I Abstract

Field asymmetric ion mobility spectrometry (FAIMS) is an atmospheric pressure analysis technique that is suitable for miniaturisation. Owlstone Ltd. has developed a nanofabricated FAIMS sensor which possesses the smallest dimensions of any such device. Following a detailed review of the theory underpinning FAIMS two separate investigations were conducted to characterise and optimise the sensor's performance.

The first case study systematically characterised the effects of modifying the pressure, humidity and magnitude of the carrier flow through the sensor. Dimethylmethylphosphonate, a simulant for the nerve agent sarin, was selected for the study. The onset of clustering, a phenomenon within FAIMS, was observed and the relationships with the modified parameters of the carrier flow were rationalised.

The second case study represented a new challenge for FAIMS - its application as a detector following the gas chromatographic separation of ethyl acetate from the main components of wine. Lessons learnt from the characterisation study were applied and as a result it was possible to negate the attenuating effects of ethanol. Ethyl acetate was successfully detected at concentrations below the human perception threshold.

Peak fitting was also explored as a method to enhance the specificity of recorded ion responses and to enable automated interpretation of generated data. Three different methods were formulated, each proved more suitable to a particular scenario than the others.

Systematic characterisation of this novel sensor, and its evaluation for non-traditional applications, has resulted in a deeper understanding of FAIMS, its limitations and capabilities. This has led to the development of new tools and methods which can aid investigations beyond these studies, ultimately enhancing the capability of the sensor for more diverse applications.

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III Owlstone Limited

The work reported within this thesis was undertaken as a joint-funded studentship between the Planetary and Space Sciences Research Institute (of The Open University) and an external company, Owlstone Ltd. Owlstone Ltd. are responsible for the development and fabrication of a field asymmetric ion mobility spectrometer on a microchip using nanofabrication techniques. Within the studentship any developed technology and intellectual rights were to be shared between the research institute and co-funding company.

Owlstone Ltd. is a spinout company from the University of Cambridge and now has offices in both the US and UK. The three founders of Owlstone, Billy Boyle, Andrew Koehl and David Ruiz-Alonso, were researchers at the University of Cambridge in the Microsystems and Nanotechnology Group and entered the 2003/2004 Cambridge University Entrepreneurs competition - which they won. Following this success substantial monetary support was secured and Owlstone Ltd. has grown into a business which now employs over thirty five people. The main application focus was initially homeland defence but revenue streams have become more diverse with investigations into industrial, food, beverage and pharmaceutical applications.

Throughout the studentship Owlstone Ltd. personnel were very generous with their time and expertise. Working alongside the most skilled researchers with the technology was extremely rewarding and benefitted the project a great deal.

IV Glossary

At times through this thesis it may be of benefit to review any stated symbol without having to find where they were first declared in the main text. They are presented here for convenience.

Symbol (English)	**Quantity**	**SI unit**
A	Permeable surface area	m^2
a	Acceleration	m/s^2
c	Concentration	$molecules/m^3$
c_v	Concentration of water vapour molecules	$molecules/m^3$
D	Diffusion coefficient	m^2/s
D_T	Duty cycle	-
E	Electric field strength	V/m
E_{max}	Maximum electric field strength	V/m
E_{min}	Minimum electric field strength	V/m
e	Fundamental/elementary charge (1.602×10^{-19} C)	C
F	Force	N
f	Frequency of waveform	Hz
g	Gap height	m
g_{eff}	Effective gap height	m
K	Mobility coefficient	$m^2/V\cdot s$
K_0	Mobility coefficient at low electric field strength	$m^2/V\cdot s$
k_b	Boltzmann's constant (1.38×10^{-23} J/K)	J/K
l	Length	m
M	Mass of gas molecule	kg
m	Mass of ion	kg
N	Molecular number density	$molecules/m^3$

Symbol (English)	Quantity	SI unit
N_A	Avrogardos constant (6.022×10^{23} molecules/mole)	molecules/mole
P	Pressure	N/m^2
P_p	Permeability coefficient	1/m·s
p	Momentum	kg·m/s
Q	Volume flow rate	m^3/s
Re	Reynolds number	-
s	Displacement	m
T	Temperature	K
T_p	Period of the asymmetric waveform	s
t	Time	s
t_1	Time of high field of waveform	s
t_2	Time of low field of waveform	s
t_{res}	Residence time of ion within separation region	s
u	Volume flow rate into exponential dilution flask	m^3/s
V	Voltage	V
$\overline{V}$	Mean velocity of neutral gas molecules	m/s
V_+	Voltage of idealised asymmetric waveform in the high field region	V
V_b	Breakdown voltage	V
V_m	Volume	m^3
$v_{//}$	Longitudinal ion velocity	m/s
$v_\perp$	Transverse ion velocity	m/s
v_d	Drift velocity	m/s
v_y	Ion velocity in the axis defined as y	m/s
$\overline{v}_r$	Mean relative velocity of ions to neutral gas molecules	m/s
$\overline{v}$	Mean velocity of ions	m/s
w	Width	m
Y	Total transverse displacement	m
y_{high}	Transverse ion displacement during the high field region of an asymmetric waveform	m

Symbol (Greek)	Quantity	SI unit
α	Alpha function	-
α_n	Alpha value	-
ε	Energy	J
ε_0	Permittivity of free space (8.854×10^{-12} F/m)	F/m
θ	Relative deflection angle of collision	°
λ	Mean free path	m
μ	Reduced mass	kg
μ_d	Dynamic viscosity	N s/m^2
ρ	Density	kg/m^3
$\nu(\bar{\varepsilon})$	Ion-neutral collision frequency	1/s
ν_k	Kinematic viscosity	m^2/s
ρ	Density	kg/m^3
τ	Mean free time between ion-molecule interactions	s
τ_v	Mean free time between ion-water vapour interactions	s
Ω	Ion-molecule collision cross section	m^2
Ω_p	Effective polar cross section	m^2

V Abbreviations

Acronym	
^{63}Ni	Nickel (63 atomic mass units)
β	Electron emission from radioactive source
CV	Compensation voltage
DC	Direct current
DF	Dispersion field
DMMP	Dimethylmethylphosphonate
EDF	Exponential dilution flask
ECD	Electron capture detector
FAIMS	Field asymmetric ion mobility spectrometry
FWHM	Full width at half maximum
GC	Gas chromatography
IMIS	Ion mobility increment spectrometry
IMS	Ion mobility spectrometry
INLDS	Ion non-linear drift spectrometry
MEMS	Micro electro mechanical system
MS	Mass spectrometry
MW	Molecular weight
NRC	National research centre
PID	Proportional - integral - differential
PR	Permeation rate
PS	Permeation source
PTFE	Polytetrafluoroethylene
SI	Le système international d'unités (international system of units)
S/N	Signal-to-noise ratio
UV	Ultraviolet