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Modeling, Fabrication, and Optimization of Niobium Cavities – Phase I: Quarterly Progress Report November 20, 2001 - February 20, 2002

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Modeling, Fabrication, and Optimization of Niobium Cavities – Phase I

Quarterly Progress Report
11/20/01 - 2/20/01

UNLV-AAA University Participation
Program

Robert A. Schill, Jr. and Mohamed B. Trabia
Principal Investigators

Purpose and Problem Statement

Multipacting is one of the major loss mechanisms in RF superconductivity cavities for accelerators. This loss mechanism limits the maximum amount of energy/power supported by the cavities. Optimal designs have been identified in others' studies. In practice, these designs are not easily manufactured. Chemical etching processes used to polish the cavity walls result in a nonuniform surface etch. A nonuniform surface etch will leave some unclean areas with contaminants and micron size particles. These significantly affect multipacting. Further, a nonuniform etch will leave areas with damaged grain structure, which is not good for superconducting properties. Typically, the depth of chemical polishing etch ranges between 10 to 150 microns.

It is the purpose of this study to examine the chemical etching process in the design of niobium cavities so to maximize the surface quality of the cavity walls while minimizing the multipacting losses. Single and multiple cavity cell geometries are to be investigated. Optimization techniques will be applied in search of the chemical etching processes, which will lead to cavity walls with near ideal properties. Figure 1 depicts a block diagram of the optimization procedure, which is intended to be fully automated among a variety of existing codes.

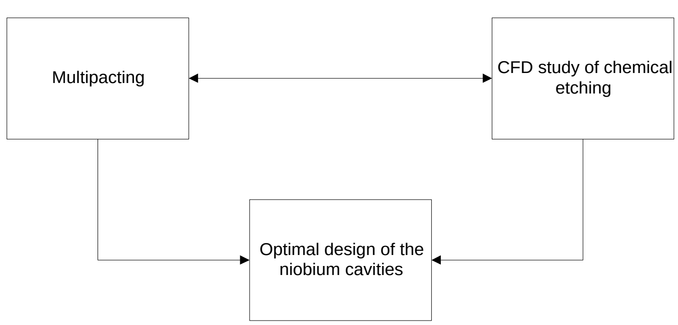


Fig. 1 Block Diagram of Optimization Procedure

Personnel

Principal Investigators:

- Dr. Robert A. Schill, Jr. (Electrical Engineering)
- Dr. Mohamed B. Trabia (Mechanical Engineering)

Research Investigator:

- Dr. Yi-Tung Chen (Mechanical Engineering)

Students:

1. Ms. Myong Holl, Undergraduate Student, (Mechanical Engineering)
2. Mr. Satishkumar Subramanian, M.S. Graduate Student, (Mechanical Engineering).
3. Ms. Qin Xue, M.S. Graduate Student, (Mechanical Engineering).

National Laboratory Contact:

- Dr. Dominic Chan, Project Leader for Superconducting RF Engineering Development and Demonstration AAA Technology Project Office at Los Alamos National Laboratory
- Dr. Tsuyoshi Tajima, Team Leader, Accelerator Physics & Engineering, LANSCE-1, Los Alamos National Laboratory

Management Progress

Budget Issues:

- N/A.

Notes:

1. Most of the major equipment budget has been spent.
2. Salary expenditures are on target.

Management Problems

N/A

Technical Progress

Dr. R. Schill and Dr. M. Trabia had a visit to LANL on January 17, 2002. During this visit Dr. Chan introduced us to Dr. Tsuyoshi Tajima. We are glad to report that we established a good working relation with Dr. Tajima. We update LANL personnel of our progress. The visit helped us better understand the concerns and interests of LANL relative to this research.

Multipacting Study

A multipacting study is essential in the design of super conducting, high power, niobium cavities for high-energy proton acceleration in linacs. Multipacting limits the quality factor of the cavity due to losses associated with secondary emission resulting from impacting resonance which is spatially localized.

