Journal of Energy

VOLUME 62 | 2013

journal homepage: http://journalofenergy.com/

Full Core Criticality Modeling of Gas-Cooled Fast Reactor using the SCALE6.0 and MCNP5 Code Packages

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ABSTRACT

The Gas-Cooled Fast Reactor (GFR) is one of the reactor concepts selected by the Generation IV International Forum (GIF) for the next generation of innovative nuclear energy systems. It was selected among a group of more than 100 prototypes and his commercial availability is expected by 2030. GFR has common goals as the rest GIF advanced reactor types: economy, safety, proliferation resistance, availability and sustainability. Several GFR fuel design concepts such as plates, rod pins and pebbles are currently being investigated in order to meet the high temperature constraints characteristic for a GFR working environment. In the previous study we have compared the fuel depletion results for heterogeneous GFR fuel assembly (FA), obtained with TRITON6 sequence of SCALE6.0 with the results of the MCNPX-CINDER90 and TRIPOLI-4-D codes. Present work is a continuation of neutronic criticality analysis of heterogeneous FA and full core configurations of a GFR concept using 3-D Monte Carlo codes KENO-VI/SCALE6.0 and MCNP5. The FA is based on a hexagonal mesh of fuel rods (uranium and plutonium carbide fuel, silicon carbide clad, helium gas coolant) with axial reflector thickness being varied for the purpose of optimization. Three reflector materials were analyzed: zirconium carbide (ZrC), silicon carbide (SiC) and natural uranium. ZrC has been selected as a reflector material, having the best contribution to the neutron economy and to the reactivity of the core. The core safety parameters were also analysed: a negative temperature coefficient of reactivity was verified for the heavy metal fuel and coolant density loss. Criticality calculations of different FA active heights were performed and the reflector thickness was also adjusted. Finally, GFR full core criticality calculations using different active fuel rod heights and fixed ZrC reflector height were done to find the optimal height of the core. The Shannon entropy of the GFR core fission distribution was proved to be useful technique to monitor both fission source convergence (stationarity) and core eigenvalue convergence (k_{eff}) to fundamental eigenmode with MCNP5. All calculations were done with ENDF/B-VII.0 library. The obtained results showed high similarity with reference results.

1 INTRODUCTION

The Gas-cooled Fast Reactor is one of the reactor concepts selected by the Generation IV International Forum (GIF) for the next generation of innovative nuclear energy systems. Several GFR fuel design concepts (plates, rod pins and pebbles) are currently being investigated [1] in order to meet the high temperature constraints characteristic for a GFR working environment. GFR has common goals as the rest GIF advanced reactor types: economy, safety, proliferation resistance, availability and sustainability. Ceramic fuels have been proposed because these materials are based on compounds of carbides and nitrides, which have a good performance in the fast neutron energy spectrum. With helium used as a coolant and high operating temperatures, the GFR is expected to have a thermodynamic efficiency of close to 50%. The GFR will use closed nuclear fuel cycle with the ability to use own depleted fuel or fuel from another reactor. This characteristic of actinides incinerator is making GFR very attractive as a sustainable technological alternative among other advanced reactors: it can be used as electric power plant, as a cogeneration plant for hydrogen production or heat production facility for any industry. Commercial availability of GFR is expected by 2030.

In this work we modeled the GFR heterogeneous core with KENO-VI/SCALE6 [2] and MCNP5 [3] Monte Carlo codes. The used codes together with nuclear data libraries are described in section 2. The GFR fuel assembly is described in section 3. Description of reactor core design is given in section 4, including: calculation of reactor core safety parameters, estimation of the axial reflector thickness, material reflector selection and estimation of the dimensions of the GFR core. Discussion of the results and effective multiplication factor (k_{eff}) of full-core criticality calculations for different active heights is given in section 5. Conclusions are given in section 6. Referenced literature is given at the end of the paper.

2 KENO-VI AND MCNP5 CODES

In this work we modeled the GFR heterogeneous core with KENO-VI/SCALE6 and MCNP5 Monte Carlo codes. Various criticality calculations for determination of reactor safety parameters were done for different heterogeneous FA models. Both codes are well established multi-functional 3D Monte Carlo codes with advanced criticality eigenvalue and shielding capabilities. KENO-VI is a functional module of CSAS6, the main analytical sequence for criticality calculations with SCALE6, while MCNP5 is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. Pointwise cross-section data [4] were used within MCNP5: auxiliary program MAKXSF prepares cross-section libraries with Doppler broadening. Multigroup neutron data in form of v7-238 were used with KENO-VI: cross-section processing was done with BONAMI (unresolved resonance energy range) and CENTRM/PMC (resolved resonance range). Both working libraries are based on the ENDF/B-VII.0 library. All the criticality calculations were performed with the following control parameters, unless told otherwise: neutron source size per cycle was 1000, initial guess for k_{eff} was 1.0, number of settling (i.e. skipped for statistics) cycles was 50 and the total cycles per run was 1000. Used CPU was QuadCore6600 with 8GB of RAM.

