# OPTIMIZATION MATHEMATICAL MODELS OF BEAM DYNAMICS IN THE INJECTION SYSTEMS WITH REAL GEOMETRY *

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**Abstract**
At the present paper new mathematical models for optimization of the intense beam dynamics in injection systems are suggested. The real geometry of the accelerating-focusing structure is considered. Optimization technique for beam formation systems is proposed. Investigations have been made for low-energy beam injection system in linear RFQ accelerator.

**Key words**
Beam control, Modeling, Nonlinear dynamics, Numerical methods

## 1 Introduction

Currently, linear and cyclic accelerators are widely used in various fields of science and technology. Increasing attention is paid to design and creation of the accelerator complexes providing precise beams. The charged particle beams formation system is an important part of an accelerator complex and largely determines its output characteristics. Increasing requirements for accelerators necessitates the development and improvement of mathematical models of beam formation systems and optimization techniques for beam dynamics [Ovsyannikov and Egorov, 1998; Ovsyannikov, Ovsyannikov, Vorogushin, Svistunov and Durkin, 2006; Kozynchenko and Svistunov, 2006].

When optimizing the dynamics of a beam, different physical (structural) parameters of the accelerating-focusing system are usually considered as control functions. To reduce the beam dynamics calculation time the external electromagnetic field at each optimization step is usually approximated by analytical expressions obtained for the simplified model of a real system. To design the accelerating-focusing structures that provide beams with required characteristics, there is a need in development of the mathematical models and beam dynamics optimization techniques, enabling the optimization in the fields, closer to real ones.

In this paper we present new mathematical models for optimizing the dynamics of intense charged particle beams in accelerating-focusing systems in which focusing and acceleration of particles is carried out by electrostatic field. Again, we propose the optimization technique where the external field at each step of optimization is defined as a solution of the boundary value problem for Laplace equation over the entire region occupied by the field. An example of nonlinear optimization problem solving for a low-energy ion beam injection system is presented.

## 2 Description of the optimization problem for non-relativistic charged particle beam formation systems

The dynamics of charged particles in the external field is considered with regard to the beam space charge, and is described by the following system of integro-differential equations

$$\left.\begin{aligned} &\frac{dX}{dt} = V,\\ &\frac{dV}{dt} = \frac{1}{m_p} f_1\left(t, X, \varphi\left(X,u\right)\right) + \\ &\quad \frac{1}{m_p}\int_{M_{t,u}} f_2\left(t, X, V, \xi\right)\rho\left(t,\xi\right)d\xi = \\ &\qquad\qquad f_3\left(t, X, V, u\right),\\ &X\left(t_0\right) = X_0,\ V\left(t_0\right) = V_0,\ \left(X_0, V_0\right) \in M_0. \end{aligned}\right\} \quad (1)$$

$$\frac{\partial\rho(t,\eta)}{\partial t} + \frac{\partial\rho(t,\eta)}{\partial\eta} f\left(t,\eta,u\right) + \rho\left(t,\eta\right) div_\eta f\left(t,\eta,u\right) = 0 \quad (2)$$

$$\rho\left(t_0,\eta\right) = \rho_0\left(\eta\right). \quad (3)$$

*THIS WORK WAS PARTIALLY SUPPORTED BY THE RUSSIAN FOUNDATION FOR BASIC RESEARCH (PROJECT 09-01-90416).

Here $t \in T_0 = [t_0\, T]$ – independent variable (time), the parameters $t_0$, $T$ are fixed; $m_p$, $X(t) \in R^3$, $V(t) \in R^3$ – mass, position, and velocity of a charged particle respectively; $u = (u_1, u_2, ..., u_p) \in D$ – vector of control parameters, where $D \subset R^p$ – limited and closed set; $\eta = (X, V) \in R^6$ – position of charged particle in phase space; $\varphi \in C^2(G)$ – potential of external electric field, where the $G \subset R^3$ – limited and open set; function $f_1(t, X, \varphi(X, u))$ describes the external field force; the selection of the function $f_2(t, \eta, \xi)$ determines the way of simulation of Coulomb interaction of charged particles; vector-function $f(t, \eta, u) = (V(t), f_3(t, \eta, u))$; $\rho(t, \eta)$ – the particles distribution density by virtue of the system (1); $\rho_0(\eta)$ – given charge distribution density in space $M_0$ at a time $t_0$ , where $M_0 \subset R^6$ – a limited and closed set of nonzero measure; $M_{t,u} = \{X(t, X_0, u), V(t, V_0, u) : (X_0, V_0) \in M_0\}$ – image of the set $M_0$ by virtue of the system (1) under the vector of control parameters $u$ in time $t$.