Commercial codes from Field Precision Inc. (Xlate, Mesh, and Wavesim), a research code (Trak_rf) developed by Stan Humphries, and various MATLAB programs developed at UNLV are used to investigate particle tracking and multipacting. The Trak_rf code is a finite element code that tracks charged particles in RF fields based on supplied initial conditions. Particles are launched when the E-field reaches a threshold value as determined by programmer to simulate field emission. This study focuses on the significant localized increases in impacting on the cavity surface and the secondary electron emission coefficients generated by each particle launched at each point of impact. Trak_rf only tracks the primary particle launched and not the secondary particles. If the primary particle exhibits some type of spatial impacting resonance and the secondary electron coefficient is greater than one at each impact, one usually interprets the impacting as multipacting. Although this is valid and satisfies the multipacting criteria, it is believed to be a special case of multipacting. If the primary particle does not exhibit a spatial resonance, then based on the multipacting criteria, we only have impacting. Although this may be true, it is possible that one of the secondary electrons emitted will result in multipacting. Because the codes do not track the emitted particles, a scheme to be able to identify potential multipacting locations based on both the spatial resonance of the primary electron and the potential spatial resonance of the secondary electron was developed.

As a first study to obtain a suitable level of confidence in the correctness of the codes, RF field resonance and particle tracking in the pillbox geometry was examined. The MATLAB generated cavity shown in Fig. 2 below has a calculated and a numerical resonant frequency of about 570 MHz for the dominant supported TM_{010} mode. Ten electrons were launched at the same initial position with the same initial particle trajectories. A subroutine (MATLAB) to plot single particle trajectories was developed to help visualize impacting and multipacting conditions for the primary particle. It is observed in Fig. 2 that the ten particles exhibit vary different particle orbits. Figure 3 shows the two dimensional front and side view of the particle orbits. This is a result of the nondeterministic or random nature of the emission calculation based on supplied secondary electron emission coefficient data. It was anticipated that two-point multipacting would exist in the region near the center of the pillbox end caps.

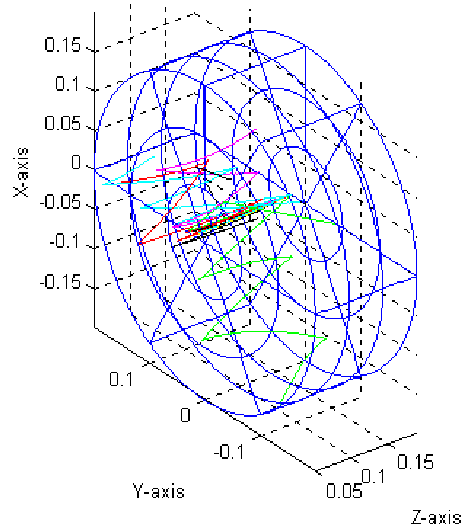


Fig. 2 Tracking of Ten Electrons with Identical Initial Conditions in a Pillbox Geometry.

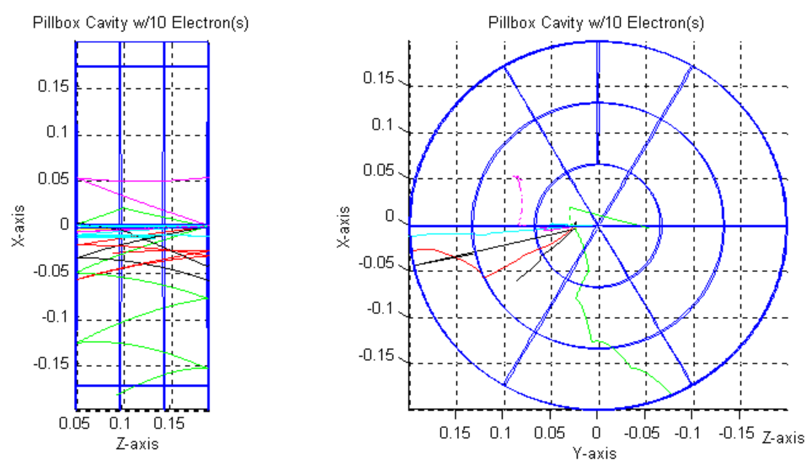


Fig. 3 Side and Front View of Figure 2.

Track_rf was modified to examine localized secondary electron emission and impacting over the cavity surface. Figures 4a and 4b illustrate the field emission statistics [maximum, minimum, average and standard deviation] for the cylindrical cavity when many electrons (50 electrons) with the same initial conditions are launched at the same time from the center of the end cap of the cylinder. Based on the statistics, a multipacting condition has not been identified for particle trajectories shown in Fig. 2.

