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ORIGINAL RESEARCH

Stable compensation voltages in differential mobility spectra by separating neutral vapors from ions in sample flow

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Abstract

In small planar differential mobility spectrometers with ambient pressure ion sources, both ions and neutral vapors of sample commonly flow from the ion source directly into and through the analyzer region. Although simple and convenient both for fabrication and operation, product ions derived from sample in this design may form clusters with neutral unreacted sample or matrix constituents particularly at vapor levels of 50 ppm or greater. Uncontrolled and changing levels of such neutrals cause concentration dependent formation of ion clusters with variations in compensation voltages of DMS spectra. Stable compensation voltages were achieved for product ions by extracting ions into a counter flow of purified gas excluding neutral vapors from ppm to percent levels. An interface with electric fields and purified air was placed between ion source and analyzer region and operated with both on-axis and orthogonal extraction of ions. Effectiveness of removal of neutrals was determined using variations in peak position for protonated monomers and proton bound dimers of dimethylmethylphosphate, significantly avoiding complications of ionization chemistry with high vapor concentrations of methylene chloride, iso-propanol, water, and methanol. *In-silico* modeling using COMSOL and SIMION clarified the flow of ions and gases in two modes of operation. Findings anticipate the development of multiple stages of DMS analyzers where vapors may be intentionally added as modifiers in one stage and removed before entering a subsequent stage.

Keywords Compensation voltage · Differential mobility spectra · Ion extraction · Neutrals

Introduction

During the first decade after the introduction of ion mobility spectrometry (IMS) as a modern analytical technique in 1970 [3, 7], a susceptibility or dependence of drift times in mobility spectra upon vapor concentrations of sample had been described [2, 8, 12]. This made measurements with these early drift tube designs somewhat unpredictable causing misunderstanding of mobility measurements and eventual disregard of IMS methods [12]. The structures for these inaugural commercial drift tubes, specifically the Beta VI from Franklin GNO, contained gaps between drift rings where neutrals could diffuse from the ion source into the drift region. Unreacted neutrals or matrices from sample in the drift region could cluster with product ions causing variations in drift times as concentrations of sample vapors changed inside the drift tube housing [2]. Nearly a decade later, such spectral instability was solved using a unidirectional flow design where the drift region was kept free of sample neutrals by a counterflow of purified air or nitrogen, the drift gas, which also vented the ion source volume [1]. This control of sample residence in the drift tube resulted in a) spectral drift times independent of sample vapor levels and b) secondary benefits of predictable times for reactions between sample vapors and reactant ions.

Small planar differential mobility spectrometers were introduced in 2000 with simple structures where ions were carried in a gas flow through an analyzer stage [13, 14]; thus, sample was passed into the ion sources and then direction into the analyzer region along with vapor neutrals of unreacted analyte and sample matrix constituents including humidity [9]. Consequently, shifts in compensation voltages of DMS spectra could be observed and were dependent on vapor concentrations of sample, i.e., unreacted sample neutrals, paralleling the 1970s history of spectral instability for IMS. This has not been widely described in DMS measurements since vapor

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concentrations of samples are routinely below ppm levels owing to ppb detection limits. Nonetheless, ion-neutral clustering and shifts in compensation voltages and the underlying mobility dependence on field (i.e., alpha functions) become noticeable at neutral concentrations of 50 ppm and above [5, 9]. Variable peak positions should be pronounced for analyzers equipped with direct sampling and membrane inlets with high transmission rates of moisture; and this may be a significant design weakness for any embodiment of DMS technology. The specific concern here is the application of DMS in environmental monitoring especially with fluctuations in atmospheric moisture or unexpected excursions of matrix concentrations. Another concern is the long-term reliability of spectral libraries, and their usefulness, across all DMS platforms and applications; this alone necessitates a correction in the existing technology design and methods of small, planar, DMS analyzers.

A final concern on unregulated flow of neutrals into DMS stages has arisen with the emergence of tandem DMS where ions are processed sequentially in multiple stages [10, 11] and the use of vapor modifiers to control peak separations in DMS [5, 17, 18] In this, polar volatile substances are added intentionally at 1 to 3% (m/v) into the gas flow enhancing peak separations though inadvertently altering ion chemistry, either in the initial step of ion formation or in subsequent analytical stages in tandem DMS. Thus, vapor modifiers added in one stage to control alpha functions may be unwelcome in latter stages and should be removed, isolating ions in a flow of purified gas. In summary, the simplicity of DMS designs during the past twenty years should be refined in a next step where ion characterization occurs in a purified and controlled gas atmosphere, regardless of sample composition. An interface technology between ion source and analytical region or between stages of a tandem DMS is envisioned as a next and simple refinement of drift tube designs in DMS.

