MONA: THERMAL AND MAGNETOHYDRODYNAMIC SOFTWARE

1. Introduction

The MONA package has been developed over the last two decades in order to be able to design the best possible cell in term of thermal and magneto-hydrodynamic cell state. MONA is designed for the determination of:

- Cell energy balance (generation of heat = heat losses)
- Steady and non stationary heat state of the cell
- Temperature field
- Heat flux distribution
- Ledge profile (including convective effects)
- Electrical potential field (bubbles effects will be implemented shortly)
- Current density distribution
- Induction magnetic field inside the cell
- Force field inside the liquids (bubbles effects will be implemented shortly)
- Velocity field in the metal
- Velocity field in the bath
- Pressure field in the liquids
- Metal surface contour (with or without constant ACD)
- Shell magnetization

The solution is determined in two adjacent 3D cells, including 3D busbars systems. Boundary conditions for the heat equations are specified as functions of the temperature and has been calibrated on many heat flux measurements around the cell. Boundary conditions for Maxwell equations are given as integral constraints on the model boundary in order not to be obliged to mesh the air. Boundary conditions for Navier-Stokes equations can be chosen as Dirichlet or Neumann conditions at the boundary of the fluids. A turbulent anisotrop viscosity model is used that was calibrated on many velocity fields measurements. The model accepts all type of materials including ferro-magnetic steel plates.

Using the steady state solution, a perturbation of all variables is assumed. The new set of equations for the first order perturbed system is solved to determine the "cell stability diagram". By analyzing this diagram, the maximum possible current in the shell, the minimum metal level and all mhd impacts are determined. Following figures give some examples of cell geometry and results.



Building a model: Collector bars



Building a model: Cathode



Building a model: Metal and bath



Building a model: Anodes



Building a model: One cell



Building a model: Neighboring cells



Building a model: Current density in a section of the neighboring cells



Building a model: Two cells as the 3D model



Example of results: Induction magnetic field

Induction magnetic field due to internal currents and external currents assuming no ferromagnetic effects.



Example of results: Induction magnetic field in presence of steel elements (shell, superstructure)



Example of results: Velocity field

velocity field



Example of results: Bath-metal surface contour



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2. Program description

Several papers published have discussed metal pad instabilities in aluminum reduction cells. Among them some are concerned with specific phenomena, as for example Kelvin-Helmoltz instabilities [1] or electrical contact problem between different materials [2]. Another one [3] deals with stability considered in its full generality and summarizes the different problems that remain to be solved. Beyond this it is somewhat surprising, at a time when most professionals are struggling to gain a few percents in efficiency, to see a new model proposed [4] that promises a 25% efficiency increase!

Stability problems can be tackled from two different points of view. The first one, which is oriented towards an understanding of the physical mechanisms that cause instability, requires approximations and simplifying assumptions to derive models that hopefully keep the essence of the studied phenomena and that are in principle technically easier to deal with.

The second approach takes advantage of the physical insights gained through the study of these simple models and considers the problem from the mathematical side. J. Descloux, M. Flueck and one of the authors use some of the powerful techniques developed in numerical analysis over the past fifty years to derive some appropriate methods and algorithms that make it possible to solve the MHD equations for geometries and busbar arrangements typical of real operating cells. The accuracy of the results is such that engineers can safely rely on them in designing new cells or improvements to existing ones.

The purpose of this document is to outline the different steps required in taking this numerical approach (see [5] and references therein), to discuss its advantages by way of some specific examples, and to compare it with some of the other ones proposed in the literature.

2.1 The steady state

It is customary when dealing with stability questions to start by computing a steady solution, i.e. a solution the values of which are, at each point in the space, time independent. One then derives and solves the equations for the time dependent fields describing small "fluctuations" around the steady solution (note that the fluctuations are also referred to as "perturbations" in the literature). Since the steady solution appears in the coefficients of the equations describing the fluctuations, it has to be determined with some accuracy; we believe that it must account for:

- the actual geometry of the cell including all the anodes and the ledge,
- the distribution of the currents in the actual busbar arrangement, and the resulting induced magnetic field,
- the presence of ferromagnetic materials,
- the anisotropic character of the flows, through an appropriate description of turbulence.

