MATHEMATICAL MODELLING OF THE PROCESS OF WATER RADIOLYSIS UNDER THE INFLUENCE OF LOW-ENERGY ELECTRONS

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Abstract*:* The radiolysis process of water under the impact of low - energy electrons (E = 1; 2:5; 5; 10 keV) was mathematically modeled using Monte-Carlo, single collision and pacing methods on the base of Mathcad program. The radiation-chemical yields of the physical (single ionized molecular orbitals - $H_2O_j^+(1a_1, 2a_1, 1b_2, 3a_1, 1b_1), e_{sub}^-$ electron - lost its energy up to a primary electron - excited energy and electron-excited states: H_2O^* (A^1B_1, B^1A_1, Rydberg state, diffusion band, dissociative excitation and plasmon- H_2O^{**})) and physicochemical(OH, e_{aq}^-, H, H_3O^+, H_2, H_2O_2, HO_2, O_2, OH^-, O_2^-, HO_2^-) phase products of the non-elastic collision of electrons and water molecules were calculated.

Keywords: Effective cross-section, excitation under, radiation-chemical yield, non-elastic collision, molecular orbitals.

1. Introduction

Low(0.05÷10 keV), moderate (10÷100 keV) or high (100÷5000 keV) energy electrons gradually loose their kinetic energy while passing through the water in elastic and non-elastic collision with water molecules. According to the mechanism of radiation energy loss at the physical phase of the non-elastic collision process ($< 10¡15$ *sec:*) intermediate particles such as $H_2O_j^+(1a_1, 2a_1, 1b_2, 3a_1, 1b_1)$, -direct single ionization of several molecular orbitals (*MO*), e_{sub}^- electron-lost its energy up to a primary electron-excited energy and electron-excited states: intermediate particles such as A^1B_1; B^1A_1 Rydberg state (*Ry*), diffusion band(*ab*), dissociative excitation (*de*) and plasmon (*ce*-collective excitation) are generating. As these particles have a strong effect on the physical, chemical, biological processes progressing in water and water solutions, it's possible to predict events which are likely to happen in the future by studying their roles in different fields of science (atomic, nuclear and plasma physics, astrophysics, modelling of atmospheric phenomena, radiochemistry, radiobiology etc.). Therefore, to theoretically and experimentally study the generation and consumption of these products is one of the main problems.
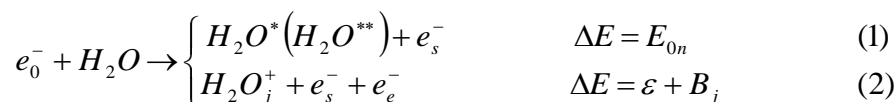
The authors of [1-6] have defined effective cross-section of ionization process of MO of water molecule$(e^-, 2e^-)$ with electron impulse, by applying various experimental methods. But the authors of [7-16] have given empiric equations in different approaches corresponded to the estimates of effective cross-section of ionization, obtained from experience, by using different theoretical approaches. There's no reference regarding water molecule excitation under an electron impact yet. Only authors [17-19] determined water electron-excitation states using a photoabsorption spectroscopy method. At the present time authors [20-24] have theoretically calculated the effective cross-section of water electron-excitation states using different polyempirical methods on the base of the experimental results. The total effective cross-section of electron-water molecule scattering was identified by authors [25-30]. While comparing the

results of the experimental and theoretical calculations it becomes evident that at the values of energy more than 30 *eV* they coincide but at lower values some deviations are observed. The radiation-chemical yields of the products generated at both phases (physical and physicochemical) of the water radiolysis process were theoretically calculated by authors [31-41] according to different approaches. There are some conformities with some errors between the theoretical and experimental results of different authors and our results. In the given work the radiolysis process of water (liquid phase) under the impact of low-energy (T = 0.5, 1.0, 1.5, 2.0 *keV*) electrons were mathematically modeled.