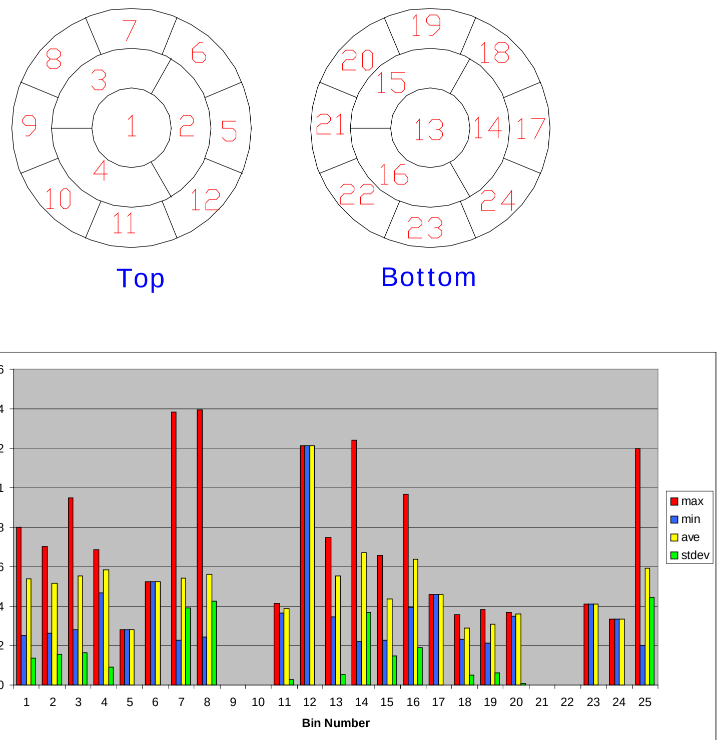


Fig. 4 a) Binning of the surface of a cylindrical cavity, and **b)** Bin statistics of secondary electron emission.

A MATLAB program was developed to draw a single cell elliptic cavity given some of the cavity's geometrical parameters. At present, a similar program is being developed for the five-cavity geometry. Wavesim has correctly determined the cavities dominant resonant frequency as compared to estimated calculations based on a cylindrical geometry. Tracking in these cavities is underway.

Discussions are underway to compare this code with baseline studies and known multipacting conditions at Los Alamos.

The secondary electron emission predicted due to impacting is only as good as the data supplied to the code. It has been shown in literature that generic secondary electron emission curves may not be the standard at all angles of incidence. Furthermore, the way the cavity surface is prepared significantly affects the secondary electron emission coefficient. Such studies have not been performed for Los Alamos cavities. Consequently, for the code to accurately predict multipacting conditions, we have submitted a proposal to experimentally study the secondary emission properties of a Los Alamos surface treated niobium target. Experimental findings are to be incorporated in the existing Trak_rf code in the future.

CFD Study of Chemical Etching

Niobium cavities are important component of the integrated NC/SC high-power linacs. Over the years researchers in several countries have tested various cavity shapes. They concluded that elliptically shaped cells and buffered chemical polishing produce good performance. The objective of this research is to study the effect of chemical etching, on the surface quality, and to optimize this process. Chemical etching of the inner surface of the cavity is achieved by circulating acid through it. As the acid interacts with the surface, it eliminates imperfections and improves surface quality. During etching, a pipe with baffles is inserted within the cavity to direct the flow along the surfaces. A finite element computational fluid dynamics model is developed for the etching process. The problem is modeled as a two-dimensional, axisymmetric, steady state fluid flow problem. This model is used to evaluate the current etching process. An alternative design with an expanding baffle is proposed. The new design is optimized to improve the chemical etching process.

