RGA modelling and simulation to include pressure dependence in the ion source

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Talk Outline

- Introduction and background
- The Binary-Encounter-Bethe (BEB) theory and approach
- Application of BEB to an electron impact (EI) source: prediction of QMS pressure dependence
- Comparison of theory with experimental results obtained from a commercial RGA
- Conclusions and future work
- Acknowledgements

Introduction and background

- Many numerical simulation techniques have been performed to study the theoretical performance characteristics of the QMS. Later research work has continued detailed investigation of mass spectra using computer simulation techniques for both hyperbolic and circular mass filters [1], [2].

- No QMS model to date that includes **pressure dependence in the ion source.**

- Reported here is a new approach to include pressure dependence in the ion source to allow better prediction of QMS instrument performance using the Binary-Encounter-Bethe (BEB) theory

The Binary Encounter Bethe (BEB) method

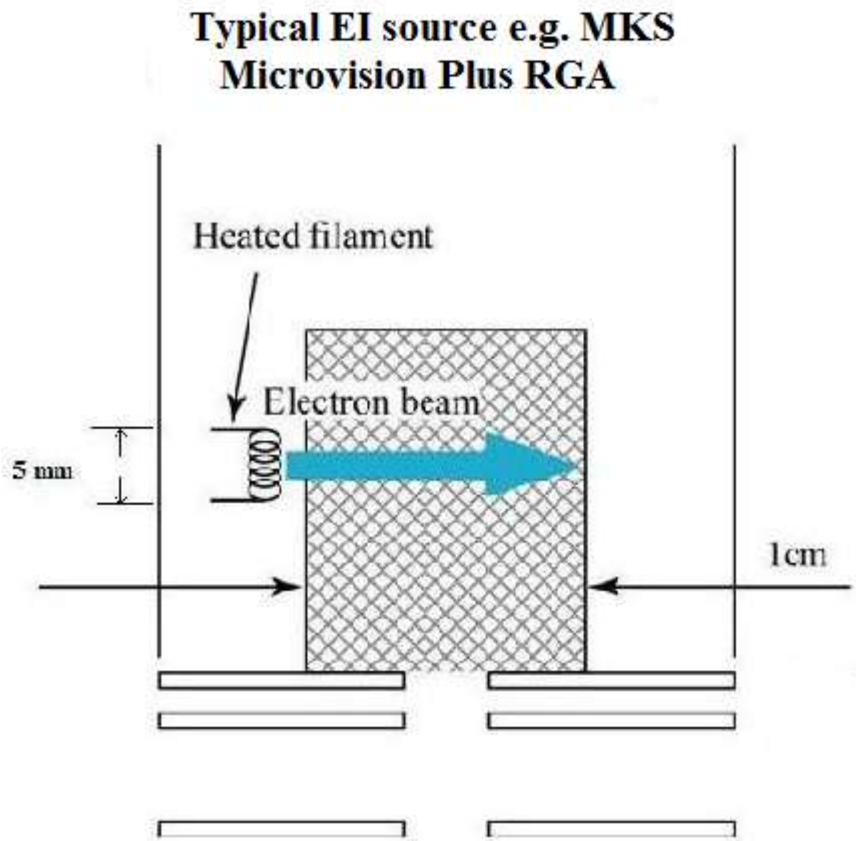
- BEB allows calculation from first principles of the total ionization cross section values as a function of electron energy.

- The BEB method allows the ion current in the source to be determined as a function of electron emission current, electron energy, and **pressure.**

- This approach was then used to model an electron ionization (EI) ion source used in a QMS RGA pressure range from 10^{-6} to 10^{-4} mbar.

- A commercial QMS residual gas analyzer, MKS MicroVision plus was used for the experiments.

Quadrupole Mass Spectrometer (QMS)



- Simulations for a filament length of 5mm, the turn density of 1000 turns/m and the filament current of 1.6mA.

- The electron beam emitted from the heated filament is directed into the mesh ionization cage where it is allowed to interact with the gas sample.

- Upon interaction between the neutral atoms and the e-beam, the neutral atoms are ionized to radical positive ions.