It may be worth noting that the shape of the aluminum/bath interface and that of the surface defined by the bottom of the anodes, which are both unknown,

have to be calculated with the help of an algorithmic procedure (see for example [6]). In the case of an anode change, up to ten iterations may be needed to reach a stationary value.

2.2 The linearized equations

Once the steady state has been computed the next step consists in solving the equations describing the fluctuations. Let us say a few words about these equations.

Although the linearized equations correctly described the fluid motion only in the time interval where its amplitude is small they contained the information which is necessary to detect all the potential instabilities which are not specifically produced by non linear effects. This possibility of characterizing the system by analyzing variations of small amplitudes only is the basis of the models that depend on linearizing the MHD equations. Linearizing here means expanding the solution around a steady solution in which, since they are very small, all the terms containing fluctuations of orders higher than one are disregarded.

We emphasize the fact that, although linearized, these equations, and consequently their solutions, retain enough information to answer the stability questions we are concerned with. It is not our purpose in this document to go into the details of the linearization process needed to derive the equations and conditions describing the fluctuations (they can be found in some of the references of [5]). Suffice it to say that the equations and conditions so obtained are linear and hence much easier to handle mathematically than the original ones. In particular it can be shown that any solution of this system can be expressed as a linear combination of some "elementary solutions", usually called modes, which are characterized by a complex frequency $\omega = \alpha + i \beta$ the time dependence of each mode is consequently of the form $\exp(i(\alpha + i \beta)t)$ an expression which shows that, according to the sign of β , the solution will either increase or decrease exponentially. It is thus clear that the system will be stable if, for all the elementary solutions, β is larger than zero.

The analysis and numerical computation of the possible modes and of their respective frequencies requires the use of a formulation, called the variational or weak formulation, which is described in the next section.

4. The variational formulation

The transformation of the problem, expressed in terms of differential equations, into a variational one is necessary in order to be able to use finite element methods in the numerical analysis. It replaces a system of differential equations with a system of algebraic ones. The advantages of this variational formulation are as follows:

- It reduces the computation of the frequencies corresponding to the different modes to the problem of finding the eigenvalues of an operator in an infinite vector space, which is more generally referred to as the spectral problem.
- It makes it possible to show that the fluctuations of the electromagnetic force field can be considered as a function of the fluctuations **U** and H

corresponding respectively to the velocity and the interface displacement in the vertical direction, and also of the frequency ω .

• The variational methods have been developed in the frame of functional analysis, a domain of mathematics that considerably generalizes the Fourier series and integrals techniques, making it possible to solve the problem without having to simplify the geometry of the cell.

At this point it is worth noting that the variational formulation for the fluctuations is again solved without approximations. It takes account particularly of:

- i) all terms remaining after the linearization process (surface current density on the interface, and all the other terms depending on U and H(see [5] for details));
- ii) the time dependence of the potential vector, and its 1/r behavior at infinity;
- iii) the geometry of a real cell, without simplification.

We also note that the variational formulation, used for the calculation of the electrical potential and of the induction magnetic field, results in an expression for the Lorentz force field in which the dependence on **U**, H and \Box appears very elegantly. With a force field (depending on **U**, H and \Box \Box the hydrodynamic equations implicitly contain, retaining its entire complexity, the elementary coupling introduced in [4].

5. Numerical calculations

What are the mathematical questions and difficulties encountered when trying to numerically compute the solutions? In particular, how can we effectively obtain the frequencies and modes?

As already mentioned above, a customary approach in numerical analysis is to make use of a finite element method. The basic idea of such a method is to approximate an infinite dimensional function space by some of its finite dimensional subspaces, the dimensions of the latter being determined by the required accuracy. With these techniques the eigenvalue problem in an infinite vector space is reduced to a classical eigenvalue problem (in a finite dimensional space). Our problem is now to pick out of the set formed by the eigenvalues only the ones that are significant, typically 12 in number, and to compute them in a way ensuring that all of them are determined with the same accuracy.

