Cascade-probabilistic methods and solution of Boltzmann type of equations for particle flow

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Abstract. A new method for calculating the spatial and temporal distributions of secondary particles and passing through a substance called cascade-probabilistic (HF) was proposed, developed and described. Original problems in the application of the original CP-technique in radiation physics, cosmic ray and positron physics was resolved. The general expression for the Boltzmann equation for the steady and unsteady cases was recorded based on an analysis of all the studies. In case of one-dimensional and three-dimensional (coordinate and angles $\vartheta$ and $\varphi$) Boltzmann equations solution goes into the previously obtained expressions for $N_m$. In addition, all previously derived analytical expressions for flow of different particles: protons, neutrons, electrons, concentration of defects, etc. are obtained after simplifying. At the same calculations give satisfactory agreement with experimental data.

1. Introduction

The intensive development of nuclear physics, especially nuclear energy, space research, the creation of various types of accelerators and nuclear reactors, obtaining materials and composites with desired properties using radiation caused interest in the study and quantitative description of the processes of interaction, education and distribution of primary and secondary particles in condensed and gaseous media \cite{1-3}. As it is known, that during the passage of particles through matter happen quite complex and diverse events that are important both theoretical and practical significance for nuclear physics, solid state physics and other fields of science and technology. First of all, it refers to the dosimetry and protection from radiation, cosmic ray physics, radiation physics, solid state physics, neutron physics and reactors, radiation chemistry, biology and medicine, radioisotope analysis, monitoring and defectoscopy, nuclear geophysics and geology and especially lately radiation technology to manufacture materials with desired physical and chemical properties \cite{4-7}.

Naturally, in order to understand and describe these phenomena, on the one hand, it is necessary to know what happens to the particles (both primary and secondary, to generate different kinds of collisions). Thus one of the main problems in this case is to establish spatio-temporal and energy distributions of the incident and the secondary particles in the environment. In addition, at the time, and also after the passage of particles through the substance almost all physical and chemical properties of the substance and its structure are changed. In the description of these processes, there is a problem of choice of theoretical research method. The most famous and widely used theoretical methods of calculation – is the Monte Carlo method, the Boltzmann equation, Focker-Planck equation, and a variety of specialized methods and models. Without belittling the well-known numerical methods and models, apparently, it can be said that the indisputable advantages over them possess analytical methods, even with their help manage only approximately describe a phenomenon \cite{1-3}.

2. The history of CP-method

The history of CP-method associated with name of the great mathematician of the last century, S.D. Poisson, particularly with the distribution of random variables, named in his honor. Poisson distribution for certain values of parameters contained in it becomes a simple cascade-probability function. Initially, it was used in calculation of angular distributions and flow of secondary particles
and meteorological factors without sufficient rigorous study. So, Goudsmit and Saunderson were able to create an approximate theory of multiple scattering in 1940, when describing angular distribution of electrons. Later, [1] using the simplest CP-functions calculations of integral multiplicities, coupling coefficients and meteorological factors and energy distribution of nucleon component of cosmic radiation in the Earth's atmosphere, as well as the neutron flow from the sun are made. In addition, energy spectrum of π-mesons in the earth's atmosphere was calculated. Despite the fact that in these studies achieved good agreement between theoretical calculations and experimental data, yet most CP-functions for different particles was not found. It is unclear role and place of these studies by comparing obtained results with CP-functions with similar distributions calculated by Monte Carlo methods and Boltzmann equation. Some clarity on these issues to a certain extent have been done in [1], in which CP-functions were derived for different stable, unstable particles and antiparticles as recurrence relations, and from Boltzmann equation, detailed mathematical analysis were done, basic physical properties, as well as the calculated spatial distribution of radiation defects in metals irradiated by electrons, protons and alpha particles were established. CP-method has been successfully used in calculation of average positron thermalization, angular distributions of annihilation photons and simulation of defects in depth with experimental data on positron annihilation [8–10].

3. Results

On the basis of general principles of cascade-probabilistic (CP) method and analysis of our fifty years research we recorded general solution of equations of unsteady cascade process (Boltzmann type) for the m-th component of any particle (including generation and elimination of phase space and their passage through substance to predetermined depth).