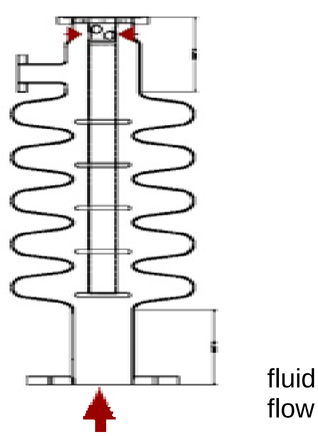


Fig. 5 Current Etching Configuration of Niobium Cavities

The following steps were taken toward understanding and modeling of this problem:

1. Continuous discussions with Dr. D. Chan, LANL, and his colleagues to understand the problem.

2. Developing a finite element model for five-cell niobium cavity with a baffle using FEMLAB software (chemical engineering module).

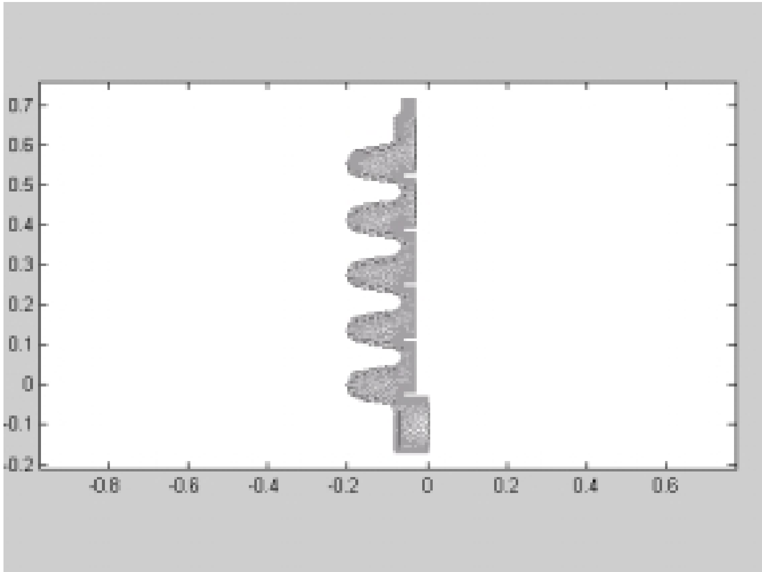


Fig. 6 Finite Element Model of the Baffle

3. Internal boundaries are created close to the inner walls of the cavity, Figure 7. Each cavity is divided into six sections as can be seen in the zoomed-in view in the same figure:
   - Bottom iris
   - Bottom straight
   - Bottom equator
   - Top equator
   - Top straight
   - Top iris

   Inlet and outlet sections are represented using one boundary each. The velocity is integrated along each section. A performance index is defined using two quantities as follows:

$$PI = F\left(\frac{v_{av}}{\frac{\sum_{i=1}^{n}\frac{\int v ds}{\int ds}}{n}}\right) + \frac{\sum_{i=1}^{n}\left[\frac{\int v ds}{\int ds} - V\right]^2}{nV} \qquad (1)$$

   where, *F* is a factor to allow combining the two quantities in the same performance index.
   v_{av} is the average inlet velocity.
   v is the velocity at any point along the internal boundaries.

n is the number of sections (total of thirty-two).
V is the average velocity along the walls of the cavity, which can be expressed as,

$$V = \frac{\sum_{i=1}^{n} \frac{\int v ds}{\int ds}}{n}$$

The first quantity describes the average velocity along the internal boundaries of the baffle while the second one defines its standard deviation. The objective of the optimization is to maximize the first and minimize the second variable.

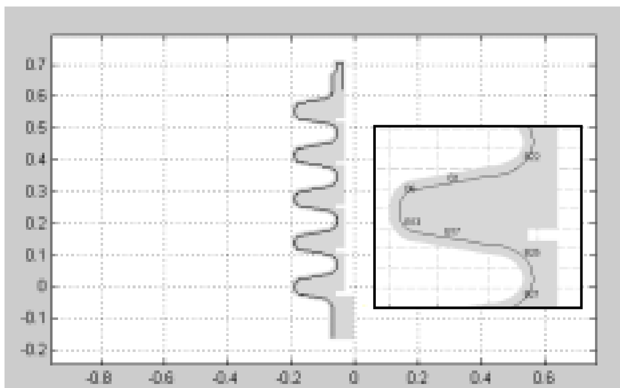


Fig. 7 Internal Boundaries of the Cavity (inset: zoomed–in view of a cavity)

4. A parametric study of the problem was conducted by varying the variables that describe the geometry and location of the baffle subject to the constraint that the baffle fits within the cavity. No case provided appreciable improvement in the performance index over the current design.

