EPSRC funded collaboration with Smiths Detection Ltd

By utilising the specialist resources and expertise from two different research environments, the Molecular Physics Research Group (University of Birmingham) and Smiths Detection Ltd (Watford, UK), we will develop an interdisciplinary and collaborative research programme providing a firm scientific understanding of the chemistry and physics involved in Ion Mobility Spectrometry (IMS), and specifically to the latest IMS technology being developed by Smiths Detection Ltd. Through the development of a unique tandem instrument, we intend to increase the dimensionality of IMS systems, investigate high field phenomena and study the importance of dopant chemistry. This will ultimately lead to a new generation of advanced chemical detectors deployed to fight crime and increase security within the UK.

Fears of terrorism and the requirement to detect dangerous agents in low concentrations is leading to an ever-increasing need, within homeland security, for reliable, real-time and sensitive detection of a wide range of substances that are a threat to the safety of our society. The chemicals needed to be detected range from explosives, through to narcotics (such as cocaine and heroin) and chemical and biological agents. The ability to quickly and accurately identify these hazardous compounds, and particularly within a complex chemical environment, is vital to our nation's needs for the fight against crime and terrorism.

Commonly used equipments for this type of security are often based on Ion Mobility Spectrometry (IMS). IMS is the base technology in a wide range of Chemical Warfare (CW) agent, drug and explosive detectors, and environmental monitors (For a description of the IMS see the Instrumentation page).

Despite their worldwide deployment and undoubted successes, the present generation of IMS based equipments should be regarded as 'first generation' and 'one-dimensional' and the exploitation of ion-molecule processes is still in its infancy. The limitations of this is highlighted in a recent National Research Council report dealing with airport security, where it is stated that "*currently deployed systems have limitations specific to the physics and chemistry of their operation*" making them unsuitable for addressing a variety of emerging threats.[3]

In order to provide the tools and knowledge allowing a fuller exploitation of IMS technology and the development of second generation, multidimensional detectors a detailed investigation of the behaviour of ions and their reactions in a high *E*-field, a phenomenon that has potential for increasing the selectivity of IMS but which is at present ill-understood, will be of great importance. Of additional importance is a fundamental study of the use of dopant gases, as present dopants have been selected almost serendipitously.

It should be noted that whilst the description of IMS given widely accepted, it is simplistic, and its implicit acceptance has been the main cause of the failure to fully exploit the potential of IMS. It is generally realised that whether a radioactive source or a corona discharge is used, the initially formed species, e.g. O^+, O_2^+, electrons, are of high energy and are very reactive, leading to complex chemistry[4] before thermalised, stable ions e.g. $H_3O^+(H_2O)_n$ or $O_2^-.CO_2$ are produced. And it is these stable ions that are known as the reactant ions. What is not generally appreciated is that these stable ions are not necessarily the 'reactant' ions and that it takes an appreciable time for them to be produced. Until these stable ions are produced, there will be a multiplicity of highly reactive ions, the nature of which will depend upon the ion source, i.e. ^{63}Ni or corona, being present in the gas stream. Since the analyte is normally introduced into the gas flow upstream of the ionisation source it, the analyte, can react with these highly reactive ions and the resulting products can be various, sometimes reacting further and sometimes appearing as ‘product’ ions. These reactions can take place in both the ionisation/reaction region or in the analysis or drift region. If the latter, then broad, ill-defined mobility peaks can be observed. Thus for optimum performance the initially formed high energy, highly reactive ions need to be converted to those of lower energy and preferably thermalised before they can react with the analyte. This can be achieved to some extent serendipitously by the high water and carbon dioxide levels in the gas in the ionisation region caused by their influx whilst sampling ambient air for the analyte. But this is not entirely satisfactory due to the natural variations in ambient water and carbon dioxide levels. Addition of a dopant can improve the situation considerably but is fraught with difficulties. Therefore a new approach has to be adopted, which is the theme of this collaboration with Smiths Detection Ltd.