MONTe-carlo Nucleon transport Code (MONC) for nucleon transport is being developed for several years. Constructive Solid Geometry concept is applied with the help of solid bodies. Union, subtraction and intersection Boolean operations are used to construct heterogeneous zones. Scaling, rotation, and translation operation of the basic bodies are allowed to construct more complex zones. Module of repetitive structure for lattice, core calculations in reactor and detector simulation is developed. Graphical User Interface along with visualization tools is developed to make input, construction and display of geometry, and analysis of output data. Low energy neutron transport module is developed using continuous linearly interpolable point neutron cross section data below 20MeV neutron energy. The code is benchmarked for simulation of accelerator driven sub-critical system, neutron shielding, heat and neutron flux distribution and keff of the critical assemblies. It is observed that results of keff are in agreement within $\sim 3\%$ with experimental results of critical assemblies as well as the values obtained from MCNP.

Keywords: Monte Carlo, Constructive Solid Geometry (CSG), Spallation, Accelerator Driven Sub-critical Systems, Critical Reactors.

I. INTRODUCTION

In past two decades development in the accelerator technology has given boost to facilitate the world with Spallation Neutron Source (SNS) and to study Accelerator Driven Sub-critical systems (ADS) [1–3]. The essential component of an ADS system is the presence of a spallation target in the core of the reactor. An external proton beam (energy 1 GeV and current tens of mA) produces spallation neutrons which drives the reactor under sub-critical conditions. Currently two types of generic target modules i.e. window and windowless concepts have been proposed [4–6]. In the window configuration, the proton beam enters the target region through a thin solid barrier (window), which isolates the beam transport pipe and the target. The spallation target is ideally conceived to be material of high atomic number (Z) or higher (N/Z) ratio and low melting point like a lead bismuth eutectic (LBE) while a few mm thick steel is used as window material. One of the critical operating conditions of the spallation target is the very high volumetric heat deposition rate. For example, 65% proton beam energy at 1 GeV is lost as ionization energy which is just heating the spallation target system. Depending on the density, the rate of heat deposition is also different for both target and window materials. The heat loss at a given energy is sum of two components; the contributions coming from direct ionization of primary beam and ionization through the hadronic interactions. At low energy, as the hadronic contribution is not very significant, the total heat loss is predominantly due to primary ionization. The longitudinal heat loss profile ($dE/dz$) as a function of $z$ has a range $r_b$ followed by a Bragg peak, an interaction process which can be described well by the Bethe formula. However, at 1 GeV proton energy, the primary ionization accounts for only 70% of the total heat loss and the remaining 30% comes due to hadronic interactions (High energy fission, charged evaporation products, $\pi^0$ decay, nuclei de-excitation, slowed down charged particles, nuclei recoil). This hadronic contribution goes up with incident beam energy and the Bragg peak is no longer visible. At 1 GeV, the $dE/dz$ shows a maximum in the spallation zone very close to the window material and decreases thereafter with increasing $z$. Since the $dE/dz$ is maximum in the window region, it is exposed to the highest temperature, hence it is important to study heat loss in the window very carefully to optimize flow and geometry parameters for effective cooling of the beam window. In an earlier work [7], we had carried out thermal hydraulic studies using computational fluid dynamics (CFD) code related to the design of a realistic LBE target for a one way coupled 750 MW thermal reactor which requires current in the range of 1-2 mA proton beam of 1 GeV energy. The input to the CFD code; the heat deposit profile was estimated using CASCADE.04 [8, 9] and FLUKA Monte-Carlo simulation codes. It was realized that the precise knowledge of energy loss $dE/dz$ in the window material is very crucial for the target design as any small variation can result in a different set of operating parameters. Therefore, in the above mentioned publication, we gave more emphasis on the study of energy deposition due to interaction of high energy proton...
in various thick targets and compared the results with available experimental measurements. As a bench mark study, the results obtained from both CASCADE.04 and FLUKA are compared with dE/dz measurements for Be, Al, Fe, Cu, Pb and Bi thick targets of proton energies 0.8 GeV, 1.0 GeV and 1.2 GeV. It was found that both FLUKA and CASCADE.04 results were comparable with the experimental measurements for heavy targets like Pb and Bi where as for targets like Be and Al, both the codes as well as experimental measurements show differences.

The CASCADE.04 code was further developed for low energy neutron transport with point data processed through NJOY (ACE format). The code was also developed for the complex geometry using boolean operation on Constructive Solid Geometrical Shapes and for repetitive reactor core/detector or any other complex structures. Reactor or ADS neutron multiplication factor/\( K_{eff} / K_{\infty} \) capabilities and GUI were developed [10]. We have also developed decay module using linear chain method. With all these development the code was released for public use through a DAE-BRNS Workshop on Monte Carlo Nucleon transport Code (MONC) BARC, Oct. 8-9, 2015 held at BARC Mumbai. We have also developed our own processing code in ROOT format files [11] under BARC-CERN collaboration for GeantV. The Decay code is extended to do reactor burnup calculations. The average cross-section for burnup is calculated during monte-carlo calculation after burnup cycle and updated for the next cycle while updating the inventory of fission fragments.

