3D-simulation of ionisation gauges and comparison with measurements

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A B S T R A C T

3D-simulations using the Vector Fields OPERA 3D software have been carried out on the CERN-type modulated Bayard-Alpert gauge. The program allows to simulate the ion creation inside the gauge and takes into account space charge effects. Parameters such as sensitivity, ion and electron path lengths inside and outside the ionisation grid, location of ion creation, collection efficiency, and potential distribution were studied as a function of emission current. This investigation resulted in a deeper understanding about the behaviour of the gauge, in particular about the effect of space charge. The achieved results were compared with experimental measurements; the results are satisfactory and encourage further studies.

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1. Introduction

In earlier simulations of ion gauges, their relevant parameters were determined from charged particle trajectories in constant potential. The modification of the potential caused by the presence of charged particles could not be addressed directly in the simulation code due to the unavailability of computational power. For the commercial Bayard-Alpert (BA) type gauges, these simulations were in good agreement with observations, since the influence of space charge in these gauges did not seem to have a significant influence under normal operation conditions [1–3]. L.G. Pittaway put into evidence the influence of electron and ion space charge in extractor type gauges and made use of it to improve the design [4]. He determined the influence of the electron emission current to the potential fields in a separate step by assuming a homogeneous charge distribution over the grid volume. The space charge was determined from the average number of electrons passing the grid volume. The availability of multi-physics software packages combined with high computation power make it possible today to include local space charge phenomenon in the simulations and study in details its effect on ion gauges. We investigated this possibility on the CERN-type BA-gauge [5,6]. Simulations were also carried out for a modified Helmer gauge [7].

2. Simulations

The simulations have been carried out using the Vector Fields OPERA software package. Within this package the SCALA module is dedicated to space charge problem resolution. Once the geometrical model of the gauge is established and the electric potentials of all boundary surfaces are defined, the electrostatic potential distribution in the volume is calculated. Electrons are emitted from the primary emitting surfaces with a predefined initial energy below 1 eV. In our case the primary emitter is always the emitting filament. The trajectories of the electrons, as well as their kinetic energies along their paths in the potential fields are then calculated. The electrons have a probability of ionising molecules in the volume or, when hitting a surface, inducing the emission of secondary particles from this surface. The possibility of simulating secondary surface emission is not applied in the simulations presented in this paper.

The generation of ions is calculated as a linear yield along the electron path. This ionisation yield \( Y_i \) is determined from the ionisation cross-section \( \sigma_i \) multiplied by the molecular density. \( \sigma_i \) is a function of the electron kinetic energy \( E_e \).

\[
Y_i = \sigma_i(E_e) \frac{P_i}{k_BT}
\]  

where \( P_i \) is the partial pressure of the gas, \( k_B \) the Boltzmann constant and \( T \) the temperature.
For hydrogen and nitrogen, we used theoretical formula for the electron-impact ionisation cross-section. The formula sums the contributions of molecular orbitals and uses the Binary-Encounter-Bethe model. The orbital constants for these molecules were determined from the NIST database [8].

For argon, which was not available in the data base, an analytical formula has been obtained following instructions in Ref. [9] and using the experimental data from Ref. [10]. The ions created are then in turn defined with their mass, charge and initial kinetic energy.

Once the electric charge distribution caused by all particles within the potential field has been determined, a new potential field is calculated taking into account such a distribution. This leads in turn to a modification in the calculated trajectories. The simulation converges once it is self-consistent, that is — when the space charge correction does not change (to a certain tolerance) the potential distribution. In case the convergence criteria is not reached, the simulation stops after a predefined number of iterations or gives an error message in case of non-convergence.

3. The CERN Bayard-Alpert gauge

In the CERN accelerators and laboratories several hundred modulated Bayard-Alpert gauges are in use. They have been developed and optimised in the 1970’s to maximise their sensitivity and minimise the X-ray residual current. The modulators allow to determine in situ the X-ray residual current, hence allow measurements down to the upper $10^{-13}$ mbar range [11]. The grid is closed on its top and bottom parts; the grid diameter is maximised to fit, together with the filaments and supports, into a standard DN63-CF aperture. The grid wire thickness is reduced to improve the transparency for the electrons, hence increasing the mean electron path length by increasing the number of passages through the grid. The collector diameter has the optimum value to minimise the transparency for the electrons, hence increasing the mean kinetic energy. The collector diameter has the optimum value to minimise the X-ray residual current and ensure sufficient ion collection efficiency (see Fig. 1).

