

# INVESTIGATION OF THE PROPERTIES OF THE NUCLEI USED ON THE NEW GENERATION REACTOR TECHNOLOGY SYSTEMS

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# INTRODUCTION

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The application fields for 14-15 MeV neutron incident energy are Accelerator-Driven subcritical Systems (ADS) for fission energy production and hybrid reactor systems which are a combination of the fusion-fission processes.

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Rubbia succeeded in a proposal of a full scale demonstration plant of the Energy Amplifier (EA) (Rubbia et al., 1995). The design of an accelerator driven system (ADS) requires precise knowledge of nuclide production cross sections in order to predict the amount of radioactive isotopes produced inside the spallation target (Rubbia and Rubio, 1996). The spallation targets can be *Pb*, *Bi*, *W* etc. isotopes and these target material can be liquid or solid. One applied field in the ADS systems is the production of neutrons from spallation reactions. The production of neutrons in spallation neutron source from ADS systems has recently gained considerable interest due to their importance in technical applications.

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- The design of a fusion-fission (hybrid) reactor and ADS systems potentialities require the knowledge of a wide range of better data.  $^{232}\text{Th}$  and  $^{238}\text{U}$  are important as fissile material in hybrid and ADS reactor systems. Thorium and Uranium (Han, 2006) are nuclear fuels and Lead (Tel et al., 2004a; 2006), Bismuth, Tungsten are the target nuclei in these reactor systems (Şarar et al., 2006; Demirkol et al., 2004).
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- The Hartree-Fock method with an effective interaction with Skyrme forces is widely used for studying the properties of nuclei (Skyrme, 1959; Vautherin and Brink, 1972). This method allows possibility to calculate many aspects of nuclei by means of quantum mechanical methods in microscopic scale. Especially the method is successfully used for a wide range of nuclear characteristics such as binding energy, RMS charge radii, neutron and proton density, electromagnetic multipole moments, etc. The Hartree-Fock description of nuclear properties yields good results not only for stable even-even spherical and deformed nuclei, but also for neutron-rich and neutron-deficient nuclei (Beiner et al., 1975; Li, 1991).
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- In this study, RMS charge, neutron radii, neutron and proton density were calculated by using the Hartree-Fock method with an effective interaction with Skyrme forces for the *U*, *Th*, *Pb*, *Bi* and *W* isotopes.
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# HARTREE-FOCK CALCULATIONS WITH SKYRME FORCE

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□ The Hartree-Fock equations and pairing equations are derived variationally from the total energy functional of the nucleus,

$$\square E = E_{\text{Skyrme}} + E_{\text{Coulomb}} + E_{\text{pair}} - E_{\text{cm}}$$

where  $E$  is the total energy of the nucleus,

$E_{\text{Skyrme}}$  is the energy of the Skyrme interaction,

$E_{\text{Coulomb}}$  is the Coulomb interaction energy,

$E_{\text{pair}}$  is the two nucleon interaction pairing energy and

$E_{\text{cm}}$  is the correction for the spurious center-of-mass motion of the mean field.

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$E_{\text{Skyrme}}$  energy is calculated by using the effective Skyrme force (Skyrme, 1959).

This force is;

$$\begin{aligned}
 V_{\text{Skyrme}} = & t_0 (1 + x_0 P_x) \delta(\vec{r}_i - \vec{r}_j) \\
 & + \frac{1}{2} t_1 (1 + x_1 P_x) \{ p_{12}^{\rightarrow 2} \delta(\vec{r}_i - \vec{r}_j) + \delta(\vec{r}_i - \vec{r}_j) p_{12}^{\rightarrow 2} \} \\
 & + t_2 (1 + x_2 P_x) \vec{p}_{12} \bullet \delta(\vec{r}_i - \vec{r}_j) \vec{p}_{12} \\
 & + \frac{1}{6} t_3 (1 + x_3 P_x) \rho^\alpha(\vec{r}) \delta(\vec{r}_i - \vec{r}_j) + i t_4 \vec{p}_{12} \bullet \delta(\vec{r}_i - \vec{r}_j) (\vec{\sigma}_i + \vec{\sigma}_j) \times \vec{p}_{12}
 \end{aligned}$$

$\vec{p}_{12} = \vec{p}_i - \vec{p}_j$  is the relative momentum

$\delta(\vec{r}_i - \vec{r}_j)$  is the delta function

$P_x$  is the space exchange operator

$\vec{\sigma}$  is the vector of Pauli spin matrices

$\vec{r} = \frac{1}{2}(\vec{r}_i + \vec{r}_j)$  and  $t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3, \alpha, w$  are Skyrme force parameters.