3 THE GFR FUEL ASSEMBLY

The geometry of GFR fuel assembly is based on a hexagonal mesh composed of 271 unit cells. The unit cell is comprised of four regions: cylindrical fuel rod in the centre (heavy metal fuel), annular cylindrical region that surrounds the fuel rod (helium gas), annular cylindrical region of cladding (silicon carbide), hexagonal outer surface that surrounds the cylindrical rod (helium gas). The fuel is composed of heavy metal uranium-plutonium carbide (80 w/o U+Pu, 20 w/o C) while mixture of silicon carbide SiC (50 w/o Si, 50 w/o C) is used for the cladding. This type of material withstands very high temperatures (> 2000 K) within high irradiation environments. Also, since SiC material is used in several reactors, a wide nuclear data-base is known based on its operating experience [5]. Helium gas is used as a coolant. All mixtures are assumed to have working temperature at T = 1200 K. Main characteristics of the unit cell and fuel assembly are taken from reference [6]. KENO-VI and MCNP5 model of heterogeneous GFR fuel assembly is depicted in Figure 1.

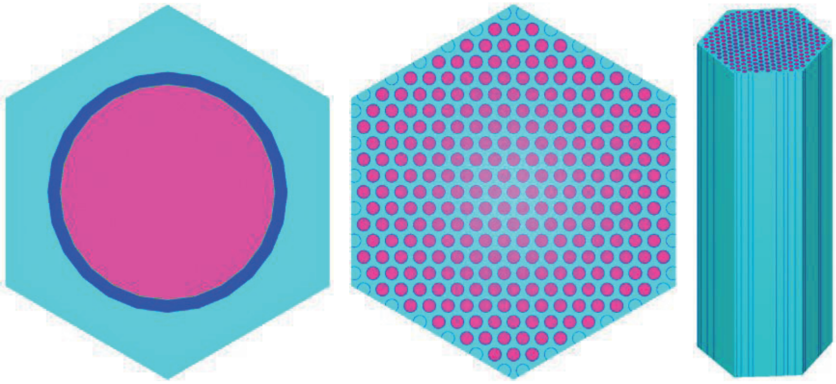

Figure 1: Elements of GFR fuel assembly (unit cell, cross sectional view, stereometric view)

4 THE GFR CORE DESIGN

In this section a calculational model of FA design is given, which includes: calculation of reactor safety parameters, estimation of the axial reflector thickness and material reflector selection. Estimation of the dimensions of the reflected GFR core is given at the end of the section [7].

4.1 Reactor safety parameters

The safety parameters which were analysed were reactivity coefficients due to variations in fuel temperature and coolant density. The first parameter is Doppler coefficient, because it is related to the resonance broadening effect when temperature of the fuel increases. The calculations were done for fuel temperatures of: 300, 400, 500, 600, 800, 900 and 1200 K. The second parameter is important for postulated loss of coolant accident (i.e. pressure drop in a core) which results in a decrease of coolant mass density. The calculations were done for He density values of: 0.01, 0.005, 0.001, 0.0001 and 0.00001 g/cm^3. Monte Carlo parameters for this part of calculations were 5000 neutrons per cycle and 1000 cycles. These calculations were done for FA of 100 cm active height and 100 cm of axial reflector (ZrC). Reflection conditions (i.e. mirror boundary) were applied on the six lateral sides and escape conditions (i.e. vacuum boundary) were applied on the two axial sides.

4.2 Estimation of the axial reflector thickness

The FA with active height of 100 cm and ZrC reflector was used for criticality calculations for different axial reflector thickness: 25, 50, 60, 75 and 100 cm. The calculations were done for cold (300 K) and hot (1200 K) conditions, with reflective conditions on six lateral sides and escape conditions on two axial sides.

4.3 Reflector material selection

The desirable characteristics of any reactor reflector are: high scattering to absorption cross-section, high logarithmic energy decrement, thermal stability and radiation endurance. For the purpose of selecting optimal material of GFR reflector, we tested three materials. ZrC (Zr 90.5 w/o, C 9.5 w/o) is a ceramic material, good reflector, candidate to be used in generation IV reactors. SiC (Si 90.5 w/o, C 9.5 w/o) is a ceramic material, at present it is a proven industrial material with production on a large scale. Unat (natural uranium) is a metallic material, in fast reactor systems it has been used as reflector/blanket material. The FA model with active height of 100 cm and 60 cm of axial reflector was used with reflective conditions on six lateral sides and escape conditions on two axial sides.