The ionic current of the given gas component (i^+) is given by [3]:

$$i^+ = \beta \times n_0 \times Q_i \times s \times i_e \qquad [A]$$

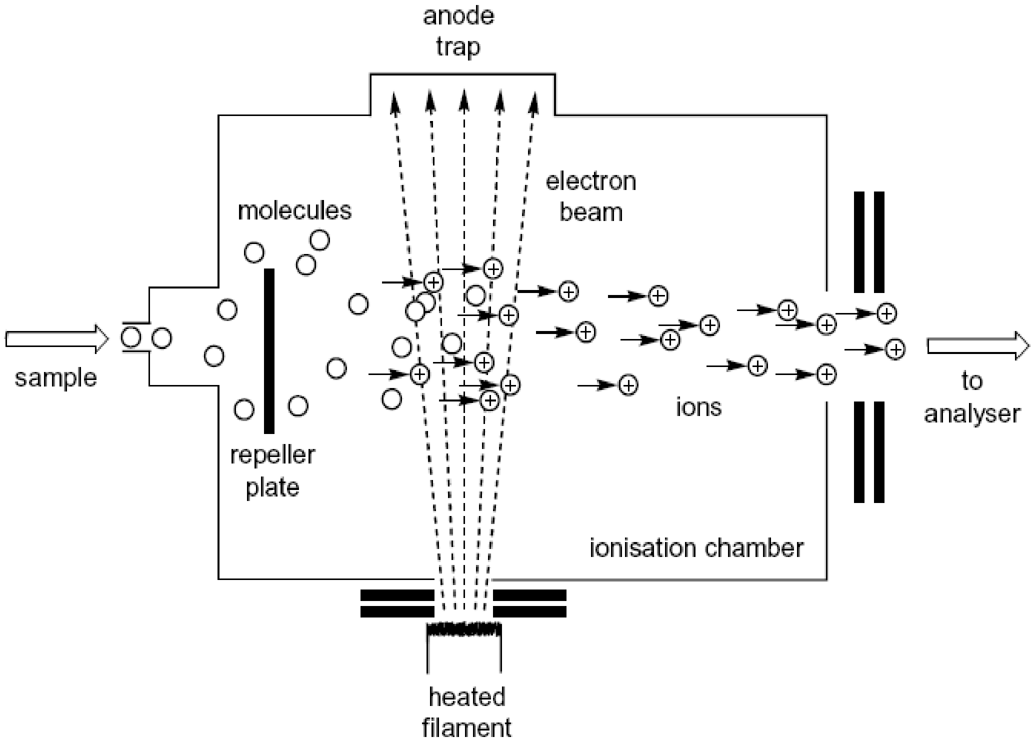
i_e – Electro

s – Effecti

Q_i – Ionizati

n_0 – Density

β – Ion extr



$$i^+ = \beta \times n_0 \times Q_i \times s \times i_e \quad [A]$$

Q_i - Ionization cross section [10^{-10}m]

Ionization cross section of a gas component in the ionic current expression above can be calculated using BEB theory [4].

$$\sigma_{BEB} = \frac{4\pi a_0^2 N \left(\frac{B}{R}\right)^2}{t+u+1}\left[\frac{\ln t}{2}\left(1-\frac{1}{t^2}\right)+1-\frac{1}{t}-\frac{l_n\, t}{1+t}\right] \qquad [10^{-10}\mathrm{m}]$$

t = *T/B*; *u* = *U/B*

B – binding energy (eV), U – orbital kinetic energy (eV), N – electron occupation number and, Q – dipole constant.