## RESULTS AND DISCUSSION

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- We used the Skyrme interaction parameters (in Table 1) in the calculations with the programme of HAFOMN. In these calculations, we took into account the pairing effects in the BCS (Bardeen-Cooper-Schrieffer) formalism by the approximation constant-force
  - The pairing equations are solved by Newton's iteration.
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# Table 1. Skyrme force parameters

Force	SI	SIII	SVI	SKM	SKM*	T3
$t_0(\text{MeV}\cdot\text{fm}^3)$	-1057.3	-1128.75	-1101.81	-2645.0	-2645.0	-1791.80
$t_1(\text{MeV}\cdot\text{fm}^5)$	235.9	395.0	271.67	385.0	410.0	298.50
$t_2(\text{MeV}\cdot\text{fm}^5)$	-100.0	-95.0	-138.33	-120.0	-135.0	-99.50
$t_3(\text{MeV}\cdot\text{fm}^{3\alpha})$	14463.5	14000.0	17000.0	15595.0	15595.0	12794.0
$t_4(\text{MeV}\cdot\text{fm}^{3\alpha})$	0.0	0.0	0.0	0.0	0.0	0.0
$x_0$	0.56	0.45	0.583	0.09	0.09	0.138
$x_1$	0.0	0.0	0.0	0.0	0.0	-1.0
$x_2$	0.0	0.0	0.0	0.0	0.0	1.0
$x_3$	1.0	1.0	1.0	0.0	0.0	0.075
$\alpha$	1.0	1.0	1.0	1/6	1/6	1/3
$w(\text{MeV}\cdot\text{fm}^5)$	0	120	115	130	130	126

Table 2. Calculated and Experimental Root-Mean-Square (RMS)  
Nuclear Charge Radii ( in fm)

	SI	SIII	SVI	SKM*	SKM	T3	Exp.
<b><sup>184</sup>W</b>	5.6504	5.7965	5.8058	5.7748	5.7702	5.7455	5.3745 ± 0.0218
<b><sup>207</sup>Pb</b>	5.4297	5.5715	5.5889	5.5076	5.4920	5.4815	5.5038 ± 0.0015
<b><sup>209</sup>Bi</b>	5.4522	5.5942	5.6124	5.5304	5.5149	5.5040	
<b><sup>232</sup>Th</b>	5.6537	5.8063	5.8156	5.7427	5.7316	5.7089	5.7195 ± 0.0367
<b><sup>238</sup>U</b>	5.7073	5.8562	5.8674	5.8023	5.7922	5.7645	5.8587 ± 0.037

Table 3. Calculated Root-Mean-Square (RMS) Nuclear Mass Radii

	SI	SIII	SVI	SKM*	SKM	T3
<b><sup>184</sup>W</b>	5.9240	6.0857	6.0448	6.1502	6.1513	6.1489
<b><sup>207</sup>Pb</b>	5.4478	5.5908	5.5952	5.5519	5.5391	5.5369
<b><sup>209</sup>Bi</b>	5.4690	5.6133	5.6197	5.5725	5.5600	5.5578
<b><sup>232</sup>Th</b>	5.6815	5.8324	5.8284	5.8039	5.7946	5.7795
<b><sup>238</sup>U</b>	5.7397	5.8859	5.8841	5.8635	5.8550	5.8363