The outline of this paper is as follows. In Sec. II we present description of Geometry. Section III contains High energy module of the code. In section IV Low energy transport module is presented. In Sec. V, the method of criticality calculations are given. In Sec. VI Criticality benchmark calculations are presented. In Sec. VII Decay and burnup calculations are presented. Section IX considers Graphical user Interface. Conclusions are given in Sec. X.

II. CONSTRUCTION OF GEOMETRY

Most important and difficult task in the Monte Carlo code is to build a complicated geometry in easiest and user friendly manner. We have chosen CSG model to build the geometry. In this model, there are simple basic geometrical bodies viz. Sphere, Cylinder, Parallel-piped, Cone, Ellipse, Hexagon etc. Boolean operations (Union, subtraction and interaction) are enabled to construct complex zones using these bodies. Fig. 1 gives an example to construct the zones from the bodies. One universe is compulsory to define that bounds the whole geometrical structures. Eight heterogeneous zones from three spherical bodies and one universe are made which can be filled with different materials.

Scaling, rotation and translation of the bodies are used in the chronological form to make more complicated structures. Repeated geometry structure has been invoked to do the lattice and core calculations of the most complicated reactor assemblies. Fig. 2 shows an example of repeated structure which are filled from different type of fuel rods. Hexagonal bounding boxes can be logical or real. Bare minimum information viz. number of rods, mean radius of ring on that rods are to be placed, and center of the repeated structures has to be provided by the user. Reflective boundary conditions are used to do single lattice or partial core calculations.
III. HIGH ENERGY PARTICLE TRANSPORT

Monte Carlo program MONC incorporates Intra-nuclear Cascade, Pre-equilibrium, Evaporation and Fission models to simulate spallation reaction mechanism for thin and thick targets. Modeling details of Intra-nuclear cascade, Pre-equilibrium particle emission are described in detail in Ref. [12,13]. Treatment of cutoff energy from Intra-nuclear to pre-equilibrium and next to evaporation stage was changed later which is described in Ref. [9]. Generalized evaporation model was developed as described in Ref. [14] and Fongs statistical fission model is used to simulate the high energy fission reaction. Fission barrier, level density parameter and inverse cross sections for pre-equilibrium/evaporation/fission model are given in detail in Ref. [8,9].

Benchmark of spallation models for experimental values of neutron, charged particles, and pions double differential production cross-sections, particle multiplicities, spallation residues and excitation functions was organized by IAEA and is given in Ref. [15]. We have used the predecessor of this code named CASCADE.04 to calculate these quantities in this benchmark. Heat Deposition algorithm for thick spallation targets and thin films was modified and benchmarked as mentioned in Ref. [7]. The code was further developed for the Neutron shielding and dosimetry applications and published [16]. The high energy part of this code can be used for single nucleus interaction in basic reaction studies and can be invoked for the thick target simulation during the transport. Energy loss of the charge particle is calculated during the transport in the thick target. The code calculates the spallation as well as fission yields which are plotted in Fig. 3. It is clear from Fig.4 that spallation products are proton rich but neutron induced fission products are neutron rich. The beauty of the spallation reaction is that it can span whole range of radio active isotopes around the stability line. Spatial distribution of any toxic/nontoxic element can be analysed and is available as an option in the input file.

Monte Carlo (MC) program CASCADE-04 (Intra-nuclear cascade - Pre-equilibrium/ Evaporation/ Fission code) realizes the particle transport in three stages: 1) sampling of particle (ion) mean free path in the medium taking into account the energy loss of a charged particle and a possible decay of non-stable particles ($\pi^0$, $\pi^\pm$). All $\pi^0$-mesons are considered to decay into $\gamma$-quanta at the point of their creation. The ionization losses of $\pi$ - mesons, protons and light ions are calculated by Sterneheims method [17] using well established Bathe formula for the average ionization loss calculations with proper density effects. Here, it is important to mention that the density effect shows reduction in ionization loss for fast charged particles due to dielectric polarization of the medium. In the lower energy region ($\gamma\ 2.0\text{MeV}$) Lindhard's approach [18] is used and a semi-phenomenological procedure [19] is applied for the heavy ions. While doing the practical simulation one has to calculate the ionization and nuclear interaction ranges and then uses the formulation to deposit heat. It is well known that heat deposition is a continuous phenomenon but in simulation one has to take some finite step size. In the earlier version (CASCADE.04) of the code we have set no limit to heat deposition step size and it may deposit total amount of heat at the ionization range point which is impractical. Of course it was provision that instead of depositing the heat at ionization range point it will deposit at the middle of last two interaction points. In this situation we found that the heat inside few centimeter depth of the target was less than the experimental data. In CASCADE.04.h we have adopted more continuous steps in which not more than 2-3% energy loss can appear at any point. In this way we could get better agreement with experimental data.

