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3D-simulation of ionisation gauges and comparison with measurements

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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].

ABSTRACT

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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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 shall only be mentioned, but 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 σ_i multiplied by the molecular density. σ_i is a function of the electron kinetic energy E_e .

$$Y_i = \sigma_i (E_e) \frac{P_i}{k_B T} \tag{1}$$

where P_i is the partial pressure of the gas, k_B the Boltzmann constant and *T* the temperature.

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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 X-rays 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 .



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).

Table 1

Dimensions of the CERN type BA gauge.

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

$$S_i = \frac{I_c}{I_e P_i} \tag{2}$$

 I_c is the ion current measured at the collector, I_e is the emission current and P_i is the partial pressure of the gas.

$$k_i = \frac{I_c - I_{cm}}{I_c} \tag{3}$$

 I_{cm} is here the measured collector current with the two modulators at ground potential.

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 σ_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 H₂ it varies about 5% within this range. A close look shows that the sensitivity has two maxima in both

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

Table 3

Table 2

Electrical p

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)	30.8 (±3.9)	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)	$0.89(\pm 0.02)$	0.89 (±0.03)

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