It has been calculated the radiation-chemical yield of initial products which can be formed in the both physical ($<10^{-15}$ san), and physical-chemical ($10^{-15} \div 10^{-12}$ san) stages of process. The radiation - chemical yields of the primary products which were likely to generate in the physical ($<10^{-15}$ san) and physicochemical ($10^{-15} \div 10^{-12}$ san) phases of the process were calculated. The more improved formula of Mott equation [7] was used to determine the effective cross – section of ionization process of molecular orbitals (*MO*), and the equations proposed by different authors were used to determine the effective cross - sections of electron - excited states of different types [13] in the model. Calculation was made on the base of Mathcad program using Monte-Carlo, single collision and pacing methods.

2. Theoretical methods and obtained results

The energy balance between low-energy electrons and water molecules during a non-elastic collision can be simply expressed by $T = E_s + \Delta E$, here *T* and E_s are accordingly kinetic energies of an electron before and after collision, ΔE is the energy transferred to water molecule by an electron during collision. This energy is used for an electron-excitation of water molecule (1) and direct single ionization (2) of molecular orbitals (*MO*) (1a$_1$, 2a$_1$, 1b$_2$, 3a$_1$, 1b$_1$)

$$e_0^- + H_2O \rightarrow \begin{cases} H_2O^*\left(H_2O^{**}\right) + e_s^- & \Delta E = E_{0n} \quad (1) \\ H_2O_j^+ + e_s^- + e_e^- & \Delta E = \varepsilon + B_j \quad (2) \end{cases}$$

Here e_0^-, e_s^- and e_e^- are accordingly incident, scattered and ejected electrons, $H_2O_j^+$, $H_2O_i^*$, H_2O^{**} –are correspondingly ionization, excitation and extreme excitation (plasmon) states of j-th MO of water molecule.

The transferred energy$\left(\Delta E\right)$ during these processes equals to an excitation energy of a molecule $\left(E_{0i}\right)$ in (1) case and the sum of the kinetic energy of an ejected electron from *j*-molecular orbital- ε and bound energy B_j of the correspondent orbital in (2) case.

Kinetic energies of scattered and ejected electrons may accordingly change $E_s = 0 \div T - B_j$, $\varepsilon = 0 \div \dfrac{T - B_j}{2}$.

A more improved formula [3,7] of Mott equation was used to calculate the effective cross - section of the single ionization of water molecule's *j-th MO*:

$$\frac{d\sigma_j(\varepsilon)}{d\varepsilon} = \frac{4\pi N_j a_0^2 R^2}{T + B_j + U_j} \left\{ \frac{1}{\left(\varepsilon + B_j\right)^2} - \frac{1}{\left(\varepsilon + B_j\right)\left(T - \varepsilon\right)} + \frac{1}{\left(T - \varepsilon\right)^2} + \frac{3U_j}{3}\left[\frac{1}{\left(\varepsilon + B_j\right)^3} + \frac{1}{\left(T - \varepsilon\right)^3}\right] \right\} \quad (3)$$

here, U_j and N_j are the kinetic energy and number of an electron correspondent to *j-th MO*, a_0-Bohr radius, $R = 13{:}61 \ eV$ is Rydberg energy. The values of B_j, N_j and U_j according to different molecular orbitals were given in Table 1.

Table 1 Radiation - chemical yield of direct single ionization corresponding to molecular orbitals (MO) of water molecule ($1a_1$, $2a_1$, $1b_2$, $3a_1$, $1b_1$) under the influence of low-energy electrons.

