ELECTROPOLISHING ON SINGLE AND MULTI-CELL: COMSOL MODELLING

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Abstract

In the framework of cavity electropolishing improvement, modelling allows evaluating some parameters not easily accessible by experiments and can also help us to guide them. At CEA Saclay, COMSOL software is used to model electropolishing of cavity in two dimensions. First, single-cell electropolishing with different shapes (TESLA, ILC Low Loss (LL_{ILC}), ILC Reentrant (RE_{ILC}) and the optional Half Re-entrant profile [1, 2]) is studied with acid inflow like in our set up. Then some improvements of both outflow and inflow of the acid are considered. This work is extended to TESLA nine-cell cavities in collaboration with KEK to understand if electropolishing process is related to some misunderstood RF performances [3, 4].

INTRODUCTION

To build the future International Linear Collider (ILC), the "cold" technology has been selected. It is based on superconducting radiofrequency (SRF) cavities. Electropolishing is presently accepted like the most efficient surface treatment to reach high gradients (40 MV/m) with niobium RF cavities. However, this technique presents the disadvantage to be not very reproducible. Experimental researches try to improve it and modelling appears like an interesting and helpful way to better understand electropolishing. In this study, COMSOL software is used to model horizontal electropolishing on 2D for single-cell and nine-cell cavities.

ELECTROPOLISHING PROCESS AND KINETICS EQUATION

COMSOL allows coupling of different physical phenomena such as chemical reaction with dynamics fluid for our purpose. It is also used in other labs; however without the introduction of chemical reactions for niobium electropolishing [5]. Generally the bath used for electropolishing is composed by a mixture of hydrofluoric and sulphuric acids (1:9 in volume) [6]. Considering that the bath is mainly composed by sulphuric acid, its characteristics (viscosity and density) have been used for modelling.

The general chemical equation for niobium oxidation is:

$$2Nb + 5H_2O \rightarrow Nb_2O_5 + 5H_2 \qquad (1)$$
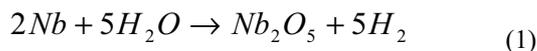
Then the pentoxide layer Nb_2O_5 is attacked by the hydrofluoric acid following the equation (2):

$$Nb_2O_5 + 10HF \rightarrow 2H_2NbOF_5 + 3H_2O \qquad (2)$$

For modelling, it is assumed that the oxide layer is continuously formed and so only equation (2) is considered. The reaction velocity v is a second order kinetics [7]; so it is equal to

$$v = k[Nb_2O_5][HF] \qquad (3)$$

where k is a kinetic constant in l/mol.s and concentrations (mol/m^3) are noticed in square brackets. If x is considered as the production of H_2NbOF_5 at a time t, α the initial concentration of Nb_2O_5 and β the initial concentration of HF, the equation (3) can be written:

$$v = \frac{1}{2}\frac{\partial x}{\partial t} = k(\alpha - x)(\beta - 10x) \qquad (4)$$

As each concentration is directly connected to the other, results for [HF] will be privileged; however [H_2NbOF_5] or [Nb_2O_5] can help to understand results.

CONVECTION DIFFUSION AND NAVIER-STOCKES EQUATIONS

Different equations are used to solve the coupling between niobium reaction and fluid dynamics:
- The mass balance equation:

$$\frac{\partial c_i}{\partial t} + \nabla N_i = R_i \qquad (5)$$

Where c_i is the concentration of the specie i (mol/l), N_i its flux (mol/l.s) and R_i its net creation rate (mo/l.s).
- The Nernst-Planck equation:

$$N_i = -D_i\nabla c_i - z_i\omega_i Fc_i\nabla\phi + uc_i \qquad (6)$$

The first term $D_i\nabla c_i$ relates the diffusion transport where D_i is the diffusion coefficient and C_i the concentration of the specie i. To determine the diffusion coefficient, the time to build up a viscous layer has been compared between experimental results on electropolished samples and its modelling with different diffusion coefficients. Then it has been found that the most optimal result of modelling is obtained for a value of diffusion coefficient equal to 10^{-8} m^2.s^{-1} [8].

