Research on control method of the Atmospheric Composition Detectors

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Abstract. The operational principle and working mode of the Atmospheric Composition Detectors (ACDs) based on the Quadrupole Mass Spectrometer (QMS) were introduced in this paper, the computer control method were detailed analyzed. Through the theoretical calculation and calibration experiment, researching results indicate that it has high resolution and performance.

Introduction

QMS is a kind of pressure measure instrument which is widely used because of its high resolution and sensitivity. QMS on board rockets and satellites is used for analyzing the planet atmosphere and the composition of soil. The composition of the planet gas plays an important part in the research of the origin and development of the planet. The analysis of isotopes can provide some valuable data for research on origin of the solar system. There are some restrictions when QMS is applied to the space exploration, the following factors must be taken into account: volume, weight, power, resolution, precision and scan speed. The ACDs based on the QMS will be presented in this paper.

Theory

The operational principle of the ACDs is similar to the ionization gauges: ionize the gas molecule and the gas pressure is proportional to ion current. The difference between QMS and ionization gauges is that QMS can separate the ion with different m/e through the Quadrupole Mass Filter. The QMS consists of four parallel cylinder electrodes with a circular cross-section, the quadrupole electric field is obtained by electrodes. The electrodes have a hyperbolic cross-section with two perpendicular zero-potential planes that lie between the electrodes and intersect along the center-line z-axis. The geometry of QMS with circular cross-section electrodes is shown in Fig.1. The two-dimensional inset indicating the polarity of the static (dc) potential used throughout this work: positive dc potential is applied to the two poles in the horizontal x-direction, while negative dc potential (of equal magnitude) is applied to the two poles in the vertical y-direction. For mass analysis both a static electric (dc) potential and an alternating (ac) potential in the rf range are applied to the electrodes of the QMS. The relative amplitudes of the dc and ac potentials control the ability of the system to mass filter a low energy beam of ions travelling along the z-axis. Assuming idealized field conditions within the structure, with vanishing component in the z direction, the potential distribution $\Phi(r, t)$ is given by

$$\Phi(r,t) = \Phi_0(t) \left( \frac{r^2}{r_0^2} \right) \cos(\omega t)$$

And

$$\Phi_0(t) = U + V \cos(\omega t)$$

where $U$ is the amplitude of the static dc potential and $V$ is the amplitude of the rf potential, which oscillates with angular frequency $\omega = 2\pi\nu$. 

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In case of a perfectly hyperbolic QMS geometry the radius \( r_0 \) is defined by the circle tangential to the four hyperbolic electrodes, and is known as the free field radius. The first two Cartesian coordinates, \( x \) and \( y \), are as shown in Fig.1. The potential satisfies the Laplace equation \( V^2 \Phi = 0 \) and is invariant in the \( z \) direction. A single ion passing through the device undergoes a motion that is a solution of Mathieu’s equations:

\[
\frac{d^2 u}{d\xi^2} + [a_u - 2q_u \cos(2\xi)]u = 0
\]

where \( \xi = \omega t / 2 \) and \( u \) represents the \( x \) or \( y \) displacement of the ion in two distinct equations; one for each dimension. The parameters \( a_u \) and \( q_u \) are related to the potentials \( U \) and \( V \) by:

\[
a_u = a_x = -a_y = -\frac{8eU}{mr_0^2 \omega^2}
\]

\[
q_u = q_x = -q_y = -\frac{4eV}{mr_0^2 \omega^2}
\]

Where \( m \) is the ion mass and \( e \) is the elementary charge. The solutions of Mathieu’s equations for motion in the \( x-y \) plane contain either a strictly growing exponential factor or an oscillatory term of finite radial extent, depending on the ion mass \( m \).

With proper choice of \( a \) and \( q \), or \( U \) and \( V \), respectively, somewhere in the stable region, ions of a corresponding \( m \) have stable trajectories, they oscillate around the \( z \) axis with finite amplitude and ultimately emerge from the end of the mass filter.

Operating under conditions of stability, only ions with a very small entrance deviation have oscillation amplitudes that can be transmitted through the QMS. Simultaneously scanning the amplitudes of \( U \) and \( V \) along a “mass scan line” of fixed ratio of \( U/V = a/2q \).

The resolution can be varied via the ratio \( U/V \), the slope of the mass scan line, measured in the factor 0.1678 = \( a/2q \). Approaching the value of \( U/V = 0.1678 \) and corresponding to a mass scan line slope, would yield highest mass resolution. The typical stable ion trajectories in the \( x \) - and \( y \)-coordinate which calculated for \( (a, q) \)-parameters of (0.23, 0.706) near the apex of the stability region.

\[
U = 1.212 \times m \times \omega^2 \times r_0^2
\]

\[
V = 7.219 \times m \times \omega^2 \times r_0^2
\]

For example, if \( \nu = 7.7 \text{MHz} \), \( r_0 = 0.0862 \text{cm} \), \( \text{mass}_{\text{max}} = 42 \text{amu} \), so \( U_{\text{max}} = 22.4 \text{V}, V_{\text{max}} = 133.6 \text{V} \).

**Control method**

According to the analysis, \( \pm (U + V \cos \omega t) \) is the amplitude of the electrodes potential, Fig.2 is the ACDs block diagram.
The sensor consists of ion source, quadrupole Mass Filter and ion detector. The MCU is the control center which including emitting current control, scanning output signal, collecting ion current and temperature signal.

The scan output signal is controlled by the MCU through control DA converter, make the $U/V$ linear change, electrometer collect the different ion with specifically $m/e$, then we can calculate the gas type and pressure according to position and intensity of the ion. In practice, we can adjust the scan signal including the rising time, falling time and scan potential. Fig. 3 shows the scan signal, which can be adjusted through the computer control software.

![Control block diagram of the ACDs](image)

![The rf scan signal](image)

1. scan amplitude $\Delta V_1$ varied from 0~5V
2. suspending amplitude $\Delta V_2$ varied from 0~5V
3. rising time $\Delta t_1$ varied from 1~15s
4. falling time $\Delta t_2$ varied from 20ms~1s
5. stopping time $\Delta t_3$ varied from 200ms~100s

**Experiment**

The experiments were conducted in our calibration laboratory. Sensor was installed on the side of the vacuum-chamber. Experimental results are shown in Fig4~Fig6: X-axis is the scan time, Y-axis is the ion voltage signal. oxygen mass spectrum is shown in Fig4, Ar mass spectrum is shown in Fig5, He $\text{CO}_2$ $\text{N}_2$ $\text{O}_2$ Ar mass spectrum is shown in Fig6.
Experimental results show that the ACDs have high resolution, sensitivity and S/N(signal-to-noise) ratio. When gas is put into the vacuum-chamber, the mass spectrum is shown on the relevant position, so we can distinguish different gases.

The latest main technical parameters and capability of the detector are listed as follows:
- Mass Resolution: 1.5 amu
- Total Ion Current: $1 \times 10^{-8} \sim 1 \times 10^{-11}$ A
- Least Detectable Ion Current: $10^{-12}$ A
Conclusion

The experimental results indicate that the ACDs based on the QMS have high resolution and sensitivity for the analysis of the atmospheric composition. It uses the adjustable computer scan method which keeps the U/V constant, changes the scan time and frequency.

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References