4.4 Reactor core dimensions

In order to investigate reactor core dimensions several test-calculations were performed: core radial size, fuel active height, reflector radial and axial thickness. The core configuration is based on two zones: the inner zone with fuel and control elements, and the outer zone with reflective elements. Different core sizes were simulated by gradually increasing the number of fuel assemblies. Therefore, an equivalent diameter of the core was estimated: hypothetical circular area is the sum of the individual areas of each fuel assembly. Former analyses of FA reflector proposed ZrC with height of 60 cm, because at that height saturation of reactivity is reached. Hence, final full-core criticality calculations with different active height were performed, including 78 fuel elements, 7 control elements and 84 reflective elements. The reference value of the k_{eff} for estimation of the active height of the GFR core was selected from values proposed by other authors [8]: the value of 6000 pcm of excess reactivity conforms active height of 100 cm. Boundary conditions for the full-core model are vacuum for all sides. Monte Carlo parameters were 5000 neutrons per cycle and 1000 cycles, with 50 cycles skipped in order to spatial fission source to converge.

5 DISCUSSION OF THE RESULTS

5.1 Results for reactor safety parameters

Negative values of fuel temperature reactivity coefficient (Table 1 and 2) and reactivity coefficient due to the pressure drop (Table 3 and 4) are shown. The negative effect in Δk_{eff} produced by the increase of fuel temperature is greater than the positive effect produced by the coolant density loss. The total combined effect is thus negative, as required by safety directions.

Table 1 Doppler results for KENO-VI

T(K)	k_{eff}	1σ (pcm)	Δk_{eff}	ΔT(K)	$(\Delta k_{eff} / k_{eff})/ \Delta T$ (pcm/K)
300	1.27033	53	0.00000	*	*
400	1.26166	48	-0.00867	100	-6.872
500	1.25588	50	-0.00578	100	-4.602
600	1.25216	55	-0.00372	100	-2.971
800	1.24343	48	-0.00873	200	-3.51
900	1.24098	51	-0.00245	100	-1.974
1200	1.23313	49	-0.00785	300	-2.122

Table 2 Doppler results for MCNP5

T(K)	k_{eff}	1σ (pcm)	Δk_{eff}	ΔT(K)	$(\Delta k_{eff} / k_{eff})/ \Delta T$ (pcm/K)
300	1.26352	54	*	*	*
400	1.25507	54	-0.00845	100	-6.733
500	1.24862	54	-0.00645	100	-5.166
600	1.24515	52	-0.00347	100	-2.787
800	1.2386	53	-0.00655	200	-2.644
900	1.23612	53	-0.00248	100	-2.006
1200	1.22963	51	-0.00649	300	-1.759

Comparison of fuel assembly k_{eff} results for KENO-VI and MCNP5 to reference MCNPX results are depicted in Fig.2. Differences in obtained k_{eff} are depicted in Fig.3.