As it is known that Boltzmann equation – the equation of kinetic theory of gases, proposed L. Boltzmann for determination particle distribution function of an ideal monatomic gas [1, 2]. Equation in dimensionless variables for the m-th component of particles:

$$\frac{\partial f_m}{\partial t} + (\nu, \nabla_v f_m) + (F, \nabla_v f_m) = \frac{1}{\varepsilon} L(f_m, f_m)$$

Here $f(x, \nu, t)$ – distribution function density of number of particles in phase space $x \otimes \nu$, $x$ – three-dimensional space coordinate, $\nu$ – speed, $t$ – time, $F$ – density of external mass forces, $\varepsilon$ – dimensionless parameter (proportional to ratio of average distance that particles pass without collision, characteristic to scale of phenomena under consideration). Collision operator $L$ in the simplest case is as follows:

$$L(f_m, f_m) = \int \left[ f_m(\nu') f_m(\nu_j') - f_m(\nu) f_m(\nu_j) \right] d \omega$$

where $\nu_1$ and $\nu$ – velocity of molecules before collision, $\nu_j$ and $\nu_j'$ – velocity of molecules after collision, $d \omega$ – element of area in a plane perpendicular to $\nu_1 - \nu$ vector.

In deriving Boltzmann equation it is assumed that evolution of $f_m(x, \nu, t)$ function is determined by its value at the time $t$ and binary collisions between gas molecules and reaction time of two molecules of collision gas is much less than time during which they move as free particles. From mathematical point of view, conclusion of Boltzmann equation is a specific algorithm for developing $L$ operator on the basis of the known laws of motion of two colliding with other gas molecules.

In equation (1) scope of variable $t$ – half: $t \geq 0$, range of variation $\nu$–all space $R^3$, range of $x$ – subdomain $\Omega$ in $R^3$ ($\Omega$ may coincide with $R^3$). Physically, function $f(x, \nu, t)$ must be non-negative and such that

$$\int f_m(x, \nu, t) \nu^2 d \nu < \infty,$$

The simplest boundary condition on $d \Omega$ is as follows:
where \( n \) – normal to \( d\Omega \). There are several different precise performances of Cauchy problem for equation (1), but existence of a whole solution of (1) natural from physical point of view of assumptions about \( L \) operator had been proved for none of them. Passing in (1) distribution function to the flow of particles in a spherical coordinate system based on an analysis [1], it is offered general solution of non-stationary equation of system of Boltzmann equations for m-th component of particles (including generation and elimination of particles from phase volume) within cascade-probabilistic method in the form of:

\[
N_m(x, y, z, \theta, \phi, E, t) = \sum_{i} \sum_{n} \int_{\nu, \nu', \nu''} N_{0i}(t = 0, x', y', z', \theta', \phi', E') \frac{1}{\lambda_0 \cos \theta_0} \cdot
\]

\[
\cdot \chi_0(x', y', z', \theta', \phi', E', t') \frac{d\sigma}{\sigma_0 d\Omega dE_0} dV_0 J_n \cdots
\]

\[
\cdot \frac{1}{\lambda_n \cos \theta_n} \chi_{0n}(x^n, y^n, z^n, \theta^n, \phi^n, E^n, t^n) \frac{d\sigma}{\sigma_n d\Omega dE_n} dV_n J_n,
\]

where, \( N_{0i}(x, y, z, \theta, \phi, E, t) \) – intensity of m-th particles at \( x, y, z \), under zenith \( \theta \) and azimuth \( \phi \); \( \chi_i \) – probability pass a way \( r_i \) at angles \( \theta, \phi \) with energy \( E \); after \( n \) interaction; \( \frac{d\sigma}{d\Omega dE} \) – differential cross section for interaction; \( dV_n(x_n, y_n, z_n) \) – volume element; \( J_n \) – Jacobian transformation; \( i, n, k \) – number of generations of interactions and reaction channels.

The integral \( \chi_{0+\chi_n} \) switches to CPF and further to Poisson distribution. At present, we calculate optimal coefficients and simple sixty fold integrals, which allow solving huge number of problems with \( \sim 15\% \) error. It is planned to calculate parameters for hundredfold and more integral. All previously derived formulas for probabilities of flows and various primary and secondary particles (stable and unstable), concentrations of defects in irradiated materials charged, neutral particles, and others were found from obtained solutions. Further, mathematical analysis of expression for flow of m-th component was performed and it was shown that asymptotic value of intensity of particles in phase space \( v(x, y, z, t) \), having a real physical meaning can be found from it [1]. Moreover, considered processes can take place both to passage of micro (nano) particles (portions) and with birth of new stable and volatile particles. It is shown that in general case, solution can be represented as a sum of multiple integrals.