The separation of gas ions from sample neutrals in air at ambient pressure has been done previously with mass spectrometry (MS) with early atmospheric pressure ionization (API)-MS instruments, specifically, pinhole inlets of early TAGA 6000 models [19] and skimmer inlets of API-III models [6] where a curtain gas of purified nitrogen was used to protect cryogenic vacuum systems from loss of pumping speed through intake of helium in ambient air. A secondary benefit was the exclusion of sample neutrals from ion flow through the curtain gas. Another development in mass spectrometry was the curtain gas filter (CGF), designed for inlets with capillary tubes of 500 μm inner diameters which are particularly vulnerable to clogging by deposition of buffers, silica, salts, or other particular matter and fouling from dissolved silica [20]. Electric fields were used to draw ions into a flow of purified gas while unionized substances and other neutral material were removed under slight vacuum [4, 21]. A limitation with this design of an ion-neutral separator was ion yield which averaged ~40% though effectiveness of removal of neutrals (vapors and salts) was 100%. Although small on the dimensions of a DMS analyzer, the CGF was designed around a capillary tube for a mass spectrometer and was not suitable for flow paths in a DMS analyzer; ion transmission of 30 to 40% were considered unviable for refined DMS technology. Another approach to transferring ions into a purified gas flow with exclusions of neutrals was described in a patent with two DMS analyzers in a stack where ions leaving a first DMS were deflected into the flow of the second DMS analyzer. While this concept demonstrates the benefits of ion deflection between gas flows, the intention was not originally as a device between the ion source and a DMS analyzer [15].

In developments described here, the design principles of the CGF were re-embodied with a new geometry suitable for DMS analyzer and termed the Neutral Excluder Stage (NES). Objectives in this work include the following:

a. explore performance of a cylindrical geometry Neutral Excluder Stage (NES) and characterize performance quantitatively using compensation voltage stability as a measure of the effectiveness of removing neutrals over a wide range of vapor concentrations.
b. determine ion yield through the NES, and.
c. demonstrate continuous DMS operation with positive and negative ions.

Dimethylmethylphosphonate with proton affinity of ~893 kJ/mol was selected for study since competitive charge exchange would be suppressed and since protonated monomers and proton bound dimers both could be used to explore influences on compensation voltages from a broad range of vapor concentrations of volatile polar compounds.

Experimental

Instrumentation

DMS Analyzer- The DMS analyzer was built in house and has been previously described [16]. The waveform was at a frequency of 1.18 MHz with Separation Voltage from +700 V to +1500 V. Compensation voltage was scanned from +30 V to −10 V over 1.8 s. Software to operate the DMS was prepared in-house using LabView. The interface card was a model 6024E ADC from National Instruments (Austin, TX).

Interface- The NES is shown in Fig. 1 as a three dimensional solid model and was comprised of four sub-components (Fig. 1A) including: 1. an aluminum inlet and ion repeller, 2. a thin washer of Teflon to electrically insulate the repeller, 3. a black ring of porous carbon foam to create a radial 360^o flow of purified gas, and 4. the aluminum body to support sub-components and join to the DMS analyzer. In Fig. 1B, a cross-section is shown with two inlets (in a

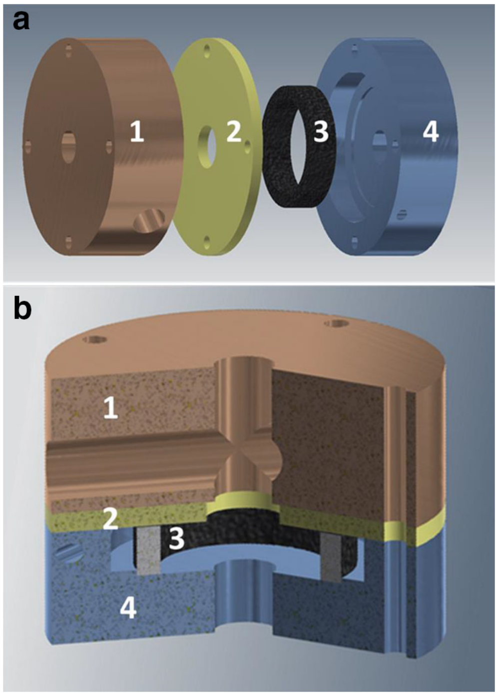

Fig. 1 Autodesk Inventor CAD model of a Neutral Excluder Stage. On the left in (**A**), the model is shown with the components pulled apart and numbered. In (**B**), an assembled model is shown with a cross-section cutaway. Parts are 1: Sample inlet and repeller electrode, 2: PTFE washer to isolate electrodes, 3: A porous carbon foam washer for equalizing purified gas inlet flow from a single point to an even, annular flow, and 4: Grounded electrode and interface to DMS

T-pattern of 6 mm diameter conduits) from the ion source for either axial injection or orthogonal extraction into a purified gas flow. Sub-components are compressed using screws which are insulated against electrical shorts between sub-components 1 and 4. An ion source of 5 mCi ^{63}Ni foil inside a 1/8" Swagelok™ union was attached to the sample chamber either on-axis or at the side of the aluminum inlet. Purified air was generated from a pressurized air supply in-house, purified in an ADDCO generator, and then polished using 5 Å molecular sieve in a column (1.5 m long × 8 cm ID). Flow was passed through a 5 μm particulate filter and contained 1 to 10 ppm moisture. Flows into the NES were controlled using mass flow controllers (Fathoms Technology, Georgetown, TX).