2) Simulation of the particle interaction with a nucleus is considered along its path. In case of inelastic interaction the CASCADE.04 code considers three stages of reaction for calculation: a) intranuclear cascade originally developed at Dubna: In this part of the calculation, primary particles can be re-scattered and they may produce secondary particles several times prior to absorption or escape from the target. Modeling of intranuclear cascades [12,13] is in general rather closer to the methods used in other transport codes. Cross-sections of the hadron-nucleus collisions are calculated based on the compilations of the experimental data [20,21]. To calculate the nucleus-nucleus cross-sections we used analytical approximations with parameters defined in ref. [22]. Criteria of transition from intra-nuclear cascade to pre-equilibrium stage are the cutoff energy (binding energy above the Fermi energy), below which the particles are considered to be absorbed by the nucleus. Particles are traced down to this cutoff energy and then the second stage, pre-equilibrium stage:
In this part of the reaction, relaxation of the nuclear excitation is treated according to the exciton model of the pre-equilibrium decay. The relaxation is calculated by the method based on the Blann's model. Proton, neutron, deuterium, tritium, 3He and 4He are considered as emitted particles in the pre-equilibrium and in the subsequent equilibrium stage. Transition from pre-equilibrium to equilibrium state of the reaction occurs when the probability of nuclear transitions changing the number of excitons \( n \) with \( \delta n = +2 \) becomes equal to the probability of transitions in the opposite direction, with \( \delta n = -2 \).

c) Equilibrium stage: This part considers the particle evaporation/fission of the thermally equilibrated nucleus.

IV. LOW ENERGY NEUTRON TRANSPORT

Low energy neutron transport code is developed recently. We have developed the package for reading pointwise cross sections for neutron in ACE (A Compact ENDF) format. The delayed neutrons are treated exclusively with their energy spectra for which data are available. Spontaneous and induced fission fragment yield are read from ENDF Fission yield libraries. The ACE library generated, mostly, using ENDF VII.0 is used for the present investigations. The free gas thermal treatment of the neutron interaction for below 4eV can be used for compound and crystal material or Thermal scattering law can be used if available in ENDF file. Probability table method is used in the un-resolved energy region.

Interaction of neutrons is considered using Monte Carlo method in the following steps. A) Identification of the initial zone number and interaction cite of the neutron, B) Selection of the collision nuclide, C) Type of interaction.

A. Identification of the initial zone number and interaction cite of the neutron

The MONC assigns the X, Y, Z, \( \cos \theta \), \( \sin \phi \), \( \cos \phi \), energy(MeV), charge, mass(MeV/C\(^2\)) coordinates with each neutron. The code identifies the zone number and geometry type of the configuration defined in the input file by calculating the surface coefficients. The method of neutron transport is as given below. The probability of interaction between \( l \) and \( l+dl \) of a neutron of given energy is defined by

\[
p(l)dl = e^{-\Sigma_t l} \Sigma_t dl
\]

Where \( \Sigma_t \) is the macroscopic total cross-section of the medium in the geometrical Zone. Mean free path for the nuclide inside the the medium of a given composition can be given as.

\[
\text{meanfreepath} = \frac{1}{\Sigma_t}; \Sigma_t = \frac{1}{n\sigma_t}
\]

Where \( n \) is the nucleon density of the selected nuclide. If \( \xi \) is random number between [0-1] then

\[
\xi = \int_0^l e^{-\Sigma_t s} \Sigma_t ds = 1 - e^{-\Sigma_t l}
\]

Thus

\[
l = -\frac{1}{\Sigma_t} \ln(1 - \xi) \equiv -\frac{1}{\Sigma_t} \ln(\xi)
\]

B. Selection of the collision nuclide

If there are \( n \) different nuclides forming the material composition in the identified zone then \( i^{th} \) nuclide is selected if

\[
\sum_{j=1}^{i-1} \Sigma_{ij} < \xi \leq \sum_{j=1}^{i} \Sigma_{ij}
\]

Where \( \Sigma_{ij} \) is the macroscopic total cross-section of the \( j^{th} \) nuclide. The MONC code needs to describe the density (g/cm\(^3\)) and nuclei weight fractions in the input file. The sum of all fractions should be normalized to one bu user otherwise code will re-normalize it to one.

C. Type of the interaction

Type (elastic, inelastic, capture, fission) of interaction with the selected nuclide is calculated directly based on the probabilities, calculated using the microscopic cross-sections. These reaction probabilities can be given as eq.

\[
\frac{\sigma_i}{\sigma_t}
\]

Where subscript ‘i’ stands for reaction type (elastic, inelastic, capture, fission, (n,xn), (n,X)) etc. and ‘t’ for total cross-section. In case of isotropic angular distribution of elastic scattered neutrons in the center of mass system, the energy has been calculated using two body collision kinematics and then converted from CM to LAB system.