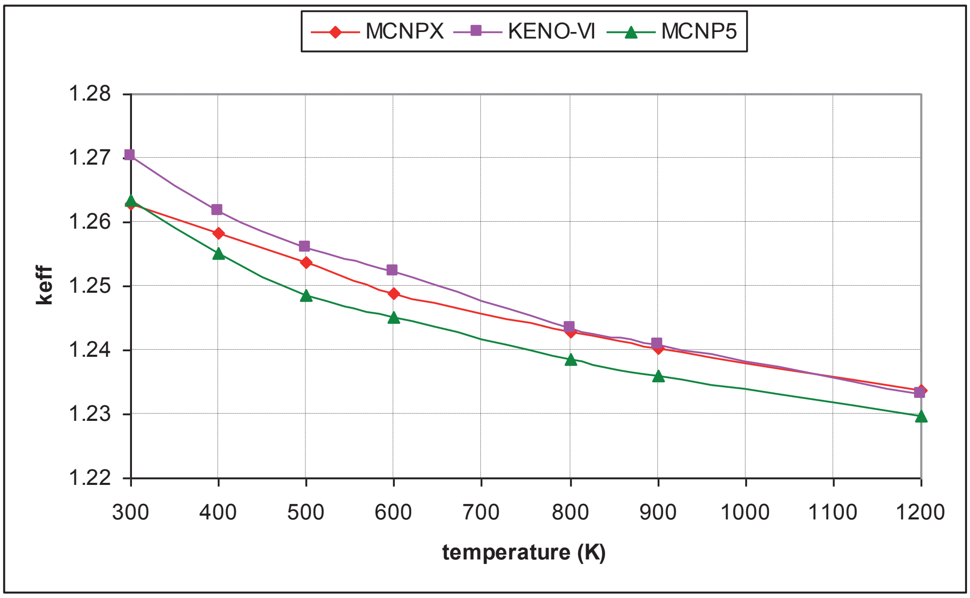

Figure 2: Comparison of KENO-VI and MCNP5 k_{eff} to MCNPX

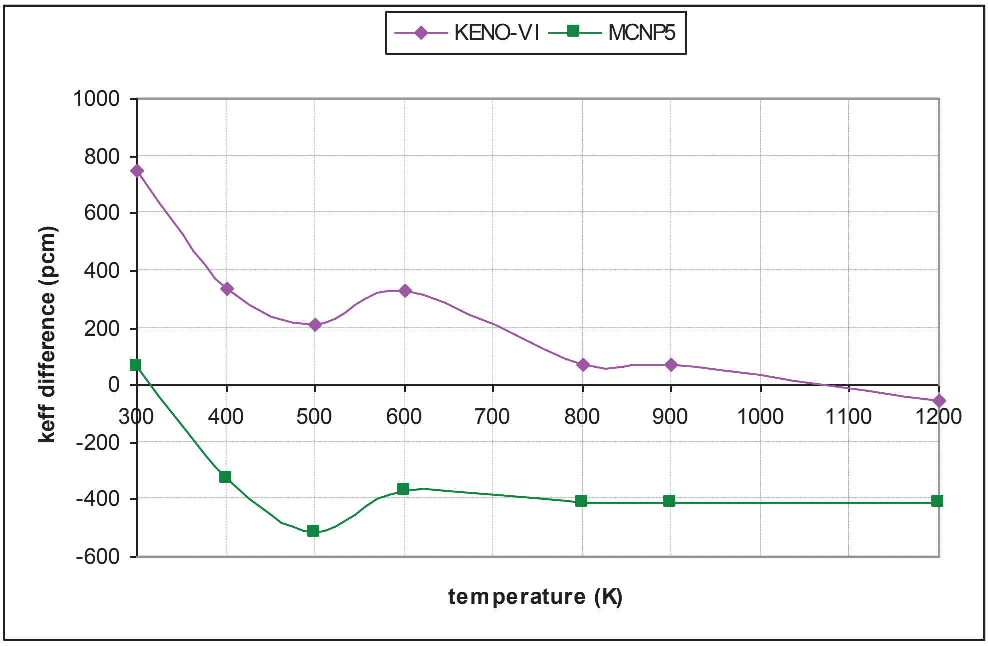

Figure 3: KENO-VI and MCNP5 k_{eff} differences to MCNPX

Table 3 Coolant density reactivity coefficient for KENO-VI

density He (g/cm^3)	k_{eff}	1σ (pcm)	$\Delta\rho$ (g/cm^3)	Δk_{eff}	$(\Delta k_{eff} / k_{eff})/ \Delta\rho$ ($1/g/cm^3$)
0.01	1.23376	22	*	*	*
0.005	1.23663	22	-0.005	0.00287	-0.574
0.001	1.23926	20	-0.004	0.00263	-0.6575
0.0001	1.24001	22	-0.0009	0.00075	-0.83
0.00001	1.2403	22	-0.00009	0.00029	-3.22

Table 4 Coolant density reactivity coefficient for MCNP5

density He (g/cm^3)	k_{eff}	1σ (pcm)	$\Delta\rho$ (g/cm^3)	Δk_{eff}	$(\Delta k_{eff} / k_{eff})/ \Delta\rho$ ($1/g/cm^3$)
0.01	1.22883	24	*	*	*
0.005	1.23203	22	-0.005	0.0032	-0.519
0.001	1.23472	24	-0.004	0.00269	-0.545
0.0001	1.23552	23	-0.0009	0.00080	-0.719
0.00001	1.23587	23	-0.00009	0.00035	-3.147

5.2 Results for axial reflector thickness

KENO-VI and MCNP5 results, for both cold (300 K) and hot (1200 K) conditions, are shown in Fig.4. Cold (300 K) and hot (1200 K) conditions are shown. One can observe high similarity between the two codes, i.e. small differences in k_{eff} are evident. Average Monte Carlo standard deviation of k_{eff} is ~ 50 pcm. Important result indicated by Fig.4 is saturation in reactivity gain [7] within reflector thickness of 60 cm. Thus, 60 cm of axial reflector thickness seems satisfactory for FA model with active height of 100 cm.