Purified air is provided to the porous carbon foam at 1.3 L/min. Under all conditions 1 L/min of this was flowing into the DMS with the remainder flowing past the insulator and venting through the conduits. Additional flow (0.25 L/min) enters the inlet from the ion source and combined flows (sample flow and excess purified air) vent at ~0.55 L/min. Voltage on the inlet was 0 to 300 V DC, providing potential gradients for ion transport through the counter-flow of purified air. In either direction of source flow (on-axis or orthogonal), flow rates and potentials were controlled to provide three modes of operation including:

a. *ion extraction*. This is the ordinary mode of operation where potential is ON, ions are pushed toward the DMS analyzer and neutrals are vented from one or more conduits. This provides exclusions of neutrals and passage of ions into a flow of purified air.
b. *no extraction*. In this mode, the potential is OFF and ions are vented from the inlet along with unreacted vapors.
c. all flow into DMS. In this mode, conduits of the inlet are capped and all sample flow from the ion source enters the DMS. Flows are controlled to keep DMS at 1 L/min

Sample Generator- Analyte vapors were generated using two methods: a) continuous flow of headspace vapors from a permeation or diffusion tube using bottles from KIN-TEK Analytical, Inc. (La Marque, TX) for orthogonal ion extraction and b) a model 5890A gas chromatograph (Hewlett-Packard Corp., Avon, PA) equipped with a splitless injector, a 10 m coiled capillary column (Restek Rtx-1701, 0.18 mm ID, 0.2 μm stationary phase) for on-axis ion introduction. The interface between GC and ion source was a 0.7 m of aluminum clad column (Supelco HT5, 0.32 mm ID, 0.1 mm film) in a stainless steel tube at 140 °C. Carrier gas was nitrogen. Chromatographic conditions were injector, 180 °C; splitless time, 30 s, initial temperature, 110 °C, program rate, 10 °C/min, final temperature,120 °C, and final temperature, 3 min. Flow from the chromatographic column (2 to 4 ml/min) was supplemented with 0.25 L/min flow of heated, purified air and passed into the ion source.

Vapor Generator- Additional vapors of small polar volatile compounds, added into the sample gas flow, were generated using a kdScientific syringe pump (KD Scientific Inc., Holliston, MA). A given volumetric flowrate of liquid reagent was added to a heated flask placed in the flow of gas which served as make up flow into the ion source. This provided a controlled vapor level of added neutrals into the NES.

Reagents and materials

Dimethyl-methyl phosphonate (DMMP) was obtained in highest purity available from Sigma-Aldrich, Inc. (St Louis, MO). Volatile compounds included iso-propanol, dichloromethane and toluene (Sigma-Aldrich, Inc., St Louis, MO). Samples at 10 ng DMMP/μL dichloromethane were prepared from a standard solution by serial dilutions in dichloromethane.

Procedures

Studies with sample flow on-axis

Concentrations of vapor modifier were varied from 0.01% to 3% m/v at a fixed flowrate using the vapor generator already described. Analyte was introduced through a GC feeding into the sample flow line and dispersion plots for each compound were plotted from a set of 9 measurements at different separation voltages. Studies of transmission efficiency were done using spectra from a measurement of purified air in three different states; once without the NES, once with the NES and a DC voltage for ion transmission, and once with an optimized 60 Hz sinusoidal voltage driving the ions.

Studies with sample flow orthogonally

In studies with flows added orthogonal to the axis of the NES and DMS, sample was taken from a diffusion source for DMMP held in a Kintek bottle with a purified air flow. This provided control over level of DMMP entering the ion source and was set to the on-set of saturation for the proton bound dimer.

Volatile organic substances or water were taken from headspace vapors over liquids in other Kintek bottles and added with the sample flow before reaching the ion source. Total flow of sample and additional neutral vapors was 0.5 L/min. Flow was drawn from the NES through the end and opposing ports of the aluminum inlet using a small diaphragm pump at 1.2 L/min. Flow of gas into the carbon ring was 1.2 L/min and flow through the DMS was 1 L/min.

Potentials were applied the inlet to establish fields in the NES using a sinusoidal waveform at 50 Hz and amplitudes of 200–300 V.

Computational/simulation

Models of the interface were built in Autodesk Inventor and imported to SIMION. Electrode potentials were specified to match experiment, and the atmospheric pressure was modeled using the Statistical Diffusion Simulation (SDS) model provided with SIMION. Ion flight experiments for the active NES were done in both on-axis and orthogonal ion introduction, with ion path overlaid on the potential contour map inside the NES. Only the DC potential was modeled with SIMION.

A model of interior volume equivalent to the SIMION model was constructed in COMSOL and used to model gas flows using the CFD module with a high-resolution mesh having 461,000 elements. The nitrogen flow media and laminar flow physics were applied to model, with the gas properties taken from the built-in COMSOL material library (Assume 68 °F gas temperature). Various sample gas & buffer gas inlet flow rates were used to explore how the system flow interactions change. See the Experimental Section for additional information. A stationary (steady-state) GMRES Iterative solver was selected and results are displayed in model "slice" format that show velocity magnitude of the gas flow to determine flow path and dynamics.