In order to do that we start by computing the so-called gravitational (or hydrodynamic) modes which correspond to the situation in which the fluids are submitted to the gravitational force field only. This set of gravitational frequencies has to be looked at as the first step of the iterative procedure, used to get the solutions, which consists in increasing the electrical current step by step from zero up to its operating value. The frequencies, calculated at each step, are plotted in the complex plane; each mode thus has its "path" in the complex plane, one extremity of which represents the frequency for the gravitational mode and the other, the frequency at the operating level of the current. We name them MHD frequencies (the corresponding solutions being MHD modes).

Three important remarks are in order:

- 1. One could in fact start the iterative process with other frequencies than the gravitational ones. We choose to start with them because these frequencies can be easily computed with an algorithmic procedure in which the first step is approximated by the trivially calculated gravitational modes corresponding to a simple cuboidal cell.
- 2. At each step the frequencies and modes are obtained with the help of an algorithm which makes use of both an "inverse power method" and a "Galerkin approximation" [8]. This algorithm delivers all the frequencies with the same accuracy; it is moreover capable (and this is quite unusual) of handling situations corresponding to a degenerate spectrum.
- 3. At each step of the algorithm the modes are elements of a subspace, of the function space mentioned above, but they are not (as one might infer from some of the published papers in this domain) linear combinations of the gravitational modes. In other words at each step of the calculation the 12 modes considered generate different subspaces of the function space. Gravitational modes are in general the only subspace the elements of which can be expressed as pure gradient fields (generally the MHD modes have both gradient and curl parts).

6. Examples

Here are the assumptions on which the model is based:

- The fluid flows are described by the classical equations of fluid dynamics: Navier-Stokes equations for the steady state and linearized Euler's equations (with the damping factor (see [7])) for the fluctuations.
- The electromagnetic fields are described by quasi-static Maxwell's equations, i.e. Faraday's (with the ∂_i B term) and Ampere's laws.
- The geometry is the exact shape of the actual cell, without any simplification.
- The ledge shape is assumed to be known, either from measurements or by calculation.
- Effects related to the generation and release of gas bubbles are ignored.

Let us now present the results of numerical calculations performed for two specific examples using code developed at the "Ecole Polytechnique Fédérale de Lausanne" in collaboration with algroup's Technology Center Chippis.

We consider the case of an end-to-end 139'000 Amps cell, shown schematically in figure 1, in two different situations: in the first one the cell is oscillating whereas in the second the cell is unstable after changing two corner anodes due to the presence of bottom crust lying on the cathode (poor bath cleaning).

a) The steady solution

We start by computing the steady solution.

Since the shape of the bath-metal interface is one of the unknowns of the problem it has to be computed; this is done iteratively as follows:

At each step one takes the approximation of the interface obtained in the preceding step, and calculates the corresponding electrical potential and

induction magnetic field. The latter, which is computed with the Biot-Savart formula, takes into account the electrical currents both inside and outside the cell.

It should be mentioned that since the interface is fixed at any given step in these calculations, (it has been obtained at the preceding step), one or other of the jump conditions has to be relaxed. The condition that has been relaxed is then automatically fulfilled when the correct interface is reached at the end of the iterative procedure (see [6] for details).

Figure 2 represents the interface obtained in this example. It shows that the assumption of a flat interface commonly used in simple models is certainly a poor approximation, especially in the neighborhood of the risers located at the extremities of the cell.