V. MONC CRITICALITY CALCULATIONS

The critical calculations in MONC are based on four methods (neutron population, Collision Estimator, Absorption Estimator, and Track Length Estimator). The
\( k_{\text{eff}} \) is a ratio between the numbers of neutrons in successive generations in a fission chain reaction. For critical systems, \( k_{\text{eff}} = 1 \), for sub-critical systems, \( k_{\text{eff}} < 1 \) and for supercritical systems, \( k_{\text{eff}} > 1 \). The number of neutrons in successive generation is obtained from number of neutrons generated by fission minus the number of neutrons absorbed and escaped from the system. Whenever \((n, x_n)\) reactions occur, the neutron generated are again transported within the fission cycle. At present fission source points as well as neutron generations are as usual allowed as other reactions but stored for the next cycle. At the end of the cycle same number of neutrons are preserved by increasing or decreasing the weight of neutrons in case of \((k_{\text{eff}} > 1)\) and \((k_{\text{eff}} < 1)\), respectively.

The critical calculation requires number of inactive cycles which need to be skipped to get the fundamental mode of fission source, active cycles for actual \( k_{\text{eff}} \), and number of source neutrons. Mono energetic neutron can be defined very easily in the input file and spectrum can be given through a separate file. In case of high energy proton or other beam, the source distribution is generated using the high energy part of the code and that is transported below 20 MeV. The value of \( k_{\text{eff}} \) is based on these low energy neutron fission reactions. The average value of \( k_{\text{eff}} \) is obtained from the maximum likelihood method applied for the values obtained from all four estimators.

A. neutron population method

The ratio of previous to next fission cycle while considering absorption and escape, gives value of \( k_{\text{eff}} \) as given below.

\[
k_{\text{eff}} = \frac{\text{neutron balance in the } i+1^{\text{th}} \text{ generation}}{\text{neutron balance in the } i^{\text{th}} \text{ generation}} \tag{7}
\]

B. Collision Estimator

It is based on the collision/fission reaction in the fission zones.

\[
k_{\text{eff}} = \frac{1}{N} \sum_i W_i \frac{\sum_k f_k \nu_k \sigma_{fk}}{\sum_k f_k \sigma_{Tk}} \tag{8}
\]

where \( i \) is summed over all collisions in a cycle if fission is possible, \( k \) is summed over all nuclides of the material involved in the \( i^{\text{th}} \) collision, \( \sigma_{Tk} = \text{total microscopic cross section, } \sigma_{fk} = \text{microscopic fission cross section, } \nu_k = \text{average number of prompt or total neutrons produced per fission by the collision nuclide at the incident energy, } f_k = \text{atomic fraction for nuclide } k, N = \text{source neutrons for cycle, and } W_i = \text{weight of particle entering collision.}

C. Absorption Estimator

It is based on the absorption in fission and other reactions in the fission zones.

\[
k_{\text{eff}} = \frac{1}{N} \sum_i W_i \nu_k \frac{\sigma_{fk}}{\sigma_{ck} + \sigma_{fk}} \tag{9}
\]

where \( i \) is summed over all fissions, \( k \) is summed over all nuclides of the material involved in the \( i^{\text{th}} \) collision, \( \sigma_{ck} = \text{capture cross section, } \sigma_{fk} = \text{microscopic fission cross section, } \nu_k = \text{average number of prompt or total neutrons produced per fission by the collision nuclide at the incident energy, } N = \text{source neutrons for cycle, and } W_i = \text{weight of particle entering collision.}

D. Track Length Estimator

This method uses length of the neutron track in the fission zones.

\[
k_{\text{eff}} = \frac{1}{N} \sum_i W_i \rho d \frac{\sum_k f_k \nu_k \sigma_{fk}}{\sum_k f_k \sigma_{Tk}} \tag{10}
\]

where \( i \) is summed over all trajectories in a cycle where fission is possible, \( k \) is summed over all nuclides of the material involved in the \( i^{\text{th}} \) collision, \( \rho = \text{atomic density in the region, } d = \text{track length.}

E. Combined \( k_{\text{eff}} \) Estimation

The average value of \( k_{\text{eff}} \) is estimated using the Maximum Likelihood method from all four estimators. It is recommended that the user should run for at least two histories (having two active and inactive cycles) to get better standard deviation. The user should also watch that the \( k_{\text{eff}} \) values by all methods should not vary more than 0.1%, also that the values should not wonder too much from the average values otherwise the number of source particles or the number inactive cycles has to be increased.

VI. BENCHMARK CALCULATIONS

A. IAEA-ADS Benchmark Problem

IAEA had organized a coordinated research project for international neutronics benchmark of an ADS with \( \text{U}^{233} \text{Th Fuel. The system is driven by an external spallation neutron source. A proton beam of energy } 1.0 \text{GeV hits Lead as spallation target placed in the center of the ADS. The spatial and energy distribution of the spallation neutrons are given in the benchmark but we have produced these neutrons from our code itself. Geometry of ADS is divided into 5 regions as shown in}
The temperature of fuel was taken as 1200K and that of Lead and steel was 900K.

The first thing is to find the $^{233}\text{U}$ enrichment for $k_{\text{eff}} = 0.98$, 0.96 and 0.94 at BOL. The enrichment % are given in Table II.

Sample input file with some comments for the high energy spallation reaction is given in FIG. 5.