Results and discussion

In-silico modeling of ion and neutral flows

Gas Flows. COMSOL models of gas flow for both modes of operation are shown in Fig. 2 for the on-axis (A, C) and the orthogonal (B, D) designs for sample flow with internal gas flow velocities shown by the heat map and corresponding streamlines. In the on-axis design, performance was sensitive to the magnitude of flow from the ion source with a break in performance at 0.3 L/min (0.9 m/s) with counter-flow of 0.3 L/min (0.4 m/s). At sample flows below 0.3 L/min, neutrals were fully excluded from the DMS analyzer, while both ions with neutrals entered the DMS above a 0.3 L/min sample flow. When sample flow was orthogonal to the axis of the DMS (Fig. 2B), neutral vapor from sample flow was removed from the NES in the opposite side of the sample chamber with no transport of neutrals into the body of the device. In this design, the excess flow from the carbon ring (3) was combined with sample flow and vented.

In both designs, COMSOL models showed patterns of flow could be arranged with little or no turbulence region between 1 and 3, and ions are transported from the sample chamber to the volume of the gas ring and on to the DMS. While the orthogonal design requires a 90° bend in ion trajectories with ions following potential contours (see below), the on-axis design required special care to avoid neutral flow into the body. For both designs the streamlines from each inlet show no flow from the sample inlet to the DMS inlet, seen by the absence of any magenta lines going to the DMS, demonstrating complete exclusion of neutrals in the flow model.

Potential Contours and Ion Flow with SIMION- Models for ion flow from SIMION are shown in Fig. 3 with potential contours, established by differences in voltages on the inlet (1) and body (4). The potential contours are independent of mode of gas flows; however, the trajectories of ions differ as shown in for on-axis (Fig. 3A) and orthogonal (Fig. 3B) sample flow. In the on-axis design, potential contours and ion flight suggest a lens effect where ions undergo an initial focusing to a point somewhat like an Einsel lens in mass spectrometry. The ion beam undergoes dispersion with convex potential contours inside the body (4). This was consistent with observed loss of ion intensity with increased voltage on the body. Increase in ion intensity with initial increases in potential are understandable as increased difference in potential contours to draw ions against the counter-flow of gas. Additionally, ion losses going into the DMS would be minimized when considering the countering effect that the flow shown in the COMSOL model would have on the ion flight trajectories in the defocusing region.

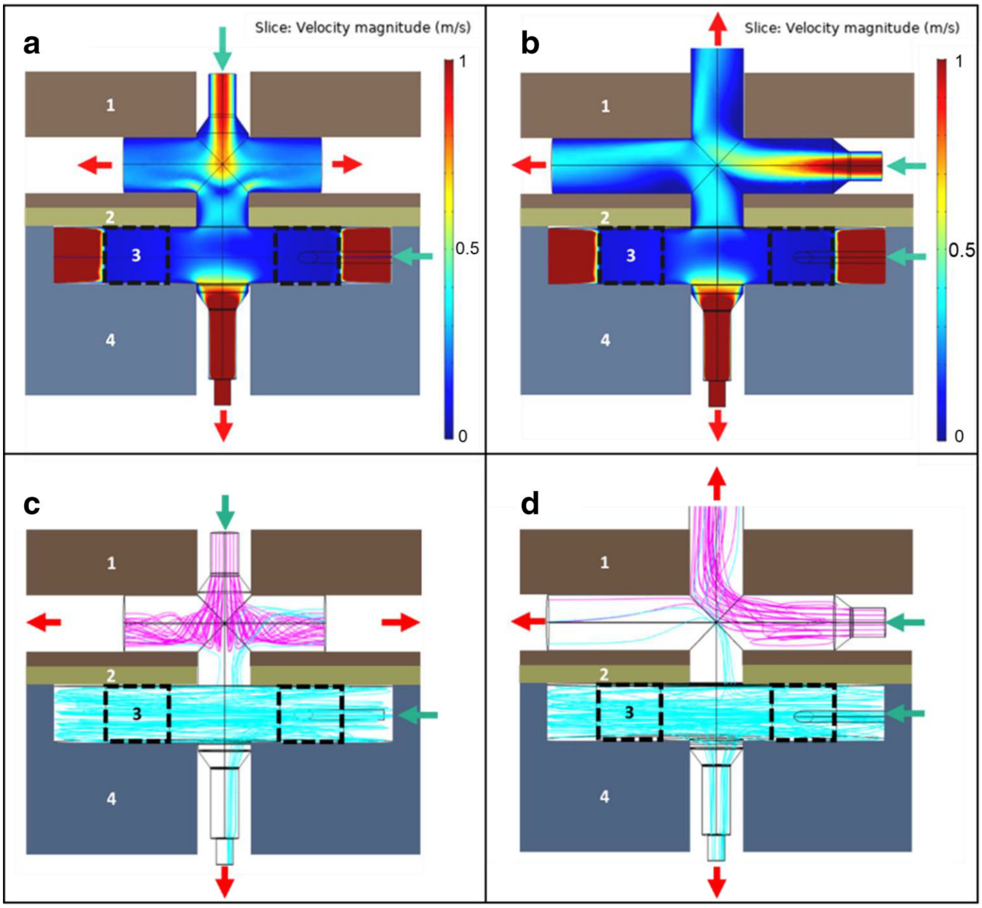

Fig. 2 COMSOL flow model of NES with sample flow on axis (left) and perpendicular (right). Plots (**A**) and (**B**) show a slice of the velocity magnitude for each design, while (**C**) and (**D**) show the corresponding gas streamlines from the two inlets in each design. Green arrows denote inlets of purified gas or sample, and red arrows are exhaust. Only the internal volume was used for the modeling in COMSOL, and matches the model used in Fig. 1