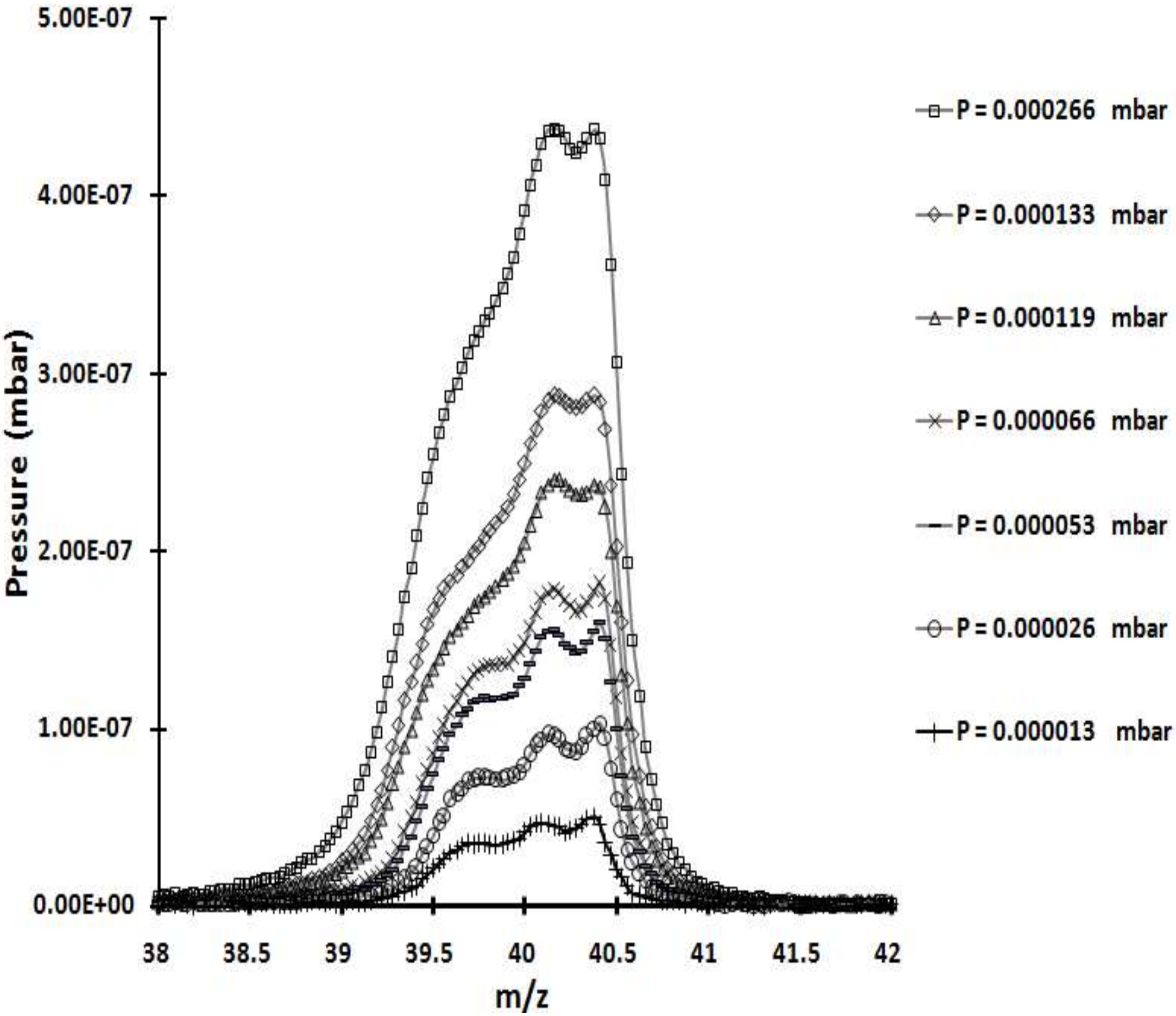
Bohr radius (a_0) – 5.29 × 10^{-11} m and Rydberg energy (R) – 13.6057 eV.

Experimental Spectral Studies:

- The calculated and experimental ionic current results of a QMS focuses on electron impact ion source including the pressure dependence.

- We show both the calculated and experimental results of Argon gas spectra obtained using an MKS001 single filter RGA. Electrode length 100mm, diameter 6.35mm and RF excitation frequency 1.8432 MHz.

Experimental mass spectrum of $^{40}Ar^{+}$



- Experimental mass peaks (m/z) of argon gas of mass 40 for an emission current of 0.35 mA, electron energy of 70 eV, and ion energy of 8.8 eV showing the variation in peak height with the applied pressure ranges between 2.6×10^{-4} and 1.3×10^{-5} mbar in the vacuum chamber.