![FIG. 4: side and Front view of the IAEA-ADS benchmark assembly](image)

![FIG. 5: Input file for spallation target](image)

### TABLE I: Nuclei densities (/barn-cm) in different regions of the ADS benchmark at BOL

| Nuclei  | region 1 | region 2 | region 3 | region 4 | region 5 |
|---------|----------|----------|----------|----------|----------|
| Th $^{232}$ | Fe $^{56}$ | Cr $^{52}$ | Mn $^{55}$ | W $^{70}$ | Pb $^{208}$ |
| 6.05E-03 | 8.10E-03 | 1.22E-03 | 4.60E-05 | 4.60E-05 | 1.77E-02 |
| 7.45E-03 | 8.87E-03 | 1.06E-03 | 5.10E-05 | 5.10E-05 | 1.56E-02 |

### TABLE II: $^{233}\text{U}$ enrichment at BOL for ENDF-B/VII.1, ENDF-B/VII.1 in the region 1 and 2.

| Participants     | $k_{\text{eff}} = 0.98$ | $k_{\text{eff}} = 0.96$ | $k_{\text{eff}} = 0.94$ |
|------------------|-------------------------|-------------------------|-------------------------|
| MONC-2.0         | 10.04                   | 9.65                    | 9.38                    |
| Russia (diffusion) | 10.01                   | 9.69                    | 9.38                    |
| Russia (MC)      | 10.26                   | 9.925                   | 9.61                    |
| Switzerland      | 9.88                    | 9.57                    | 9.25                    |
| Italy            | 10.29                   | 9.96                    | 9.63                    |
| France           | 10.27                   | 9.94                    | 9.61                    |
| German           | 10.00                   | 9.68                    | 9.36                    |
| Netherlands      | 10.13                   | 9.81                    | 9.49                    |
| Japan            | 9.7                     | 9.4                     | 9.1                     |
| Belarus          | 10.50                   | 10.17                   | 9.85                    |
| Sweden           | 10.419                  | 10.095                  | 9.771                   |
| Average          | 10.17                   | 9.85                    | 9.53                    |
| MCNT/ORIGEN2     | 9.99                    | 9.672                   | 9.353                   |
| ANDOTOR          | 10.265                  | 9.948                   | 9.629                   |
FIG. 6: Different Spherical and Cylindrical Critical assemblies

5) The Enriched U-235 (14.11%) Cylinder of radius = 26.65 cm, Height = 44.239 cm and density = 18.41 g/cc. Remaining material is U-238. The geometry for problems 1-5 are shown in fig. 6.

\[ k_{eff}^{(MONC)} = 0.9905 \pm 0.0018 \]

\[ k_{eff}^{(MCNP)} = 0.9908 \pm 0.0006 \]

6) The Enriched Pu-239 (100.0%) Cylinder of radius = 4.935 cm, Height = 17.273 cm and density = 15.8 g/cc.

\[ k_{eff}^{(MONC)} = 1.0142 \pm 0.0005 \]

\[ k_{eff}^{(MCNP)} = 1.0157 \pm 0.0003 \]

7) The Enriched Pu-239 (100.0%) Cylinder of radius = 4.935 cm, Height = 6.909 cm and density = 18.80 g/cc. Uranium Reflector Thickness = 5 cm, Height = 6.909 cm.

\[ k_{eff}^{(MONC)} = 0.8879 \pm 0.0018 \]

\[ k_{eff}^{(MCNP)} = 0.8865 \pm 0.0001 \]

8) The Enriched Pu-239 (100.0%) Cylinder of radius = 4.935 cm and density = 15.8 g/cc. Uranium Reflector Thickness = 5 cm all around (radially and axially).

\[ k_{eff}^{(MONC)} = 1.0225 \pm 0.0004 \]

\[ k_{eff}^{(MCNP)} = 1.0248 \pm 0.0006 \]

9) The Enriched U-235 93.5% sphere of radius = 7.3984 cm and density = 18.6 g/cc. The sphere is surrounded by graphite of thickness = 5.1 cm. The geometry for problems 6-8 are shown in fig. 6.

\[ k_{eff}^{(MONC)} = 0.9983 \pm 0.0001 \]

\[ k_{eff}^{(MCNP)} = 0.9981 \pm 0.0029 \]

10) The Enriched U-235 97.67% sphere of radius = 6.5537 cm consisting of 22.16 kg mass and density = 18.794 g/cc. The sphere is surrounded by water tank of radius = 30 cm and height = 70 cm. The geometry for problems 9-10 are shown in fig. 8.

\[ k_{eff}^{(MONC)} = 0.9981 \pm 0.0007 \]

\[ k_{eff}^{(MCNP)} = 0.9956 \pm 0.0011 \]

11) Three interacting enriched U-235 93.2% cylinders of radius = 10.15 cm and height = 41.4 cm in an aluminum container of thickness = 0.15 cm. The density of Alu-
**TABLE III: \( k_{eff} \) values for different radii of the \(^{235}\)U sphere.**