The model for orthogonal ion injection demonstrates the consequence of bending ions 90° over a gap without a sharp focus point though with less dramatic defocusing in the body. The principle of operation still is the same: gas ions are drawn by potential contours against a flow of purified air and ions that pass the mid-point of the carbon ring are carried by gas flow into the DMS analyzer. Unreacted sample neutrals, vapor modifiers, and other material in flow from the ion source are vented from the conduits.

Removal of neutrals from source flow

On-axis Design. In Fig. 4, spectra are shown for DMMP in purified air (top spectrum) and in excessive levels of solvents, dichloromethane (DCM), toluene, and isopropanol (IPA) using the on-axis design. The spectra are comprised of the proton bound dimer (at −0.5 V), the protonated monomer (6 V), and the reactant ion (16 V) in purified air (top spectrum, Fig. 4A and B). In 0.14% DCM, the ion peak is

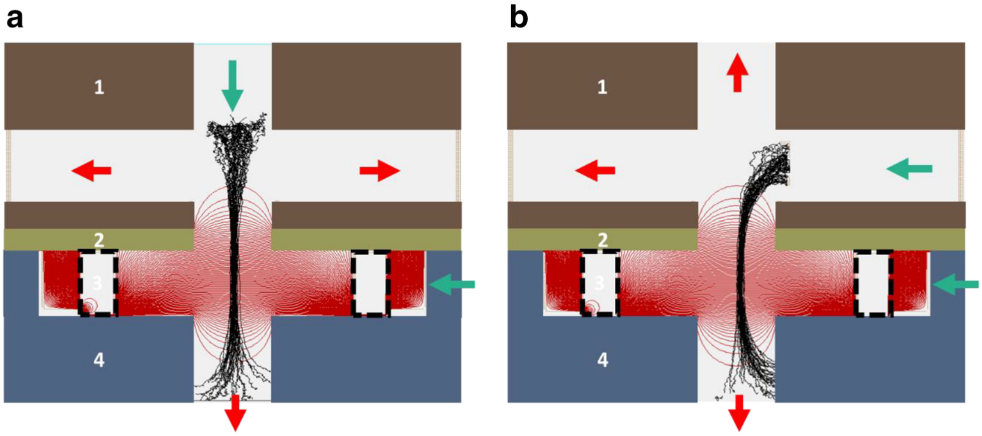

Fig. 3 A SIMION model of the NES with ion flight from sample introduction on axis (**A**) and orthogonal (**B**). Potential contours are also shown in the red lines, established by a 300 V DC field applied to the repeller electrode, (1). This model was directly imported from the Autodesk 3d model in Fig. 1

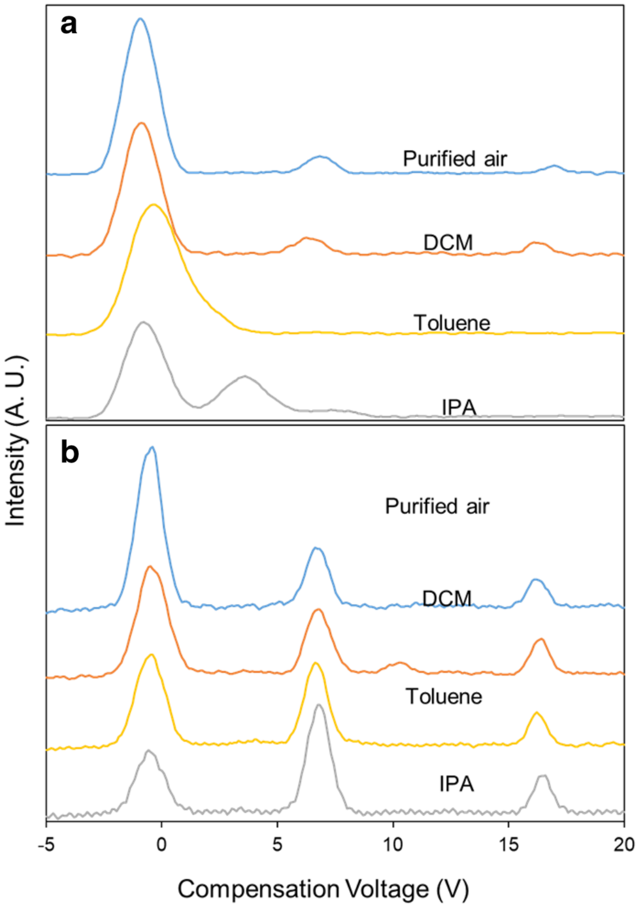

Fig. 4 Spectra of DMMP taken in purified air and 3 vapor modifiers at 0.1% *w*/w of vapor modifier, without use of the NES (top) and with use of the NES (bottom)