Molecular Orbitals	N_j	B_j, eV	U_j, eV	T, keV			
				0.5	1	1.5	2.0
$1a_1$	2	539.7	793.4	1.661	1.596	1.561	1.541
$2a_1$	2	36.88	70.71	1.056	1.028	1.011	0.997
$1b_2$	2	19.83	48.36	0.578	0.570	0.564	0.560
$3a_1$	2	15.57	59.52	0.187	0.201	0.207	0.214
$1b_1$	2	12.61	61.91	0.000	0.0005	0.0011	0.0020

If we integrate the (3) expression for all possible values of ejected electrons'energies, i.e. from $\varepsilon = 0$ up to $\varepsilon_{max} = \dfrac{T - B_j}{2}$, we can get the expression describing the dependence of ionization effective cross - section on the kinetic energy of a primary (Fig.1) electron during non-elastic collision corresponding to *j-th MO*:

$$\sigma_j(T) = \int\limits_0^{\varepsilon_{max}} \frac{d\sigma_j(\varepsilon, T)}{d\varepsilon} d\varepsilon \qquad (4)$$
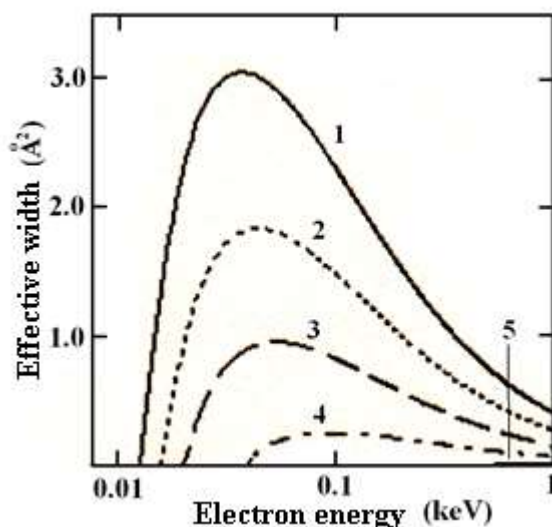

Fig. 1. Dependence of the effective cross - section of a direct single ionization corresponding to j-th MO of water molecules on its kinetic energy under the impact of low – energy electrons

In order to get the total effective cross - section of ionization (Fig.1, curve 2) we should to sum the (4) expression according to the number of molecular orbitals (*MO*) [11]:

$$\sigma_{ion}(T) = \sum_{j=1}^{N_{MO}} \sigma_j(T) \qquad (5)$$

Here $N_{MO} = 5$ is the number of molecular orbitals (*MO*) of a water molecule.

During non-elastic collision between electrons and water molecules the effective cross-section of electron transformation from a ground state (0) to (n) excited state was calculated on the base of Cobut's formula of Kutcher and Green's equation:

$$\frac{d\sigma_i(T,\varepsilon)}{d\varepsilon} = \rho(T,\varepsilon)f_i(T)ln\left[\frac{\alpha(T)T}{\varepsilon}\right]\varepsilon \tag{6}$$

here, $\rho(T,\varepsilon) = \frac{4\pi a_0^2}{T}\left(\frac{R}{\varepsilon}\right)^2$, $\alpha(T) = 4 - e^{-\frac{T-E_{0,i}}{\alpha_i}}$, $f_i(T) = f_{0,i}\sqrt{\frac{\alpha_i}{\pi}}e^{[-\alpha_i](T-E_{0,i})^2}$ are constants corresponding to junction and $E_{0,i}$ [13] is an excitation energy. If we integrate (6) expression according to electron energy $0 \rightarrow n$ junction

$$\sigma_{0,n}(T) = \int_{E_{0,i}}^{T-E_{0,i}} \frac{d\sigma_i(T,\varepsilon)}{d\varepsilon}d\varepsilon \tag{7}$$

we will get the value of effective cross-section..Constants for each junction were choosen according to the values of radiation-chemical yield obtained from experiments. The value of constants $(f_{0,i}, \propto_{0,i})$ and E_{0n}, used in calculations were given in table 2. In Fig.2 the dependence of effective cross-sections of electron-excitation states (A^1B_1, B^1A_1, Rydberg state, diffusion band, dissociative excitation and plasmon (ce)) in water on their kinetic energy under the influence of low energy electrons calculated according to expression(7) were described.