Fig.1 Calculated charge density of  $^{184}\text{W}$

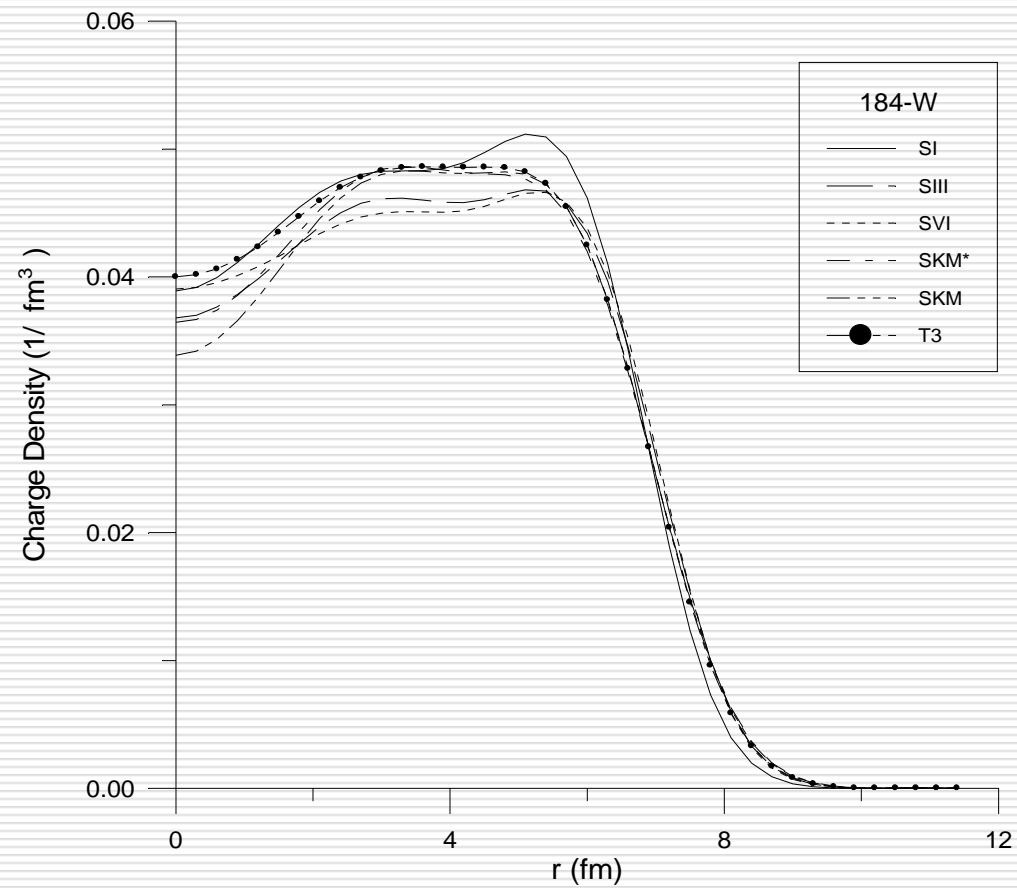


Fig.2 Calculated charge density of  $^{209}\text{Bi}$

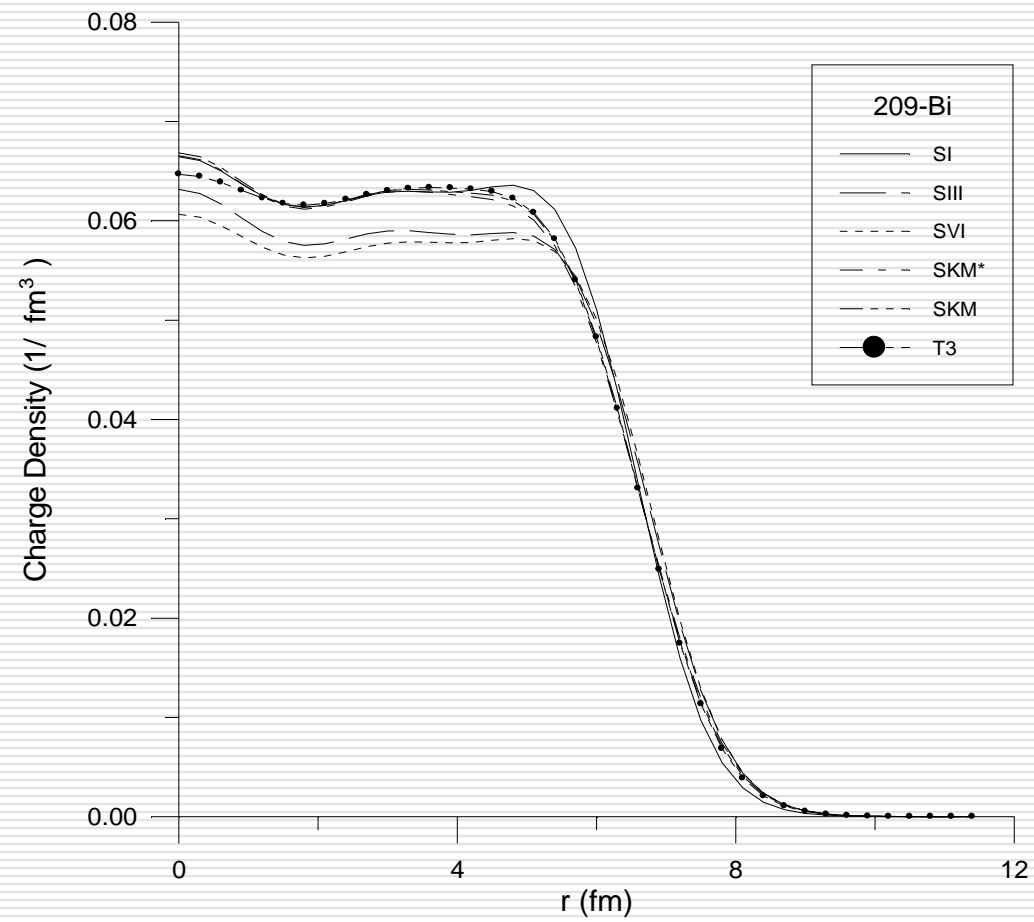


