De-Convolution of Complex Residual Gas Spectra at JET

T. Coyne, S. Davies, N. Balshaw, A. Miller, C. Robertson, C. Whitehead and EPDA JET contributors

1EURATOM/UKAEA Fusion Association, Culham Science Centre, Oxon. OX14 3DB, UK
2Plasma & Gas Analysis Division, Hiden Analytical Ltd., 42b Europa Boulevard, Warrington, WA5 7UN, UK

INTRODUCTION

At JET, fusion fuel most commonly used in the tokamak is deuterium. Purity of the fuel is vital to ensure the data obtained from plasma pulses is useful, and that pulse recipe repeatability is not compromised.

Our primary goal was to determine the purity of the fueling gas, deuterium, and confirm that we did not have any contamination from helium (He). Analysis using our quadrupole Residual Gas Analysers (qRGA) in the conventional way was not possible due to the overlapping masses of the two species at 4 atomic mass units (amu).

Here, we present and demonstrate the approach we used to solve this problem; a complimentary technique, Threshold Ionization Mass Spectrometry (TIMS), operating on the qRGA mass spectrometer in a mode allowing control over the energy of the electrons emitted within the ionization source.

Recognising the potential to identify more complex compounds which have brought uncertainty when attempting to interpret data from the torus primary vacuum vessel we have applied this technique across a broad range of gases that exhibit overlapping masses in the laboratory.

JET is unique due to the many interacting species.

• 2 isotopes of helium: 3He, 4He
• 3 isotopes of hydrogen: hydrogen, deuterium and tritium.
• 6 isotopes of oxygen, 18O/16O, and super heavy water, T2O.
• 6 Tonnes of carbon tiles, complex carbon / hydrogen isotope interactions.

Baking the vessel to 320°C further complicates an already difficult task due to dissociation of C2H4 and C2H6 species from the vessel wall.

Experimental Details of TIMS at JET

The Hiden Analytical qRGA system at JET is operated in a mode where the energy of the electrons emitted within the ionization source is variable. Different elements have defined ionization energies required to ionise the electrons emitted by the ionization source.

Here, we present and demonstrate the approach we used to solve this problem; a complimentary technique, Threshold Ionization Mass Spectrometry (TIMS), operating the qRGA mass spectrometer in a mode allowing control over the energy of the electrons emitted within the ionization source.

Our primary goal was to determine the purity of the fuelling gas, deuterium, and confirm that we did not have any contamination from helium (He). Analysis using our quadrupole Residual Gas Analysers (qRGA) in the conventional way was not possible due to the overlapping masses of the two species at 4 atomic mass units (amu).

Experimental Aims

• Mix D2 and 1He and control ratio of the mixture with MFC’s. Investigate the possibility of de-convolution of D2 from 4He at 4amu in the mass spectrum, and real-time quantification analysis techniques using the qRGA TIMS technique, combined with BEB ionization cross section (c) theory.
• Mix D2 with the hydro-carbon mixture to investigate the possibility of TIMS de-convolution of complex H2D0, C2H4, C2H6, and preliminary real time qualitative data analysis. Investigate D2O formation and de-convolution at 20amu.

Results: TIMS De-convolution of 4He/D2 Gas Mixture at JET

The figure below shows real time mass flow controlled ratio of 4He/D2 gas mixture displayed within qRGA software. The inset on the left shows the corresponding raw qRGA data [at 4amu] taken as a function of time. The two traces represent Ni(D2) and Ni(D2 + 4He) at 19eV and 31eV respectively. The real time qRGA data on the right shows the true 4He/D2 abundance ratio Ni(D2)/Ni(4He) after applying BEB theory in the qRGA software.

Application of the BEB threshold ionization cross section theory to qRGA data:

From theory, Ni(D2) is the D2 partial pressure signal measured at 19eV and Ni(D2 + 4He) is the D2 and 4He partial pressure signal combined, measured at 31eV in the qRGA. Now, Ni(D2) and Ni(4He) are the real abundance densities of D2 and 4He in the sample gas. To obtain the ratio, Ni(D2)/Ni(4He) from the measured partial pressure signals Ni(D2) and Ni(4He), one must determine Ni(D2) from Ni(D2) + Ni(4He) at 31eV; i.e., to a first approximation it can be given as:

Ni(D2) = A1 [NI(D2) + TH1] ηD2 (1),

and similarly, 
Ni(D2 + 4He) = A1 [NI(D2 + 4He) + TH1] ηD2 + A2 [NI(D2 + 4He) + TH1] η4He (2)

A1 is the instrument (qRGA) factor which is the same for both D2 and 4He as the signal is measured at m/z = 4amu. It is also independent of electron ionization energy between energies of 19 and 31eV. Also, we define the ionization cross sectional coefficients for D2 and He as ηD2 and η4He respectively: Solving (1) and (2) yields;
The figure below shows separation of small (<1%) quantities of heavy water from chamber residual Argon. Neon (Ne) at mass 20 has also been separated in this way. The two spectra above show the raw data curve (top) and the derivative (bottom) clearly demonstrating the separation of the D$_2$O at 12.6eV and Ne at 21.5eV, both sharing the same mass at 20amu. Separation of these masses will prove a useful tool at JET as the vessel interspaces are filled with neon so detection of a leak from one of these into the torus can be identified easily.

**Conclusions and Future Work**

Using the qRGA TIMS technique, de-convolution of the mass spectra obtained at JET could lead the way to providing a better understanding of the chemistry within the vacuum vessel, as well as providing invaluable diagnostic information during vessel conditioning.

Initial TIMS has proved encouraging, demonstrating discrimination of D$_2$/He (1amu) and D$_2$O/Ar$^{++}$ (20amu). De-convolution of C$_x$H$_y$ and C$_x$D$_y$ molecules in the mass spectrum is ongoing, with initial results de-convoluting CH$_4$ formation of C$_x$H$_y$ and C$_x$D$_y$ molecules. For example at 16amu, overlapping species are

<table>
<thead>
<tr>
<th>Species Major m/z</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_4$</td>
</tr>
<tr>
<td>CO$_2$</td>
</tr>
<tr>
<td>C$_2$H$_6$</td>
</tr>
<tr>
<td>C$_3$H$_8$</td>
</tr>
<tr>
<td>C$_4$H$_10$</td>
</tr>
</tbody>
</table>

This work was funded jointly by the United Kingdom Engineering and Physical Sciences Research Council and by the European Communities under the contract of Association between EURATOM and UKAEA. The views and opinions expressed herein do not necessarily reflect those of the European Commission. This work was carried out within the framework of the European Fusion Development Agreement.

**References**

(1). Coyne, T. RIGAs Used At JET, RGA-8, Culham (2008)