The horizontal components of the steady velocity field, in the middle of the aluminum layer, are shown in figure 3.

b) The frequency spectrum

As explained in the previous sections the computation of the frequency spectrum starts by calculating the gravitational frequencies and modes. They are represented in figure 4 by small triangles located along the real axis. The MHD frequencies and modes corresponding to the operating values of the electrical current are reached through an analytic continuation during which the current is slowly increased from zero up to its operating value. The paths followed by the frequencies in the complex plane during this analytic continuation process are represented in the same figure. It is important to note that this picture represents calculations of the frequencies performed without the damping factor used in [7]. The effect of the latter corresponds to the straight green line parallel to the real axis. One can see that the cell is stable, the most critical frequency of 0.029s⁻¹ at full operating current being well away from the stability limit.

c) The anode current (oscillating cell)

In order to check the validity and the accuracy of the computed frequency spectrum we compare the values obtained with those resulting from anode current recordings performed on the cell for which the calculations were made. Figure 5 shows an anode current recording in a cell showing MHD instability unrelated to anode change, and figure 6 the Fast Fourier Transform of that current, which gives the frequency spectrum. There is very good agreement between the main peak in the FFT at 0.027s⁻¹ and the corresponding calculated critical frequency of 0.029s⁻¹ shown in figure 4.

d) The frequency spectrum (after anode change)

In the second example we consider the same cell after two corner anodes have been changed, under the assumption that some bottom crust is lying on the cathode because of poor bath cleaning. As in the previous case we look again at the spectrum and at the anode current. The computed frequencies are shown in figure 7.

A comparison with figure 4 shows that the frequencies have shifted and the shapes of their paths have altered (note that in figure 6 the variable is the frequency v new whereas this variable is $\omega = 2\pi v$ in figure 7). In particular, the imaginary part of the spectrum has changed drastically, with the path at 0.0388s⁻¹ reaching the instability limit. The cell did in fact become unstable after this double corner anode change, confirming the prediction.

e) The anode current (after anode change)

Figures 8 and 9 are analogous to figures 5 and 6 above.

Again a comparison between figure 7 and figure 9 shows excellent agreement between the main peak of the Fourier analysis of recordings and the unstable frequency given by the numerical computations.

From these results we draw some important conclusions:

- 1. The numerical simulations predict frequency values that agree exceptionally well with the observations made on the actual cells.
- 2. The actual effects of changing the two corner anodes are accurately mirrored in the stability diagram. The fluid motion has reached an unstable state.
- 3. The frequency spectrum reflects the state of the cathode

A further numerical simulation of operation after corner anode changing with proper bath cleaning predicted that the cell would remain stable, and this prediction was in fact confirmed in practice.

7. Physical phenomena

Up to now the stability question has been considered from a mathematical point of view only. Although physical laws have been important in deriving this model, as well as in the variational formulations and in the choice of the algorithms, our main goal has always been to write a computer program capable of calculating frequencies and modes accurately enough to help engineers in their tasks.

Let us now turn to the physical aspects of the mechanisms generating instabilities. It is legitimate to ask: is it possible to obtain some physical insights from the variational formulations used to solve the stability problem? Before trying to answer this question let us begin with an important remark.

As is proved in [5] the variational formulations are obtained from the set of differential equations and conditions describing the fluctuations through some mathematical manipulations. Conversely it can be shown that (under reasonable regularity conditions) the system of differential equations and conditions can be fully recovered from the variational formulation. This formulation thus clearly contains the same physical information as the differential equations we started with. It may be worth keeping in mind that in physics, laws expressed in terms of differential equations are generally derived from variational formulations too. In fact the differential and the variational formulations complement each other and can be considered as equivalent.

As with linearization we will not go into details here. We will however mention that when one gets acquainted with variational formulations, physical phenomena can be studied by introducing appropriate subspaces of the function space in which the solutions are computed. In this way it is for example possible to recover the results obtained from the very simple model derived in [9], but in a more general context.

Although it is rather difficult to identify in the variational formulation the different physical mechanisms generating instabilities (one should note that this is equally true of a description in terms of differential equations), one can study, with the help of the numerical simulation that has been developed, the influence of the different field contributions on the imaginary parts ($\Box \Box \Box \Box$ of the frequencies and consequently on the stability. Qualitatively the behavior of $\Box \Box$ can be summarized as follows.