A comparison is performed with MONC-2.0 and MCNP-4c.

| R, cm | \( k_{eff} \) (MONC-2.0) | \( k_{eff} \) (MCNP-4c) |
|-------|-----------------|-----------------|
| 2.5   | 0.3163±0.0014   | 0.3172±0.0003   |
| 5.0   | 0.6295±0.0057   | 0.6291±0.0001   |
| 8.9   | 1.0531±0.0002   | 1.0522±0.0001   |
| 15.0  | 1.5017±0.0004   | 1.5025±0.0006   |
| 25.0  | 1.8736±0.0003   | 1.8746±0.0004   |
| 50.0  | 2.1485±0.0002   | 2.1485±0.0003   |

**FIG. 10:** \( k_{eff} \) values for Sub-critical, Critical and Super-critical \(^{235}\)U spherical assemblies

Minium is 2.71g/cc and density of UO\(_2\) F\(_2\) water solution is 1.131g/cc. The cylinders were set on equilateral triangle with 0.38cm surface separation. The atomic density of material was 0.0021345 (U-235), 0.00015382 (U-238), 0.33383 (Oxygen), 0.65930 (Hydrogen) and 0.0045756 (Fluorine) in atoms/barn. The geometry for problem 11 is shown in Fig. 11.

\( k_{eff} \) (MONC) = 0.9993 ± 0.0003
\( k_{eff} \) (MCNP) = 0.9991 ± 0.0011

The \(^{235}\)U sphere of different radii (2.5cm - 50cm) are simulated for the sub-critical, critical and super-critical cases to verify the algorithm of weight adjustment. The \( k_{eff} \) values are plotted in the Fig. 10. Numerical values are given in Table III.

Problem #13 A 2x2x2 un-reflected array of 93.2% enriched \(^{235}\)U metal cylinders as described in 28 and shown in Fig. 12 is considered for \( k_{eff} \) calculation. The surface separation in x-y direction is 2.244cm and it’s 2.245cm in z-direction. Height and diameter of the cylinders are 10.765cm and 11.496cm respectively. The repeated structure of MONC is employed. The sample input file is given in Fig. 11. \( k_{eff} \) (MONC) = 1.0012 ± 0.00121
\( k_{eff} \) (MCNP) = 0.9999 ± 0.0009

**FIG. 11:** MONC input file for 2x2x2 array of 93.2% enrich uranium cylindrical assembly.

\( k_{eff} \) (KENO) = 0.9996 ± 0.0011

Problem #14 A 2x2x2 paraffin reflected array of 93.2% enriched \(^{235}\)U metal cylinders as shown in Fig. 14 is considered for \( k_{eff} \) calculation. The surface separation in x-y direction is 11.984cm and it’s 11.985cm in z-direction. Height and diameter of the cylinders are 10.765cm and 11.496cm respectively. The arrangement of uranium cylinders is surrounded by 15.24cm thick paraffin of density 0.93cm. The repeated structure of MONC is employed. The sample input file is given in Fig. 15.

\( k_{eff} \) (MONC) = 0.9975 ± 0.00337
\( k_{eff} \) (MCNP) = 0.9990 ± 0.0011
\( k_{eff} \) (KENO) = 1.0009 ± 0.0013

Problem #15 This is same problem as problem #14 except the paraffin thickness of 30.48cm instead of 15.24cm.

\( k_{eff} \) (MONC) = 0.9975 ± 0.00337
\( k_{eff} \) (MCNP) = 0.9995 ± 0.0027
\( k_{eff} \) (KENO) = 1.0210 ± 0.0009
The details of the PHWR 19 and 37 rod fuel assembly are taken from Ref. [29] and are given below. The 19-rod fuel assembly has 1+6+12 central, first ring and second ring arrangement as shown in Fig. 16 and 37-rod fuel assembly has (1+6+12+18) structure as given in Fig. 17.
TABLE V: Initial material composition

| Nuclide | Weight (%) | No. Density /\text{cm}^3 |
|---------|------------|-------------------------|
| Fuel    |            |                         |
| $^{234}$U | 0.0688    | 1.82239E+19            |
| $^{235}$U | 8.5946    | 2.26826E+21            |
| $^{238}$U | 79.4866   | 2.07128E+22            |
| $^{16}$O | 11.8500   | 4.59686E+22            |
| Cladding|            |                         |
| O       | 0.125      | 3.08281E+20            |
| Cr      | 0.1        | 7.58663E+19            |
| Fe      | 0.21       | 1.48338E+20            |
| Zr      | 98.115     | 4.24275E+22            |
| Sn      | 1.45       | 4.81835E+20            |
| Coolant |            |                         |
| $^1$H   | 11.19      | 6.66295E+22            |
| $^{16}$O| 88.81      | 3.33339E+22            |

The dimensional and natural uranium fuel parameters for 19-rod fuel lattice assembly are given in Tables VI and VIII. The $K_{eff}$ values at t=0 without any load is 1.136 and 1.133 for 19 and 37 pin assemblies, respectively. Detailed burnup calculations are underway.