The gauge has two filaments, but only one is emitting during operation. The second one is a spare; it is at the same potential as the emitting one. More detailed information on the relevant dimensions can be found in Table 1.

The electrical potentials applied to the different parts of the gauge are shown in Table 2.

The two main characteristics of the gauge that need to be determined are the sensitivities $S_i$ and the modulation factors $k_i$.

### 4. Results of simulations and measurements

A comparison of the values for $S_i$ and $k_i$ as determined by simulations with the statistical average from calibrations is shown in Table 3.

The values in brackets indicate approximate values for the uncertainties. The indicated uncertainty of 15% in the simulations takes into account the uncertainty in the calculated theoretical $s_i$ of better than 10% as stated in Ref. [8] and the variation of the calculated $S_i$ with different simulated emission currents (Fig. 2).

The uncertainty in the measured values correspond to the 68% standard deviation of all calibrations for the three gases carried out at CERN since the 1990s. This includes more than 250 gauges. Those gauges have been calibrated in the range between $10^{-10}$ to $10^{-6}$ mbar. All simulations were carried out for a pressure of $10^{-10}$ mbar.

Simulations and measurements agree reasonably. Additional measurements have been carried out on a particular gauge on a dedicated set-up. While changing parameters on the test gauge the pressure was monitored with a second gauge to make sure that the pressure remained stable during the measurements. The measured sensitivity is rather stable with changing emission current up to about 10 mA (see Fig. 3). For H$_2$ it varies about 5% within this range. A close look shows that the sensitivity has two maxima in both

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**Table 1**

Dimensions of the CERN type BA gauge.

| Part             | Dimensions [mm] |
|------------------|-----------------|
| Grid             | φ 35 × 45, pitch 2, wire φ 0.13 |
| Grid covers      | pitch 3, wire φ 0.13 |
| Modulator        | φ 0.7, length 42 (inside grid) |
| Filament         | Wire φ 0.18, height 30 |
| Collector        | φ 0.05, length 42 (inside grid) |
| Vacuum chamber wall | φ 63 |

**Table 2**

Electrical potentials applied on the CERN type BA-gauge.

| Part                  | El. Potential [V] |
|-----------------------|-------------------|
| Grid                  | 150               |
| Modulator             | 150 (or 0 during modulation) |
| Filaments             | 50                |
| Collector             | 0                 |
| Vacuum chamber wall   | 0                 |

**Table 3**

Simulated and measured sensitivity and modulation factors for 3 different gases.

|                     | H$_2$       | N$_2$       | Ar         |
|---------------------|-------------|-------------|------------|
| Simulated $S$ [mbar$^{-1}$] | 15.5 (±2.3) | 38.0 (±5.7) | 45.1 (±6.7) |
| Average measured $S$ [mbar$^{-1}$] | 13.8 (±2.3) | 30.0 (±5.9) | 39.5 (±4.4) |
| Simulated $k$        | 0.84 (±0.13) | 0.85 (±0.13) | 0.85 (±0.13) |
| Average measured $k$ | 0.85 (±0.03) | 0.89 (±0.02) | 0.89 (±0.03) |

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Fig. 1. Photo of a CERN-type BA-gauge and corresponding geometrical model used in the simulations (a filaments, b grid, c collector, d modulators).
measurement and simulation. This has its origin in the deformation of the electrostatic potential caused by the electrons space charge. Fig. 4 illustrates the change of the electrical potential profile with emission current.

