IRSTI 29.15.19

https://doi.org/10.26577/RCPh.2024v89i2-01



R-MATRIX CALCULATIONS OF THE DEUTERIUM-TRITIUM FUSION CROSS SECTION BASED ON PRECISE COULOMB FUNCTIONS

Due to the availability of fuel, favorable kinetics, and high output energy, the deuterium-tritium (D-T) fusion reaction is dominantly used in thermonuclear fusion. This paper presents a detailed, step-by-step theoretical calculation of the D-T fusion cross-section within the framework of the phenomenological R-matrix method. The fundamental principles of the phenomenological R-matrix method are outlined. Nuclear and Coulomb interactions are addressed by the R-matrix formalism, which classifies the configuration space into internal and external regions, respectively. Precise Coulomb functions are utilized in the calculations, essential for the accurate determination of the penetration and shift factors. Precise Coulomb functions for the D+T, ⁴He+¹²C systems have been calculated. The penetration and shift factors for the D+T system for a given angular momentum have been obtained. Two different R-matrix models with parameters from recent scientific papers are employed to calculate D-T fusion cross-sections and reaction rates, which are then compared with those obtained from the ENDF/B-VIII.0 library data. Within a crucial low-energy range (from 0 to 0.1 MeV), important for fusion technology, our results show quite good agreement with experimental data, while in a high-energy range, the obtained results are slightly underestimated due to non-resonant ⁵He levels not being taken into account. These findings indicate that the models can be used for future thermonuclear fusion applications.

Key words: thermonuclear fusion, R-matrix, Coulomb functions, penetration factor, shift factor, cross section, reaction rate.

O.C. Баяхметов^{*}, С.К. Сахиев Ядролық физика институты, Алматы қ., Қазақстан *e-mail: <u>bayakhmetov.o.s.92@gmail.com</u>

Нақты Кулон функцияларына негізделген дейтерий-тритий синтезі қимасының R-матрицалық есептеулері

Отынның қолжетімділігіне, қолайлы кинетикасына және жоғары энергия шығымына байланысты дейтерий-тритий (D-T) синтез реакциясы ядролық синтез мәселелері саласында әсіресе қолданылады. Бұл мақалада феноменологиялық R-матрицалық әдіс шеңберінде D-T синтез реакциясы қимасының егжей-тегжейлі, қадамдық теориялық есептеуі берілген. Феноменологиялық R-матрицалық әдістің негізгі принциптері көрсетілді. Ядролық және кулондық өзара әрекеттесу R-матрицалық формализмнің көмегімен өңделеді, оған сәйкес конфигурация кеңістігі сәйкесінше ішкі және сыртқы аймақтарға бөлінеді. Есептеулерде туннельдік және ығысу коэффициенттерін нақты анықтау үшін нақты Кулон функциялары пайдаланады. D+T, ⁴He+¹²C жүйелері үшін нақты Кулон функциялары есептелді. D+T жүйесі үшін туннельдік және ығысу коэффициенттері берілген бұрыштық импульс үшін анықталды. D-T термоядролық реакцияларының қимасы мен жылдамдығын есептеу үшін қазіргі заманғы ғылыми жұмыстардағы параметрлері бар екі әр түрлі R-матрица моделі пайдаланылады, және олардың нәтижелері ENDF/B-VIII.0 кітапханасының деректерінен алынған эксперименталдық нәтижелермен салыстырылады. Термоядролық синтез технологиясы үшін өте маңызды төмен энергия диапазонында (0-ден 0.1 МэВ-қа дейін) біздің нәтижелер тәжірибелік деректермен жақсы сәйкестігін көрсетеді, ал жоғары энергия диапазонында алынған нәтижелер ⁵Не ядросының резонанстық емес деңгейлерін есептеулерде есепке алынбауына байланысты біршама төмен бағаланады. Алынған нәтижелер осы мақалада қолданылған моделдердің болашақ термоядролық қосымшалар үшін пайдалануға болатынын көрсетеді.

Түйін сөздер: термоядролық синтез, R-матрица, Кулон функциялары, туннельдеу коэффициенті, ығысу коэффициенті, қима, реакция жылдамдығы.

