

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

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ABSTRACT

The application fields of the fast neutron are Accelerator-Driven subcritical Systems (ADS) for fission energy production and hybrid reactor systems. The technical design hybrid reactor and ADS systems potentialities require the knowledge of a wide range of better data and much effort. Thorium (*Th*) and Uranium (*U*) are nuclear fuels in these reactor systems. Lead (*Pb*), Bismuth (*Bi*) and Tungsten (*W*) are the target nuclei in the ADS reactor systems. The Hartree-Fock (H-F) method with an effective interaction with Skyrme forces is widely used for studying the properties of nuclei such as binding energy, Root Mean Square (RMS) charge radii, mass radii, neutron density, proton density, electromagnetic multipole moments, etc. In this study, by using H-F method with interaction Skyrme RMS charge radii, RMS mass radii, neutron density and proton density were calculated for the ^{232}Th , ^{238}U , ^{207}Pb , ^{209}Bi and ^{184}W isotopes used on the new generation reactor systems. The calculation results of charge radii have been compared with experimental data and obtained other results have been discussed for hybrid and ADS reactor systems.

Keywords: ADS systems, Hybrid reactor, Skyrme force, Neutron density, Charge radii,

1. INTRODUCTION

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. 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. The precision of models to estimate residue production cross sections is still far from the performance required for technical applications. 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. ADS systems can be used for production of neutrons in spallation neutron source and they can act as an intense neutron source in accelerator-driven subcritical reactors, capable of incinerating nuclear waste and of producing energy (Takizuka et al., 1995). Another field of interest, which is presently discussed, is the technical application of nuclear-collision processes for the energy production and the transmutation of nuclear waste in hybrid reactor systems which work as a fission reactor where an additional high-energetic proton or ion beam serves to increase the neutron flux in the reactor in a controlled way. The fusion-fission hybrid is a combination of the fusion and fission processes (Şahin et al., 1986, 2002a, 2002b, 2003, 2005; Übeyli and Tel, 2003). The fusion plasma is surrounded with a blanket made of the fertile materials (^{238}U or ^{232}Th) to convert them into fissile materials

(^{239}Pu or ^{233}U) by transmutation through the capture of the high yield fusion neutrons. The fertile materials may also undergo a substantial amount of nuclear fission, especially, under the irradiation of the high energetic 14.1 MeV- (D,T) neutrons. In addition to that some of the bred fissile material burns in the hybrid blanket “*in situ*” (Übeyli and Acir 2007; Yıldız and Acir, 2005).

The design of a fusion-fission (hybrid) reactor and ADS systems potentialities require the knowledge of a wide range of better data. ^{232}Th and ^{238}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 (Şarer et al., 2006; Demirkol et al., 2004). 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). 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.

2. HARTREE-FOCK CALCULATIONS WITH SKYRME FORCE

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

$$\mathbf{E} = \mathbf{E}_{\text{Skyrme}} + \mathbf{E}_{\text{Coulomb}} + \mathbf{E}_{\text{pair}} - \mathbf{E}_{\text{cm}} \quad (1)$$

where E is the total energy of the nucleus, $\mathbf{E}_{\text{Skyrme}}$ is the energy of the Skyrme interaction, $\mathbf{E}_{\text{Coulomb}}$ is the Coulomb interaction energy, \mathbf{E}_{pair} is the two nucleon interaction pairing energy and \mathbf{E}_{cm} is the correction for the spurious center-of-mass motion of the mean field. The Coulomb interaction's infinite range makes it very consuming to evaluate the exchange part exactly and makes the exchange contribution only a small fraction of the total Coulomb energy, thus to preserving the simplicity of the Skyrme - Hartree-Fock with equation the Coulomb-exchange part treated in the Slater approximation (Vautherin and Brink, 1972, Beiner et al., 1991). The Coulomb energy is given by

$$E_{\text{Coul}} = \frac{1}{2} e^2 \int d^3r d^3r' \rho_c(\vec{r}) \frac{1}{|\vec{r} - \vec{r}'|} \rho_c(\vec{r}') + E_{\text{Coul,exch}} \quad (2)$$

$$E_{\text{Coul,exch}} = -\frac{3}{4} \left(\frac{3}{\pi}\right)^{1/3} 4\pi \int_0^\infty dr r^2 \rho_{pr}^{4/3} \quad (3)$$

where e is the charge of the electron, $\rho_c(r)$ is the charge density and ρ_{pr} is the proton density.