The second term $z_i\omega_i Fc_i\nabla\Phi$ expresses the transport by electromigration. z_i represents the valence of the specie i, ω_i its mobility and Φ the electrostatic potential. F is the Faraday constant As for electropolishing in case of high concentrated

electrolyte, the transport of species is mainly due to diffusion and convection, electromigration can be neglected [9,10].

The last term uc_i represents the convection where u is the velocity of specie (m/s).

By combining equations (5) and (6), the general equation to solve is:

$$\frac{\partial c_i}{\partial t} + \nabla(-D_i\nabla c_i - z_i\omega_i Fc_i\nabla\phi + uc_i) = R_i \qquad (7)$$

where R_i is calculated thanks to the velocity of the chemical reaction in equations (3,4).
- The equation (7) is coupled to Navier-Stockes equation (8) for an incompressible fluid (9), to model the fluid dynamics in the cavity:

$$\rho\frac{\partial u}{\partial t} - \eta\nabla^2 u + \rho(u.\nabla)u + \nabla p = G \qquad (8)$$

$$\nabla.u = 0 \qquad (9)$$

η is the dynamic viscosity (10^{-3} kg/m.s)
u the fluid velocity (m/s)
p the pressure (N/m^2)
G (N/m^3), the resultant force, only the gravity is considered here.

Acid concentration [HF] (mol/m^3) during time is studied. It is considered that at time t=0, the cavity is full with acid. Maximal time (20 000 s, ~ 6 hours), corresponds to a standard electropolishing (100 µm). Acid concentration is calculated for a so long period, because a simple defect in acid attack would be easily detected. Velocity fluid (m/s) is also used to help us in the understanding of electropolishing process.
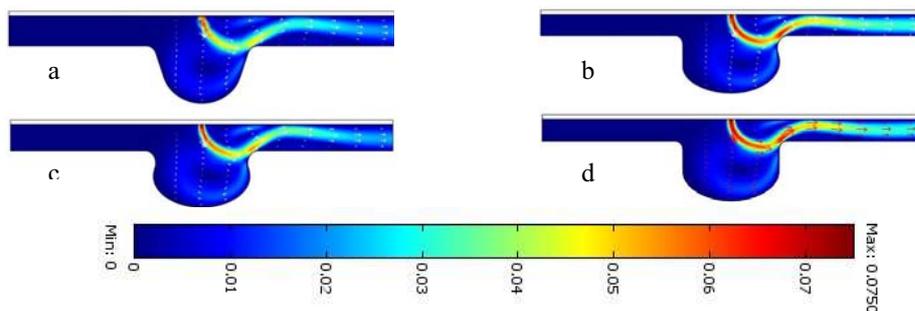
SINGLE-CELL

First studies have been motivated by the optimisation of electropolishing set up for single-cell cavities at Saclay: the acid inflow comes by a hole in the middle of the cathode and exits from the "right" beam tube. The flow rate is 2 l/mn. This type of horizontal electropolishing has been modelled on different cavities shapes. For each shape, acid rebounds on the "right" iris and the "left" beam tube is very bad renewed in acid (figures 1 and 2). For LL and half RE profiles, there is an impoverishment of acid in one side of the cell and the "left" beam tube is less renewed than for the two other shapes (TESLA and RE profiles).

A modification of the acid inflow has been studied on TESLA shape to improve the electropolishing on the left beam tube: the acid arrives from the left beam tube and goes out by the right one with a flow rate of 10 l/mn (figures 3a and 3b). This new configuration is beneficial for both beam tubes; however the acid sweeps badly the cell. A protuberance cathode has been added to force the acid to sweep the bottom of the cell (figures 3c and 3d). It improves electropolishing in the cell however it creates a little dissymmetry of acid attack in the beam tubes comparing to the previous solution. The best way seems to be the one developed for the nine-cell cavities with an inflow in the middle of the cathode and the outflow on both beam tubes (figure 4). As consequence of this result, we plan to modify our electropolishing set-up in such direction. However, irises have a higher acid attack than other parts of the cavity.