О.С. Баяхметов^{*}, С.К. Сахиев

Институт ядерной физики, г.Алматы, Казахстан *e-mail: <u>bayakhmetov.o.s.92@gmail.com</u>

R-матричные расчеты сечения дейтерий-тритиевого синтеза на основе точных кулоновских функций

Благодаря доступности топлива, благоприятной кинетике и высокому уровню выхода энергии реакция синтеза дейтерия-трития (D-T) преимущественно используется в области задач термоядерного синтеза. В данной статье представлен подробный, пошаговый теоретический расчет сечения D-T синтеза в рамках метода феноменологической R-матрицы. Изложены фундаментальные принципы феноменологического метода R-матрицы. Ядерные и кулоновские взаимодействия рассматриваются с помощью формализма R-матрицы, согласно которому конфигурационное пространство делится на внутреннюю и внешнюю области, соответственно. В расчетах используются точные кулоновские функции, необходимые для точного определения коэффициентов туннелирования и сдвига. Рассчитаны точные кулоновские функции для систем D+T, ⁴He+¹²C. Получены коэффициенты туннелирования и сдвига для системы D+T для заданного углового момента. Две разные модели R-матрицы с параметрами из современных научных работ используются для расчета сечений и скоростей реакций слияния D-T, результаты которых затем сравниваются с данными, полученными из данных библиотеки ENDF/B-VIII.0. В важном для термоядерной технологии диапазоне низких энергий (от 0 до 0.1 МэВ) наши результаты показывают достаточно хорошее согласие с экспериментальными данными, тогда как в диапазоне высоких энергий полученные результаты несколько занижены из-за нерезонансных уровней ядра ⁵Не, которые не учитываются в расчетах. Полученные результаты показывают, что модели могут быть использованы для будущих приложений термоядерного синтеза.

Ключевые слова: термоядерный синтез, R-матрица, кулоновские функции, коэффициент туннелирования, коэффициент сдвига, сечение, скорость реакции.

Introduction

Thermonuclear fusion reactions play a significant and vital role in both fundamental and applied physics [1]. Firstly, these processes are widely recognized as the primary mechanisms responsible for the formation of elements in the Universe, known as nucleosynthesis [2]. Secondly, the significant energy release from thermonuclear fusion reactions has enabled the practical application of nuclear fusion technologies for producing energy [3]. Nuclear fusion has consistently attracted humanity due to several fundamental features: it reaches remarkably high power densities; it depends on plentiful fuel sources; it emits no greenhouse gases throughout its operations and shows minimal carbon impact across its lifecycle [4]; its intrinsic safety arises from the absence of chain reactions (where reactants differ from reaction products, preventing uncontrolled fusion escalation if control is lost). Progressing in our comprehension of nuclear fusion reactions and overcoming technical challenges, nuclear fusion presents the potential to become a new and effective energy source in the future.

Although various thermonuclear fusion fuel options exist, modern fusion reactors mostly use deuterium and tritium as fuel. The main reasons are the abundant availability of these isotopes, favourable reaction kinetics, high energy release, and the relatively lower temperature requirements essential for achieving controlled and efficient nuclear fusion [5]. In addition, taking into account the present level of technological advancement and the particular requirements of controlled fusion reactions, the use of deuterium and tritium enhances the opportunity of nuclear fusion to become a viable energy source.

In this article, we consider a step-by-step calculation of the resonant deuterium-tritium fusion cross section within the framework of the phenomenological R-matrix method. The main formalism of the R-matrix method is presented, precise Coulomb functions for the D+T, ${}^{4}\text{He}+{}^{12}\text{C}$ systems have been calculated, the penetration and shift factors for the D+T system have been obtained, and the cross sections and reaction rates for the deuterium-tritium fusion reaction have been determined by choosing different R-matrix models with parameters obtained from modern scientific papers.

Methods

R-matrix formulation

The general detailed formalism of the R-matrix theory is shown in works [6-7]. In this paper, we consider the main principles of the R-matrix method as well as the main mathematical calculations essential for the determination of the fusion cross sections and reaction rates.

In the framework of the R-matrix method, the configuration space is divided in two parts [8]. The first is the internal region, characterized by a radius a, where it is important to consider the nuclear interaction between the colliding nuclei. The second is the external region, where there is only the Coulomb interaction. The physics of the problem is derived from real and energy-independent parameters E_{λ} and γ^{λ} , known as the energy and the reduced width of pole λ [8].