Fig.3 Calculated charge density of  $^{207}\text{Pb}$

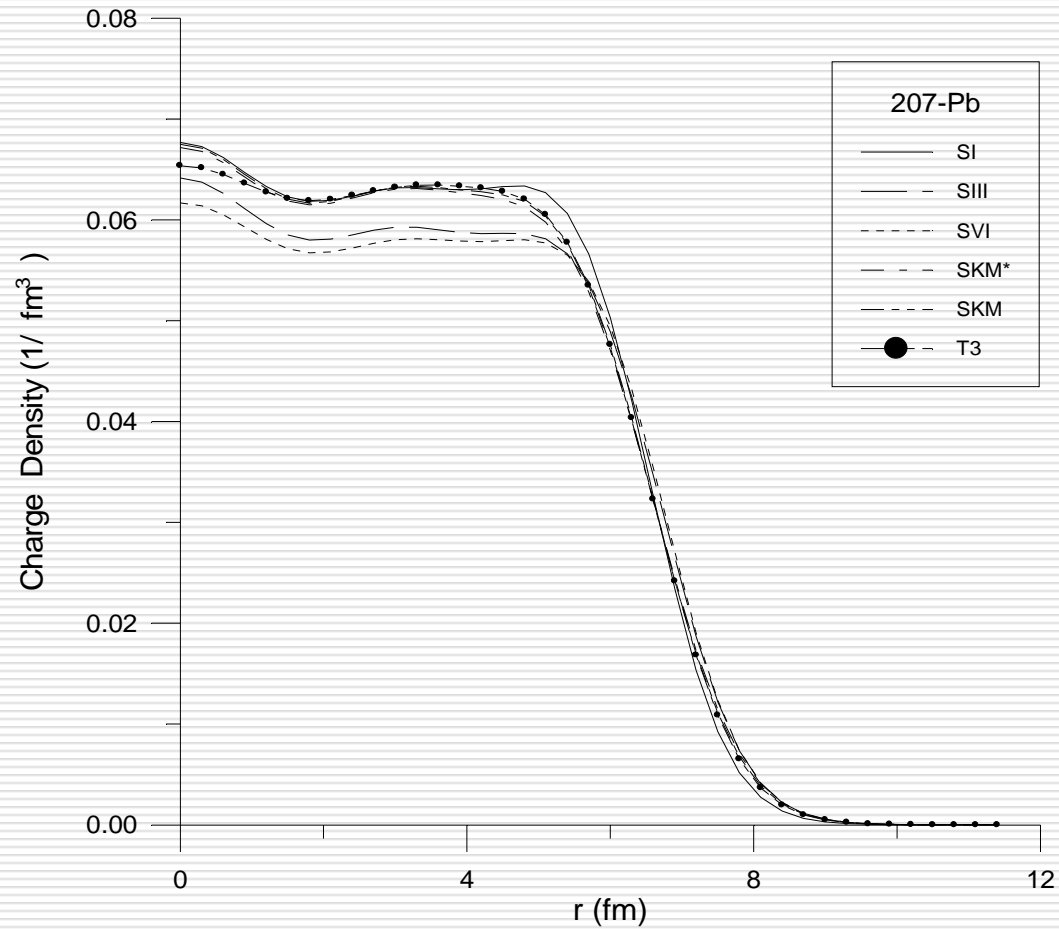


Fig.4 Calculated neutron density of  $^{184}\text{W}$