5. To verify the accuracy of FEMLAB software as modeling tool, we created a model for the problem of a flow above a square cavity that was presented by [1]. Results for both low and high Reynolds Number show close correspondence. This study also helped in better tuning of the software variables to produce better results.

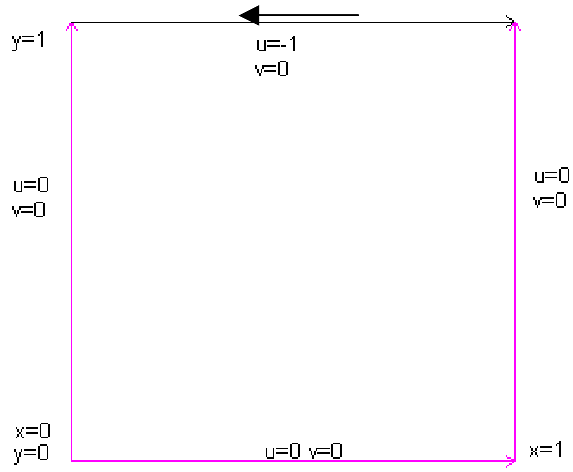


Fig. 8 Geometry and Boundary conditions for cavity flow

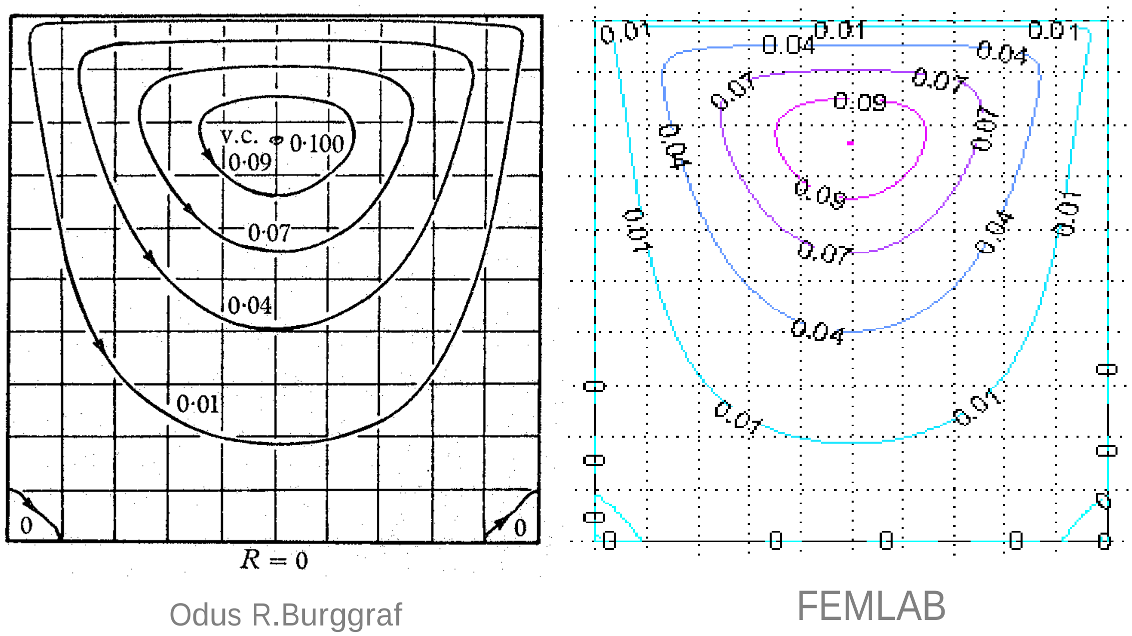
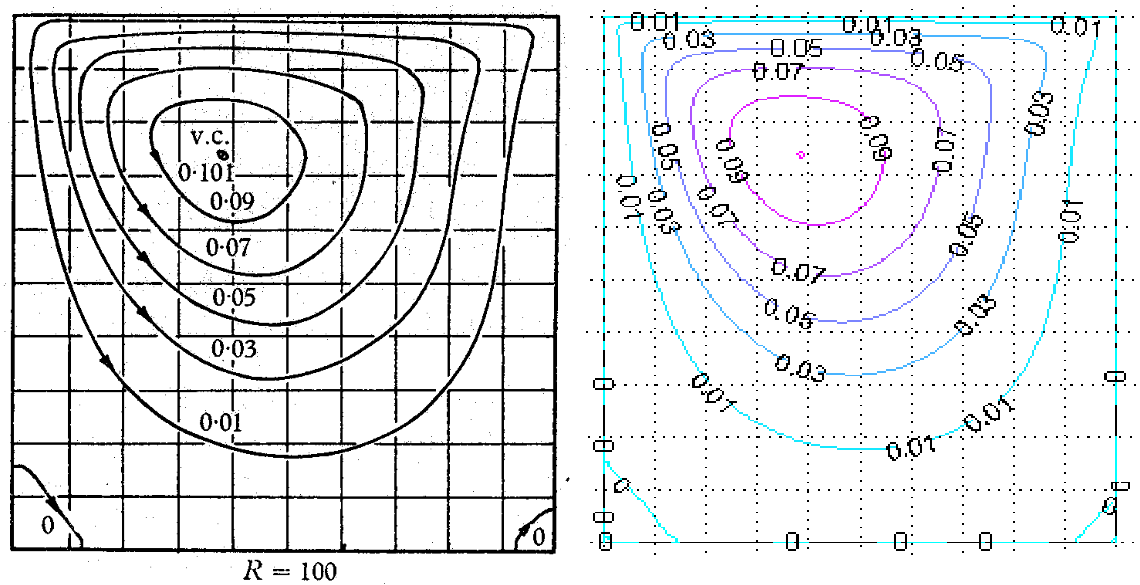