In order to obtain totally effective cross-section (figure 3) of electron-excitation, (7) expression should be summed according to the number of excitation states.

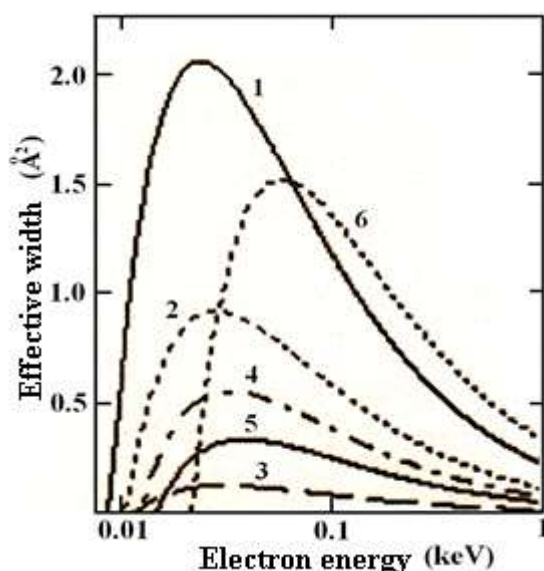$$\sigma_{exc}(T) = \sum_n \sigma_{0,n}(T) \tag{8}$$

Fig. 2. The dependence of effective cross-sections of electron-excitation states (1- A^1B_1, 2- B^1A_1, 3-Rydberg state (Ry), diffuse band (db), dissociative excitation (de) and plasmonic (ce)) of water molecules under the influence of low energy electrons on their kinetic energy

Primary electrons or δ-electrons of a new generation formed by them lose part of their energy during each non-elastic collision and this process continues till the next non-elastic collision of an electron energy. The amount of the moderate energy ΔE (T) lost during each non-elastic collision of the electron with T energy with a water molecule was taken as an equivalent to the following expression [38, 39, 41]:

$$\Delta E(T) = \sum_n P_{0n}(T)E_{0n} + \sum_j P_j(T)\varepsilon_i(T) \tag{9}$$

Here: $P_{0n}(T) = \dfrac{\sigma_{0n}(T)}{\sigma_{tot}(T)}$ is the probability of transformation into n-excited state, $P_j(T) = \dfrac{\sigma_j(T)}{\sigma_{tot}(T)}$ is the probability of event occurrence corresponding to ionization of j-th MO, $\sigma_{tot}(T) = \sum_n \sigma_{0n}(T) + \sum_j \sigma_j(T)$ - is totally effective cross-section (figure 3), $\varepsilon_j(T) = \int_{B_j}^{T} \varepsilon \dfrac{d\sigma_j(T)}{d\varepsilon} d\varepsilon$ – is the moderate energy calculated for forming of one electron-positive ion pair in j-th MO by the electron with T energy.

On the base of model the calculations were made for the single ionization of five molecular orbitals and six electron-excitation states of water molecules. The calculated values of the single ionization correspondent to 1a1, 2a1, 1b2, 3a1, 1b1 molecular orbitals (*MO*) were given in Table 1, and in Table 2 the calculated values of the radiation-chemical yields of *A*1*B*1, *B*1*A*1, Rydberg state (*Ry*), diffusion band (*db*), dissociative excitation (*de*) and plasmon (*ce*) electron-excited states were given.
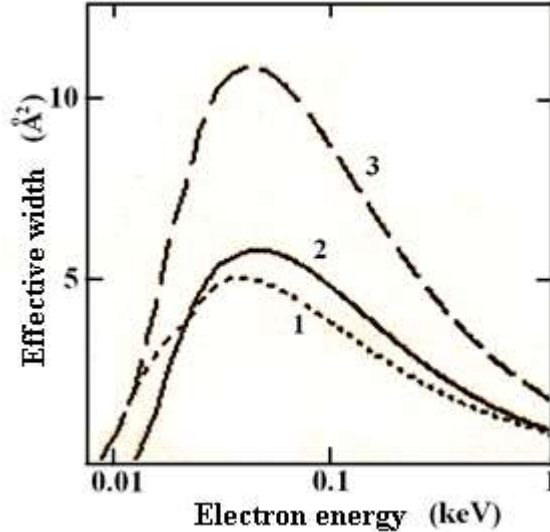