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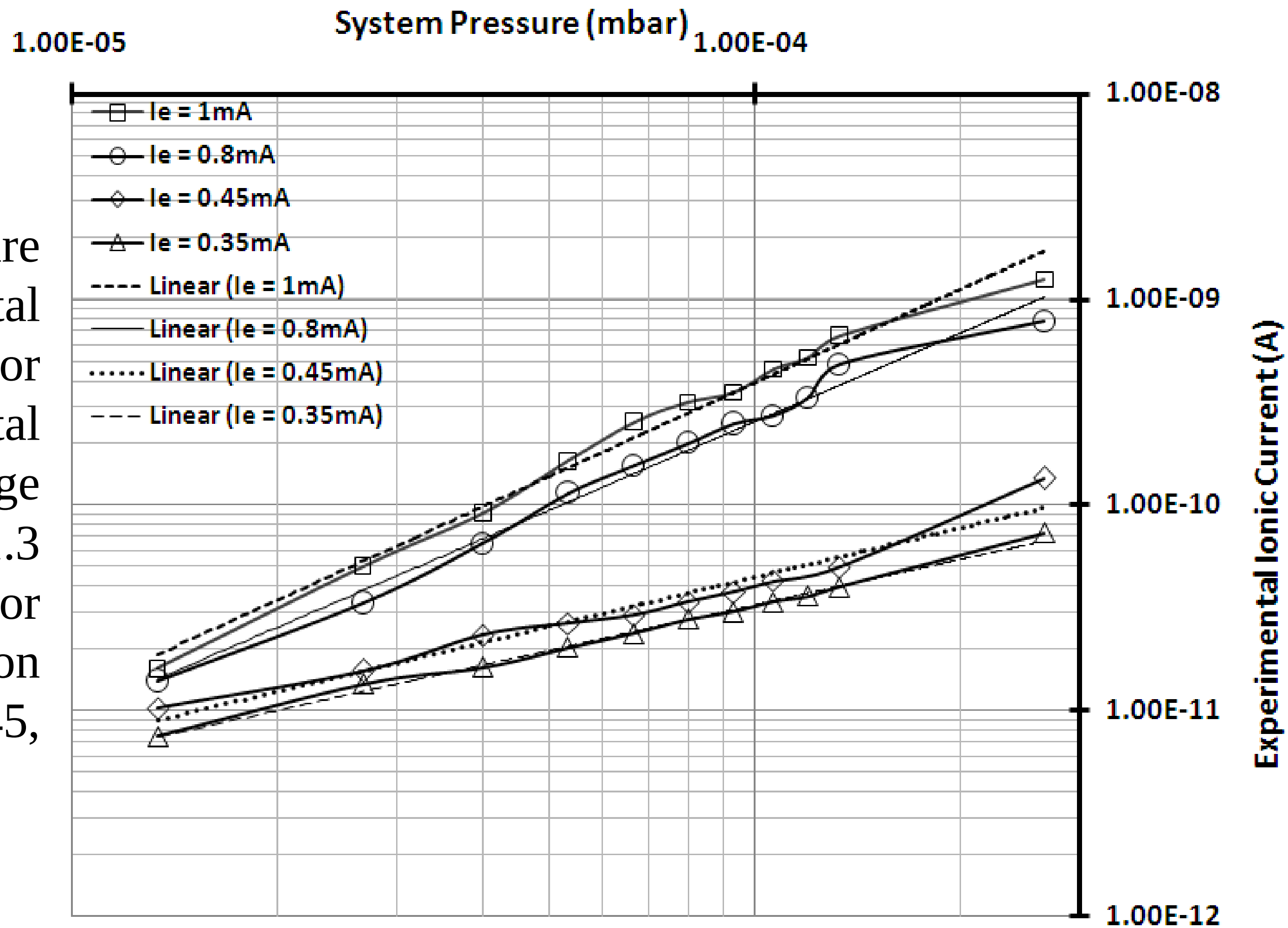
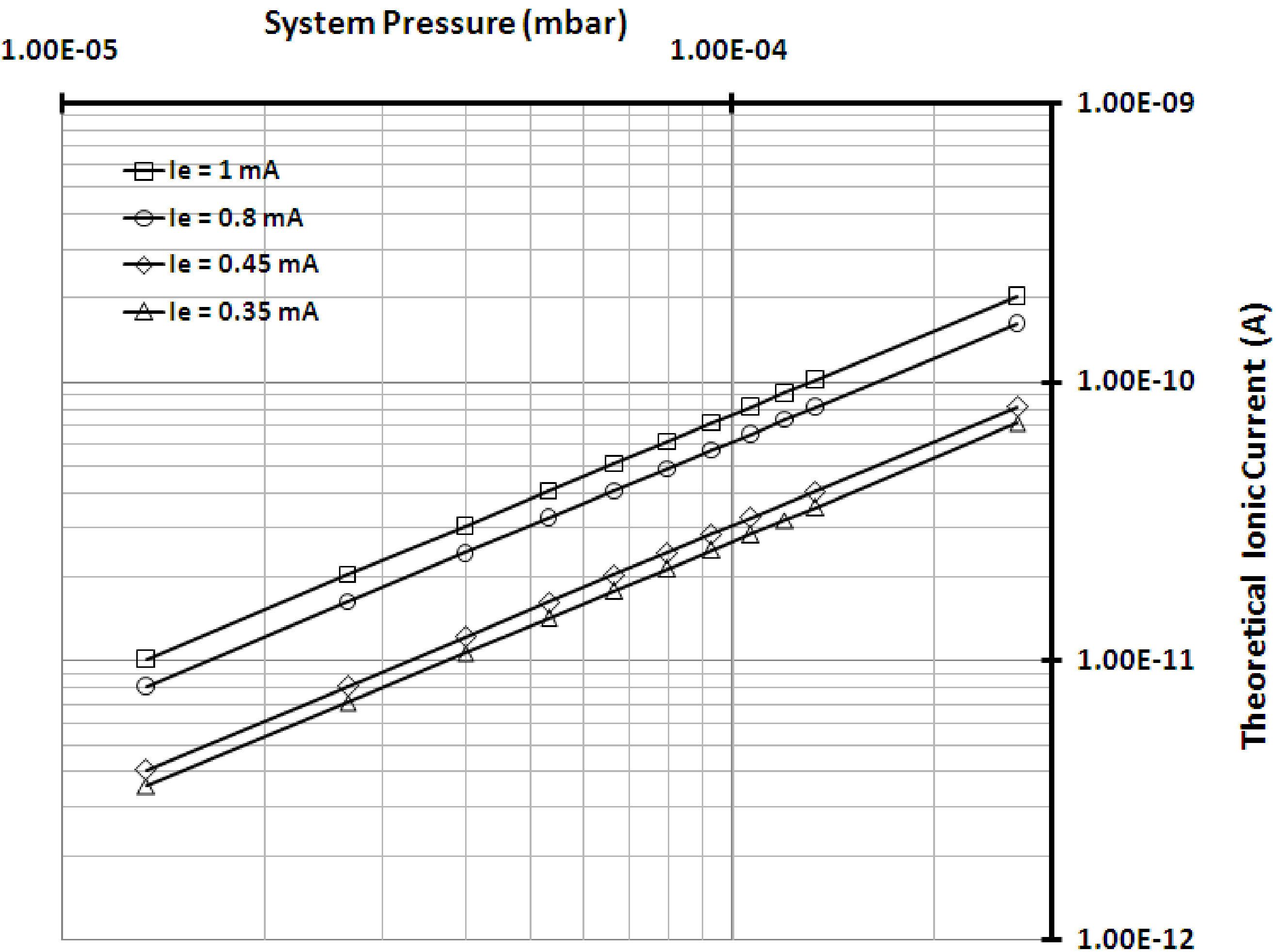
Experimental argon ionic current with increasing pressure for different electron emission currents (*Ie*)