The R-matrix in the case of a multichannel problem with N poles can be expressed as

$$R_{ij}(E) = \sum_{\lambda=1}^{N} \frac{\gamma_i^{\lambda} \gamma_j^{\lambda}}{E_{\lambda} - E},$$
(1)

where E_{λ} and γ_i^{λ} are the energy and reduced width in channel *i*. As it is shown in work [6], from Eq. (1) one can easily deduce the collision matrix *U* as follows

$$U(E) = (Z^{*}(E))^{-1}Z(E), \qquad (2)$$

where the matrix Z(E) is expressed as

$$Z_{ij}(E) = I_i(E)\delta_{ij} - a\sqrt{k_ik_j}R_{ij}(E)I'_j(E).$$
 (3)

In Eq. (3), k_i and k_j are the wave numbers in channels *i* and *j*, respectively, and the ingoing Coulomb function $I_i(E)$ is given by

$$I_i(E) = e^{i\omega_i}[G_i(E) - iF_i(E)], \qquad (4)$$

where ω_i is the Coulomb phase shift, $F_i(E)$ and $G_i(E)$ are the regular and irregular Coulomb functions, respectively, calculated at $k_i a$ (the derivative $I'_j(E)$ is also calculated with respect to this value). The outgoing Coulomb function is defined as

$$O_i(E) = I_i^*(E). \tag{5}$$

In the case of a two-channel reaction using the singlepole approximation (N = 1) [8], we can assume that

$$R_{12}^2 = R_{11}R_{22}. (6)$$

Using Eq. (6), we easily obtain the elements of the collision matrix U

$$U_{11} = \frac{I_1}{O_1} \frac{1 - R_{11}L_1^* - R_{22}L_2}{1 - R_{11}L_1 - R_{22}L_2'},$$
$$U_{22} = \frac{I_2}{O_2} \frac{1 - R_{11}L_1 - R_{22}L_2^*}{1 - R_{11}L_1 - R_{22}L_2},$$
(7)

$$U_{12} = U_{21} = \frac{2ia\sqrt{k_1k_2}\sqrt{R_{11}R_{22}}}{O_1O_2(1 - R_{11}L_1 - R_{22}L_2)}$$

where the function $L_i(E)$ is given by

$$L_{i}(E) = k_{i}a \frac{O_{i}'(E)}{O_{i}(E)} = S_{i}(E) + iP_{i}(E).$$
(8)

In Eq. (8), $S_i(E)$ is the shift-factor, and $P_i(E)$ is the penetration factor.

The nuclear fusion cross section corresponds to the transfer cross section from channel 1 to channel 2, and, in the case of partial wave J^{π} [8], it can be obtained as

$$\sigma_{1\to 2} = \frac{\pi}{k_1^2} \frac{(2J+1)(1+\delta)}{(2J_1+1)(2J_2+1)} |U_{12}|^2, \qquad (9)$$

where J_1 and J_2 are the spins of the colliding nuclei, δ is the Kronecker delta, equal to 1 or 0 for symmetric and nonsymmetric systems, respectively. Using Eq. (7), one can easily obtain the value of $|U_{12}|^2$ as

$$|U_{12}|^2 = \frac{4a^2k_1k_2R_{11}R_{22}}{(G_1^2 + F_1^2)(G_2^2 + F_2^2)|1 - R_{11}L_1 - R_{22}L_2|^2}.$$
(10)

For more convenience, we have omitted the explicit energy dependence of the Coulomb functions and R-matrices in Eq. (10). Now, introducing the formulas for the penetration factors P_1 and P_2

$$P_1 = \frac{k_1 a}{G_1^2 + F_1^2}, \quad P_2 = \frac{k_2 a}{G_2^2 + F_2^2}, \quad (11)$$

and, using Eq. (8), deriving that

$$|1 - R_{11}L_1 - R_{22}L_2|^2 = (1 - R_{11}S_1 - R_{22}S_2)^2 + (R_{11}P_1 + R_{22}P_2)^2,$$
(12)

we can rewrite Eq. (10) as follows

$$|U_{12}|^2 = \frac{4P_1P_2R_{11}R_{22}}{(1 - R_{11}S_1 - R_{22}S_2)^2 + (R_{11}P_1 + R_{22}P_2)^2}.$$
(13)

Choosing the one-pole, two-channel R-matrix, given by Eq. (1), one can simply obtain

$$|U_{12}|^2 = \frac{4P_1P_2\gamma_1^2\gamma_2^2}{(E_1 - E - \gamma_1^2S_1 - \gamma_2^2S_2)^2 + (\gamma_1^2P_1 + \gamma_2^2P_2)^2}.$$
(14)

Eq. (14) can be expressed in a more concise form by introducing the total width and the level shift, considered below in this paper.