At a given vector $u = \tilde{u}$, the electric field potential $\varphi$, defined and continuous in $\overline{G}$, is the solution of the boundary value problem for the Laplace equation

$$\Delta\varphi(\zeta, \tilde{u}) = 0, \quad \zeta \in G, \tag{4}$$

$$\varphi(\zeta, \tilde{u})_{\Gamma_G(u)} = \varphi_0(\zeta). \tag{5}$$

Here $\Gamma_G(\tilde{u}) = \bigcup_k \Gamma_k$ – border of the region $G$, consisting of piecewise smooth curves $\Gamma_k$; $\varphi_0(\zeta)$ – known function.

In the cross-sections of a beam of trajectories the following functional is involved, which characterizes the dynamics of the beam

$$I(u) = \int_0^T \int_{M_{t,u}} \Phi(t, \eta_t, \mu_{ks}^{(1,1)}, ...\mu_{ks}^{(i,j)}, ..., \mu_{ks}^{(N_t,N_t)}) d\eta_t dt, \tag{6}$$

where $\Phi$ – the function of parameters $t$, $\eta_t$ and $\mu_{ks}^{(i,j)}$; $\mu_{ks}^{(i,j)} = \int_{M_{t,u}} (\eta_i - \overline{\eta}_i)^k (\eta_j - \overline{\eta}_j)^s \rho(t, \eta_t)\, d\eta_t$ – moments of orders $k$, $s$ of the coordinates $\eta_i$, $\eta_j$; $\overline{\eta}_i = \int_{M_{t,u}} \eta_i \rho(t, \eta_t)\, d\eta_t$ – average values of coordinates $\eta_i$, $i, j = \overline{1, N_t}$; $N_t$ – number of particles in the beam at $t \in [t_0, T]$.

We will consider the problem of finding the vector $u^0 \in D$, delivering a minimum or maximum to the functional (6) under constraints

$$\left.\begin{array}{l} I \leq A^0, w_T = B^0, N_L \leq C^0 N_0, u_i \leq C^i, \\ i = \overline{1, p_1}, p_1 \leq p, \\ \frac{\left|u_{j+1}^e - u_j^e\right|}{z_j^e} < E_{pr}, \\ -\sum_{k=0}^{n^e} q_p \left(u_{k+1}^e - u_k^e\right) = w_T, \\ j = \overline{1, n^e - 1}, r^{\max} \leq D^0 r^a. \end{array}\right\} \tag{7}$$

or

$$\left.\begin{array}{l} I \geq A^0, w_T = B^0, N_L \leq C^0 N_0, u_0 \leq C^i, \\ i = \overline{1, p_1}, p_1 \leq p, \\ \frac{\left|u_{j+1}^e - u_j^e\right|}{z_j^e} < E_{pr}, \\ -\sum_{k=0}^{n^e} q_p \left(u_{k+1}^e - u_k^e\right) = w_T, \\ j = \overline{1, n^e - 1}, r^{\max} \leq D^0 r^a. \end{array}\right\} \tag{8}$$

Here $w_T$ – energy of the beam at the output of accelerating-focusing system; $N_0$ – number of beam particles at the inlet of accelerating-focusing system; $N_L$ – beam losses in an accelerating-focusing system; $r^{\max}$ – maximum beam radius; $r^a$ – radius of an aperture; $u_j^e$, $z_j^e$ – potentials and distances between the electrodes, respectively; $n^e$ – number of electrodes of accelerating-focusing system; $E_{pr}$ – given breakdown intensity of vacuum; $q_p$ – particle charge; $A^0$, $B^0$, $C^i$, $D^0 < 1$ – given values.

## 3 The problem of minimization of the non-relativistic beam emittance growth at the output of a beam formation system

Consider the problem of minimization of the beam emittance growth at the output of a beam formation system. This problem is described by the mathematical model (1) – (7), in which the functional (6) at the outlet of the accelerating-focusing system is defined as

$$I = \frac{A_3\sqrt{\tilde{D}_x^T \tilde{D}_{x'}^T - \tilde{K}_{xx'}^T{}^2} + A_4\sqrt{\tilde{D}_y^T \tilde{D}_{y'}^T - \tilde{K}_{yy'}^T{}^2}}{A_1\sqrt{\tilde{D}_x^0 \tilde{D}_{x'}^0 - \tilde{K}_{xx'}^0{}^2} + A_2\sqrt{\tilde{D}_y^0 \tilde{D}_{y'}^0 - \tilde{K}_{yy'}^0{}^2}} \tag{9}$$