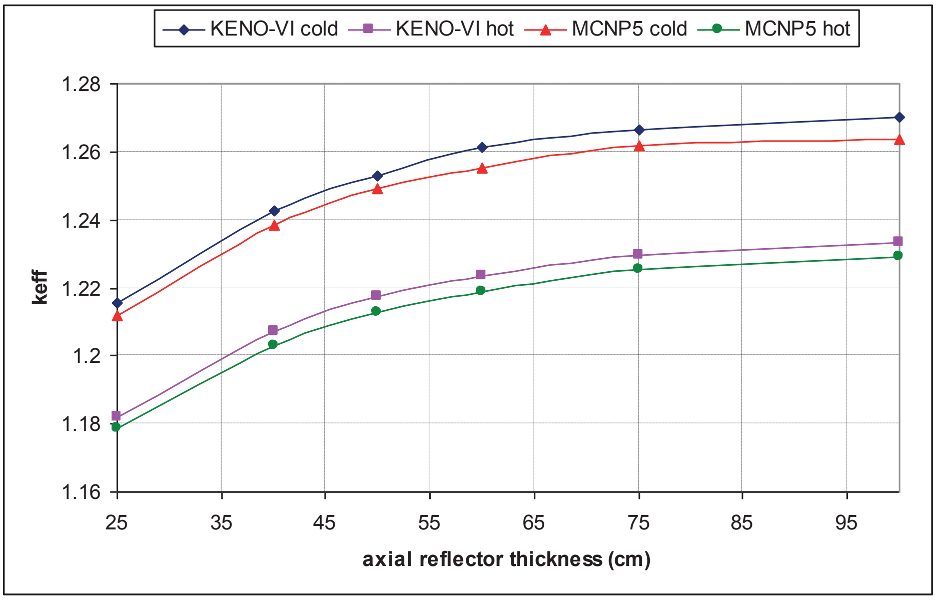

Figure 4: Axial reflector thickness results for KENO-VI and MCNP5 (300K and 1200K)

5.3 Results for reflector material

The results depicted in Fig.5 are for a model of FA with 100 cm of active height and an axial reflector thickness of 60 cm. Three reflector materials were tested (ZrC, SiC and Unat), but only ZrC and SiC reveal good reflector characteristics. Calculations for cold and hot conditions were done. In summary, ZrC is the material with the largest contribution to reactivity of the critical system and was selected as a reflector for full-core modeling.

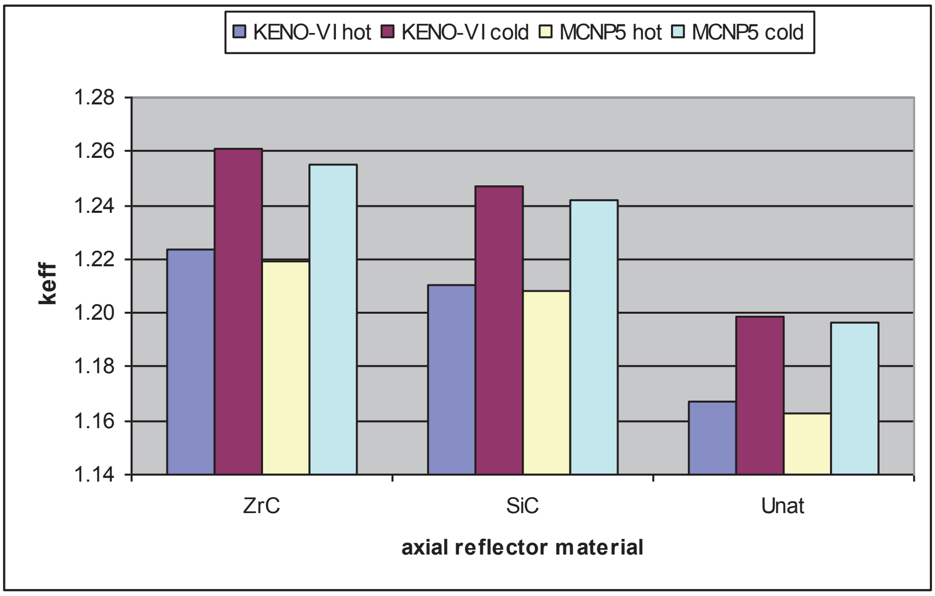

Figure 5: Reflector material results for KENO-VI and MCNP5 (300 K and 1200 K)

5.4 Results for reactor core dimensions

In order to investigate reactor core dimensions, several test-calculations were performed using KENO-VI and MCNP5 codes. Hot temperature condition (1200 K) was applied with escape conditions on all core sides. Initial calculations with bare and later reflected core suggested equivalent core diameter of 180-220 cm, which matches 61-91 FA in core. Again, saturation in reactivity is observed for equivalent diameter greater than 180 cm, so final proposed size of a reflected GFR core was 78 FA (eq.diameter of 207.04 cm). Additionally, seven preliminary locations of control assemblies were selected with control rods totally withdrawn from the core (He in active volume). The lateral core reflector comprises 84 reflective assemblies (ZrC in active volume). The GFR radial core configuration is shown in Fig.6.