In the direct term, the nuclear charge distribution includes in folding with the finite size of the proton. The exact nuclear ground state should be a state with a total momentum zero. The mean field, however, localizes the nucleus and thus breaks translational invariance, so that the center-of-mass of the whole nucleus can oscillate in the mean field. The correction is;

$$E_{cm} = \frac{\langle P_{cm}^2 \rangle}{2Am},$$

$$\langle P_{cm}^2 \rangle = \sum (w_\beta \langle \varphi_\beta | p^2 | \varphi_\beta \rangle - \sum (w_\alpha w_\beta + \sqrt{w_\alpha(1-w_\alpha)w_\beta(1-w_\beta)}) \langle \varphi_\alpha | p | \varphi_\beta \rangle)^2 \quad (4)$$

where $P_{cm} = \sum_i p_i$ is the total momentum operator of center-of-mass, p is the momentum operator, A is the nucleon number, m is the average nucleon mass, The occupations probability of the β state is w_β and isospin label q runs over $q \in \{pr, ne\}$ (pr = proton and ne= neutron). The φ_β is the single-particle wave function of β state and $|\varphi_\beta\rangle$ is the eign vector of the β state and $\langle \varphi_\beta |$ the complex conjugate of β state of $|\varphi_\beta\rangle$. Equation (4) includes the two-body operator, which leads to a double-sum over single-particle states. It would be time consuming to evaluate the center-of-mass correction, and so this correction is computed after variation, and does not contribute to the Hartree-Fock equations. Finally, the zero-point energy of the nearly harmonic oscillations of the center of mass is subtracted as in Equations (1). Pairing energy is given by;

$$E_{pair} = \sum_q G_q \left[\sum \sqrt{w_\beta(1-w_\beta)} \right]^2 \quad (5)$$

where G_q and w_β are the pairing matrix elements and the pairing weights of the proton and neutron, respectively (Campi and Sprung, 1972). The varying the Equation (2), energy functional, with respect to the pairing weights w_β , yields the BCS equations (Li, 1991). The pairing weights become as

$$w_\beta = \frac{1}{2} \left(1 - \frac{\varepsilon_\beta - \varepsilon_{F,q}}{\sqrt{(\varepsilon_\beta - \varepsilon_{F,q})^2 + \Delta_q^2}} \right) \quad (6)$$

The pairing gap Δ_q and Fermi energy $\varepsilon_{F,q}$ are obtained by simultaneous of the gap equation is

$$\frac{\Delta_q}{G_q} = \sum_{\beta \in q} \sqrt{w_\beta (1 - w_\beta)} \quad (7)$$

and the particle-number condition is

$$A_q = \sum_{\beta \in q} w_\beta \quad (8)$$

where A_q is the desired number of protons ($q = \text{pr}$) or neutrons ($q = \text{ne}$). E_{Skymrme} energy is calculated by using the effective Skyrme force (Skymrme, 1959). This force is

$$\begin{aligned}
V_{\text{Skyrme}} = & t_0(1 + x_0 P_x) \delta(\vec{r}_i - \vec{r}_j) \\
& + \frac{1}{2} t_1 (1 + x_1 P_x) \{ p_{12}^2 \delta(\vec{r}_i - \vec{r}_j) + \delta(\vec{r}_i - \vec{r}_j) p_{12}^2 \} \\
& + t_2 (1 + x_2 P_x) \vec{p}_{12} \bullet \delta(\vec{r}_i - \vec{r}_j) \vec{p}_{12} \\
& + \frac{1}{6} t_3 (1 + x_3 P_x) \rho^\alpha(\vec{r}) \delta(\vec{r}_i - \vec{r}_j) + i t_4 \vec{p}_{12} \bullet \delta(\vec{r}_i - \vec{r}_j) (\vec{\sigma}_i + \vec{\sigma}_j) \times \vec{p}_{12}
\end{aligned} \tag{9}$$

where $\vec{p}_{12} = \vec{p}_i - \vec{p}_j$ 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. These Skyrme force parameters are given in Table 1. These parameters values and the other Skyrme force parameters can be find from the reference (Li, 1991).