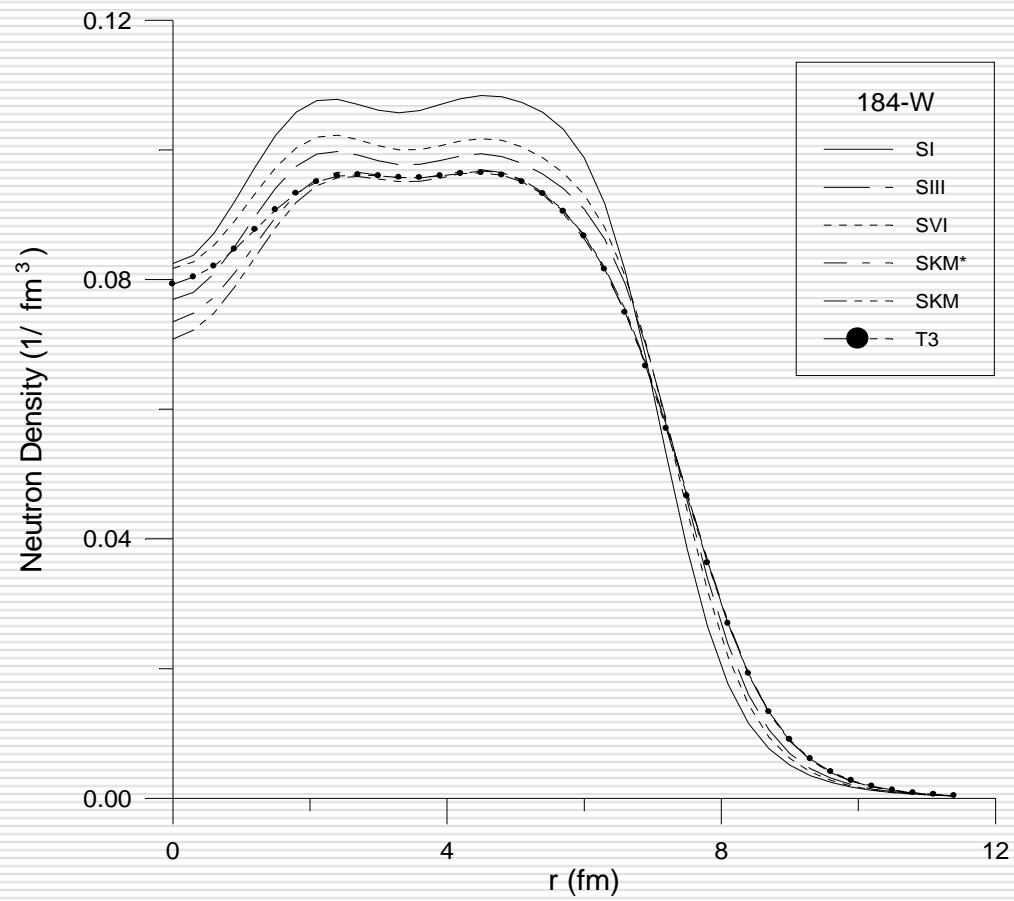


Fig.5 Calculated neutron density of  $^{207}\text{Pb}$

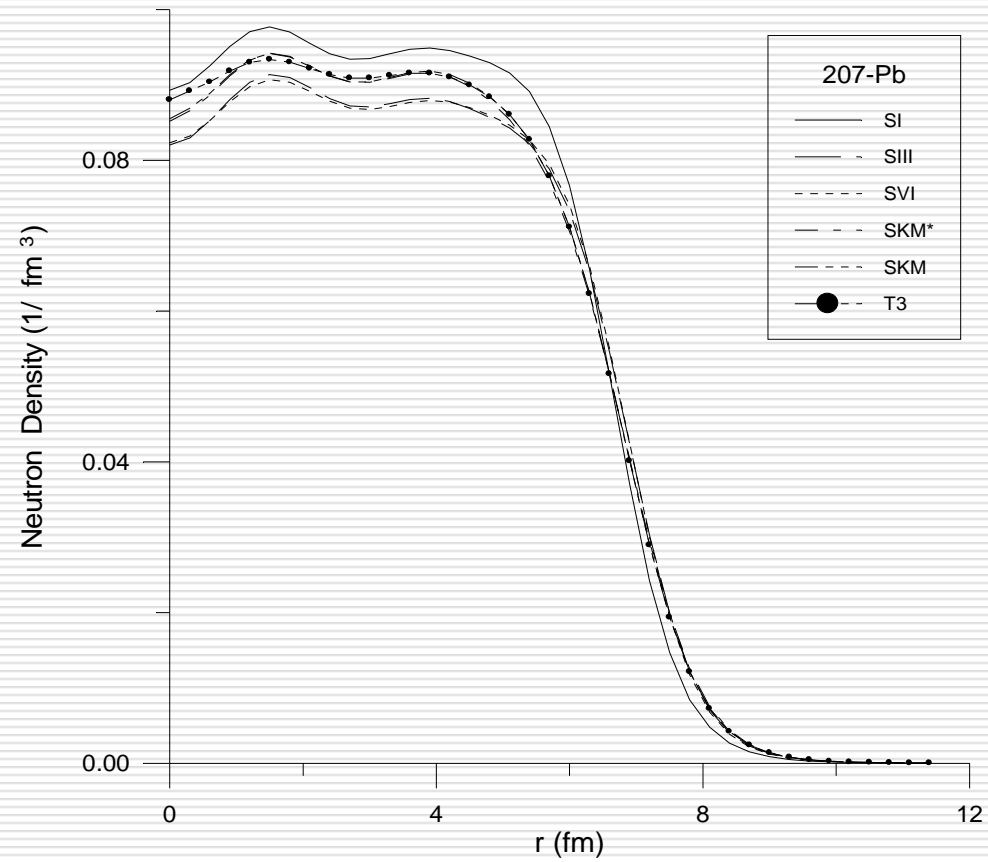


Fig.6 Calculated neutron density of  $^{209}\text{Bi}$