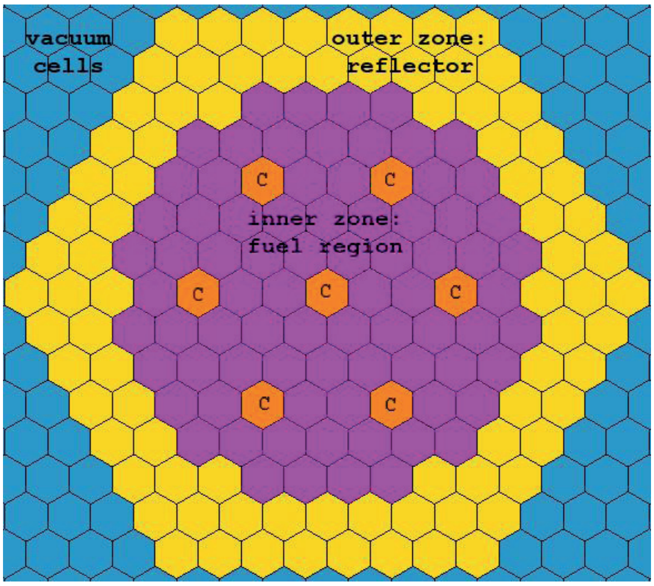

Figure 6: The GFR core axial midplane (C – control assembly)

Results for full-core criticality calculations with KENO-VI and MCNP5 with different core heights are shown in Table 5 together with reference results obtained with TRIPOLI-4. The reference value of the k_{eff} for estimation of the active height of the GFR core was selected from values proposed by other authors: the value of 6000 pcm of excess reactivity conforms active height of 100 cm. It is evident that active height of 100 cm is a satisfactory value in terms of reactivity gain.

Table 5 Core criticality results for different active heights

core active height (cm)	*H/D*	TRIPOLI-4		KENO-VI		MCNP5	
		k_{eff}	1σ (pcm)	k_{eff}	1σ (pcm)	k_{eff}	1σ (pcm)
50	0.24	0.92998	29	0.94059	26	0.93571	25
60	0.29	0.97113	30	0.98006	25	0.97573	26
70	0.34	1.00451	32	1.01172	30	1.00674	26
80	0.39	1.03035	31	1.03524	28	1.03147	26
90	0.43	1.05181	33	1.05607	25	1.05155	25
100	0.48	1.07075	34	1.07255	29	1.06811	26

The parameter *H/D* (height-to-diameter) is related to the pressure drop inside the core [7], thus proposed core of 100 cm and *H/D* of 0.48 has a pressure drop of ~ 1 bar. Differences between KENO-VI and MCNP5 to reference TRIPOLI-4 results are shown in Fig.7. Constant offset of cca 500 pcm is observable for all core active height, although MCNP5 values are in better agreement to TRIPOLI-4. The values of k_{eff} for different core heights are shown in Fig.8. Typical CPU run time for full-core criticality calculation with KENO-VI and MCNP5 was about 4 h on average.