3. RESULTS AND DISCUSSION

We used the Skyrme interaction parameters (in Table 1) in the calculations. In these calculations, we took into account the pairing effects in the BCS formalism in the approximation constant-force with $G_{pr} = \frac{22\text{MeV}}{A}$, $G_{ne} = \frac{29\text{MeV}}{A}$ where A is the total nucleon number of a nucleus. A commonly accepted parameterization of gap is

$$\Delta_q = 11.2\text{MeV} / \sqrt{A}$$

where, $A = A_{pr} + A_{ne}$ is the total number of the nucleons. The pairing equations are solved by Newton's tangential iteration.

For description of the systems consisting of an odd number of particles, we used the filling approximation. The Hartree-Fock and pairing equations are coupled, and they are solved by simultaneous iteration of the wave functions and the occupation weights. Completely filled shells have $w_{\beta} = 1$, but fractional occupancies occur for nonmagic nuclei, these are determined by pairing scheme discussed in equation (Skyrme, 1959; Vautherin and Brink, 1972; Beiner et al., 1991; Li, 1991).

An even simpler approach to the center-of-mass correction was used in early applications. One can take the one-body part of equation (4), $P_{cm}^2 = \sum_i p_i^2$, and thus express centre-of-mass correction as a modification of the nucleon mass

$$\frac{\hbar^2}{2m} \rightarrow \frac{\hbar^2}{2m} \left(1 - \frac{1}{A} \right)$$

In this study, We have calculated by using the Hartree-Fock method with an effective interaction with Skyrme forces parameters (in given by Table 1) for the *U*, *Th*, *Pb*, *Bi*, *W* isotopes and compared with experimental data experimental Root-Mean-Square (RMS) nuclear charge radii in Table 2. Experimental values were taken from Atomic Data and Nuclear Data Tables (Nadjakov et al., 1994). The nuclear charge radii and nuclear charge density are the most useful observable for analyzing nuclear structure. The nuclear charge radii and nuclear charge density provide information about the nuclear shape and can be determined by clear-cut procedures from the cross section for

elastic electron scattering. To compute the observable charge density from the Hartree-Fock results, one has to take into account that the nucleons themselves have intrinsic electromagnetic structure. Thus one needs to fold the proton and neutron densities from the Hartree-Fock method with the intrinsic charge density of the nucleons.

The Root-Mean-Square (RMS) radii of neutron, proton, charge and mass distributions can be evaluated from these densities;

$$r_q = \langle r_q^2 \rangle^{1/2} = \left[\frac{\int r^2 \rho_q(r) dr}{\int \rho_q(r) dr} \right]^{1/2}$$

where q represent neutron, proton, charge and mass. It can be seen that the experimentally measured nuclear charge RMS radii increases from ^{184}W to ^{238}U (from $Z=74$ to $Z=92$) as the proton number increases in Table 2. Theoretically calculated charge RMS values, except for ^{184}W , are quite consistent with experimental values. For ^{184}W , theoretical calculations are slightly higher than experimental values.

The character of the nuclear deformation can be seen in the mass regions $150 < A < 190$ and $A > 220$, which correspond respectively to the rare-earth and actinide elements. In these regions, the energies of the first excited states are smaller than those of other nuclei and they have large values of quadrupole moments as such nuclei are far away from closed-shell configurations (Okuducu and Ahmadov, 2003; Tel et al., 2004). The ^{184}W have character the strongest nuclear deformation in these nucleuses. The Skyrme - Hartree-Fock method is the useful for calculating of the spherical nuclei because this force is central and has zero range interactions. These means that the interactions are

only dependence of radial and there is not dependence of angular. So this method dose not give well results for calculating of the with deformation nuclei.

We have calculated by using the Hartree-Fock with Skyrme forces parameters for the *U*, *Th*, *Pb*, *Bi*, *W* isotopes RMS nuclear mass radii without discriminating neutron and proton in Table 3. Target nuclei of ^{207}Pb and ^{209}Bi values for nuclear mass RMS radii calculated are very close to each other because these nuclei have near to each other mass number($A= 207$, $A=209$). The nuclear mass RMS radii calculated have near to each other in fuel nuclei of ^{238}U and ^{232}Th . But in the ^{184}W , nuclear mass RMS radii are higher than ^{207}Pb and ^{209}Bi . The method doesn't useful for calculating with strong deformation nuclei.

