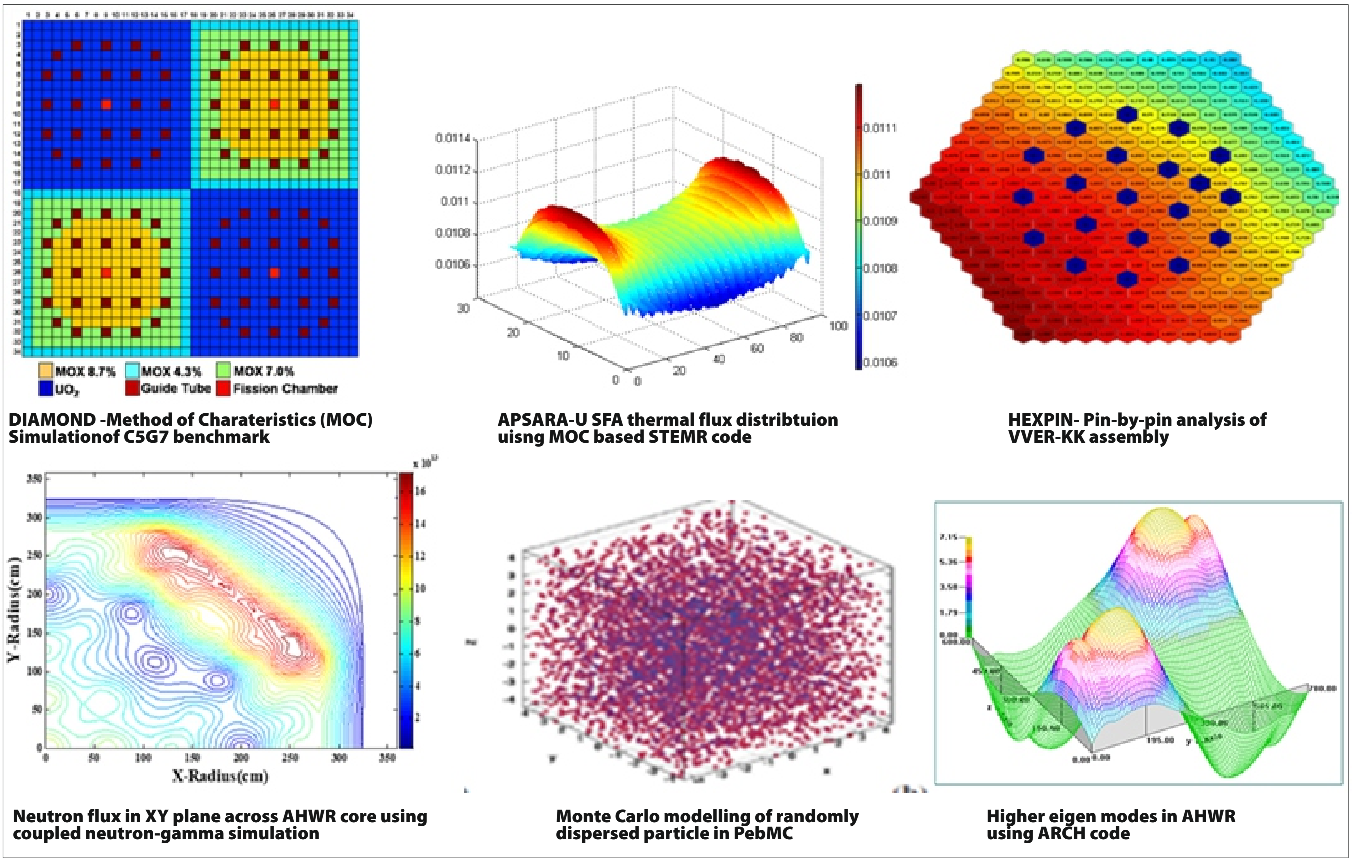
ARCH is a diffusion theory-based 3D core analysis code using finite difference techniques developed for both square and hexagonal geometries [28]. New multi-physics modules ARCH-TH has been introduced in this code and it also has been coupled with thermal hydraulics in a code system PROMISIN.