The penetration and shift factors based on precise Coulomb functions

In this section, we explore the penetration and shift factors, which play an important role in the obtaining of the fusion cross sections at low energies. These energies correspond to so-called stellar conditions. Generally, in this range of energies the scattering of charged nuclei mostly depends on the Coulomb interaction [2]. Therefore, we can neglect the inner structure of nuclei. Thus, we have a two-body Coulomb problem defined by the following radial Schrödinger equation at the center-of-mass energy E for a given angular momentum l:

$$-\frac{\hbar^2}{2\mu m_N} \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right) g_l(r) + \frac{Z_1 Z_2 e^2}{r} g_l(r) = E g_l(r), \tag{15}$$

where \hbar is the reduced Planck's constant, μ is the reduced mass of the colliding nuclei, μ_N is the nucleon mass, Z_1 and Z_2 are the charge numbers, e is the elementary charge, $g_l(r)$ is the radial wave function, which depends on the magnitude of the relative coordinate r.

The regular and irregular Coulomb functions, $F_i(E)$ and $G_i(E)$, respectively, shown in Section 2, are the solutions of Eq. (15). In terms of the dimensionless parameters ρ and η , we have $g_l(\eta, \rho)$, and Eq. (15) becomes

 $g'' + \left[1 - \frac{2\eta}{\rho} - \frac{l(l+1)}{\rho^2}\right]g = 0,$

where
$$\rho = kr$$
, $k = \sqrt{2\mu m_N E/\hbar^2}$, $\eta k = Z_1 Z_2 e^2 \mu/\hbar^2$, and $' \equiv d/d\rho$. Therefore, we can rewrite Coulomb functions as $F_l(\eta, \rho)$ and $G_l(\eta, \rho)$, respectively, defining the Sommerfeld parameter η given by

$$\eta \approx 0.1575 Z_1 Z_2 \sqrt{\frac{\mu}{E}},\tag{17}$$

where μ is measured in MeV.

The regular Coulomb function $F_l(\eta, \rho)$, expressed with hyper-geometric functions [9], is given by

$$F_{l}(\eta,\rho) = C_{l}(\eta)\rho^{l+1}e^{i\omega\rho}{}_{1}F_{1}(1+l+i\omega\eta;2l+2;-2i\omega\rho),$$
(18)

where $\omega = \pm 1$, and the normalizing Gamow factor $C_l(\eta)$ can be obtained as follows

(16)

$$C_{l}(\eta) = 2^{l} \exp\left[\frac{-\pi\eta + \left[\ln\left(\Gamma(1+l+i\eta)\right) + \ln\left(\Gamma(1+l-i\eta)\right)\right]}{2} - \ln\left(\Gamma(2l+2)\right)\right], \quad (19)$$

where the natural logarithm of the gamma function $\ln(\Gamma(z))$ is implied.

The irregular Coulomb function $G_l(\eta, \rho)$ is calculated as follows

$$G_l(\eta,\rho) = \frac{F_l(\eta,\rho)\cos(\chi) - F_{-l-1}(\eta,\rho)}{\sin(\chi)}, \quad (20)$$

where $\chi = \sigma_l - \sigma_{-l-1} - (l+1/2)\pi$ and $\sigma_l(\eta) = (\ln(\Gamma(1+l+i\eta)) - \ln(\Gamma(1+l-i\eta)))/(2i)$. Here $\sigma_l(\eta)$ is the Coulomb phase shift [9].

Although the analytical expressions for the Coulomb wave functions in Eq. (18)-(20) may appear to be simple, their numerical computation presents significant challenges. Consequently, numerous papers have explored the computation of the Coulomb wave functions [10-15]. Nonetheless,

significant parts of the complex plane have not been investigated due to both numerical and theoretical limitations. In this paper, we have applied a precise method to compute the Coulomb wave functions with all of its arguments complex, as detailed in [9].

