Algorithm for Solving the Optimization Problem for the Temperature Distribution on a Plate

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Abstract. The work describes the maximization problem regarding heating of an area on the surface of a thin plate within a given temperature range. The solution of the problem is applied to ion injectors. The given temperature range corresponds to a required pressure of a saturated gas comprising evaporated atoms of the plate material. In order to find the solution, a one-parameter optimization problem was formulated and implemented leading to optimization of the plate’s specific geometry. It was shown that a heated area can be increased up to 23.5\% in comparison with the regular rectangle form of a given plate configuration.

1 Introduction

The work describes the maximization problem regarding heating of an area on the surface of a thin plate within a given temperature range. The plate serves for injecting the working species (atoms of the plate material evaporated from its surface) into the working space of the ion source \cite{1}. The plate is heated by the flux of electric current passing through it. The injection starts when the temperature reaches the required value depending on the material of the plate. The temperature range and the working area of the surface respectively are defined by the required pressure of a saturated vapor above the surface of the plate.

In this work a model of the plate and a one-parameter variation of its geometry are discussed (see Fig. 1). In the existing technical device the plate has a rectangular form (Fig. 1a). In order to maximize the working area on its surface we suggested to change the geometry in the following way. A new shape has been derived from the regular one by removal of rectangular parts from the corners. Thus rectangular wing-like structures (further referenced as wings) appear on the both sides of the plate (Fig. 1b with their length being specified by us as a free parameter. Our simulations have shown that the working area of the plate has approximately a rectangular shape for the used set of parameters. The shape of the plate has been optimized by varying the length of these wings in order to reach a maximum of the working area. The procedure has been applied under the condition that the highest temperature has to be significantly less than the melting temperature of the plate material.

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Figure 1: The geometry of the plate. Here $2L$ is a length of the plate, $2w$ is a width of the plate, $2l$ is a length of the wings, $2w_w$ is a width without wings, $S$ is a working area of the plate surface heated to the required temperatures, $2d$ is a length of the working area. Left and right sides are connected to the temperature terminal.

2 Main Equation and Conditions

The stationary temperature distribution in the plate could be modelled by the following equation [2]:

$$\frac{\partial}{\partial x} \left( \lambda(T) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial z} \left( \lambda(T) \frac{\partial T}{\partial z} \right) + \frac{I^2 \chi(T)}{S_C^2} = 0,$$

(1)

where the thermal conductivity $\lambda(T)$ and the resistivity $\chi(T)$ are non-linearly dependent on a sought-after function (temperature), $S_C$ is a cross-sectional area, and $I$ is an electric current.

Due to the symmetry at the middle of the plate along the $x$- and $z$- axes solving the problem on a quarter of the full domain is sufficient (see Fig. 2):

$$\begin{cases}
\frac{\partial T}{\partial n} = 0 & \text{if } (x, z) \in \partial \Omega \setminus \{(x, z) | z = L\}, \\
T = T_0 & \text{if } (x, z) \in \{(x, z) | z = L\}.
\end{cases}$$

(2)

The right side of the plate is connected to the temperature terminal with $T_0 = 78$ K. At the boundary of the domain the temperature flow equals to zero: along the $x$- and $z$- axes because of the symmetry and at the other points because the plate is placed inside the vacuum chamber.

The problem (1)–(2) can be solved by various methods, we have chosen the method considering a solution of the elliptic equation (1) as a stationary solution of the parabolic one (3):

$$\rho(T) c_V(T) \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \lambda(T) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial z} \left( \lambda(T) \frac{\partial T}{\partial z} \right) + \frac{I^2 \chi(T)}{S_C^2},$$

(3)

here the density is $\rho(T)$, the heat capacity is $c_V(T)$, and $X(T) = \chi(T)/S_C^2$. The solution of the elliptic equation (1) is the stationary solution of the heat equation (3). In order to solve the equation (3) we have chosen the initial condition to be:

$$T = T_0 \quad \forall (x, z) \in \Omega.$$

(4)