- The total pressure versus experimental total ionic current for $^{40}Ar^{+}$ with the total pressure in the range from 2.6 × 10^{-4} to 1.3 × 10^{-5} mbar for different emission currents of 0.35, 0.45, 0.8, and 1.0 mA.

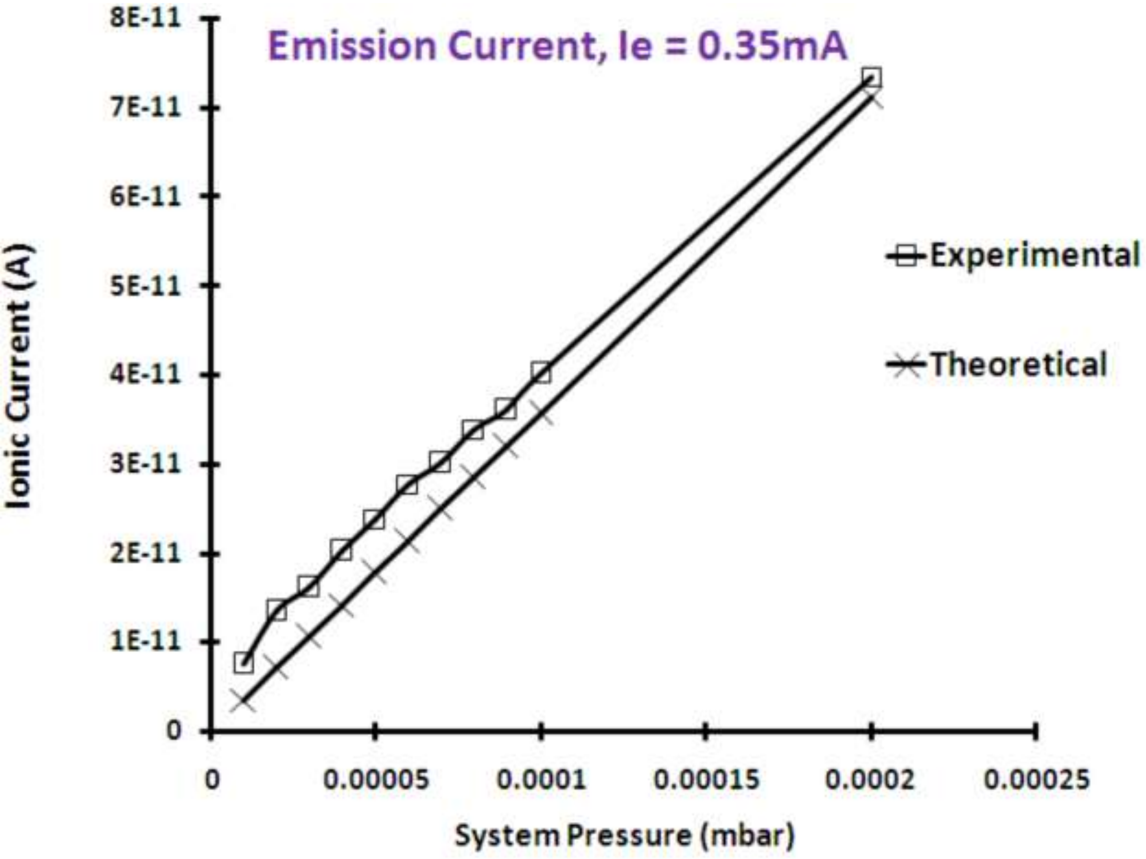


Predicted argon ionic current with pressure for different values of the electron emission current (*Ie*)



- The theoretical total ionic current for $^{40}Ar^{+}$ as a function of the total pressure in the range from 2.6 × 10^{-4} to 1.3 × 10^{-5} mbar for different emission currents of 0.35, 0.45, 0.80, and 1.00 mA.