Fig. 3. Dependence of electron-excitation (1) $\sigma_{exc}(T) = \sum_n \sigma_{0n}(T)$, *MO ionization (2)* $-\sigma_{ion}(T) = \sum_j \sigma_j(T)$

states in water under the influence of low energy electrons and the totally effective cross-section
(3) $-\sigma_{tot}(T) = \sigma_{exc}(T) + \sigma_{ion}(T)$ *on their energies*

The calculated values of single ionization correspondent to 1a_1, 2a_1, 1b_2, 3a_1, 1b_1 molecular orbitals (MO) were given in the Table 1 and in Table 2 the calculated values of the

radiation-chemical yield of A^1B_1, B^1A_1, Rydberg state (Ry), diffuse band (db), dissociative excitation (de) and plasmonic (ce) electron-excited states were given.

Table 2 Radiation-chemical yield of electron-excited states (A^1B_1, B^1A_1, Rydberg state (Ry), diffusion band (db), dissociative excitation (de) and plasmon (ce)) formed in the water under the influence of low-energy electrons

Electron-excitation states	Electron-excitation energy, eV	Constants		T, keV			
		f_i	α_i	0.5	1.0	1.5	2.0
A^1B_1	8.4	0.2770	3	0.906	0.869	0.857	0.845
B^1A_1	10.1	0.1400	4	0.419	0.407	0.376	0.359
Ry	12.26	0.0205	6	0.058	0.054	0.045	0.035
ab	12.93	0.1000	4	0.275	0.271	0.248	0.240
de	14.1	0.0840	2	0.211	0.211	0.212	0.214
ce	21.4	0.5300	0.8	1.050	1.093	1.118	1.134

Physical phase products at the next physicochemical phase: at the result of e_{sub}^- - electrons' elastic collision and dipole relaxation and transform into thermal electrons and consequently solvates ($e_{sub}^- \rightarrow e_{aq}^-$), H_2O+ ions transform into $H3O+$ ion and OH radical at the result of an ion-molecular reaction, and electron-excited molecules generate their next products due to relaxation, auto- ionization and dissociation.

The next products which were likely to be generated by the products of the physical phase in the course of $\sim 10^{-12}$ sec were given in Table 3.

Table 3 The percentage of products which are likely to be generated in physical-chemical stage by products of physical phase in water

Physical stage products	$\dfrac{G}{100eV}$	Forming channels	Percentage, %
e_{sub}^-	3.4	e_{aq}^-	100
H_2O^+	3.4	$H_3O^+ + OH$	100
A^1B_1	0.869	$\begin{cases} H_2O \\ H + OH \end{cases}$	$\begin{cases} 35 \\ 65 \end{cases}$
B^1A_1	0.407	$\begin{cases} H_2O \\ H_2 + H_2O_2 \\ H_3O^+ + OH + e_{aq}^- \\ H + OH \\ 2H + O \end{cases}$	$\begin{cases} 23 \\ 3.1 \\ 50 \\ 20 \\ 3.9 \end{cases}$
(Ry, db, de)	0.536	$\begin{cases} H_2O \\ H_3O^+ + OH + e_{aq}^- \end{cases}$	$\begin{cases} 50 \\ 50 \end{cases}$
ce	1.093	$\begin{cases} H_3O^+ + OH \\ H^* + OH \end{cases}$	$\begin{cases} 92.2 \\ 7.8 \end{cases}$

In the calculation carried out by us the radiation- chemical yield of products generated in the physical and physicochemical phase of the radiolysis process progressing in the course of $\sim 10^{-12}$sec were determined and obtained results (Table 4) were given in comparison with the theoretical [31,42] and experimental [43,44,50,51] ones obtained by different authors.