ADWITA is a fuel cycle analysis code developed for spent fuel analysis which estimates actinide concentration, activity of actinides and fission products and radiotoxicities [29]. This has been validated with experimental results decay heat and PHWR discharged fuel of both uranium and thorium cycle. Codes based on probabilistic methods have also been developed. The general geometry continuous energy Monte




**State-of-the-art reactor physics analysis tools developed for analysis and design of thermal reactors**

*Fig.12: Reactor Physics code basket developed by RPDD.*




**DIAMOND -Method of Charateristics (MOC) Simulationof C5G7 benchmark**

**APSARA-U SFA thermal flux distribtuion uisng MOC based STEMR code**

**HEXPIN- Pin-by-pin analysis of VVER-KK assembly**

**Neutron flux in XY plane across AHWR core using coupled neutron-gamma simulation**

**Monte Carlo modelling of randomly dispersed particle in PebMC**

**Higher eigen modes in AHWR using ARCH code**

*Fig.13: A few simulation results from advanced neutronics codes.*

Carlo code M3C, multi-group Monte Carlo code PATMOC and time dependent Monte Carlo code KINMC have been developed and validated extensively and used for routine simulations [30,31,32]. McBURN - a Monte Carlo based burnup simulation tool has been integrated with the indigenous Monte Carlo codes and tested for burnup simulations of PHWRs and VVERs. An overview of the reactor physics codes developed recently is shown in Fig.12.

VISWAM, a versatile neutron transport code for lattice geometries has been developed with several options of solution methods. TRANPIN and HEXPIN, core simulation tools have been developed for triangular geometries for a detailed pin-by-pin analysis [33]. Transport theory codes are used for more exact simulation of highly heterogenous cores. 2D MOC codes for neutron transport DIAMOND and STEMR have also been developed. Some of the other codes that have been developed based on advanced methods and techniques are in-core fuel management code CARS based on genetic algorithms and ANN [34], PebMC, a Monte Carlo method for treating fuel pebbles in high temperature reactors, SAARA, code for fuel management in MSRs, MSDyn, a circulating fuel salt analysis code and codes based on modal analysis. Multi-physics modeling in MSDyn and ARCH-TH have been verified with experiments and results have agreed very well [35,36]. Some of the selected results from the simulations using advanced codes and methods are presented in Fig.13. A varied set of codes cratering to several different applications have been developed and tested over the years.

## Summary

The physics challenges are manifold for future energy systems. Reactor physics design and the engineering development are complimentary and they influence each other. Multi-physics modelling is very important to determine the safety and estimate the feedbacks more accurately. Experimentation on fuel and processes will help in reducing margins and validate the neutronic tools. Post irradiation examination of irradiated fuel will throw light on the fuel behavior especially for high burnups. Material challenges are varied and new materials have to be developed and experimentally qualified for its high irradiation stability and durability. To quote a few specialized tasks, better neutron transport methods to estimate the tritium breeding in ITER blanket, use of more foil irradiation coupons to cover the entire energy range to estimate the fluence in reactor pressure vessel (RPV) in LWRs, and study of fuel thermo-mechanical behavior both with deterministic and AI techniques.

In order to estimate the neutron counts in highly sub-critical phases, better physics methods will be required and signature of the emerging particles should be captured more accurately and out-of-core detection systems also should be enhanced. Newer detectors for estimation of in-core fluxes are required for the different types of neutron spectra that will be encountered in future.

On the nuclear physical constants, for neutron and particle induced cross sections, more precise measurements are required with cutting edge technology. Elastic scattering cross section of new compound materials is the need of the day even for current generation reactors. High energy cross sections are difficult to measure and require more precise instrumentation. Neutron and gamma shielding will also play a major role in these new and hybrid energy systems and Monte Carlo based particle transport methods will be required and will be tested to their ultimate capabilities in order to develop cost effective shields. Irradiation behavior is not fully understood for new fuel types and will require long irradiation campaigns, detailed post irradiation examination and accelerated testing in accelerators.

New generation power reactors are being designed with diverse objectives and require newer materials and better simulation methods. On the research reactor front, the challenge will be to achieve high neutron fluxes for material characterization and design several features for extracting the neutron for basic research. This will also involve the development of many engineered systems such as neutron guides, detectors and spectrometers and high energy probes. These novel experimentation efforts will induce reactor technologists to take up more challenges. The excitement in reactor design is driven by deep understanding of the basic physics of nuclear interactions and its interplay with other processes.

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