Fig. 9 Comparison of Stream Function Contours for Re=1



Odus R.Burggraf FEMLAB

Fig. 10 Comparison of Stream Function Contours for Re=100

Optimization Study

1. While the idea of having a baffle inside the cavity partially succeeded in directing the flow inside the cavity, a different design configuration may be necessary to get the flow closer to the equator regions. The modified baffle design has the following features:
   - The baffle is angled near the inlet of each cavity.
   - The baffle is modified so it can be extended inside the cavities. This design has the baffle made of four sections. Each section can be expanded or retracted by rotating a cam that moves a spring-loaded follower, which is attached to the baffle section.
   - Flow exit is now parallel to flow inlet.
   - Each baffle is centered along the equator of a particular cavity.

   Six design variables are identified. Table I presents description of these variables.

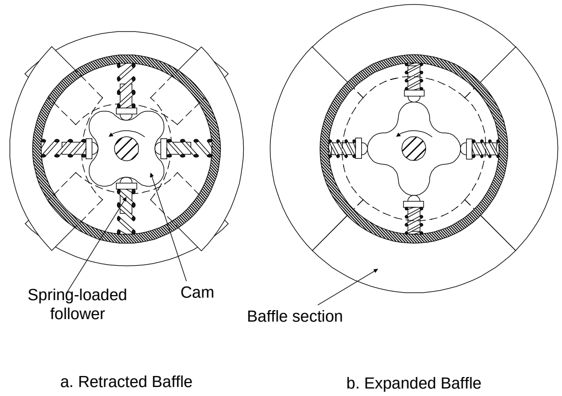


Fig. 11 Possible Design for an Expanding Baffle

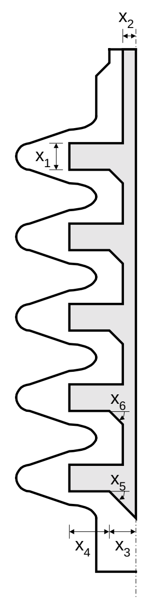


Fig. 12 Design Variables of the Expanding Baffle

Table I. Variables of the Modified Baffle Design

Variable	**Description**
x_1	Thickness of the baffle
x_2	Radius of the baffle pipe
x_3	Radius of the fixed portion of the baffle
x_4	Length of the extended portion of the baffle
x_5	Baffle angle at the first cavity
x_6	Baffle angle at the second through fifth cavities