3 Formulation of Optimization Problem

The optimization problem has been formulated to maximize the working area. Temperature values range from $T_{\text{low}} = 678$ K to $T_{\text{high}} = 778$ K. $T_{\text{high}}$ has been chosen to be significantly less than the melting point of the plate material. The maximum temperature constraint is applied to the hottest point on the surface of the plate which is located at its center due to plate’s homogeneity and symmetry.
The size of the working area is proportional to \( d \). Thus the maximum of the working area is reached for the maximum of \( d \). Note, that the width of the plate \( 2w \) is a constant and has a maximum possible value based on the technical requirements. The relation \( w/h \) is fixed. Being dependent on the semilength of the wings \( l \) (see Fig. 3) for the given temperature \( T_{\text{low}} \), \( d \) is the solution of the following equation for \( z \):

\[
T(x = 0, z; l) - T_{\text{low}} = 0, \quad (5)
\]

when we choose the source coefficient \( I \) (electrical current) satisfying the maximum temperature constraint.

Therefore, the maximum of the working surface area \( S \) corresponds to the maximum of \( d(l) \):

\[
d(l^*) = \max_{0 \leq l \leq l} |d(l)|. \quad (6)
\]

An implementation of the optimization problem requires solving of the heat conduction problem (2)–(4) numerous times.

### 4 Numerical Algorithms

#### 4.1 Solving of Direct Problem

The finite difference method has been chosen to solve the heat conduction problem (2)–(4):

\[
\rho_{i,j} c_{V_{i,j}} \frac{\tilde{T}_{i,j} - T_{i,j}}{\tau} = \Lambda_x (\tilde{T}_{i,j}) + \Lambda_z (T_{i,j}) + I^2 X_{i,j}, \quad (7)
\]

\[
\begin{cases}
\Lambda_x (\tilde{T}_{i,j}) = \frac{1}{h_i^2} \left[ \Lambda_{i+\frac{1}{2},j} \tilde{T}_{i+\frac{1}{2},j} - \Lambda_{i-\frac{1}{2},j} \tilde{T}_{i-\frac{1}{2},j} \right], \\
\Lambda_z (T_{i,j}) = \frac{1}{\eta_j^2} \left[ \Lambda_{i+\frac{1}{2},j+\frac{1}{2},j} T_{i+\frac{1}{2},j+\frac{1}{2},j} - \Lambda_{i-\frac{1}{2},j+\frac{1}{2},j} T_{i-\frac{1}{2},j+\frac{1}{2},j} \right],
\end{cases} \quad (8)
\]

where \( i = 1 \ldots N_j - 1, \ j = 1 \ldots M_j - 1, \ h_i = x_i - x_{i-1}, \eta_j = z_j - z_{j-1}, \ h_i = (h_{i+1} + h_i)/2, \eta_j = (\eta_{j+1} + \eta_j)/2, T_{i,j} = T(x_i, z_j, t_k), \tilde{T}_{i,j} = T(x_i, z_j, t_{k+1}), c_{V_{i,j}} = c_v(T_{i,j}), X_{i,j} = X(T_{i,j}), \lambda_{i+\frac{1}{2},j} = \lambda \left( T_{i,j} + T_{i+1,j} \right)/2, \lambda_{i,j+\frac{1}{2}} = \lambda \left( T_{i,j+1} + T_{i,j} \right)/2.