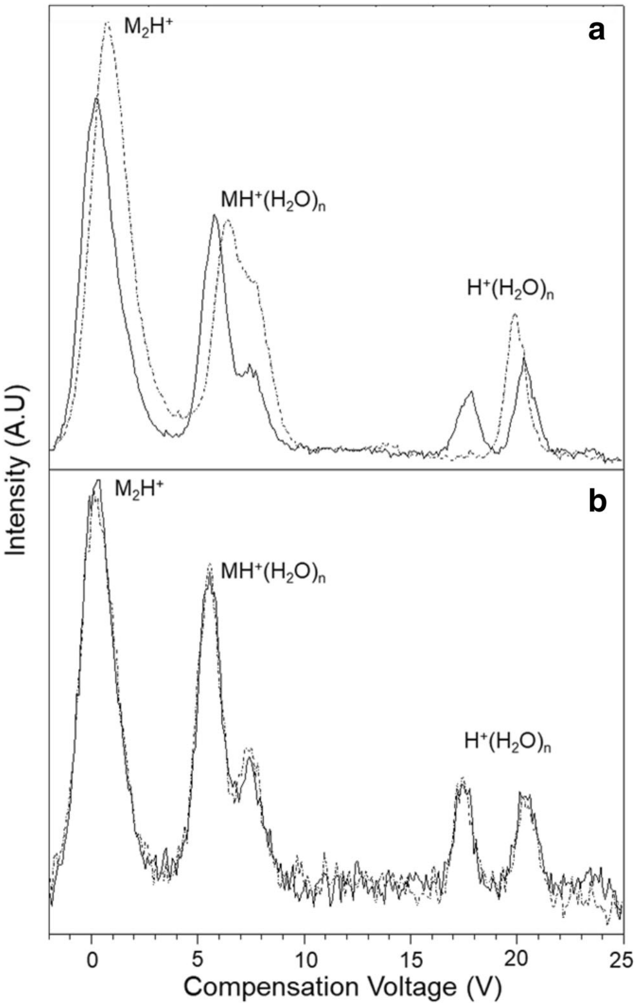

Fig. 5 DMS spectra of DMMP at 0.5 ppm in moisture of 100 ppm (solid) and 7000 ppm (dotted) without (top) and with (bottom) a NES unit

little changed suggesting negligible formation of ion-neutral clusters in positive polarity. In contrast, 0.10% of toluene causes broadening of the proton bound dimer and possibly the shift of the protonated monomer, becoming a shoulder peak on the proton bound dimer. The spectrum with 0.12% IPA is unlike that in purified air with formation of ion-molecule clusters or modification of the alpha function. In contrast, the DMS equipped with the NES shows the same spectra regardless of neutral vapors with agreement in the positions of the dimer, monomer, and RIP better than 0.02 V in compensation voltage. Differences in relative abundances of product ions were observed and pronounced for IPA; nonetheless, compensation voltages for all ion peaks, RIP, protonated monomer and proton bound dimer were distinct and recognizable at these extreme solvent vapor levels.

Orthogonal extraction

Effects with water, a strongly polar molecule, are shown in overlaid spectra (Fig. 5A) for DMMP in purified air with ~ 100 ppm moisture (solid black line) and purified air with 30% relative humidity or moisture of ~7000 ppm (dotted line). A mixture of spectral effects are evident including loss of one ion peak at 18 V, changes in relative abundance of ion peaks at 4 to 9 V, and shifts in compensation voltages for all peaks. Significantly, even the proton bound dimer (M_2H^+) exhibits some displacement on the CV scale and more significant changes are seen with the protonated monomer ($MH^+(H_2O)_n$) and the reactant ion peak, $H^+(H_2O)_n$, both able to easily hydrate. The alignment of DMS spectra demonstrates a stability of spectra with independence of moisture in sample flow due to hydration. Suppression of ion formation in the ion source is an additional topic not addressed in this work. An immediate benefit of this capability is independence of DMS spectra from the influences of changes in moisture in an open loop inlet design or any DMS design where excursions in moisture may be expected including membrane equipped instruments. DMS analyzers without impacts from moisture in ambient air can now be designed and employed.