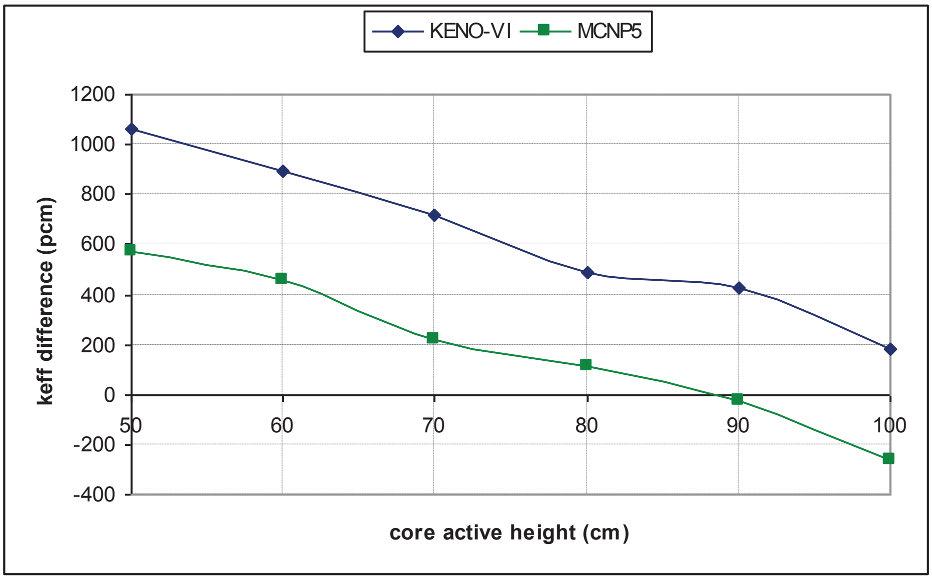

Figure 7: Differences of k_{eff} for KENO-VI and MCNP5 to TRIPOLI-4

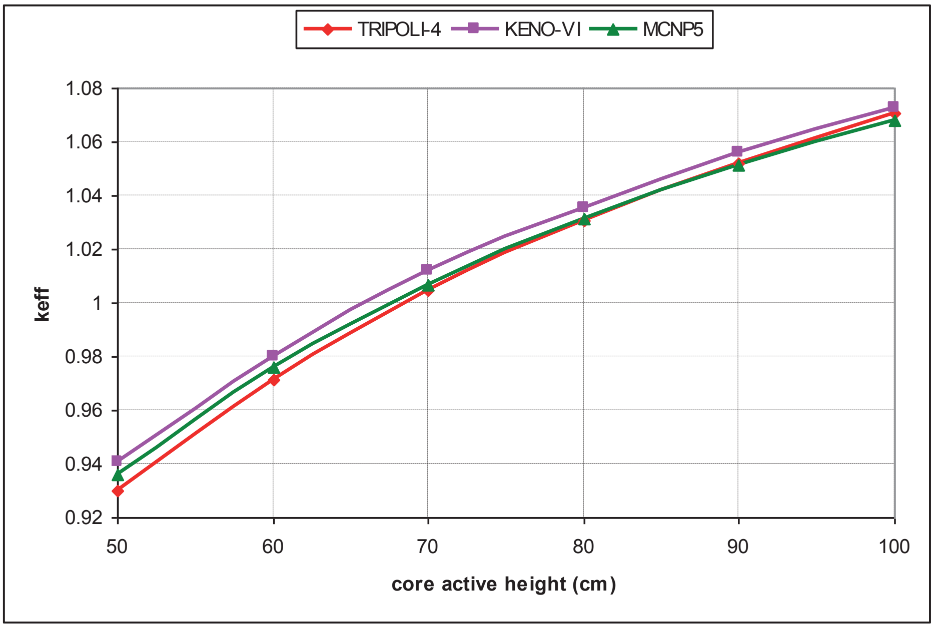

Figure 8: Values of k_{eff} for TRIPOLI-4, KENO-VI and MCNP5

Calculations of track length volume fluxes of GFR core were also done with MCNP5 (FMESH card) for criticality part, the tallies are for one fission neutron being born in the system at the start of a cycle. The user mesh was 100x100x100 cells over entire core with 100 cm height. The volume flux mesh tally is shown in Fig.9 for axial and radial midplane.