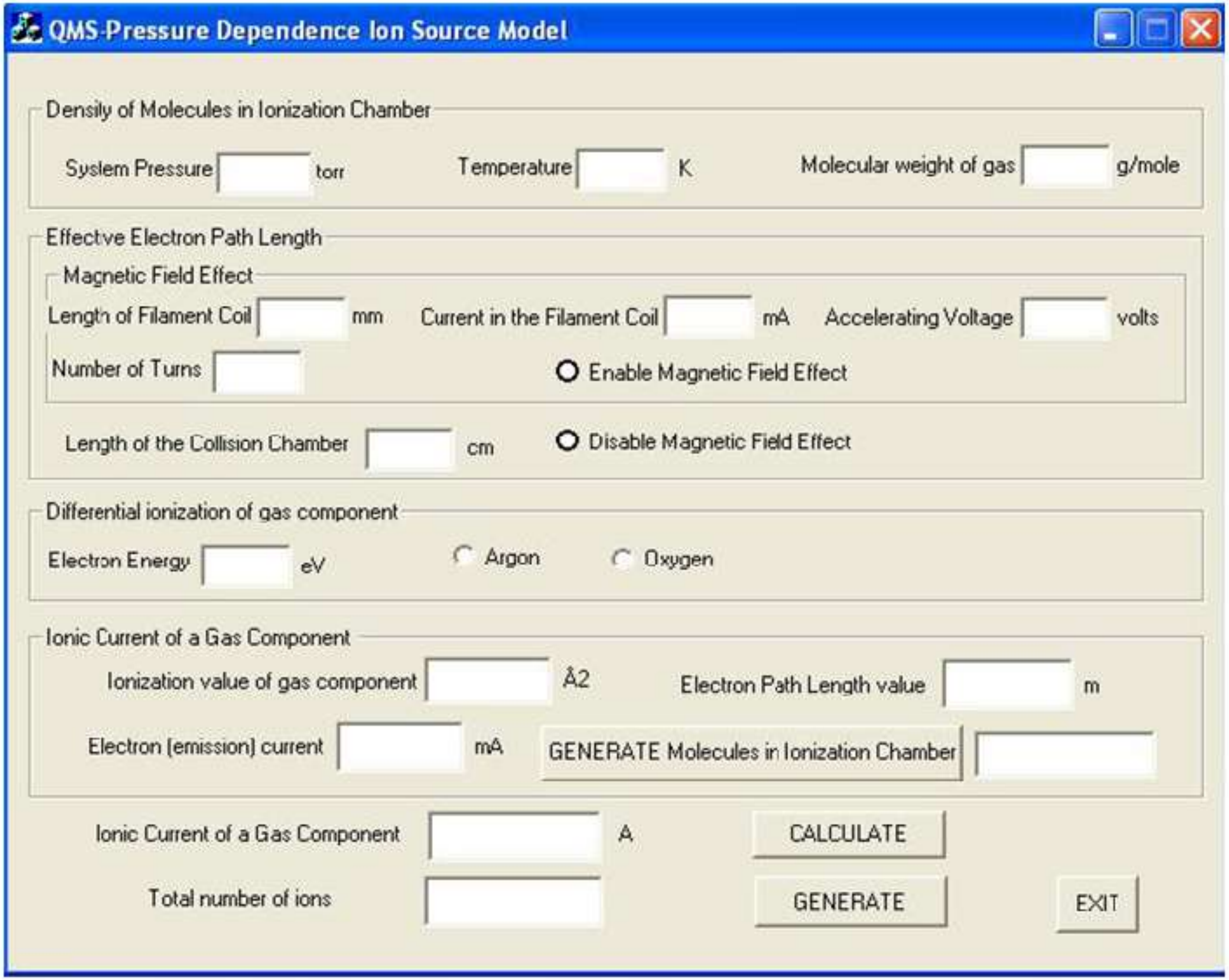
Comparison of calculated and experimental total ionic current for $^{40}Ar^{+}$ as a function of system pressure for an emission current, Ie = 0.35mA



- The comparison of the calculated and experimental total ionic current for argon gas (*m/z 40*) with the total pressure in the range from 2.6×10^{-4} to 1.3×10^{-5} mbar for an emission current of 0.35 mA .