We have drawn the charge, mass, proton and neutron densities for the *U*, *Th*, *Pb*, *Bi*, *W* isotopes in figure 1-3. The density values at the center of ^{207}Pb and ^{209}Bi nuclei are close to each other while charge, mass, proton and neutron densities in ^{184}W are the lowest calculated at the center (at $r = 0$) in figure 1 and 2. These densities at the central densities of ^{238}U and ^{232}Th fuel nuclei indicate similar values in figure 3. The neutron density of target nuclei ^{184}W , ^{207}Pb and ^{209}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 in figure 2. The calculated densities are constant from about to 2 fm radii value than 5-6 fm radii value while they decreases drastically to zero after 5-6 fm for ^{238}U and ^{232}Th fuel nuclei in figure 3. Values close to zero are about in the vicinity of 8-9 fm. These can be explained that all the Skyrme interactions we have used fairly well the nuclear saturation properties. Hence the density in the central region of heavy nuclei and

consequently the effective mass come very close to their corresponding nuclear matter values.

We have drawn the comparison of the calculated using only the T3 parameter charge, mass, neutron and proton densities of ^{238}U and ^{232}Th in figure 4. The T3 force has the interaction parameter the many than other Skyrme force. It can be seen that ^{232}Th in the centre is higher than ^{238}U while neutron density of ^{238}U is higher than ^{232}Th as moving forward to surface regions.

4. SUMMARY AND CONCLUSIONS

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:

1. The experimentally measured nuclear charge RMS radii increases from ^{184}W to ^{238}U (from $Z=74$ to $Z=92$) as the proton number increases. Theoretically calculated charge RMS values, except for ^{184}W , are quite consistent with experimental values. For ^{184}W , theoretical calculations are slightly higher than experimental values.
2. Target nuclei of ^{207}Pb and ^{209}Bi values for nuclear mass RMS radii calculated without discriminating neutron and proton are very close to each other. In the

- ^{184}W , nuclear mass RMS radii are higher than ^{207}Pb and ^{209}Bi . These values calculated in fuel nuclei of ^{238}U and ^{232}Th are near to each other.
3. The calculated charge and proton densities of each nuclei used in this study exhibits nearly equal values to each other.
 4. Density values at the center of ^{207}Pb and ^{209}Bi nuclei are close to each other while charge, mass, proton and neutron densities in ^{184}W are the lowest calculated at the center (at $r = 0$). Besides, values at the central densities of ^{238}U and ^{232}Th fuel nuclei indicate similar values.
 5. Neutron density of target nuclei ^{184}W , ^{207}Pb and ^{209}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 to 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.
 6. When the neutron densities calculated for ^{238}U and ^{232}Th are compared, ^{232}Th in the center is higher than ^{238}U while neutron density of ^{238}U is higher than ^{232}Th as moving forward to surface regions.

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Figure Captions

Fig.1. Calculated charge and mass densities of ^{184}W , ^{207}Pb and ^{209}Bi

Fig.2. Calculated neutron and proton densities of ^{184}W , ^{207}Pb and ^{209}Bi

Fig. 3. Calculated charge, mass densities and neutron densities of ^{232}Th and ^{238}U

Fig. 4. Comparison of the calculated using the T3 parameter charge, mass, neutron and proton densities of ^{232}Th and ^{238}U