where $A_1$, $A_2$, $A_3$, $A_4$ – given values, $\tilde{D}_x^T$ , $\tilde{D}_{x'}^T$, $\tilde{K}_{xx'}^T$, $\tilde{D}_y^T$, $\tilde{D}_{y'}^T$, $\tilde{K}_{yy'}^T$, $\tilde{D}_x^0$, $\tilde{D}_{x'}^0$, $\tilde{K}_{xx'}^0$, $\tilde{D}_y^0$, $\tilde{D}_{y'}^0$, $\tilde{K}_{yy'}^0$ determined by the formulas

$$\left.\begin{array}{l} \tilde{D}_x = \frac{1}{mes(M_{T,u})} \int_{M_{T,u}} x^2 \rho(t, \eta_T)\, d\eta_T, \\ \tilde{D}_{x'} = \frac{1}{mes(M_{T,u})} \int_{M_{T,u}} x'^2 \rho(t, \eta_T)\, d\eta_T, \\ \tilde{K}_{xx'} = \frac{1}{mes(M_{T,u})} \int_{M_{T,u}} x x' \rho(t, \eta_T)\, d\eta_T, \\ x' = v_x / v_z, \end{array}\right\} \tag{10}$$

$$\left.\begin{array}{l}\tilde{D}_y=\frac{1}{mes(M_{T,u})}\int_{M_{T,u}} y^2\rho\left(t,\eta_T\right)d\eta_T,\\ \tilde{D}_{y'}=\frac{1}{mes(M_{T,u})}\int_{M_{T,u}} y'^2\rho\left(t,\eta_T\right)d\eta_T,\\ \tilde{K}_{yy'}=\frac{1}{mes(M_{T,u})}\int_{M_{T,u}} yy'\rho\left(t,\eta_T\right)d\eta_T,\\ y'=v_y/v_z.\end{array}\right\} \quad (11)$$

The problem of finding the vector $u^0 \in D$, delivering a minimum to the functional (9) under the constraints (7), is considered.

## 4 The problem of matching of the non-relativistic beam at the output of beam formation system with acceptance of the following accelerating-focusing structure.

Consider the problem of matching of the non-relativistic beam at the output of the formation system with a given acceptance of the following accelerating-focusing structure. At the output of a formation system the following functional is considered

$$I(u)=\int_{M_{T,u}}\Phi_1\,\Phi_2\,dx_T dx'_T dy_T dy'_T, \quad (12)$$

where

$$\Phi_1\left(x_T,x'_T\right)=\begin{cases}1, & \left(x_T,x'_T\right)\in G_1\\ 0, & \left(x_T,x'_T\right)\notin G_1\end{cases}, \quad (13)$$

$$\Phi_2\left(y_T,y'_T\right)=\begin{cases}1, & \left(y_T,y'_T\right)\in G_2\\ 0, & \left(y_T,y'_T\right)\notin G_2\end{cases}, \quad (14)$$

$$G_1=\left\{\left(x_T,x'_T\right):S_1\left(x_T,x'_T\right)<1\right\}, \quad (15)$$

$$G_2=\left\{\left(y_T,y'_T\right):S_2\left(y_T,y'_T\right)<1\right\}, \quad (16)$$

$x'_T=v_{xT}/v_{zT}, y'_T=v_{yT}/v_{zT}$; $S_1\left(x_T,x'_T\right)=1$ and $S_2\left(y_T,y'_T\right)=1$ – ellipses, describing the given acceptance of the accelerating-focusing system, following the beam formation system, in planes $xx'$ and $yy'$ respectively.

The problem of finding of the vector $u^0 \in D$ delivering a maximum to the functional (12) under the constraints (8) is considered.

For solving the applied problems of optimization of injection systems for linear accelerators and cyclotrons, described by the mathematical model (1) – (8), at the present paper we propose the following optimization techniques, namely, based on the average gradient, Box-Wilson [Box and Draper, 1987; Law and Kelton, 2000; Montgomery, 2005] and ridge-valley [Gel'fand and Tsetlin, 1961] methods.