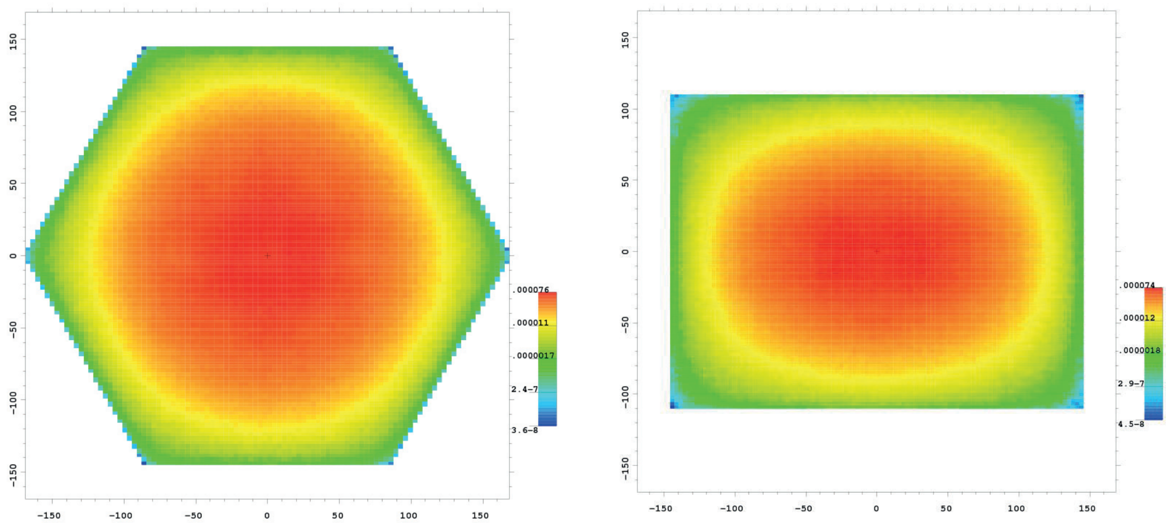

Figure 9: Track length volume flux for GFR core (MCNP5 results)

These tally quantities (i.e. user desirable results) are accumulated only after the inactive cycles are finished, after the spatial fission distribution attained eigenmode. To assist user in assessing the convergence of the fission source spatial distribution, MCNP5 computes a Shannon entropy[3,9] of the fission source distribution H_{src}. It is a well-known concept from information theory, and provides single cycle-wise number for convergence characterization. As the source distribution approaches stationarity the Shannon entropy converges to a single steady-state value. To calculate H_{src}, source distribution must be discretizied over 3D mesh grid with N_s elementary boxes to track a number of normalized fission sites P_j in it. Then, the Shannon entropy of a fission source distribution for every cycle is:

$$H_{src} = -\sum_{j=1}^{N_s} P_j \cdot \ln_2(P_j).$$

H_{src} varies between 0 for a point distribution to $\ln_2(N_s)$ for a uniform distribution. Plot of Shannon entropy vs. cycle number for core height of 100 cm is shown in Fig.10. Selected number of inactive cycles (50) in this paper was more than conservative, since stationarity of a source is reached about cycle 10.

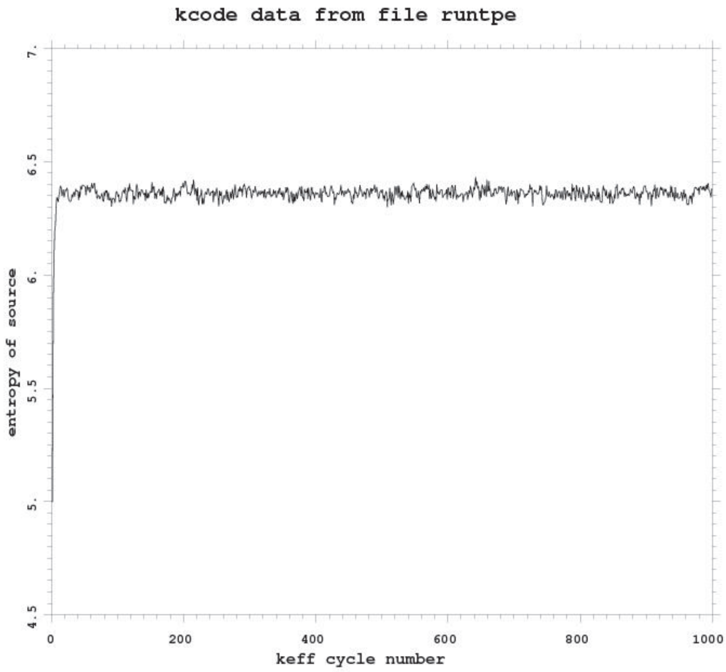

Figure 10: Shannon entropy of fission source distribution (MCNP5 results)

6 CONCLUSIONS

In this work we modeled a pin-type GFR heterogeneous FA (U+Pu carbide fuel, SiC clad, He coolant), and later full-core with KENO-VI and MCNP5 Monte Carlo codes. Calculational results of reactor safety parameters, axial reflector thickness and material reflector selection are first given and compared. The combined temperature reactivity effect is negative since Doppler effect is dominant over loss of coolant density case. A good value of axial reflector thickness was found to be 60 cm, since saturation in reactivity is observed. Zirconium carbide (ZrC) was selected as a best reflector material. Finally, the results of critical GFR core dimensions are given. Equivalent core diameter was found to be 207.04 cm, which corresponds to core of 78 fuel elements, 7 control elements and 84 reflector elements. Thus, proposed GFR core has an active height of 100 cm with ZrC axial reflector of 60 cm.

Overall, the obtained results are showing high similarity with reference results (MCNPX for FA calculations and TRIPOLI-4 for core calculations). Also, fission source distribution stationarity with Shannon entropy check in MCNP5 was found to be quite useful technique to determine number of inactive cycles in Monte Carlo criticality calculations.

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