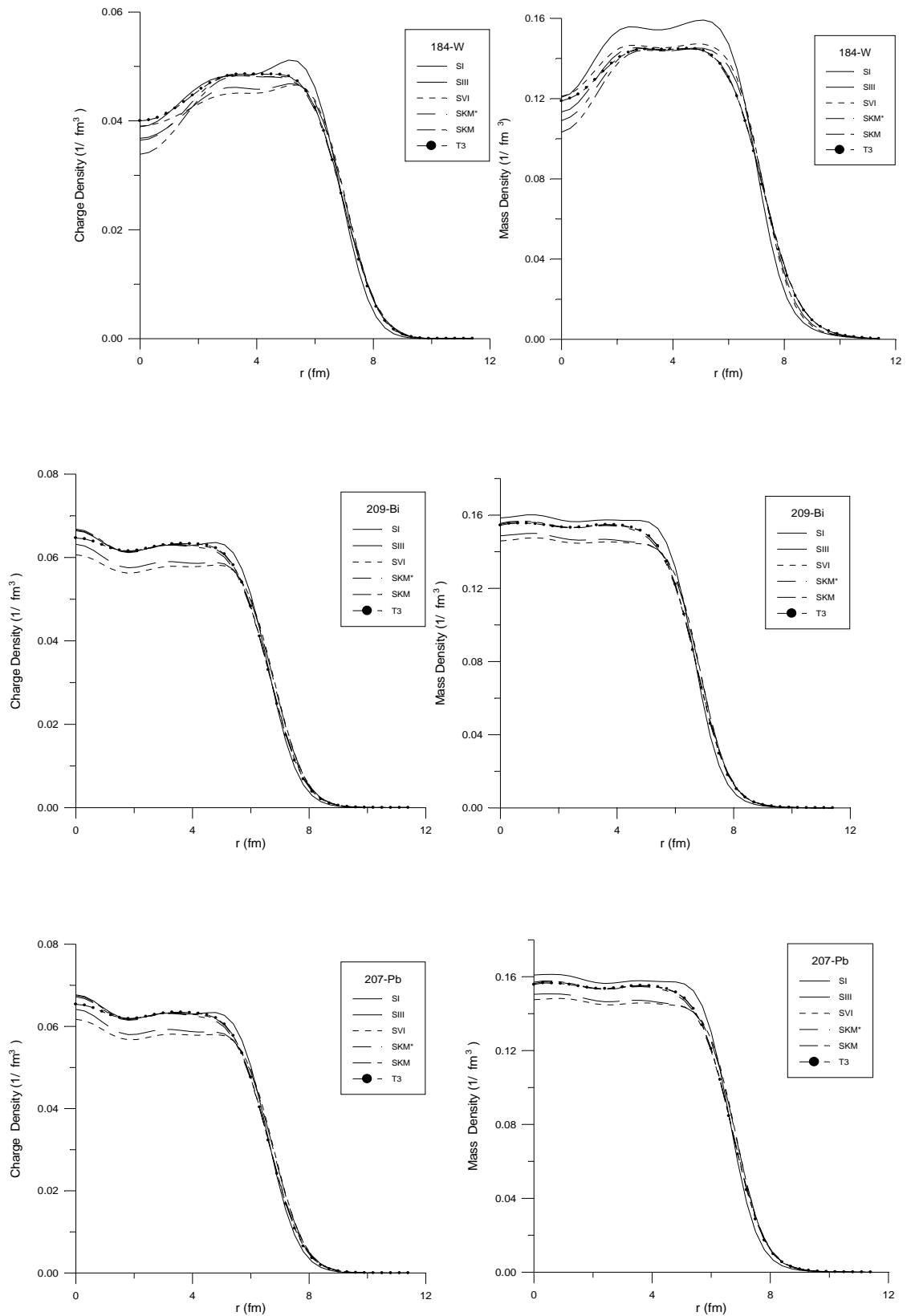


Fig.1. Calculated charge and mass densities of ¹⁸⁴W, ²⁰⁷Pb and ²⁰⁹Bi