- The ionic current was calculated neglecting the axial magnetic field experienced by the heated coil.

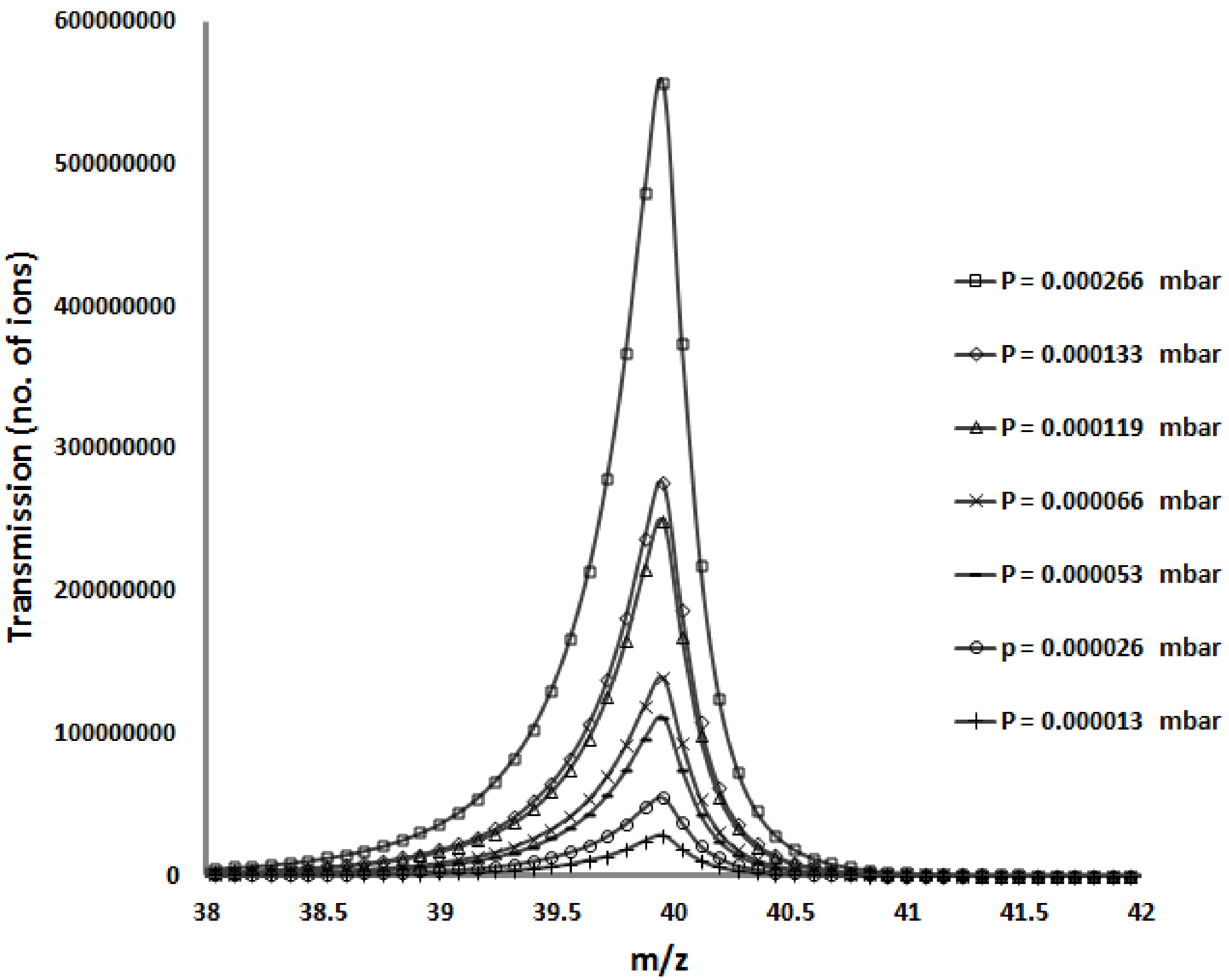
QMS2-Pressure Dependence Ion Source Model