Table 4 Radiation - chemical yield generated in the physicochemical phase ($10^{-15} \div 10^{-12}$san) of the radyolysis prosess processing in the steam under the influence of low-energy electrons

Initial products	Turner [42]	Kaplan [31]	Experimental results [31,42]	Our results
OH	8.4	5.85	5.9	5.52
e_{aq}^-	6.3	5.16	4.7	4.875
H	2.1	0.61	0.7	0.765
H_3O^+	6.3	5.16	4.8	4.875
H_2	0.3	0.39	0.45	0.029
H_2O_2	0.3	0.39	-	0.013

The results obtained for the radiation-chemical yields of the active intermediate products generated in the physical and physicochemical phases of the radiolysis process progressing in water, calculated on the base of our model from the theoretical calculations and experiments conducted by different authors according to different approaches conform with some errors. The processes progressing in water and water solutions under the impact of ionizing radiation (electron and γ -quantum) can be calculated on the base of this model. The model can be used to determine the processes progressing in aerosols of the atmosphere under the effect of space rays, changes in water and water solutions used in atomic and nuclear power-engineering as an energy-carrier or for different purposes, the nano-, micro and total absorption dose during radiating ancological patients by electrons and γ quantum in the same and different directions as well as for the minimum selection of by-effects.

References

1. M.A.Bolorizadeh, M.E.Rudd, Phys.Rev.A, 1986, 33, 882-6
2. K.W.Hollman, G.W.Kerby, M.E.Rudd, J.H.Miller, S.T.Manson , Phys.Rev.A 1988, 38, 3299
3. B.G.Lindsay and M.A.Mangan, in Photon and Electron Interactions with Atoms, Molecules and Ions, Landolt- Börnstein Vol. I/17, Subvolume C, edited by Y. Itikawa (Springer, New York, 2003)
4. H.C.Straub, B.G.Lindsay, K.A.Smith, and R.F.Stebbings, J.Chem. Phys.,1998, 108, 109
5. M.V.V.S.Rao, I.Iga, and S.K.Srivastava, J.Geophys. Res., 1995, 100, 26421
6. J.Schutten, F.J. de Heer, H.R.Moustafa, A.J.H. Boerboom, and J.Kistemaker, J.Chem.Phys., 1966, 44, 3924
7. Y.-K.Kim, M.E.Rudd, Phys.Rev.A 1994, 50, P.3954-3967
8. M.Coplan, J.H.Moore, J.P.Doering, Rev.Mod.Phys. 1994, 66, P.985
9. Y.-K.Kim, W.Hwang, N.M.Weinberger, M.A.Ali, M.E.Rudd, J.Chem.Phys., 1997, 106 (3), 1026-1033
10. Dingfelder, D.Hantke, M.Inokuti, H.G.Paretzke, Radiat.Phys.Chem., 1998, 53, 1-18
11. Y.-K.Kim, W.R.Johnson, M.E.Rudd, Phys.Rev.A 2000, 61, 032702
12. M.A.Haynes, B.Lohmann, J.Phys.B, 2000, 33, 4711
13. Y.-K.Kim, J.P.Desclaux, Phys.Rev.A 2002. 66. 012708-12