Figure 1: Velocity (m/s) in single-cell for different shapes (1a: TESLA, 1b: half RE, 1c: RE and 1d: LL)


Figure 2: [HF] (mol/m^3) in single-cell for different shapes at time = 20 000 s
(2a: TESLA, 2b: half RE, 2c: RE and 2d: LL)

Fluid
Velocity

[HF]
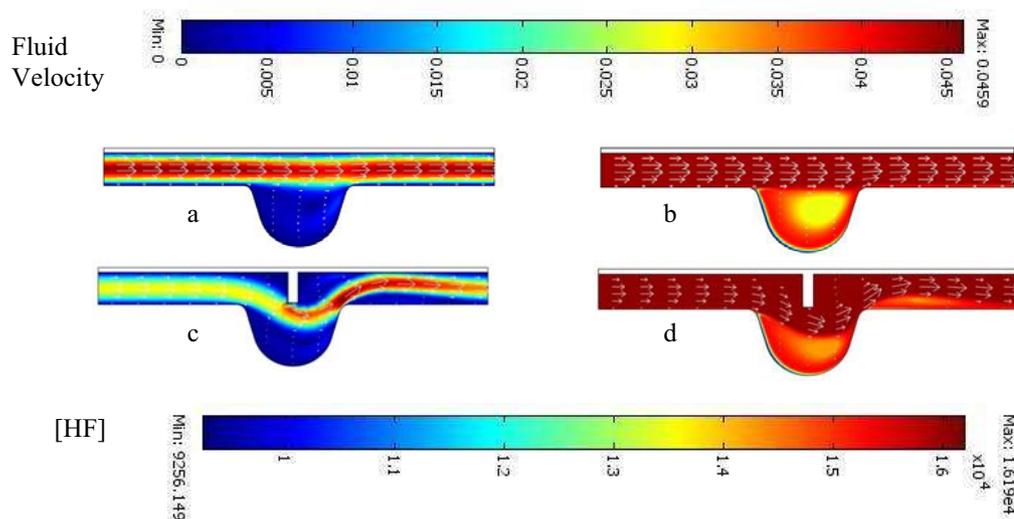
Figure 3: Fluid velocity (m/s) for new acid arrival (3a and 3c) and [HF] (mol/m^3) at time = 20 000s (3b and 3d)

Fluid
Velocity

[HF]
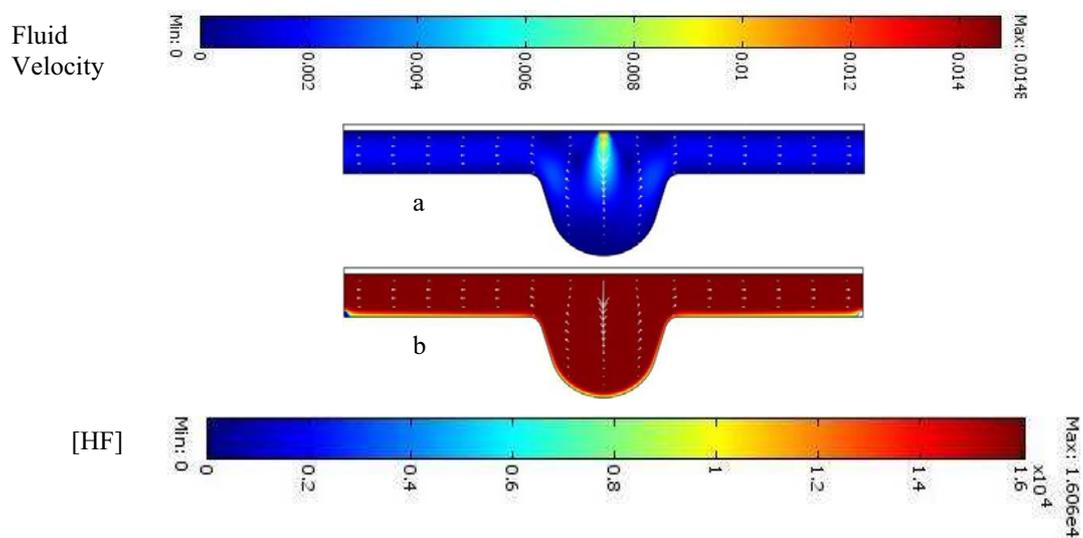
Figure 4: Fluid velocity (m/s) (4a) and [HF] (mol/m^3) at time =20 000s (4b) for exit on both beam tubes