At low emission current, the flat maximum close to the grid wire allows more ions to escape from the grid. This fact is illustrated in Fig. 5, which shows the location of ion creation with respect to their final destination (collected by the ion collector or escaped from the grid) for 1 mA and 10 mA emission current. The parameter that relates the number of ions collected \( N^c \) to the number of ions created inside the grid \( N^t \) is the collection efficiency \( \mu \).

\[
\mu = \frac{N^c}{N^t} \quad (4)
\]

Simulation allows to determine this parameter. Figs. 4 and 5 may suggest that the collection efficiency decreases with lower emission current, which is indeed the case. Therefore, for the sensitivity to remain rather stable (see Fig. 3) with emission current, there must be a compensating mechanism. At low emission current, i.e. flatter potential gradient, the mean path length of the electrons inside the grid is longer (see Fig. 6, triangles) and more electrons penetrates close to the centre of the grid at a high kinetic energy. Therefore more ions are created near the collector. At high emission current (Fig. 4-d), the increased electron space charge provokes a lower generation of ions near the collector, because less electrons reach that area; in addition, ionisation is also reduced, due to a lower ionisation cross-section at lower kinetic energy. The reduced ion generation and the increased collection efficiency caused by the effect of space charge nearly compensate, resulting in a rather stable sensitivity with emission current over a wide range (Fig. 6).

The collection efficiency has been measured following the method proposed by Benvenuti and Hauer [6]. There, it is assumed that in modulation mode all ions that are created inside the grid are collected either on the collector or on the modulators. With the additional assumption that during modulation the same number of ions is created as during normal operation, the ratio of the collector
current during normal operation $I_c$ over the sum of collector current $I_{cm}$ plus modulator current $I_{mm}$ in modulation mode gives a possibility to estimate experimentally the collection efficiency $\mu_{\text{exp}}$.

$$\mu_{\text{exp}} = \frac{I_c}{I_{cm} + I_{mm}}$$  (5)

Simulation showed that these assumptions are rather rough approximations as the modulation can affect the mean electron path and ionisation yield up to 20% compared to normal operation. This may be the cause of the difference between the two curves in Fig. 7, which shows the measured collection efficiency using (5) and the simulated one determined using (4). The shapes of the two curves, however, are in good agreement.

5. Helmer gauge

Simulations of a Helmer gauge have also been compared with measurements on gauges as described in Ref. [7]. Two gauges were available for measurements. One is the improved Helmer gauge (H$\beta$) manufactured in 1980 and described in Ref. [7] and one is a newly built gauge at CERN (H$\beta$C, Fig. 8), which is very close to the design of the H$\beta$.

The sensitivity versus deflection voltage $U_{\text{defl}}$ is reported in Fig. 9. The simulation reproduces quite well the experimental curves. Both gauges show the maximal sensitivity at an emission current around 1.5 mA (Fig. 10). This maximum is not clearly reproduced by the simulation. The tendency of the sensitivity to decrease with emission current is also found. For unperturbed electrical potentials one would not expect such a change in sensitivity; this change is attributed to space charge.

Fig. 8. Main components of the Helmer gauge; on the right with opened cage. (a filament, b grid, c cage, d inner deflector, e outer deflector, f suppressor, g collector). The yellow line indicates the ion trajectory from the grid volume towards the collector. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 9. Measured and simulated sensitivity for nitrogen as a function of (negative) deflector voltage at an emission current of 1.5 mA ($U_{\text{grid}}$: 250 V, $U_{\text{fil}}$: 100 V; outer deflector and cage are at ground potential). Both simulation and measurements for a pressure of $10^{-10}$ mbar. The simulation did not include the suppressor.
6. Discussion and conclusion

The simulations carried out so far for the CERN-type modulated BA-gauge showed that the space charge caused by the electron emission current significantly modifies the electrical potential profile. However, the resulting increase in the ion collection efficiency at higher emission current is to a certain extent compensated by a reduced ionisation rate inside the grid, in such a way that the gauge sensitivity remains rather stable over a wide range of emission currents. This behaviour may be specific for this gauge, because of its very thin collector. Commercial gauges have much thicker collectors by more than a factor two. An increase of collector diameter results also in a steeper potential gradient closer to the grid. BA-gauges with thicker collector diameters are therefore less sensitive to the space charge caused by the emission current.

The Helmer gauge showed a strong reduction of the sensitivity with increasing emission current. This tendency could also be reproduced by the simulation.

Encouraged by the results of the simulations so far, this work will be continued. As the software allows to simulate electron and ion induced desorption, it would be of interest to include secondary surface emission in the simulations and study ion gauges at their pressure limit. The space charge caused by ions is included in the simulation, but has not been analysed in details yet.

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