14. D.Emaietzoglou,K. Karava, G.Papamichael, M.Moscovich, Phys.Med.Biol., 2003, 48, 2355
15. W.Hwang, Y.-K. Kim, and M. E. Rudd, J.Chem.Phys., 1996, 104, 2956
16. C.Champion, J.Hanssen, and P.A.Hervieux, J.Chem.Phys., 2002,117, 197
17. W.F.Chan, G.Cooper, and C.E.Brion, Chem.Phys., 1993, 178, 387
18. Gürtler, V. Saile, and E.E.Koch, Chem.Phys. Lett., 1977, 51, 386
19. Chutjian, R. I. Hall, and S. Trajmar, J.Chem.Phys.,1975, 63, 892
20. D. Gorfinkiel, L.A.Morgan, and J.Tennyson, J. Phys. B, 2002, 35, 543
21. W.A.Goddard III and W.J.Hunt, Chem.Phys.Lett., 1974, 24, 464
22. N.W.Winter, W.A.Goddard III, and F.Bobrowicz, J.Chem.Phys., 1975, 62, 4325
23. J.J.Olivero, R.W.Stagat, and A.E.S.Green, J.Geophys.Res., 1972, 77, 4797
24. M.Zaider, D.J.Brenner, and W.E.Wilson, Rad.Res., 1983, 95, 231
25. C.Szmytkowski, Chem.Phys.Lett., 1987, 136, 363.
26. A.Zecca, G.Karwasz, S.Oss, R.Grisenti, and R.S.Brusa, J.Phys. B. 1987, 20, 1253
27. H.Nishimura and K.Yano, J.Phys.Soc.Jpn., 1988, 57, 1951
28. Z.Saglam and N.Aktekin, J.Phys. B. 1990, 23, 1529
29. Z.Saglam and N.Aktekin, J.Phys. B. 1991, 24, 3491
30. M.Kimura, O.Sueoka, A.Hamada, and Y.Itikawa, Adv.Chem.Phys., 2000, 111, 537
31. I.G.Kaplan and V.Y.Sukhonosov. Radiat.Res., 1991, 127:1-10,
32. M.Dingfelder, M.Inokuti, H.G.Paretzke // Radiat.Phys.Chem., 2000, 59, 255
33. D.Emaietzoglou // Radiat.Phys.Chem., 2003, 66. 373
34. C.Champion, J.Hanssen, P.A.Hervieux, Phys.Rev.A, 2001, 63, 052720
35. C.Champion, J.Hanssen, P.A.Hervieux // Phys.Rev.A, 2002, 65, 022710
36. D.S.Milne-Brownlie, S.J.Cavanagh, B.Lohmann, C.Champion, P.A.Hervieux, J.Hanssen Phys.Rev.A, 2004, 69, 032701
37. Y.-K.Kim // Phys.Rev. A, 2001, 64, P.032713
38. A.A.Garibov, Y.D.Jafarov, Ye..A.Shirshov 4-th International Confrence "Nuclear and Radiation Physics" Almaata, 2003, p. 335-337
39. Y.D.Jafarov,A.A.Garibov, International Confrence "Physical-chemical processes in Nonorganic Materials, Kemerevo, Russia, 2004, v.1, p. 32-34
40. S. Uehara, H. Nikjoo, J.Radiat.Res., 2006, 47, 69-81
41. Y.D.Jafarov, M.R.Hasanova, F.N.Nurmammadova The fifth Eurazian conference Nuclear science and its application Ankara, 2008, 95-96
42. Y.D.Jafarov Mathematical modelling of radiolysis proses of water under the impact of low-energy electrons, Problems of atomic science and technology, 2011, N5, Series: Nuclear Physics Investigations (56), 42-47
43. J.E.Turner, R.N.Hamm, H.A.Wrighr, R,H.Rachie, J.L.Magee, A.Chatterjee, W.E.Bolch Radiat. Phys. Chem., 1988, 32, 503
44. H.G.Paretzke, J.E.Turner, R.N.Hamm, H.A.Wright, R.H.Ritchie, J.Chem.Phys., 1986, 84:3182
45. E.A.Bigildeev and V.Michalik. Radiat.Phys.Chem., 1992, 47:197
46. S.M.Pimblott and A.Mozumder, J.Phys.Chem., 1991, 95:7291
47. Ballrini F.,Biggi M.,Merzagova M.,Ottolenghi A.,Dingfelger M.,Friedland W.,Jacob P. and Peretzke H.G. Radiat.Environ.Biophys.,2000, 39, 179
48. G.J.Kutcher and A.Green, Radiat.Res., 1976, 67:408
49. V. Cobut, Y. Frongillo, J. P. Patau, T. Gouler, M.-J. Fraser, J.-P. Jay-Gerin, Radiat. Phys. Chem., 1998, 51, 229-43
50. A.K.Pikayev, Modern radiation chemistry. Radiolysis of basin and liguids. M.: Science, 1986, p. 440