TABLE VI: 19-rod unit cell model parameters

| parameters                           | Values |
|--------------------------------------|--------|
| Diameter of fuel rod (cm)            | 1.437  |
| Fuel pellet (UO$_2$) diameter (including gap) | 1.445  |
| Fuel element diameter (including sheath) | 1.521  |
| 1$^{st}$ ring Pin Circle Diameter (cm) | 3.302  |
| 2$^{nd}$ ring Pin Circle Diameter (cm) | 6.358  |
| Stack length (cm)                    | 48.118 |
| Fuel bundle length (inclusive both end plates)(cm) | 49.53  |
| Inner diameter of pressure tube (cm)  | 8.26   |
| Outer diameter of pressure tube (cm)  | 9.0    |
| Air gap thickness (cm)               | 0.85   |
| Inner diameter of calandria tube (cm) | 10.80  |
| Outer diameter of calandria tube (cm) | 11.06  |
| Lattice spacing (square)(cm)         | 22.86  |

VII. DECAY OF THE RADIO-ACTIVE ELEMENT

Monitoring of decay heat, radio-activity of spent fuel, fission products and minor Actinides is an important task for spent fuel management, reprocessing and permanent disposal. The decay and burnup calculations are required for estimation of inventory of accelerator or reactor produced nuclear waste. The generalized Bateman’s eq. \cite{27} is solved exactly with linear chain method. This kind of
TABLE VIII: 37-rod unit cell fuel element parameters

| parameters                                      | Values       |
|------------------------------------------------|--------------|
| Diameter of fuel rod (cm)                      | 1.218        |
| Fuel pellet-clad air gap (cm)                  | 0.008        |
| Fuel pellet (UO$_2$) diameter (including gap)  | 1.308        |
| Fuel element diameter (including sheath)       | 1.521        |
| 1$^{st}$ ring Pin Circle Diameter (cm)         | 2.978        |
| 2$^{nd}$ ring Pin Circle Diameter (cm)         | 5.750        |
| 3$^{rd}$ ring Pin Circle Diameter (cm)         | 8.660        |
| Stack length (cm)                              | 48.118       |
| Fuel bundle length (inclusive both end plates)(cm ) | 49.5    |
| Inner diameter of pressure tube (cm)           | 10.338       |
| Outer diameter of pressure tube (cm)           | 11.238       |
| Air gap thickness (cm)                         | 1.694        |
| Inner diameter of calandria tube (cm)          | 12.932       |
| Outer diameter of calandria tube (cm)          | 13.212       |
| Lattice spacing (square)(cm)                   | 28.60        |
| Specific power (kW/ kg of U)                   | 26.58        |

method is also used in other codes like CINDER [28] and BISON [29] while ORIGEN [30] uses matrix exponential method to solve the equations. The Bateman equation for decay in n-nuclide series in linear chain describing $n^{th}$ nuclide concentration at time t is given by

$$N_n(t) = \frac{N_1(0)}{\lambda_n} \sum_{i=1}^{n} \lambda_i \alpha_i \exp(-\lambda_i t) \quad (11)$$

Here $N_1(0) \neq 0$ and $N_i(0) = 0$ when $i > 1$, means inventory of all daughters are assumed zero at time zero, $\lambda_i$ is the decay constant of $i^{th}$ nuclide. This equation is valid if the decay constants are different otherwise it becomes infinite. Very small difference in decay constants also may lead to biased numerical results. We have artificially shifted the decay constants to get the approximate solutions as these kind of problems are not with too many isotopes in the chain. In case of transmutation due to particle flux, the modified decay constant is used as follows

$$\lambda_{i,j} = b_{i,j} \lambda_j + \sum_{x=n,p,\alpha,..} \int \phi_x \sigma_{ij}^x(E) dE \quad (13)$$

where $b_{i,j}$ is branching ratio of decay through some decay channel of nuclide j to nuclide i. $\phi_x$ is particle flux and $\sigma_{ij}^x$ is production cross-section of nuclide i through reaction with j by particle x. In other words one can replace the decay constant $\lambda \Rightarrow \lambda + \sigma \phi$. ENDF-B decay data library is used to extract decay properties (half life, decay type ($\beta^-$, $\beta^+$, $\alpha$, EC, decay heat, decay spectra etc.) of the radio-active/stable isotopes.

FIG. 18: Decay of $^3$H

FIG. 19: Decay of $^{14}$C

Decay of $^3$H, $^{14}$C, $^{99}$Tc, $^{152}$Eu, $^{233}$Pa are given in Fig. [18][19][20][21][22].