The precise Coulomb functions in the deuterium-tritium (D+T) system are shown in Figure 1. The center-of-mass energy is E = 0.064 MeV, the relative orbital momentum of the colliding nuclei is l = 0, and the dimensionless parameter ρ is in the range from 0 to 12. In addition, we have used the Coulomb amplitude A_l given by



Figure 1 – Precise Coulomb functions for the deuterium-tritium (D+T) system. The red solid line corresponds to $F_l(\eta, \rho)$, the blue solid – to $G_l(\eta, \rho)$, and the black dashed – to the amplitude $A_l(\eta, \rho)$.

Using the parameters, indicated in Eq. (16)-(17), the penetration and shift factors, at a radius a, can be obtained by

$$P_l(E,a) = \frac{ka}{F_l^2(\eta,ka) + G_l^2(\eta,ka)}$$

$$S_{l}(E, a) = [F_{l}(\eta, ka)F'_{l}(\eta, ka) + G_{l}(\eta, ka)G'_{l}(\eta, ka)]P_{l}(E, a), (22)$$

where the derivatives of the Coulomb functions are calculated at ka.

The penetration factors $P_l(E, a)$ for a deuteriumtritium (D+T) system are illustrated in Figure 3. From the Figure 3, it can be inferred that, depending on the increase of the radius *a*, the penetration factor for the D+T system in the S-wave state (l = 0) negligibly varies, and, in contrast, in the D-wave state (l = 2) slightly grows.

The shift factors $S_l(E, a)$ for the D+T system in the S-wave (l = 0) and D-wave (l = 2) states are shown in Figures 4 and 5. As in the case of the penetration factor, it can be noticed from Figure 4 that the values of the S-wave state shift factor

$$A_{l} = \sqrt{F_{l}^{2} + G_{l}^{2}}.$$
 (21)

As an additional example, we also provide here the graph for the precise Coulomb functions in the case of the ⁴He+¹²C system (see Figure 2). The center-of-mass energy is E = 3 MeV, the relative orbital momentum of the colliding nuclei is l = 0, and the dimensionless parameter ρ is in the range from 0 to 20.



Figure 2 – Precise Coulomb functions for the ⁴He+¹²C system. The red solid line corresponds to $F_l(\eta, \rho)$, the blue solid – to $G_l(\eta, \rho)$, and the black dashed – to the amplitude $A_l(\eta, \rho)$.

insignificantly increase depending on the growth of the radius a. In the D-wave state (see Figure 5) the values of the shift factor grow gradually with an increase in the radius a.



Figure 3 – Penetration factors for the D+T system. The blue solid line corresponds to l = 0, a = 5 fm, the green solid – to l = 2, a = 5 fm, the red dotted – to l = 0, a = 6 fm, and the green dashed – to l = 2, a = 6 fm.



Figure 4 – Shift factors for the D+T system in the Swave state (l = 0). Solid and dashed lines correspond to a = 5 fm and a = 6 fm, respectively.



Figure 5 – Shift factors for the D+T system in the D-wave state (l = 2). Solid and dashed lines correspond to a = 5 fm and a = 6 fm, respectively.

Results and Discussion

D-T fusion cross section

The integrated fusion cross section of the $J^{\pi} = 3/2^{+} {}^{3}\text{H}(d,n)^{4}\text{He}$ nuclear reaction in the one-level, two-channel R-matrix approximation [16] can be defined as

$$\sigma_{dn}(E) = \frac{\pi}{k_d^2} \frac{2J+1}{(2J_1+1)(2J_2+1)} |S_{dn}|^2, \quad (23)$$

where k_d and *E* are the center-of-mass deuteron wave number and energy, respectively, $J_1 = 1$ and $J_2 = 1/2$ are the spins of the colliding nuclei (deuteron and tritium), and J = 3/2 is the resonance spin, $|S_{dn}|$ is the scattering matrix element. In Eq. (23), the scattering matrix element [16] is given by

$$|S_{dn}|^{2} = \frac{\Gamma_{d}\Gamma_{n}}{(E_{1} + \Delta - E)^{2} + (\Gamma/2)^{2}},$$
 (24)

where E_1 is the level eigenenergy, Γ_d and Γ_n are the partial widths of the ³H+d (l = 0) and ⁴He+n (l = 2) channels, Γ is the total width, Δ is the level shift. The total width and the level shift are given by