2. We investigated the possibilities of improving this modified baffle design. Inequality constraints are used to ensure realistic solution. The problem is subject to several constraints including:

$$0.005 \le x_1 \le 0.044 \quad \text{m} \tag{2}$$

$$0.01 < x_2 < 0.04 \quad \text{m} \tag{3}$$

$$0.01 < x_3 < 0.06 \quad \text{m} \tag{4}$$

$$0 \le x_4 \le 0.8 x_3 \quad \text{m} \tag{5}$$

$$0 \le x_5 \le \frac{\pi}{3} \quad \text{rad.} \tag{6}$$

$$0 \le x_6 \le \frac{\pi}{3} \quad \text{rad.} \tag{7}$$

The upper bound in the fourth set of constraints indicates a physical limit on the length of the extended portion of the baffle. Additional constraints ensure that baffle does not intersect the internal boundaries of Figure 3. These constraints are created by representing each segment of the internal boundaries of the cavity and the baffle using the parametric form of a curve:

$$\begin{Bmatrix} x \\ y \end{Bmatrix} = \begin{Bmatrix} x_s \\ y_s \end{Bmatrix} + u \begin{Bmatrix} f(x_s, x_f) \\ f(y_s, y_f) \end{Bmatrix} \qquad 0 \le u \le 1 \tag{8}$$

where, (x_s,y_s) and (x_f,y_f) are the starting and final point of segment respectively. Possibility for intersection between two segments, *a* and *b*, is checked by solving their parametric equations simultaneously. If both u_a and u_b are between *zero* and *one*, intersection occurs. All constraints are included in the objective function using penalty terms. Since the quality of the mesh changes for each set of variables, an additional constraint is needed to ensure that the results of the finite-element model are reasonable. The following constraint compares the flow rate in the inlet and the exit of the cavity as follows,

$$\left| Q_i - Q_e \right| \le 0.02\, Q_i \tag{9}$$

where, Q_i and Q_e are the flow rates at inlet and exit of the cavity respectively. Flow rate at exit, Q_e, is calculated by integrating velocity over exit area. Constraints are incorporated in the objective function using the bracket function. The modified objective function is,

$$\begin{aligned} &\text{minimize,} \qquad FC = PI + \sum_{i=1}^{m} \Omega_i \\ &if\ \ g_i(x) \le 0 \quad \Omega_i = R * g_i(x)^2 \\ &if\ \ g_i(x) > 0 \quad \Omega_i = 0 \end{aligned} \tag{10}$$

3. The algorithm reached the following solution after *738* function evaluations:

$$\{x\}^T = \{0.044, 0.013, 0.060, 0.048, 0.005, 0.004\}^T$$

Average velocity in this case is equal to 0.0553 m/s while the standard deviation is 0.1854.

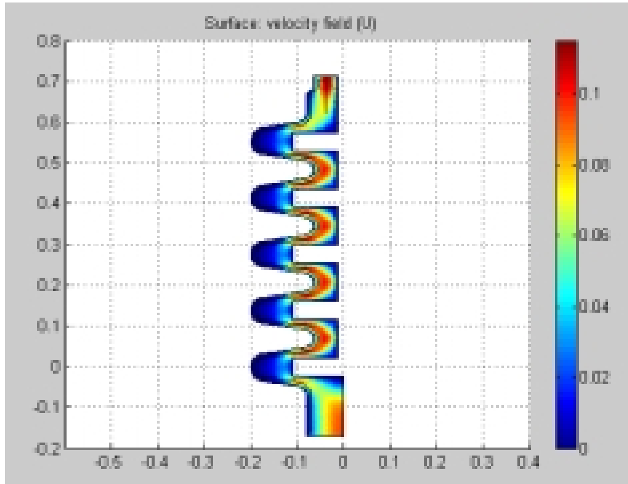


Fig. 13 Velocity Field for the Optimized Modified Baffle Design

Research Outcome:

We have a paper under review for publication in the International Congress on Advanced Nuclear Power Plants (ICAPP). The paper title is, "Modeling and Optimization of the Chemical Etching Process in Niobium Cavities." The abstract is already accepted and we were invited to submit a full paper.

References:

[1] Odus R. Burggraf, Analytical and numerical studies of the structure of steady separated flows, J. Fluid Mech. (1966), vol.24, part1, pp113-151.