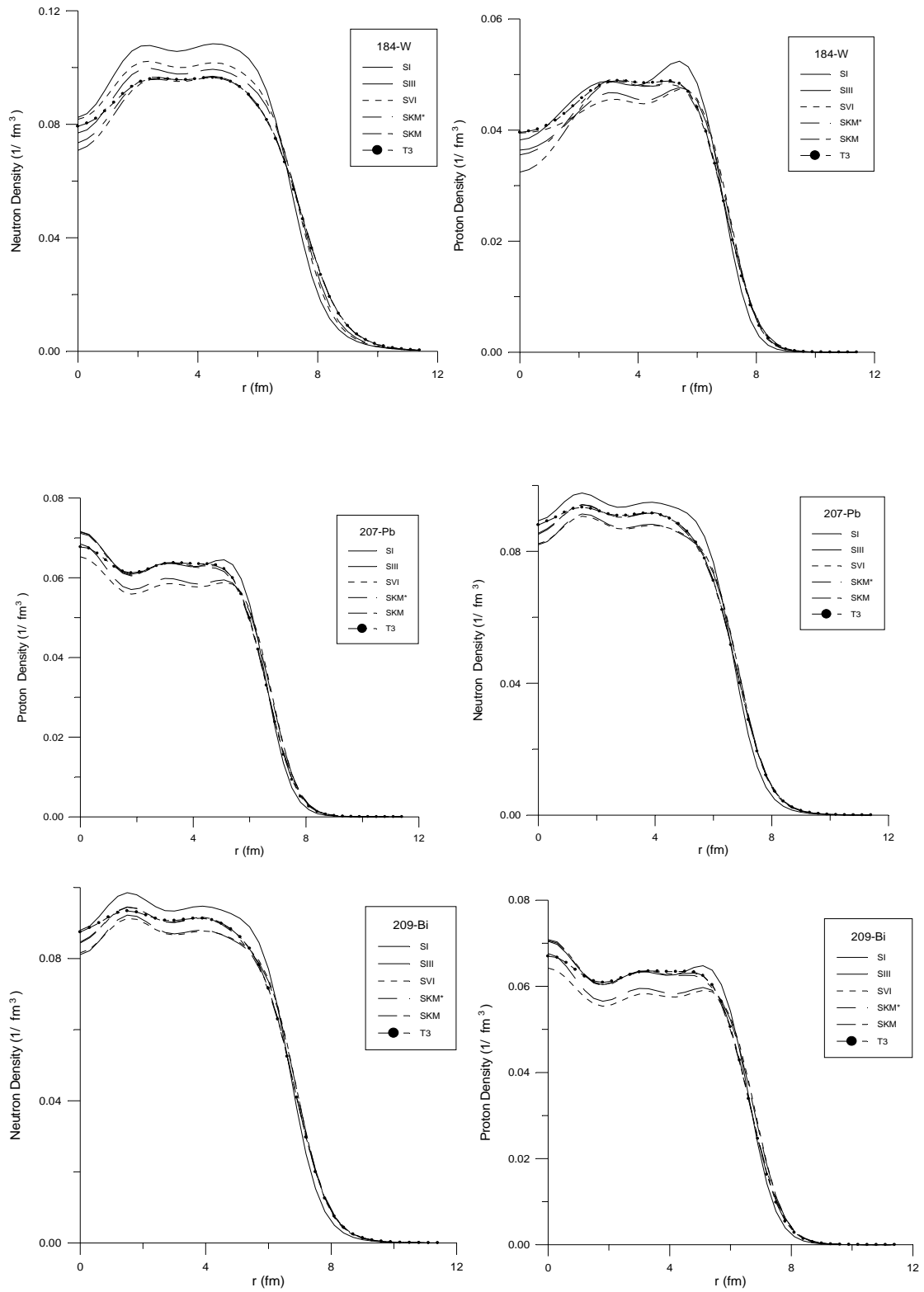


Fig.2. Calculated neutron and proton densities of ^{184}W , ^{207}Pb and ^{209}Bi