The difference scheme (7)–(8) has been solved by Thomas algorithm (3)–(4):

\[
\alpha_i = \frac{-C_i}{B_i + A_i \alpha_{i-1}}, \quad \beta_i = \frac{F_i - A_i \beta_{i-1}}{B_i + A_i \alpha_{i-1}}, \quad \tilde{T}_{i,j} = \alpha_i \tilde{T}_{i+1,j} + \beta_i. \quad (9)
\]

The coefficients \( A_i, B_i, C_i, \) and \( F_i \) are defined from the difference equation (7):

\[
\begin{align*}
A_i &= -\frac{\lambda_{i+\frac{1}{2},j}}{h_i h_i}, \\
B_i &= \frac{1}{h_i} \left[ \frac{\lambda_{i+\frac{1}{2},j}}{h_i} + \frac{\lambda_{i+\frac{1}{2},j}}{h_{i+1}} \right] + \frac{\rho_{i,j} c_{V_{i,j}}}{\tau}, \\
C_i &= -\frac{\lambda_{i+\frac{1}{2},j}}{h_i h_{i+1}}, \\
F_i &= \frac{\rho_{i,j} c_{V_{i,j}}}{\tau} T_{i,j} + \Lambda_z \left[ T_{i,j} \right] + I^2 X_{i,j}.
\end{align*} \quad (10)
\]
The boundary conditions (2) in Thomas algorithm could be approximated as following:

\[ \alpha_0 = \frac{2 \lambda_{0,j} \tau}{h^2 \rho_{0,j} c_{V0,j} + 2 \lambda_{0,j} \tau}, \quad \beta_0 = \frac{\rho_{0,j} c_{V0,j} T_{0,j} + \tau (\Lambda [T_{0,j}] + \rho^2 X_{0,j})}{h^2 \rho_{0,j} c_{V0,j} + 2 \lambda_{0,j} \tau}, \]

(11)

\[ \hat{T}_{N,j} = \frac{4 - \alpha_{Nj-2}}{3 - \alpha_{Nj-1}} \beta_{Nj-1} - \beta_{Nj-2}. \]

(12)

Corresponding to (4) the initial condition is \( T_{i,j} = T_0 \) \( \forall \ i,j \).

The difference scheme (7)–(12) is the second order approximation of the heat conduction problem (2)–(4) by spatial steps while being the first order by time-step. The scheme is unconditionally stable relating to spatial step \( h \) and conditionally stable relating to \( \eta_j \):

\[ \tau \leq \frac{\min |\eta_j^2|}{2} \cdot \frac{\min |\rho(T)c_{V}(T)|}{\lambda(T)}. \]

(13)

4.2 Algorithm for Solving Optimization Problem

The algorithm comprises the following steps: 1) the length of wings \( l \in [0, L] \) is sampled with a number \( N_{\text{wings}} \); 2) for each \( l \), the source problem is solved and \( d(l) \) is calculated; 3) the value of \( l^* \) is found according to the maximum value of \( d \).

The value of the electric current \( I \) varies in the range of \([0, I_{\text{max}} = 500 \text{ mA}]\). If \( I \) equals to \( I_{\text{max}} \), the temperature in the central point of the plate exceeds the maximum temperature constraint for all \( l \in [0, L] \). In order to find the only solution existing within the defined range of \( I \), the bisection method is used.

The algorithm for solving the optimization problem is described by the pseudo code following below.

4.3 Parallel Algorithm

The parallel algorithm was implemented with the usage of Message Passing Interface (MPI) [6]. The main loop of the algorithm (line 2) was parallelized. For each \( l \), the source problem is solved by a separate parallel process. The parallel algorithm may be executed up to \( N_{\text{wings}} \) times faster in comparison with the non-parallel one.

5 Results

The results are presented for the plate made of Thulium. Generally, the algorithm has been developed for temperature values depending on thermal coefficients, but for the present simulations the thermal coefficients [7, 8] are assumed to be constant for the considered temperature range: the conductivity is \( \lambda = 0.169 \text{ J/(cm s K)} \), the specific heat is \( c_V = 0.16 \text{ J/(g K)} \), the density is \( \rho = 9.33 \text{ g/cm}^3 \), and the ratio resistivity to square of the cross-section area is considered to be the same throughout the whole plate \( \chi/S_C^2 = 10^3 \times 10^3 \text{ Ohm/cm}^3 \). The fixed size of the plate is the following \( L = 1 \text{ cm}, w_b = 0.05 \text{ cm} \) and \( w = 0.125 \text{ cm} \) (see Fig. 1b). The sampling number \( N_{\text{wings}} = 10 \).