Extreme levels of polar volatile compounds (iso-propanol, IPA; acetone, and ethanol) were measured using dispersion curves over a range of separation voltages (Fig. 6) for the

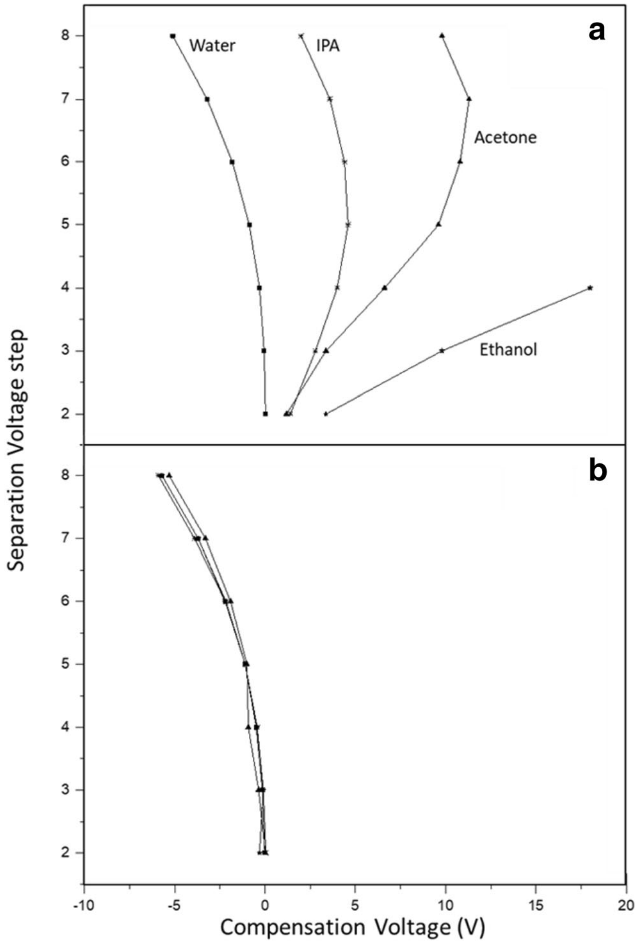

Fig. 6 Dispersion plots for proton bound dimer of DMMP with four neutral vapors (see inset) and without (top) and with (bottom) the NES. The scale on separation voltage/field range is from

proton bound dimer (PBD) of DMMP, which exhibits a negative alpha function. The dispersion curves for the PBD of DMMP are shown with vapor levels at saturation levels in Fig. 6A. The dispersion curve for water exhibits a negative alpha function and results above suggest this could be affected slightly. The plots for IPA, acetone, and ethanol show extreme influence on the dispersion plots, both in the shape of the dispersion curves and the absolute CV values with the orthogonal design. This astonishing result is likely more than action as a vapor modifier only and may also include decomposition of the proton bound dimer into a solvated protonated monomer (MH + S) where S is the volatile vapor modifier per Eq. 1:

$$(\mathrm{DMMP})_2\mathrm{H}^+ + \mathrm{S} \leftrightarrow (\mathrm{DMMP})\mathrm{H}^+\mathrm{S} + \mathrm{DMMP} \tag{1}$$

While this is energetically unfavorable with thermalized ions, the dissociation of the PBD is possible at fields as low 15,000 V/cm per Eq. 2.

$$(\mathrm{DMMP})_2\mathrm{H}^+ \longleftrightarrow^{E/N} (\mathrm{DMMP})\mathrm{H}^+ + \mathrm{DMMP} \tag{2}$$

Once dissociated, solvation of the protonated monomer is statistically favored and the solvated protonated monomer should have a significant positive alpha function as seen in Fig. 6A.

When the interface is inserted between ion source and DMS analyzer and activated, the removal of neutrals is evident in Fig. 6B where dispersion plots for all solvents in Fig. 6A are shown with the same pattern and absolute CV scales, within experimental error. That is the ion was effectively separated from the neutral solvent vapors and characterized in purified air free of solvent (estimated sensitivity of 50 ppm threshold for influence). This concept is tested below with quantitative vapor levels for the monomer alone.

Dependence of CV for protonated monomer on neutral vapors concentration

While excessive levels of neutral vapors are likely uncommon, concentrations from 0 to 0.5% were explored using the protonated monomer of DMMP. Measurements of CV were taken at constant SV at steps in vapor concentration as shown in Fig. 7. The monomer of DMMP was clearly affected by the changes in concentration with CV changes from 3 to 12 V. In contrast, the compensation voltage for the protonated monomer with the NES was constant (within error) at 6.2 V. Under these relatively low levels of IPA, compensation voltages for the proton bound dimer were unaffected.

Efficiency of ion transmission

Orthogonal Extraction. In a DC mode of operation, the interface exhibited a decrease in peak intensity as shown in Fig. 8 and the loss in intensity was attributed to charging of dielectric, possibly the Teflon insulator. Overall efficiency was determined as 80% or better for ion

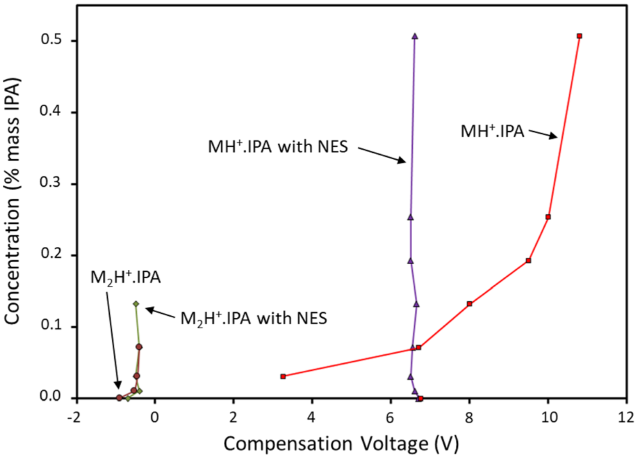

Fig. 7 Plot of the peak position of DMMP monomer and dimer with increasing concentration of IPA with and without the NES, using on-axis sample introduction