- □□□□ strongly depends on the steady electrical current distribution, which is also one of the main factors determining the shape of the bath-metal interface.
- □□□□is strongly affected by the presence of the linearized convection terms. In some cases their effects are even stronger than those of the steady electrical current distribution. This contribution is almost certainly related to the Kelvin-Helmoltz instability studied in [1].
- 3. The so-called induced currents (the contribution to the electrical current density resulting from the motion of the fluid in the presence of the induction magnetic field) are also responsible for some significant contributions to
- 4. Finally and surprisingly enough the time derivative of the induction magnetic field, which appears in Faraday's law, cannot be disregarded. It may induce up to 50% variation in the factor □□ In the frequency variable this term enters the variational formulation through the expression i□A which appears in the current density.
- **8.** Discussion and conclusions

As we have seen in the above examples the chosen variational formulation has several advantages.

- It is immediately suitable for a numerical approach using a finite element method.
- With the use of this method the values of the frequencies turn out to be the solutions of an eigenvalue problem. Making use of rather sophisticated techniques the physically significant frequencies are obtained with a special algorithm that can handle degeneracy and also compute all the frequencies with the same accuracy.
- Studying the spectrum makes it possible to predict the maximum current at which the cell can be run without becoming unstable.
- Some disturbances of particular practical importance can be numerically studied, such as anode changing, tapping metal or the presence of bottom crust.
- When approximations of the model are required in order to throw light on particular mechanisms that may affect stability, the variational formulation is particularly suitable because it can be done in a way that ensures that the basic physical phenomena are taken account of.

An approach similar to the one presented in this paper has been introduced in [10]. As far as we are aware, however, the authors of that paper neglect some of the effects we include.

As pointed out in the introduction, two different points of view can be adopted in the study of instability problems. Our purpose here is neither to give an exhaustive list nor a detailed account of the recently published papers. We however would like to clearly state that, as shown in the previous sections, the effects of the different fields on stability cannot be easily disentangled, for all of them are significant. This means that work like [1] which focusses on some particular aspects of instabilities must depend on very simple models that can throw light on some of the underlying mechanisms leading to instability. Results obtained in this way are clearly of a qualitative nature only.

In conclusion we see that, with the help of a variational formulation and some of the powerful tools developed in numerical analysis, we have been able to build a numerical simulation that describes the behavior of the cell and yields results that agree exceptionally well with direct observations of the actual cell.

This unique tool can be used for instance in designing modifications to existing cells and in the study of cell voltage behavior. Furthermore, it can be used to test ideas for improving the MHD of the cell which would otherwise require costly, time-consuming and perhaps risky experimental campaigns in operating potlines.

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The authors

Michel.V. Romerio studied at the University of Neuchâtel, Switzerland, where he graduated in Physics in 1962, earning his Ph.D in 1969. He did postdoctoral studies in theoretical physics at Cornell University, USA from 1969 to 1972. He then became Assistant professor in theoretical physics at the University of Neuchâtel. Between 1980 and 1984 he did private consulting work for industry. From 1979 to 1989 he was "chargé de cours" in mathematics at the University of Fribourg, Switzerland. In 1984 he joined the Department of Mathematics at the "Ecole Polytechnique Fédérale de Lausanne", Switzerland where he is presently teaching and working on industrial research.

Jacques Antille took his degree in physics in 1974 at the University of Lausanne (CH). After his Ph.D. thesis Jacque Antille worked for some years at the European Center of Nuclear Research (CERN). Postdoctoral studies at the Nuclear Physics Institute of the University of Lausanne followed. Since 1984 Jacques Antille is with Alusuisse Technology and Management Technology Center, where he is project leader in the electrolysis group (Modelling) and in charge of magneto-hydrodynamic problems.



Figure 1 : Example of cell geometry used for mhd calculations







scale : i 15 cm/s

Figure 3: Horizontal velocity field within the metal



Figure 4: Stability diagram: the x corresponds to the paths of the frequencies at the different steps of the iterative procedure.



Figure 5: Recording of the anode current in a cell showing MHD instability unrelated to anode change



Figure 6: FFT of the current represented in figure 5.



Figure 7: Stability diagram (after anode change).



Figure 8: Recording of the anode current in a cell showing MHD instability related to anode change



Figure 9: FFT of the current represented in figure 8.