The optimization of beam dynamics is performed by choosing the physical (structural) parameters of an accelerating-focusing system. At each step of optimization process, instead of being approximated by analytical expressions, the external field is determined as a result of the solution of boundary value problem for the Laplace equation over the entire area occupied by the field in the accelerating-focusing system. The search for the extremum of the functional $I(u)$ is performed by the following ways:

- in the case of an arbitrary number of control parameters, the average gradient and ridge-valley methods are used in tandem. The average gradient method is applied in the first phase of the search for the rough localization of the functional extremum region. In the second stage by using the ridge-valley method, the more precise study of the extreme region is performed.
- in the case of a small number of control parameters ($p \leq 5$) the Box-Wilson gradient design method can be applied.
- in the case of a large number of optimization parameters, the coordinate descent method is applied followed by the ridge-valley method or the Box-Wilson technique (for the optimization with a part of parameters).

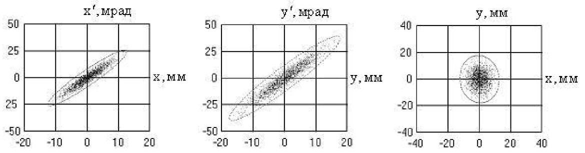
## 5 Matching of the low-energy $H^-$ ion beam at the output of the injection system with the acceptance of RFQ

Consider the problem of matching of the ion beam at the output of the injector with acceptance of linear accelerator with RFQ, described by the mathematical model in the form (1) – (5), (12) – (16).

We shell investigate the accelerating-focusing structures, consisting of five elliptical electrodes. At the input of the electrode system, the elliptical beam of ions $H^-$ with initial energy of 17 keV and current of 17 mA is considered. The characteristics of this beam are presented in Fig. 1. The beam energy at the injection system output is 100 keV. The set $M_0$ has the form

$$\begin{array}{l}M_0=\{(x,y,z,v_x,v_y,v_z):\\ \qquad |x|\leq 0.012,\ |x'|\leq 0.025,\\ \qquad |y|\leq 0.012,\ |y'|\leq 0.025,\\ \qquad c_0\leq |z|\leq c_0+0.018,\\ \qquad v_z=\sqrt{\frac{5.45\cdot 10^{-20}}{m\left(1+(x')^2+(y')^2\right)}},\\ \qquad v_x=x'v_z, v_y=y'v_z, c_0=const\}\end{array} \quad (17)$$

We consider the potentials of the electrodes, half-axis of the minimum electrode cross-sections, the distances between the electrodes, as well as the parameters that determine the shape of electrodes as components of the vector u. During the process of optimization, the parameters of the electrode system, not included in the vector $u$, had been taken constant.




(a) (b) (c)

Figure 1. Characteristics of an elliptic beam of ions $H^-$ at the outlet of the plasma-surface ion source Dudnikov type. (a) – the phase portrait of the beam in the plane $xx'$, (b) – the phase portrait of the beam in the plane $yy'$, (c) – particles density distribution in the plane $xy$.

Under given vector $u = \tilde{u}$ the external three-dimensional electrostatic field is determined as a result of solving the problem (4), (5) by finite-difference method [8] with the number of grid nodes $N^{sg} \approx 2000000$. The area, limited by dotted line as shown in Fig. 2, is considered as the region $G$. The boundary $\Gamma_G(\tilde{u}) = \bigcup_{i=1}^{n_\Gamma} \Gamma_i$ is defined by end points of the sections, such as segments of straight lines, arcs and circles, etc. Here $n_\Gamma$ is the given value. In order to eliminate gaps between electrodes, the segments of straight lines (for example, the section $\Gamma_q$ in Fig. 2) are used. On the various parts of the boundary $\Gamma_G$ (see Fig. 2) the boundary conditions (5) will be given by the following relations

$$\varphi(x, y, z_0)_{\Gamma_1} = \Phi_0, \tag{18}$$

$$\varphi(x_0, y_0, z)_{\Gamma_2} = \Phi_0 + (U_1^e - \Phi_0)\frac{z - z_1}{z_2 - z_1}, \tag{19}$$

$$\varphi(x, y, z)_{\Gamma_p} = U_j^e, \quad j = \overline{1, n_e}, \tag{20}$$

$$\varphi(x_0, y_0, z)_{\Gamma_q} = U_{i-1}^e + \left(U_i^e - U_{i-1}^e\right)\frac{z - z_{i-1}}{z_i - z_{i-1}}, \tag{21}$$

$$\varphi(x_0, y_0, z)_{\Gamma_{n_\Gamma - k}} = U_{n_e}^e - U_{n_e}^e \frac{z - z_{n_\Gamma - k - 1}}{z_{n_\Gamma - k} - z_{n_\Gamma - k - 1}}, \tag{22}$$

$$\varphi(x, y, z_0)_{\Gamma_{n_\Gamma - k + 1}} = \Phi_1, \tag{23}$$

where $x_0$, $y_0$, $z_0$ are given.

