

# Application and Progress of Single Particle Aerosol Time-of-Flight Mass Spectrometry in Fine Particulate Matter Research



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**Abstract:** The idea of single particle aerosol mass spectrometry was first proposed in the 1970s and then developed quickly in recent two decades. Because it can simultaneously provide much information including particle size distribution, composition of multiple chemical species and mixing state for each single particle with high-time resolution, single particle aerosol mass spectrometry has been widely applied in the area of environmental monitoring and fine particulate matter research. This review aims to (1) provide an introduction of the development history and progress of single particle aerosol time-of-flight mass spectrometry, (2) summarize its principle, methods for data analysis, output of results and its applications in environmental measurement and research using two major commercialized instruments (ATOFMS and SPAMS), and (3) provide suggestions for future research.

**Key Words:** Single particle aerosol mass spectrometry; Fine particulate matter; On-line source apportionment; Review

## 1 Introduction

Regional air pollution has become more serious with rapid economic growth in China. Frequent hazy weather and serious air pollution episodes have attracted great attention in China and abroad. The invention and development of aerosol measurement techniques especially on-line measurements have enhanced our understanding of the characteristics of aerosols and atmospheric pollution<sup>[1]</sup>.

On-line aerosol mass spectrometry has been widely deployed because of its high time resolution and low detection limit. There are mainly two types of online aerosol mass spectrometry, one for bulk measurement and the other for single particle measurement. Aerosol mass spectrometer (AMS), aerosol chemical speciation monitor (ACSM) and thermal desorption chemical ionization mass spectrometer

(TDCIMS) are in the category of on-line aerosol bulk measurement instruments. Particles are first vaporized by heating and then ionized by different ionization methods such as electron impact, chemical ionization and optical ionization. On the contrary, aerosol time-of-flight mass spectrometry (ATOFMS) and single particle aerosol mass spectrometry (SPAMS) are two commercial single particle instruments which can measure size distribution, chemical composition and mixing state of single particle at the same time<sup>[2]</sup>.

In this paper, the basic principle, data processing methods and outputs of the two commercial on-line single particle aerosol time-of-flight mass spectrometers, ATOFMS and SPAMS were introduced. Main research and application areas of on-line single particle time-of-flight mass spectrometry (single particle aerosol mass spectrometry for short in following text) were also summarized with suggestions for future research direction.

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## 2 Development of single particle aerosol mass spectrometry

Friedlander<sup>[3,4]</sup> proposed that ideal aerosol instrument could measure the size, chemical composition and shape of every single particle simultaneously. At the beginning stage, researchers<sup>[5,6]</sup> tried to use metal filament (*e.g.* rhenium and tungsten) to vaporize and ionize aerosol. By this way, chemical composition of single particle was measured. In the 1980s and 1990s, with the rapid development of techniques such as laser, time-of-flight chamber, and ion trap and so on, the on-line single particle aerosol mass spectrometry technique had great progresses. In 1996, Prather *et al.*<sup>[7]</sup> invented aerosol time-of-flight mass spectrometry (ATOFMS). The invention and later commercialization of ATOFMS made this technique widely applied in the atmospheric science and many other fields.

## 3 Introduction of commercial single particle aerosol mass spectrometry

### 3.1 Operation principles

The basic operation principle of single particle aerosol mass spectrometry is that atmospheric aerosols are first induced into ion source region, then vaporized/ionized, and finally detected by a detector<sup>[5]</sup>. Specifically, atmospheric particles are first converged to a very narrow particle beam by converging nozzle or aerodynamic lens system. After size measurement, every single particle is vaporized/ionized to charged fragments and finally detected by time-of-flight chamber and micro channel plates (MCPs) detector. As the commercial single particle aerosol mass spectrometers, ATOFMS and SPAMS include four major systems: vacuum system, aerosol sizing system, ionization system and mass spectrometry detection system<sup>[8]</sup>. Aerodynamic lens and high energy laser ionization system are deployed in both two commercial single particle aerosol mass spectrometers. Detailed operation principles and parameters can be seen in Prather<sup>[7]</sup> and Li *et al.*<sup>[9,10]</sup>.

### 3.2 Calibration methods

The calibration of single particle aerosol mass spectrometry includes size and mass calibration. Size calibration is to assure the accuracy of size measurement. Polystyrene latex spheres (PSLs) with standard size (0.2, 0.3, 0.5, 0.72, 1.0, 1.3 and 2.0  $\mu\text{m}$ ) are generated through atomization and then induced into spectrometer. Mass calibration, including calibration with standard materials or ambient air, is to assure the accuracy of mass spectra of particles. Standard materials or ambient air are induced into SPAMS to calibrate the shift of the mass to charge ratios ( $m/z$ ) of some fragments in spectrum (*e.g.*  $^{23}\text{Na}^+$ ,  $^{39}\text{K}^+$ ,  $^{208}\text{Pb}^+$ ,  $^{46}\text{NO}_2^-$ ,  $^{62}\text{NO}_3^-$ ,  $^{97}\text{HSO}_4^-$ ).

## 3.3 Methods for data analysis

Direct extraction and clustering analysis are the two main methods to analyze the single particle data.

### 3.3.1 Direct extraction of physical and chemical properties of single particles

Particle size affects the deposition velocity and residence time in the air. SPAMS and ATOFMS can be used to analyze aerosol sample and provide size distributions of particles in accumulation mode. The measurement range of particle size is 0.2–2.0  $\mu\text{m}$  for SPAMS and 0.1–3.0  $\mu\text{m}$  for ATOFMS. Moreover, ultrafine ATOFMS can measure nucleation mode particles in the size range of 50–300 nm<sup>[11,12]</sup>.

Particle counts and relative areas for certain components can be obtained by some specific spectra analysis. Particle counts are used to show the number of particles containing some specific fragments, while relative area is to reflect the intensity of certain fragments. Thirty-minute is often chosen as the time resolution to obtain reliable and representative data.

Response of individual species varies in SPAMS due to the difference in ionization energy of components and matrix effects. For instance,  $\text{K}^+$  could be 5 times more sensitive than  $\text{Na}^+$ <sup>[13]</sup>. Furthermore, fragments with the same  $m/z$  might be from different ions. As a result, to minimize the interference from other ions, signal intensity, stable isotopes and oxidants of specific components are often considered together when identifying particles containing certain ions. For example, fragments of  $m/z$  –79 might be from  $\text{Br}^-$ ,  $\text{PO}_3^-$  or other ions, so only fragment with high signal of  $m/z$  –79 and –81 at the same time is identified as bromine containing particles to reduce the interference of  $\text{PO}_3^-$ <sup>[14]</sup>. Furthermore, because more than one fragment can be produced when a standard is analyzed or ionized by single particle aerosol mass spectrometry, till now there is no unified standard way to identify a specific chemical species. Taking nitrate for example, with  $m/z$  30<sup>[15]</sup>, 62<sup>[16]</sup>, 30 or 46 or 62 or 108<sup>[17]</sup> were all used to identify whether a particle contains nitrate or not. Fu *et al.*<sup>[18]</sup> summarized the ways to identify sulfate, nitrate, ammonium, EC and OC containing particles and found that it was very method-dependent. Thus, it is quite important to consider the method differences in determining certain components and to choose the best method when analyzing raw data from single particle aerosol mass spectrometry.

### 3.3.2 Particle clustering analysis

With such a large dataset, particles can be classified into different types on the basis of the similarity of their spectra. Typical ion clustering and algorithm clustering are two major methods for particle clustering analysis. As for clustering with typical ions, certain particles with specific fragments are selected

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