One can see from the Fig. 4a that the temperature profile is sensitive to the length of the wings. The function \( d(l) \) and the temperature field for \( l^* \) are shown in Fig. 4b and Fig. 4c respectively. The maximum \( d \) corresponds to \( l^* = 0.6 \text{ cm} \).
Algorithm 1 The algorithm for Solving Optimization Problem (6)

1: procedure SolveOCP
   \(\triangleright\) Solve (6)
   \(\textbf{Input:}\) \(L\) – the finite set of \(l_i\) values, where \(i = 0 \ldots N_{\text{wings}} - 1\)
   \(\textbf{Output:}\) A value of \(l_i\) corresponding to \(\sup \{D\}\) (maximal value of parameter \(d\))
2: \hspace{2em} for all \(l_i \in L\) do
3: \hspace{4em} \(d_i = \text{SolveSCP}(l_i)\) \(\triangleright\) See lines 8–18
4: \hspace{2em} end for
5: \hspace{2em} \(\text{ind} = \text{FindMax}(D)\)
6: \hspace{2em} return \(l_{\text{ind}}\) and \(d_{\text{ind}}\)
7: end procedure

8: procedure SolveSCP\((l_i, I_{\text{min}}, I_{\text{max}})\)
   \(\textbf{Input:}\) \(l_i, I_{\text{min}} = 0\) and \(I_{\text{max}} = 500\)
   \(\textbf{Output:}\) A value of \(d_i\) for corresponding value of \(l_i\)
9: \hspace{2em} while \(|T(0, 0, l_i) - T_{\text{high}}| \geq \varepsilon\) do
10: \hspace{4em} \(I = (I_{\text{min}} + I_{\text{max}}) / 2\)
11: \hspace{4em} \(T(x, z, l_i) = \text{SolveDP}(I, l_i)\) \(\triangleright\) Solve direct problem for heat equation (2)–(4)
12: \hspace{4em} if \(T(0, 0, l_i) > T_{\text{high}}\) then \(I_{\text{max}} = I\)
13: \hspace{4em} else \(I_{\text{min}} = I\)
14: \hspace{4em} end if
15: \hspace{2em} end while
16: \hspace{2em} \(d_i = \text{SolveEq5}(T(0, z, l_i))\) \(\triangleright\) Solve equation (5)
17: \hspace{2em} return \(d_i\)
18: end procedure

Fig. 5 illustrates the performance of the parallel algorithm depending on the number of CPUs – \(n_p\). The calculations have been carried out on HybriLIT heterogenous cluster (CPU – Intel Xeon E5-2695). Fig. 5a shows the calculation time \(t_{n_p}\), Fig. 5b – the speedup of calculations \(t_1/t_{n_p}\), and Fig. 5c – the efficiency of parallelization \(t_1/(n_p \times t_{n_p})\).

(a) Temperature profiles for different lengths of wings  
(b) Parameter \(d\) for different length of wings  
(c) Temperature field in quota of the plate

Figure 4: Results of solving the source problem as a function of \(l\)
6 Summary and Conclusion

In order to maximize the working area we have suggested changing the plate geometry. A new shape has been derived from the regular one by removal of rectangular parts from its corners. The simulations have been carried out in order to find the optimal plate geometry. For that the algorithm for solving the one-parameter optimization problem has been developed and its parallel version has been implemented.

The optimal geometry of the plate has been found ($l^* = 0.6$ cm) allowing to increase the working area up to 23.5% in comparison with the one of the regular plate. The value of the electric current corresponding to the maximum working area has been found and equals to $I = 385$ mA.

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