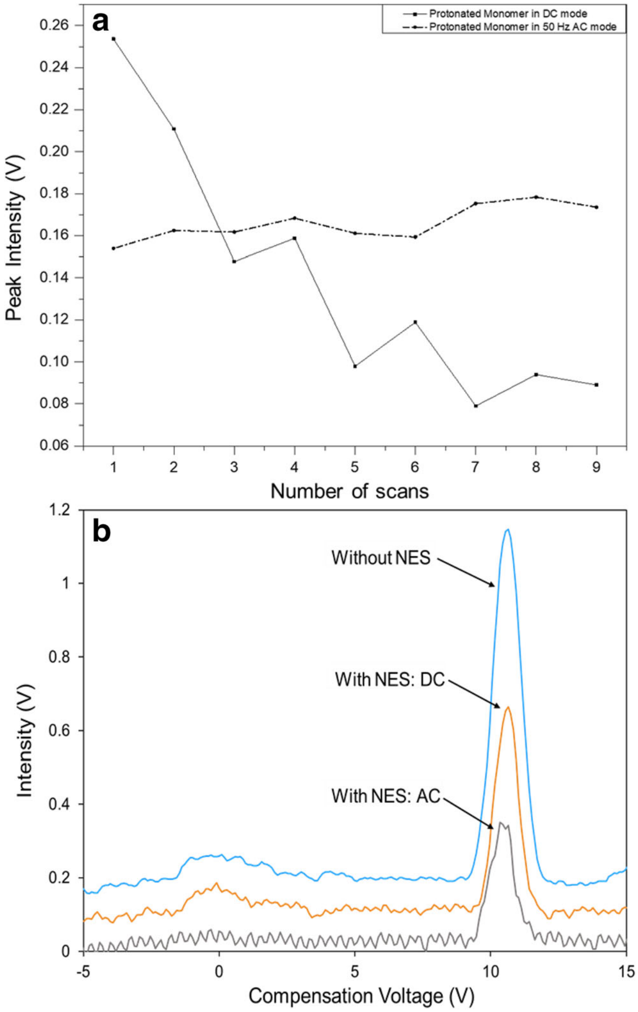

Fig. 8 Ion transmission efficiency for orthogonal (**A**) vs on-axis (**B**) sample introduction using both DC and AC voltages applied on the repeller electrode. For orthogonal sample introduction (A), charging issues reduced long term transmission efficiency of the NES, but with AC mode the charging issue was not a problem. For on-axis flow, no charging was observed. For both, the efficiency of AC mode was roughly half the efficiency of the DC mode, as would be expected

transmission. In both AC and DC modes the ions were only present upon application of field, providing initial confirmation of the functionality of the curtain gas in excluding molecules from the ion source region.

On-axis Design. In the DC mode there is 59% transmission, a stable peak in one polarity and no additional noise. In the AC mode a waveform is used to propel ions of both polarities through the counterflow. This functions with 36% ion transmission, alongside significant noise introduction through the presence of the 60 Hz waveform in the detector signal. The AC voltage mode was of special interest for its use of both polarities simultaneously, enabling the full analytical capability of the DMS (only positive is shown here). Despite these advantages, the current embodiment did not have sufficient performance in AC mode, and optimization was left to future work after demonstrating proof of concept. All other studies here described use only the first two modes; without NES and with the NES operating under +300 V DC.

Conclusions

An embodiment of a NES was designed and characterized for ion-neutral separation prior to a DMS analyzer. Loss of response and selectivity due to clustering effects was eliminated, validating the technology as a functional proof of concept and laying the groundwork for future experiments and applications for sample introduction methods requiring ion-neutral separation.

Vapor levels of small polar molecules can be removed at ~100% efficiency using two flow embodiments of a neutral excluder stage. Ion yield was roughly 70% with orthogonal ion extraction and 40% with on-axis design. Ions with the vapor neutrals removed exhibit common dispersion behavior suggesting that the gas atmosphere was controlled within measurement error and that stability of ion peak position can be assured. Significantly for the development of tandem DMS, experiments with reagents and modifiers can be made in various stages of an analyzer and ions restored to controlled gas atmospheres for characterization further in latter stages of the instrument.

The success of the NES in ion-neutral separation was demonstrated, but ionization chemistry remained a point of concern for chemical identification in mixtures using a NES-DMS. Relative reactivities or abundances of chemicals could suppress detection of the desired analyte, demonstrated especially with the IPA, where at high concentrations in the ion source the analyte signal was suppressed and eventually completely gone.

Next embodiments of the NES will need to address multiple issues. A primary goal would be to design for the AC mode, as it would allow full use of the DMS capabilities for detection. Changes in geometry toward improved field and flow would be another main goal, especially given the scattering effect that simulations show could be responsible for significant ion losses. Additionally, studies would be necessary for transmission efficiencies and ion bias with frequency and field strengths in AC mode, something unexplored in this work.

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