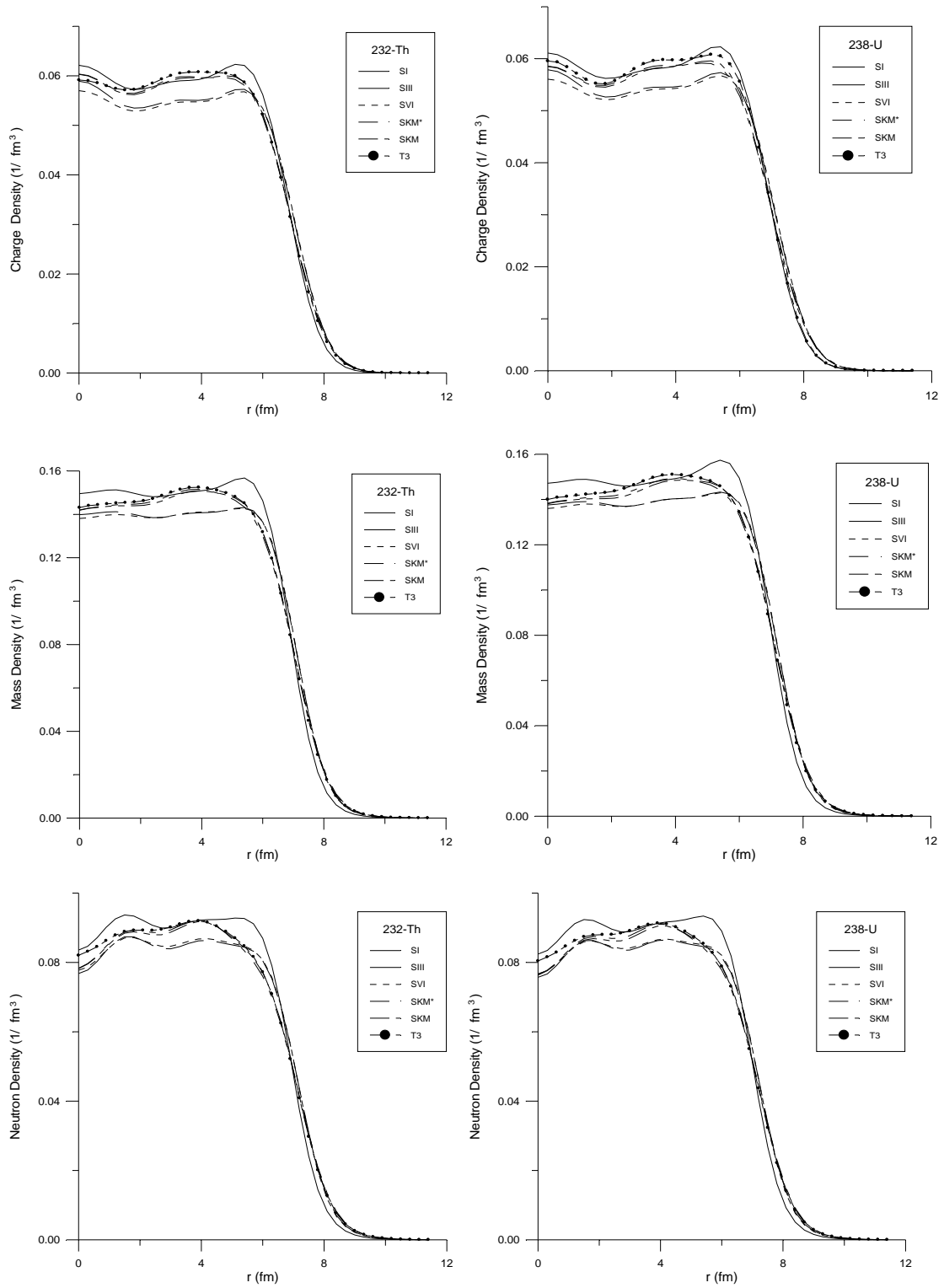


Fig. 3. Calculated charge, mass densities and neutron densities of ^{232}Th and ^{238}U