$$\Gamma = \sum_{c} \Gamma_{c}, \ \Gamma_{c} = 2\gamma_{c}^{2}P_{c},$$
$$\Delta = \sum_{c} \Delta_{c}, \ \Delta_{c} = -\gamma_{c}^{2}(S_{c} - B_{c}), \qquad (25)$$

where γ_c^2 is the reduced width, P_c and S_c are the penetration and shift factors, respectively, defined in Section 3, and B_c is the boundary condition parameter. Assuming that $B_c = 0$, the square scattering matrix element $|S_{dn}|^2$ can be easily obtained, using Eq. (14), defined in Section 2. Thus, we have presented the complete step-by-step calculation of the resonant deuterium-tritium nuclear fusion cross section. In addition, it should be noted that we have not shown the results for the penetration and shift factors for the ⁴He+n system (these properties can be easily calculated as it is shown in Section 3). Nevertheless, we have accurately included these results into our calculations.

In this paper, we have used two different Rmatrix models with parameters obtained in recent papers [17-18]. The channel radii were chosen to be equal in model 1 [17], whereas, in model 2 [18], these radii are different. The full list of the R-matrix parameters is shown in Table 1. The obtained deuterium-tritium fusion cross sections are illustrated below in Figure 6. To compare our results with modern evaluated data, we have also included the results obtained from the ENDF/B-VIII.0 library [19]. In the range from 0 to 0.1 MeV, the results of both models are in good agreement with the ENDF/B-VIII.0 library data. However, since our calculations only consider the resonant level $J^{\pi} = 3/2^+$, fusion cross sections are slightly underestimated for energies exceeding 0.1 MeV. Consequently, it is important to include non-resonant levels of 5He in future calculations. Nevertheless, the energy range from 0 to 0.1 MeV is the most significant for nuclear fusion technology. Therefore, the results from both models are suitable for future considerations within the context of thermonuclear fusion applications.

Model	a _d , fm	a_n , fm	B_d	B _n	E ₁ , MeV	$\gamma_d^2,$ MeV	γ_n^2 , MeV
Model 1 [17]	7	7	-0.59	-2	0.179	0.324	0.0122
Model 2 [18]	5.56	3.633	-0.2721	-0.3874	0.0420	3.23	0.133

 Table 1 – Parameter values for one-level twochannel R-matrix



Figure 6 – Deuterium-tritium fusion cross sections in different R-matrix models. The blue solid line corresponds to model 1 [17], the orange solid – to model 2 [18], the green solid – to the results of the ENDF/B-VIII.0 library [19]

Thermonuclear reaction rates

The reaction rate is obtained as follows [20]

$$N_A \langle \sigma v \rangle = N_A \frac{(8/\pi)^{1/2}}{\mu^{1/2} (k_B T)^{1/2}} \int_0^\infty \sigma(E) E \exp(-E/k_B T) dE,$$
(26)

where N_A is the Avogadro number, k_B is the Boltzmann constant, T is the temperature, v is the relative velocity. Integration is executed utilizing energies within the center-of-mass framework, while the distribution of nuclei conforms to a Maxwellian pattern.

Thermonuclear reaction rates for the D-T nuclear fusion reaction, obtained in different R-matrix models, are illustrated in Figure 7. As mentioned earlier, we have employed two models and examined the results from the ENDF/B-VIII.0 library [19]. Between temperatures ranging from 0 to 0.1 MeV (0 to $1.1604 \cdot 10^9$ K), the results of both models demonstrate a strong alignment with the ENDF/B-VIII.0 library data. However, at higher temperatures, the models appear to deviate slightly from the reference data. In general, the obtained results are in a good agreement with the ENDF/B-VIII.0 library results.

Conclusion

In this paper, we have presented a detailed analysis of the resonant deuterium-tritium (D-T) fusion cross section in the framework of the phenomenological R-matrix method. The main focus has been on using precise Coulomb functions to accurately determine penetration and shift factors, essential for the calculation of the fusion cross sections and reaction rates. We have outlined the fundamental principles of the R-matrix formalism,



Figure 7 – Thermonuclear reaction rates for the D-T fusion reaction in different R-matrix models. The blue solid line corresponds to model 1 [17], the orange solid – to model 2 [18], the green solid – to the results of the ENDF/B-VIII.0 library [19]

showing step-by-step calculations for the D-T fusion reaction. The precise Coulomb functions for the D+T systems have been calculated. Based on these functions, the penetration and shift factors for the D+T system have been obtained, providing accurate inputs for further calculations of the D-T fusion cross sections and reaction rates. In addition, we have calculated the precise Coulomb functions for the ${}^{4}\text{He}+{}^{12}\text{C}$ system.