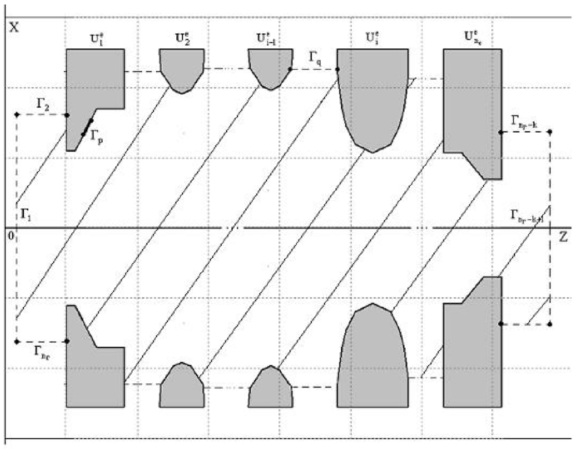



Figure 2. The cross section of electrode system by the plane $y = 0$. Region $\bar{G}$ of modeling of electrostatic field is restricted by dotted line and shaded.

In the equation system (1) the force $F_1 = f_1(t, X, \varphi(X, u))$ is determined by external fields, and $F_2 = \int_{M_{t,u}} f_2(t, X, \eta_t)\, \rho(t, \eta_t)\, d\eta_t$ – by interaction of charged particles. One of the common methods of Coulomb interaction modelling is the method of large particles.

Under solution of the given optimization problem, the beam is modelled by an ensemble of $N_{mod} = 2000$ large particles – uniformly charged balls. The equations of motion of model particles ensemble are integrated using the Runge-Kutta fourth-fifth order method with automatic step-size control [Press, Teukolsky, Vetterling and Flannery, 2002]. Functional (12) is chosen as

$$I(u) = \sum_i \Phi_1 \left(x_{iT}, x'_{iT}\right) \Phi_2 \left(y_{iT}, y'_{iT}\right), \qquad (24)$$

where $\Phi_1\left(x_T, x'_T\right)$, $\Phi_2\left(y_T, y'_T\right)$ are calculated according to formulas (12) – (15). In the formula (8) $A_0 = 0,75$, $w_T = 100$, $C^0 = 0,25$ and $D^0 = 0,8$.

The optimized $H^-$ ion beam injection system is shown in Fig. 3, which produces the final beam with the given characteristics, and having $78\,\%$ of particles involved in subsequent acceleration process in linear accelerator (Fig. 4).

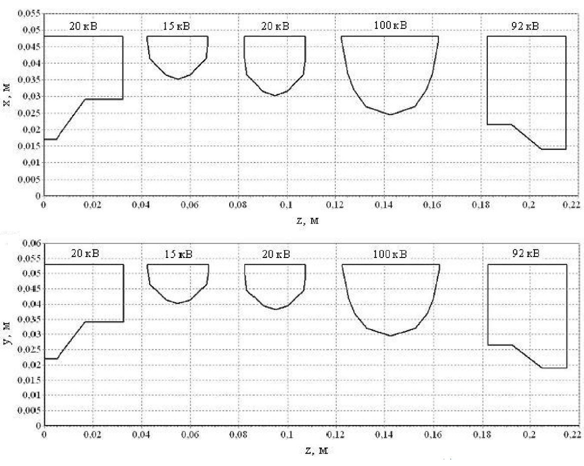
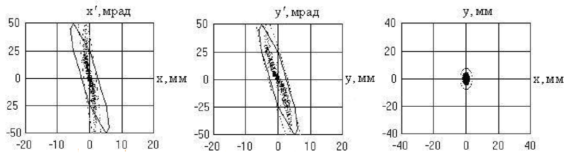



Figure 3. The injection system of RFQ for elliptical beams of ions $H^-$ .

## 6 Conclusion

As the computer simulation has shown, the presented mathematical models and optimization technique appears to be practicable in the considered particular case and can be applied in the future to solve similar problems with different number of control parameters. The injection system, presented in Fig. 3, produces beams with the required characteristics at an acceptable level of losses.




(a) (b) (c)

Figure 4. Characteristics of an elliptic beam of ions $H^-$ at the output of the injection system, shown in Fig. 3. On the figures (a) and (b) the acceptance of RFQ is shown kneeling solid ellipse. (a) – the phase portrait of the beam in the plane $xx'$, (b) – the phase portrait of the beam in the plane $yy'$, (c) – particles density distribution in the plane $xy$.

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