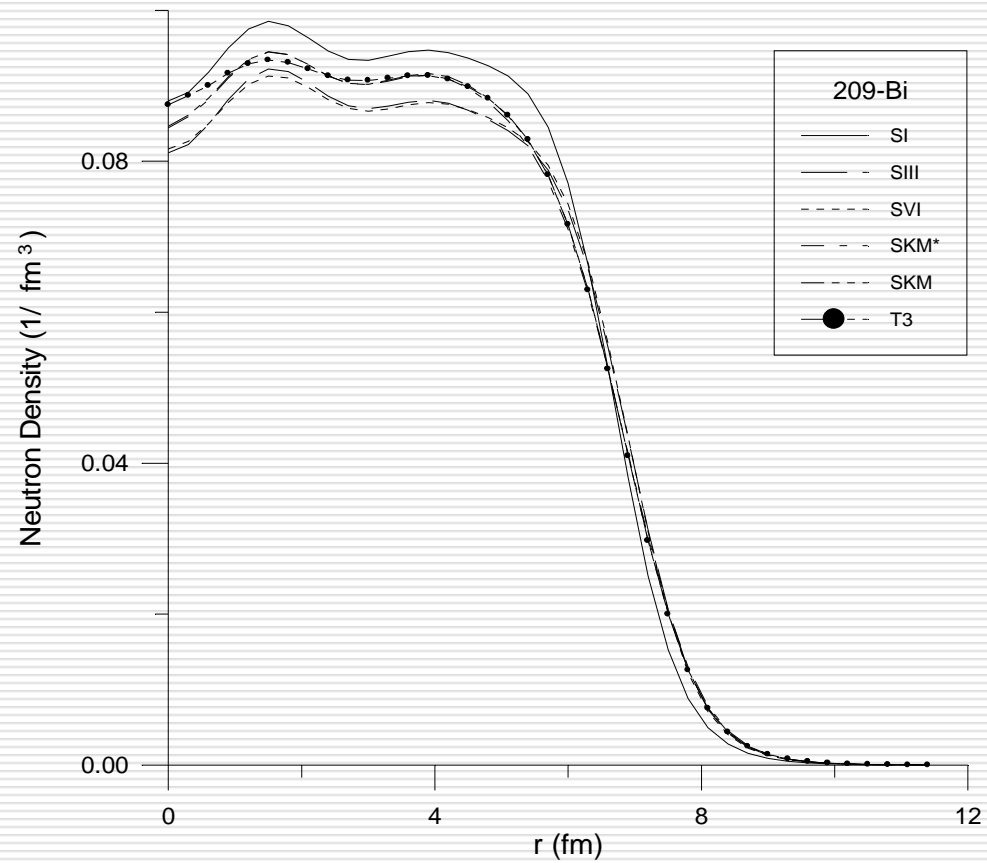


Fig. 7 Comparison of the calculated using the T3 parameter charge and mass densities of  $^{232}\text{Th}$  and  $^{238}\text{U}$