The D-T fusion cross sections and reaction rates have been calculated using different R-matrix

models. Two different models with parameters from recent scientific papers have been used, and the obtained results have been compared with the ENDF/B-VIII.0 library [19] data. The cross sections and reaction rates in the low-energy range from 0 to 0.1 MeV (0 to $1.1604 \cdot 10^9$ K in units of temperature) are in good agreement with the reference data. However, at higher energies the results in both models are slightly underestimated, since non-resonant levels of ⁵He have not been considered in our calculations. Nevertheless, as mentioned earlier,

energies in the range from 0 to 0.1 MeV are especially crucial in nuclear fusion technology. Therefore, the results of both models are appropriate for future considerations in thermonuclear fusion applications.

Acknowledgments

This research was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP14871936).

References

1 Lw W., Duan H., Liu J. Enhanced deuterium-tritium fusion cross sections in the presence of strong electromagnetic fields // Phys. Rev. C. – 2019. – Vol. 100. – P. 064610.

2 Descouvement P. Nuclear Reactions of Astrophysical Interest // Front. Astron. Space Sci. – 2020. – Vol. 7. – N $_{2}$ 9. – P. 1-15.

3 Meschini S., Laviano F., Ledda F., Pettinari D., Testoni R., Torsello D., Panella B. Review of commercial nuclear fusion projects // Front. Energy Res. – 2023. – Vol. 11. – P. 1157394.

4 Banacloche S., Gamarra A.R., Lechon Y., Bustreo C. Socioeconomic and environmental impacts of bringing the sun to earth: A sustainability analysis of a fusion power plant deployment // Energy. – 2020. – Vol. 209. – P. 118460.

5 Abdou M. et al. Physics and technology considerations for the deuterium–tritium fuel cycle and conditions for tritium fuel self sufficiency // Nucl. Fusion -2021. - Vol. 61. - P. 013001.

6 Lane A.M., Thomas R.G. R-Matrix Theory of Nuclear Reactions // Rev. Mod. Phys. – 1958. – Vol. 30. – P. 257-353.

7 Descouvement P., Baye D. The R-matrix theory // Rep. Prog. Phys. – 2010. – Vol. 73. – P. 036301.

8 Angulo C., Descouvemont P. R-matrix parametrizations of low-energy transfer reactions // Nucl. Phys. A. – 1998. – Vol. 639. – P.733-747.

9 Michel N. Precise Coulomb wave functions for a wide range of complex l, eta and z // Comput. Phys. Comm. – 2007. – Vol. 176. – P. 232-249.

10 Tamura T., Rybicki F. Coulomb functions for complex energies // Comput. Phys. Comm. – 1969. – Vol. 1. – P. 25-30.

11 Takemasa T., Tamura T., Wolter H.H. Coulomb functions with complex angular momenta // Comput. Phys. Comm. – 1979. – Vol. 17. – P. 351-355.

12 Barnett A.R. Continued-fraction evaluation of Coulomb functions $F\lambda(\eta, x)$, $G\lambda(\eta, x)$ and their derivatives // J. Comput. Phys. – 1982. – Vol. 46. – P. 171-188.

13 Thompson I.J., Barnett A.R. COULCC: A continued-fraction algorithm for Coulomb functions of complex order with complex arguments // Comput. Phys. Comm. – 1985. – Vol. 36. – P. 363-372.

14 Seaton M.J. Coulomb functions for attractive and repulsive potentials and for positive and negative energies // Comput. Phys. Comm. – 2002. – Vol. 146. – P. 225-249.

15 Noble C.J. Evaluation of negative energy Coulomb (Whittaker) functions // Comput. Phys. Comm. – 2004. – Vol. 159. – P. 55-62.

16 Barker F.C. 3/2+ levels of 5He and 5Li, and shadow poles // Phys. Rev. C. - 1997. - Vol. 56. - P. 2646-2653.

17 Hale G.M., Brown L.S., Paris M.W. Effective field theory as a limit of *R*-matrix theory for light nuclear reactions // Phys. Rev. C. – 2014. – Vol. 89. – P. 014623.