51. V.L.Bugaenko, V.M.Byakov, V.L.Grishkin// Second All-Union. Conf. of theor. J. Radiation chemistry. Obninsk, Proc. rep. M .: Research Institute tech.- studies, 1990, p. 29.

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ПРОЦЕССА РАДИОЛИЗА ВОДЫ ПОД ВЛИЯНИЕМ НИЗКОЭНЕРГЕТИЧЕСКИХ ЭЛЕКТРОНОВ

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***Резюме*:** Процесс радиолиза воды под воздействием низкоэнергетических электронов (E = 1; 2: 5; 5; 10 кэВ) математически моделируется методом Монте-Карло, однократным столкновением и методом стимуляции на базе программы Mathcad. Были вычислены радиационно-химические выходы физических (однократно ионизированных молекулярных орбиталей $H_2O_j^+(1a_1, 2a_1, 1b_2, 3a_1, 1b_1)$, e_{sub}^- электрон - потерял свою энергию до первичного электрона – возбужденные энергетические и электронно-возбужденные состояния: H_2O^* (A^1B_1, B^1A_1, Ридберговское состояние, диффузионная полоса, диссоциативное возбуждение и плазмон H_2O^{**})) и физико-химические (OH, e_{aq}^-, H, H_3O^+, H_2, H_2O_2, HO_2, O_2, OH^-, O_2^-, HO_2^-) фазовые продукты неупругого соударения электронов и молекул воды.

Ключевые слова: Эффективное сечение, случаи возбуждения, радиационно-химический выход, неупругое соударение, молекулярные орбитали.

KİÇİK ENERJİLİ ELEKTRONLARIN TƏSİRİ ALTINDA SUYUN PARÇALANMASI PROSESİNİN RİYAZİ MODELLƏŞDİRİLMƏSİ

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Xülasə: Kiçik enerjili elektronların təsiri altında suyun parçalanması prosesi (E = 1; 2:5; 5; 10 keV) Monte Karlo, sadə toqquşma və addımlama metodlarından istifadə edilərək Matchad proqramı əsasında riyazi modelləşdirilmişdir. Su molekulları və elektronların qeyri elastik toqquşmasının fiziki (sadə ionlaşdırılmış molekulyar orbitallar- $H_2O_j^+(1a_1, 2a_1, 1b_2, 3a_1, 1b_1)$, öz enerjisini əsas elektron həyəcanlanma enerjisinə qədər itirmiş e_{sub}^- elektronu və elektron həyəcanlanma halları: H_2O^* (A^1B_1, B^1A_1, Ridberq halı, diffuzyon zolaq, dissosiativ həyəcanlanma və plazmon-$H2O^{**}$)) və fiziki-kimyəvi (OH, e_{aq}^-, H, H_3O^+, H_2, H_2O_2, HO_2, O_2, OH^-, O_2^-, HO_2^-) faza məhsullarının radiasiya-kimyəvi çıxımı hesablanmışdır.

Açar sözlər: Effektiv en-kəsiyi, həyəcanlanma halları, radiasiya-kimyəvi çıxış, qeyri elastik toqquşma, molekulyar orbitallar.