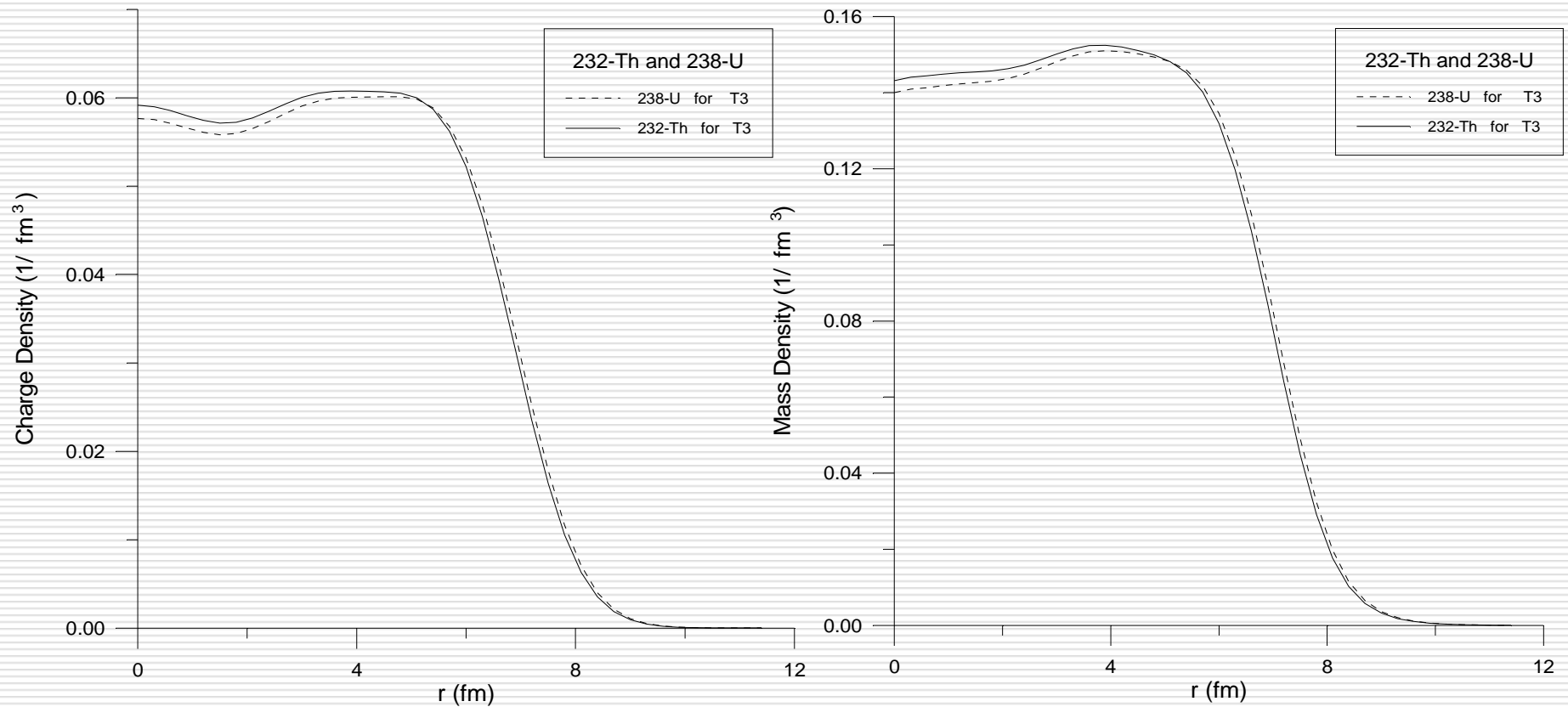
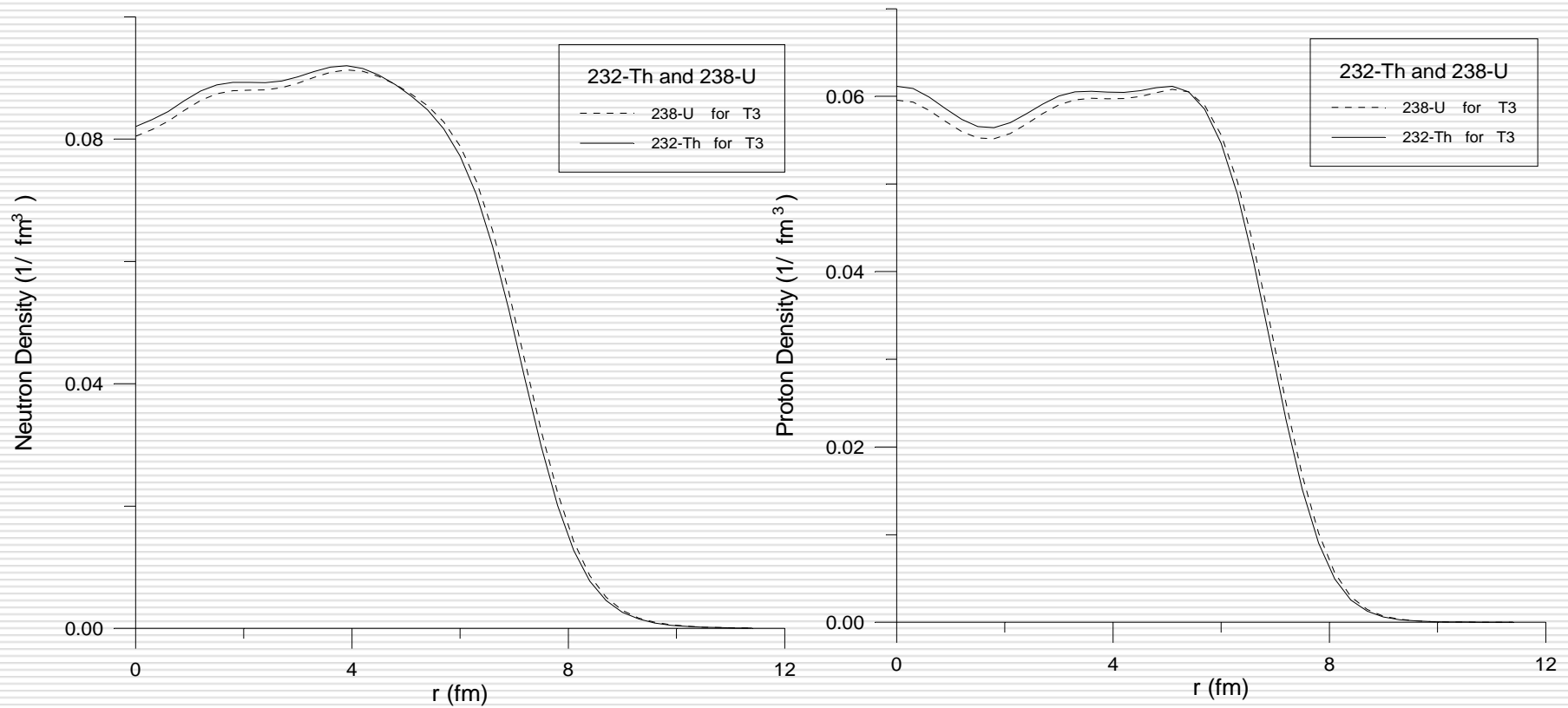