18 de Souza R.S., Boston S.R., Coc A., Iliadis C. Thermonuclear fusion rates for tritium + deuterium using Bayesian methods // Phys. Rev. C. – 2019. – Vol. 99. – P. 014619.

19 Brown D.A, Chadwick M., Capote R., Kahler A., Trkov A., Herman M. et al. ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data // Nucl. Data Sheets. – 2018. – Vol. 148. – P. 1-142.

20 Descouvemont P., Adahchour A., Angulo C., Coc A., Vangioni-Flam E. Compilation and R-matrix analysis of Big Bang nuclear reaction rates // At. Data Nucl. Data Tables. – 2004. – Vol. 88. – P. 203-236.

References

1 W. Lw, H. Duan, J. Liu, Phys. Rev. C, 100, 064610 (2019).

2 P. Descouvemont, Front. Astron. Space Sci., 7 (9), 1-15 (2020).

3 S. Meschini, F. Laviano, F. Ledda, D. Pettinari, R. Testoni, D. Torsello, B. Panella, Front. Energy Res., 11, 1157394 (2023).

- 4 S. Banacloche, A.R. Gamarra, Y. Lechon, C. Bustreo, Energy, 209, 118460 (2020).
- 5 M. Abdou et al., Nucl. Fusion, 61, 013001 (2021).
- 6 A.M. Lane, R.G. Thomas, Rev. Mod. Phys., 30, 257-353 (1958).
- 7 P. Descouvemont, D. Baye, Rep. Prog. Phys., 73, 036301 (2010).
- 8 C. Angulo, P. Descouvemont, Nucl. Phys. A, 639, 733-747 (1998).
- 9 N. Michel, Comput. Phys. Comm., 176, 232-249 (2007).
- 10 T. Tamura, F. Rybicki, Comput. Phys. Comm., 1, 25-30 (1969).
- 11 T. Takemasa, T. Tamura, H.H. Wolter, Comput. Phys. Comm., 17, 351-355 (1979).
- 12 A.R. Barnett, J. Comput. Phys., 46, 171-188 (1982).
- 13 I.J. Thompson, A.R. Barnett, Comput. Phys. Comm., 36, 363-372 (1985).
- 14 M.J. Seaton, Comput. Phys. Comm., 146, 225-249 (2002).
- 15 C.J. Noble, Comput. Phys. Comm., 159, 55-62 (2004).
- 16 F.C. Barker, Phys. Rev. C, 56, 2646-2653 (1997).
- 17 G.M. Hale, L.S. Brown, M.W. Paris, Phys. Rev. C, 89, 014623 (2014).
- 18 R.S. de Souza, S.R. Boston, A. Coc, C. Iliadis, Phys. Rev. C, 99, 014619 (2019).
- 19 D.A. Brown, M. Chadwick, R. Capote, A. Kahler, A. Trkov, M. Herman et al. Nucl. Data Sheets., 148, 1-142 (2018).

20 P. Descouvemont, A. Adahchour, C. Angulo, A. Coc, E. Vangioni-Flam, At. Data Nucl. Data Tables, 88, 203-236 (2004).

Article history:

Received 01 April 2024 Received in revised form 13 June 2024 Accepted 15 June 2024 **Мақала тарихы**: Түсті – 01.01.2024 Түзетілген түрде түсті – 13.06.2024 Қабылданды – 15.06.2024

Information about authors:

1. **Olzhas Bayakhmetov** (corresponding author) – PhD, Institute of Nuclear Physics (Almaty, Kazakhstan, email: <u>bayakhmetov.o.s.92@gmail.com</u>).

2. **Sayabek Sakhiyev** – Doct. of Phys. and Math. Sc., Prof. Institute of Nuclear Physics (Almaty, Kazakhstan, email: <u>s.sakhi@inp.kz</u>).

Авторлар туралы мәлімет:

1. Олжас Баяхметов (автор корреспондент) – PhD, Ядролық физика институты (Алматы қ., Қазақстан, email: bayakhmetov.o.s.92@gmail.com).

2. Саябек Сахиев – физ.-мат.ғыл. докт, проф., (Алматы қ., Қазақстан, email: <u>s.sakhi@inp.kz</u>).