The mathematical analysis of the found expression for the particle flow was performed.

1. From (2) it follows that \( x = x', y = y', z = z' \) and \( t = 0 \)

\[
N_m(x, y, z, \theta, \phi, E, t) = N_{0i}(t = 0, x, y, z, \theta', \phi', E'),
\]

where \( N \) – flow of particles, \( x, x', y, y', z, z' \) and \( t \) – coordinates and time, \( \theta \) and \( \phi \) – zenith, azimuthal angles. In this case, the flow is equal to flow of primary particles.

2. From obtained equation (2) with \( x \to \infty \), or \( y \to \infty \), or \( z \to \infty \), or \( t \to \infty \), follows that

\[
N_m(x, y, z, \theta, \phi, E, t) \to 0.
\]

This is easy to show, because each cascade-probability function has an exponent (with negative exponent), which for infinite values of parameters in each term of sum tends to zero.

3. If (2) to put \( i = 0, n = 0 \) and \( k = 0 \), case of vertical incidence of one type of particles on substance (such as plates), we obtain:

\[
N_m = N_{0e} e^{- \frac{n}{\lambda_0}}.
\]
4. In case of one-dimensional and three-dimensional (coordinate and angles $\theta$ and $\varphi$) Boltzmann equations solution (2) goes into the previously obtained expressions for $N_m$ (formulas 1.36 and 1.40 from [1]).

5. In addition, all previously derived analytical expressions for flow of different particles: protons, neutrons, electrons, concentration of defects, etc. are obtained after simplifying (2). At the same calculations give satisfactory agreement with experimental data [1].

4. Conclusion

1. General solution of the nonstationary Boltzmann type equations for the $m$-th component of particles (including the generation and elimination of particles from the phase volume) within the cascade-probabilistic method was proposed.

2. It is shown that for $x = x', y = y', z = z'$ and $t = 0$

$$N_m(x, y, z, \theta, \varphi, E, t) = N_{0m}(t = 0, x', y', z', \theta', \varphi', E').$$

and for $x \rightarrow \infty$, or $y \rightarrow \infty$, or $z \rightarrow \infty$, or $t \rightarrow \infty$ on the basis of mathematical analysis of expression for particles flow.

3. After simplifying (2) it is possible to get all the previously derived analytical expressions for particles flows that give satisfactory agreement with experiment.

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References

[1] Boos E G, Kupchishin A I, Kupchishin A A, Shmygalev E V and Shmygaleva TA 2015 Relations to Markov chains (Almaty: Abay KazNPU. RINCT, al-Farabi Kazakh National University, LLP "Kama") 388

[2] Vinogradov Ed IM 1977 Mathematical Encyclopedia "Soviet Encyclopedia" V.1 (M.) 1152

[3] Boltzmann L 1956 Lectures on theory of gases/translated from german (M.)

[4] Kupshishin A I, Potatyi K V and Chukurova R M 1987 Cryst. Latt. Defects and Amorphous Mater. I3 (34) 157 – 162

[5] Klimenko I V, Zhuravleva T S, Lenenko N D and Zhuravleva Yu V 2009 Zhurnal Physicheskoihimii 83 346 –350

[6] Harnutova E P, Petrov E I 2004 Journal Materials Research 19(7) 1924

[7] Lappan U, Fuchs B, Geifiler U, Scheler U, Lunkwitz K 2003 Rad. Phys. Chem. 67 (4) 447

[8] Boos E G, Kupchishin A I 1988 The solution of physical problems by cascade-probabilistic method (Alma-Ata: Nauka) Part 1 112 Part 2 144

[9] Kupchishin A A, Kupchishin A I and Shmygaleva T A 2007 Computer modeling of radiation-physical problems (Almaty: Kazakh University) 432

[10] Kupchishin A I, Lisitsin A A and Kupchishin A A 2014 The interaction of high-energy radiation with matter (Tomsk: Tomsk Polytechnic University) 153