Fig. 8 Comparison of the calculated using the T3 parameter neutron and proton densities of  $^{232}\text{Th}$  and  $^{238}\text{U}$



## SUMMARY AND CONCLUSIONS

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- In this study, charge RMS radii, mass RMS radii, neutron and proton density have been calculated by using the Hartree-Fock method with an effective interaction with Skyrme forces for the *U*, *Th*, *Pb*, *Bi*, *W* isotopes and compared with experimental data, and the following conclusions can be summarized as follows:
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- The experimentally measured nuclear charge RMS radii increases from  $^{184}\text{W}$  to  $^{238}\text{U}$  (from  $Z=74$  to  $Z=92$ ) as the proton number increases. Theoretically calculated charge RMS values, except for  $^{184}\text{W}$ , are quite consistent with experimental values. For  $^{184}\text{W}$ , theoretical calculations are slightly higher than experimental values.
  - Target nuclei of  $^{207}\text{Pb}$  and  $^{209}\text{Bi}$  values for nuclear mass RMS radii calculated without discriminating neutron and proton are very close to each other. In the  $^{184}\text{W}$ , nuclear mass RMS radii are higher than  $^{207}\text{Pb}$  and  $^{209}\text{Bi}$ . These values calculated in fuel nuclei of  $^{238}\text{U}$  and  $^{232}\text{Th}$  are near to each other.
  - The calculated charge and proton densities of each nuclei used in this study exhibits nearly equal values to each other.
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- Density values at the center of  $^{207}\text{Pb}$  and  $^{209}\text{Bi}$  nuclei are close to each other while charge, mass, proton and neutron densities in  $^{184}\text{W}$  are the lowest calculated at the center (at  $r = 0$ ). Besides, values at the central densities of  $^{238}\text{U}$  and  $^{232}\text{Th}$  fuel nuclei indicate similar values.
  - Neutron density of target nuclei  $^{184}\text{W}$ ,  $^{207}\text{Pb}$  and  $^{209}\text{Bi}$  at the center (at  $r = 0$ ) appear to give maximum with the value near to about 2 fm radii value than its lowest value. Calculated densities are constant from about 2 fm radii value than 5-6 fm radii value while they decreases drastically to zero after 5-6 fm. Values close to zero are about in the vicinity of 8-9 fm.
  - When the neutron densities calculated for  $^{238}\text{U}$  and  $^{232}\text{Th}$  are compared,  $^{232}\text{Th}$  in the center is higher than  $^{238}\text{U}$  while neutron density of  $^{238}\text{U}$  is higher than  $^{232}\text{Th}$  as moving forward to surface regions.
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Thank You For Your Kind  
Attention