One group cross-sections are calculated for transmutation/burnup calculations. (n,$\gamma$), (n,f), (n,2n), (n,3n), (n,4n), (n,$\alpha$), (n,p) reactions are included in the burnup. Flux normalization is used and normalization factor is based on the following equation [14]

$$FN = \frac{P}{\sum_{i}^{n} V_i \sum_{j}^{m} N_{ij} Q_j \int \sigma_{ij}(E) \phi_i(E) dE} \quad (14)$$

where P is total power,

where $V_i$ is volume of zone i,

$N_{ij}$ is number density of actinide j in zone i,
or alternatively by the following eq. \[ Q(Z,A)(\text{MeV/fission}) = 1.29927 \times 10^{-3} Z^2 A^{0.5} + 33.12 \]

\[ FN = \frac{P_{\nu}}{Q.K_{\text{eff}}} \] (15)

VIII. GRAPHICAL USER INTERFACE

Graphical User Interface (GUI) along with data visualization is a powerful tool required for supporting such ambitious software. The GUI and the visualization modules are developed to support cross-platform usage. Development of these modules is done in Python language using the base libraries of Visualization Toolkit [9] for visualization and WxPython for GUI. The communication between the GUI and the Monte-Carlo code is through loose coupling, i.e. both these modules are independent of each other and the communication is through external files. The GUI and visualization modules are developed for cross-platform usage, so that they can be run on all Windows and Linux platforms. Construction and display of geometry, making the input file (defining the material properties and filling the material in different zones, defining the number of events and description of the output tallies etc.) and analysis of the output data are handled in this GUI. A snapshot of the MONC GUI depicting multiple concentric cylinders is shown in Fig.23 running under 32-bit Ubuntu Linux environment.

To construct geometry, all Boolean operations viz. union, subtraction, intersection are available in this framework to make the complex zones from the basic bodies. Scaling, rotation and translation of the basic bodies is supported here. This information is saved in the input file and the Monte-Carlo code can be run either through terminal or from the GUI itself. Standard features viz. showing 3D-axis around bodies, tak-
FIG. 23: GUI showing concentric geometrical assembly

Boolean operations Union, subtraction and intersection are mapped to operators +, - and * respectively, the construction of a geometry is mapped to a simple mathematical expression. Computational Geometry Algorithm Library (CGAL) is used for implementing the Boolean operations and converting them to equivalent triangulated meshes. The CGAL created meshes are converted to equivalent VTK filter objects and are joined into the VTK rendering pipeline consisting Mapper, Actor, Renderer and RenderWindow objects. Currently the code supports only five basic building bodies namely box, Cone, cylinder, hexagon and sphere. From these five basic building bodies, any number of complex geometries using Boolean operations. For visualization, tessellation of the geometry is mandatory and thus the basic building blocks are all complex polyhedrons in nature. A complex polyhedron is defined as a closed object whose boundary is manifold i.e. in the Euler Characteristic equation for polyhedrons X=V-E+F, X must be equal to 2, where V is the number of vertices forming polyhedral, E is the number of edges and F is the number of faces forming the polyhedral. Though Python being an interpreter based language is slower compared to performance of the compiled executable files, it is used owing to its inherent features supporting rapid application development. In order to offset the inferior performance of the Python running mathematically intense calculations, the classes which are intense in terms of computations are developed in C++ and are compiled into dynamic libraries. Using Python-C++ wrapper libraries information is exchanged between C++ and Python and vice-versa. Cross-platform development is done in two phases.

The first phase, i.e. the development of code is done using the ANSI standards of the C++, so that the compilation is smooth on all platforms like Windows and Linux. The second phase is to support compilation procedure on all platforms. The Linux Make files and Windows Project files have to be created properly. This is achieved by writing higher level CMake scripts. The Menu structure is divided into four groups namely File, Properties, Insert and Help. File menu consists of opening and saving of the MONC scripts as well as saving the screen shots. Properties menu handles all the property pages which can be modified by the users for supporting various simulations. Insert menu gives control over the insertion of bodies and construction of geometries using the complex mathematical expressions consisting of multiple Boolean operations. Help menu provides a detailed help system which is developed using the advanced HTML help engine supporting searching of the key words, indexing of the help items as well. A tool bar useful with frequently used operations is provided. Standard three button mouse interactions are implemented viz. left-button controls the rotation, middle-button is for translation and the right-button is for scaling. The most important aspect of GUI is to visualize and correct the geometry in 3-dimensions. Overlapping regions (if any) after scaling, rotation, and translation can be easily identified and corrected before running the Monte-Carlo code.

IX. CONCLUSION

The Monte Carlo code MONC has been developed for ADS, Spallation reactions, reactor, dosimetry, and shielding applications. New CSG model with Union, Subtraction and Intersection Boolean operations is developed to make the heterogeneous zones. Scaling, rotation, and translation operations are used to make more complex zones. Repeated geometry model has been developed for simulation of any complex reactor designs as well as the detector simulations. The pointwise cross section data for neutrons below 20MeV are used. The S(α, β) scattering matrices for neutron energy < 4eV is used if it is available in the library for the given compound element otherwise Fermi-gas treatment is used. The code has been benchmarked for K_{eff} of many experimental simple assemblies and is under extensive benchmark for different other assemblies including real Thorium Plutonium MOX fuel based AHWR system. List of fission product and their spatial distribution can be analyzed using this code at any given time. MONC uses MPI architecture and has been tested for more than 1000 nodes.

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