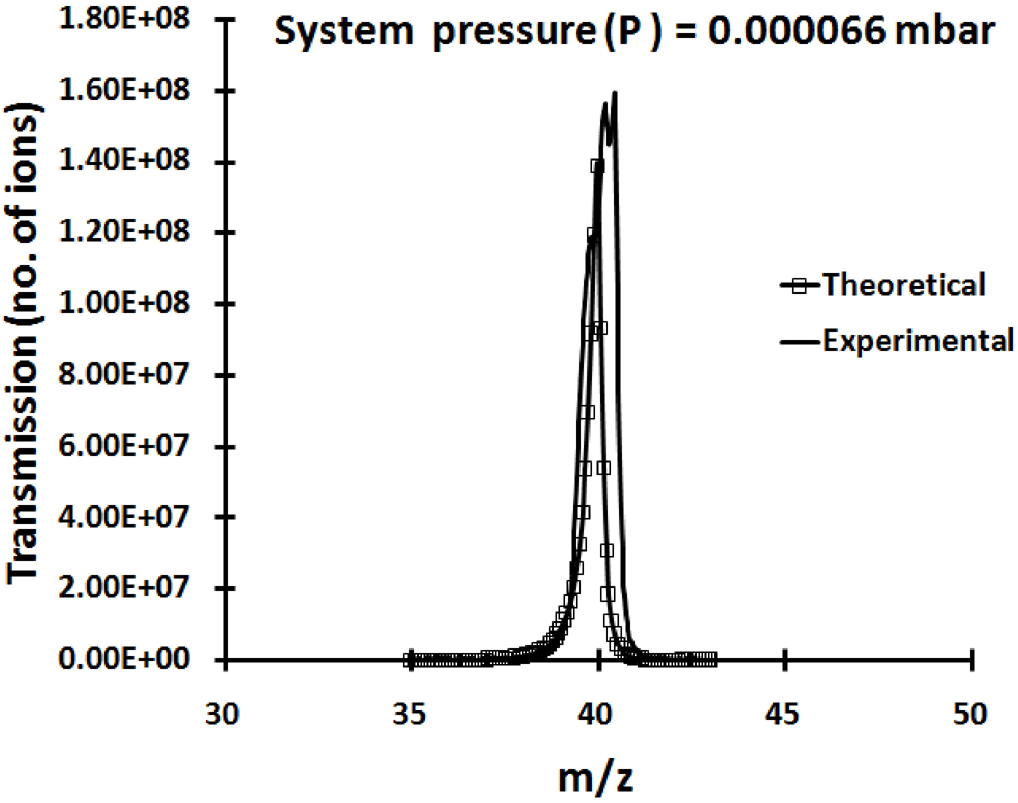
Simulated mass spectrum of $^{40}Ar^{+}$

***QMS2* computer simulation test conditions**

QMF PARAMETER	CONDITION
Length	100 mm
r_0	2.76 mm
Frequency	1.8432 MHz
U/V	100
Detector radius	10 mm
Ion Source	
Ion energy	8.8 eV
Ion source radius	0.55 mm
Ion energy spread	0
Ion angular spread	0
Ion species	40 m/z



Comparison of simulated and experimental mass spectrum of $^{40}Ar^{+}$



- The experimental mass peak for $^{40}Ar^{+}$ ions obtained from a commercial QMS residual gas analyzer (MKS MicroVision Plus RGA) operated for an electron current of 0.35 mA with a pressure is 6.6 × 10^{-5} mbar.

- The simulated mass peak for $^{40}Ar^{+}$ ions is generated using QMS2-Hyperbolic and QMS2-EI ion Source pressure-dependence programs.

Conclusions

- The QMS2-EI ion source pressure dependence theoretical model has been developed using the visual C++ environment.
- The model as a function of electron energy calculates the electron-impact total ionization cross-sections from first principles using the BEB theory.
- The calculated theoretical ionic currents are compared with the ionic current of the experimental results obtained from a commercial QMS residual gas analyzer and show good agreement
- Experimental mass spectra have been successfully simuluated for argon gas in the pressure range from 10^{-6} to 10^{-4} mbar for different emission currents 0.35, 0.45, 0.80, and 1mA.

Future work

- Testing of the model with different gases
- Quantify the performance characteristics experimentally
- Use the model to investigate different modes of operation e.g. for obtaining spectra at different values of electron energy in the EI source.

References

[1] J. Gibson, S. Taylor, and J. H. Leck, “Detailed simulation of mass spectra for quadrupole mass spectrometer systems,” *J. Vac. Sci. Technol. A, Vac. Surf. Films*, vol. 18, no. 1, pp. 237–243, Sept. 2000.

[2] J. R. Gibson and S. Taylor, “Prediction of quadrupole mass filter performance for hyperbolic and circular cross section electrodes,” *Rapid Commun. Mass Spectrom.*, vol. 14, no. 18, pp. 1669–1673, July 2000.

[3] Charles A. McDowell, *Mass spectrometry*, Krieger, Huntington (N.Y.), 1979.

[4] Y.-K. Kim and M.E. Rudd, Phys. Rev. A 50, 3954 (1994).

[5] T.J.Hogan, QMS2- Hyperbolic User Guide, Revision 1.0, 2006.

Acknowledgements

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