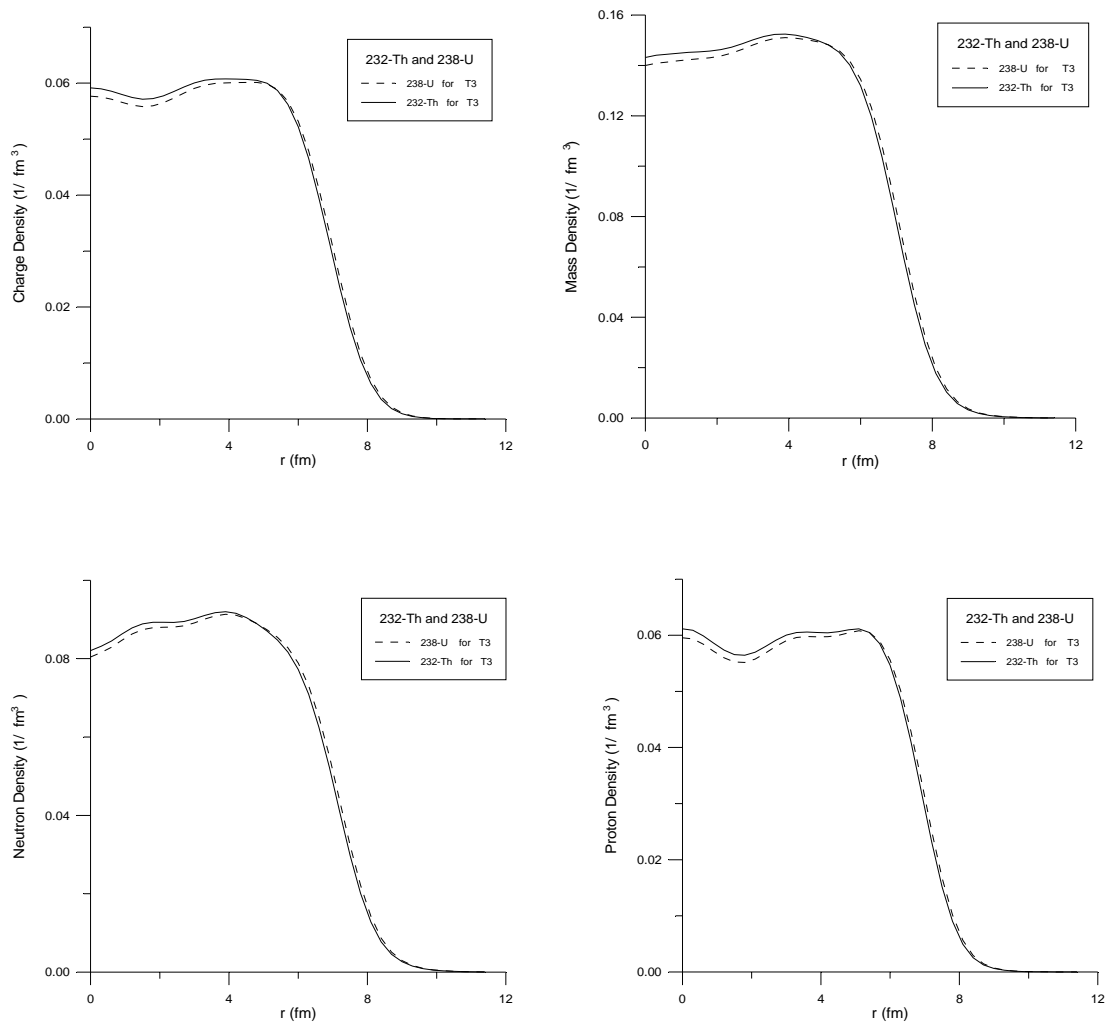


Fig. 4. Comparison of the calculated using the T3 parameter charge, mass, neutron and proton densities of ^{232}Th and ^{238}U

Table 1. Skyrme force parameters

Force	SI	SIII	SVI	SKM	SKM*	T3
$t_0(MeV.fm^3)$	-1057.3	-1128.75	-1101.81	-2645.0	-2645.0	-1791.80
$t_1(MeV.fm^5)$	235.9	395.0	271.67	385.0	410.0	298.50
$t_2(MeV.fm^5)$	-100.0	-95.0	-138.33	-120.0	-135.0	-99.50
$t_3(MeV.fm^{3\alpha})$	14463.5	14000.0	17000.0	15595.0	15595.0	12794.0
$t_4(MeV.fm^{3\alpha})$	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
α	1.0	1.0	1.0	1/6	1/6	1/3
$w(MeV.fm^5)$	0	120	115	130	130	126

Table 2. Calculated and experimental Root-Mean-Square (RMS) Nuclear Charge

Radii (in fm). Experimental values were taken from ref (10)

	SI	SIII	SVI	SKM*	SKM	T3	Exp.
¹⁸⁴ W	5.6504	5.7965	5.8058	5.7748	5.7702	5.7455	5.3745 ± 0.0218
²⁰⁷ Pb	5.4297	5.5715	5.5889	5.5076	5.4920	5.4815	5.5038 ± 0.0015
²⁰⁹ Bi	5.4522	5.5942	5.6124	5.5304	5.5149	5.5040	
²³² Th	5.6537	5.8063	5.8156	5.7427	5.7316	5.7089	5.7195 ± 0.0367
²³⁸ U	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
¹⁸⁴ W	5.9240	6.0857	6.0448	6.1502	6.1513	6.1489
²⁰⁷ Pb	5.4478	5.5908	5.5952	5.5519	5.5391	5.5369
²⁰⁹ Bi	5.4690	5.6133	5.6197	5.5725	5.5600	5.5578
²³² Th	5.6815	5.8324	5.8284	5.8039	5.7946	5.7795
²³⁸ U	5.7397	5.8859	5.8841	5.8635	5.8550	5.8363