Computational Evaluation of an Ion Peak Compression Concept for Ion Mobility Spectrometry

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Overview

- Methods to reduce the physical width of an ion mobility packet due to diffusional broadening were explored.
- A concept using intermittent non-linear potential gradients in an otherwise linear potential gradient in a drift tube was explored.
- Such periodic ion peak compression is shown to potentially enable greatly extended lossless ion mobility separations using cyclic separations to achieve very long drift length separations.

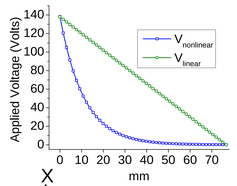
Introduction

- IMS coupled with MS has immense potential for biological analysis,[1] but performance is limited by the drift path length[2]
- SLIM[3,4] allow building of longer drift length devices, and particularly cyclic designs with effectively unlimited path lengths
- However ion packet diffusion ultimately limits cyclic separations.
- A device that can periodically compress ion packets would facilitate extended path lengths

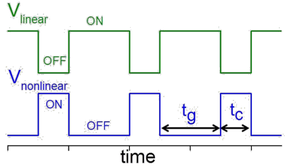
Methods

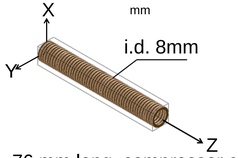
- Initial linear drift field: 18 V/cm
- initial drift length: 87cm
- Time for application of non linear profile for time: t_c
- Time between two compressions: t_g

Two voltage profiles



generic timing diagram



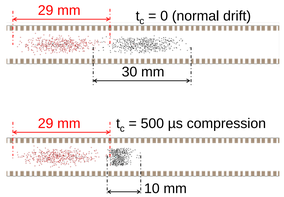


76 mm long compressor cell

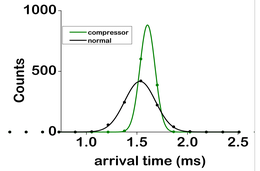
- SIMION simulations
- SDS collisions model[4]
- Pressure : 4 torr,
- RF voltage : 200 Vp-p

Results

Effect of Compressor on a Single Peak



Snapshot of ion compression

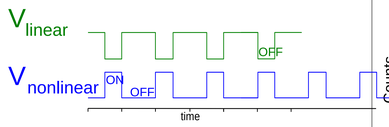


arrival time distribution

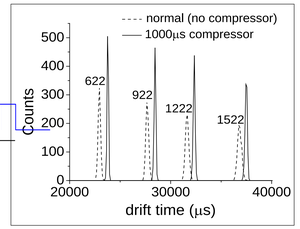
Red dots: **Initial ion distribution**
Black Dots: **Ion distribution after 500 µs**

Results continued...

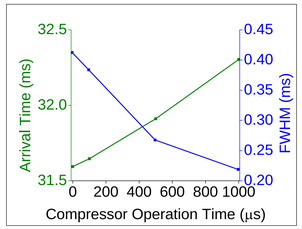
Ion Compression over a Broad Mobility Range



t_g ~4 ms ; t_c < 1 ms

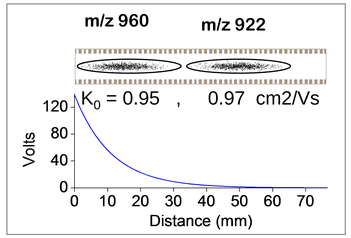


Simulated spectrum

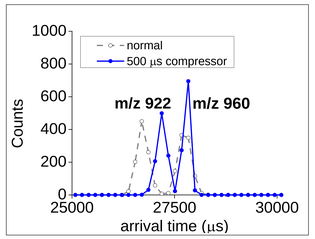


Arrival Time and FWHM

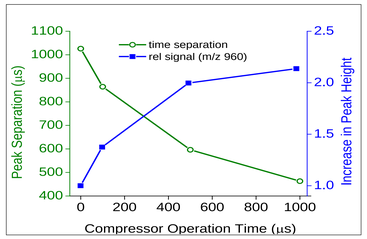
Effects over a Narrow Mobility Range



Initial relative position of ion packets with respect to the applied potential profile



Simulated spectra of two simultaneously compressed ion peaks



Effect of compression on signal intensity and peak resolution

- When switching occurs to a non-linear (e.g. curved) gradient profile, the leading and trailing parts of an ion packet experience different fields resulting in peak compression after the linear gradient profile is resumed.
- The slower mobility ion packet experiences a stronger field in the non-linear profile, and e.g. increased peak height with increased time in the compressor field.
- There is some loss of peak separation with increasing compression time, but the small loss of separation power is recoverable with reasonable additional drift length (e.g. in a conventional linear field gradient).

Conclusions

- SIMION 8.1 simulations were used to evaluate a concept for ion peak compression.
- Intermittent switching between linear and nonlinear profiles is shown to enable ion packet compression.
- The compression led to increased peak height and decreased peak widths.
- When optimized, the loss of separation can be recovered quickly while retaining the benefits of compression i.e. decreased peak widths and increased peak intensities.
- Peak compression is particularly attractive for use in cyclic ion mobility designs where periodic ion packet size reduction can enable essentially unlimited cycle times and resolution.

Acknowledgements

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References

1. E.S. Baker, T. Liu, V.A. Petyuk, K.E. Burnum-Johnson, Y.M. Ibrahim, G.A. Anderson, R.D. Smith, Genome Medicine, 2012, 4 : 63
2. E.S. Baker, B.H. Clowers, F.M. Li, K. Tang, A.V. Tolmachev, D.C. Prior, M.E. Belov, R.D. Smith, Journal of American Society for Mass Spectrometry, 2007,
3. I.K. Webb, S.V.B. Garimella, A.V. Tolmachev, TC Chen, X.Y. Zheng, R.V. Norheim, S.A. Prost, B. LaMarche, G.A. Anderson, Y.M. Ibrahim, R.D. Smith, Analytical Chemistry, 2014
4. S.V.B. Garimella, Y.M. Ibrahim, I.K. Webb, A.V. Tolmachev, X.Y. Zheng, S.A. Prost, G.A. Anderson, R.D. Smith, Journal of American Society for Mass Spectrometry, 2014

Career Opportunities: For potential openings in Integrative Omics Group at PNNL please visit http://omics.pnl.gov/careers

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