Fluid
Velocity

[HF]
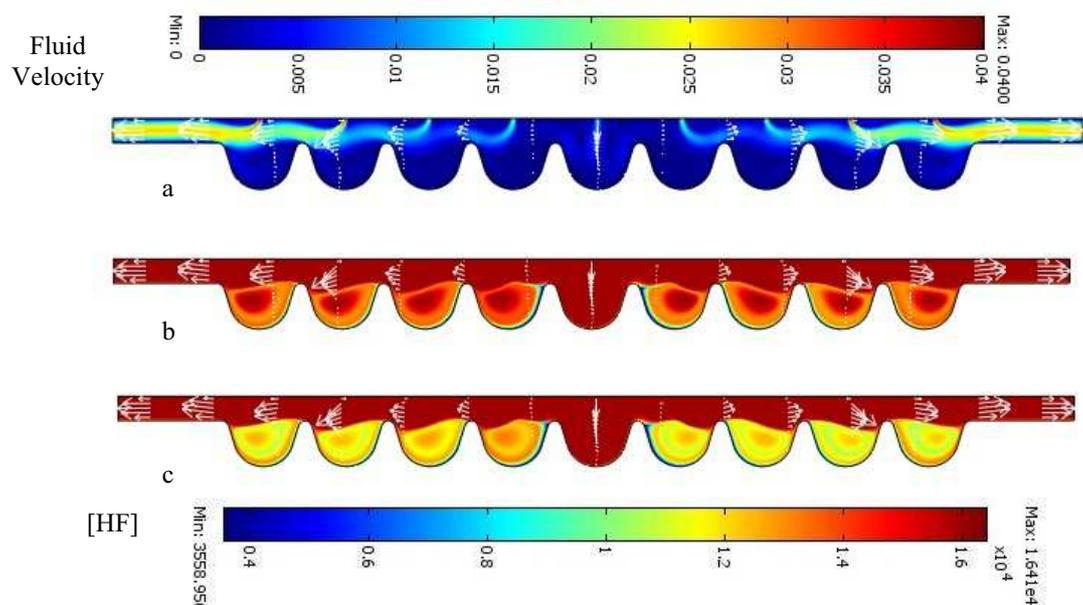
Figure 5: Velocity fluid (m/s) (5a) and [HF] (mol/m^3) at time 4 000s (5b) and 20 000s (5c) for TESLA nine-cell.

NINE-CELL TESLA CAVITIES

Then work has been extended to TESLA nine-cell cavities, with an electropolishing similar as KEK set up [4]. Acid arrives by 9 holes located in the middle of each cell and goes out from both beam tubes. Size of the hole is higher in the central cell (10 mm in cell 5) and decreases (down to 6 mm) in the direction of the beam tubes to optimise the sweeping of each cell. Modelling allows showing an asymmetric acid attack of cells. That could be an explanation to the field flatness degradation experimentally observed after electropolishing [3].

Cell 5 is well swept by the acid, arguing for a good electropolishing compared to an impoverishment for the others cells.

In our model, we noted on figure 5 a tiny right-left dissymmetry in the acid flow and attack, this can be explained by a dissymmetry of the mesh in the central part of the cell 5 (figure 6).
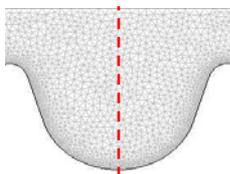

Figure 6: Mesh repartition of the cell for modelling

CONCLUSION

First results on modelling are promising and show that electropolishing is heterogeneous in single and nine-cell cavities. These results can give explanation to disparate RF test and degradation of field flatness after electropolishing. Further parameters have to be introduced to perform a more realistic modelling of cavity electropolishing: rotation, temperature. 3D modelling is currently under consideration too (figure 7).
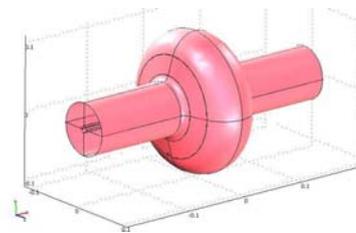

Figure 7: 3D single cell cavity

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