Reducing Impact Fragmentation with a Novel Inlet on a Closed Source Neutral Mass Spectrometer.

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Introduction: Closed-source neutral mass spectrometers are often used on flyby missions to characterize the molecular components of planetary exospheres. For example, the upper atmosphere of Enceladus and Titan were analyzed using an Ion and Neutral Mass Spectrometer (INMS) on the Cassini space probe [1]. In a typical closed source, neutrals are thermalized through multiple bounces within a spherical antechamber prior to ionization and mass anlaysis. The closed source improves sensitivity via a ram pressure enhancement.

A limitation of existing closed-source inlets is that the neutrals are traveling at high speeds (5-20 km/s) when they enter the thermalization chamber, and the high kinetic energy of impact leads to fragmentation before molecules enter the ionization region of the mass spectrometer. Due to this fragmentation the original composition of the molecule may have been altered, giving incorrect composition of the exosphere and possibly missing important compounds that were present. Jaramillo-Botero *et al.* used quantum mechanical based simulatons to determine the velocities at which molecular fragmentation occurs [2]. They showed that dissociative adsorption and scattering occurs at about 6 km/s with the inelastic scattering being the dominate pathway up to 8 km/s. Adiabatic sputtering, implantation, and nonadiabatic fragmentation occur at 15 km/s [2].

Knowing that fragmentation occurs, and even knowing some or all of the fragmentation pathways, does not allow deconvolution of flight data to give correct composition. Only stable, volatile fragments will be observed in the subsequent mass spectrometer. Different organic compounds will likely give similar fragmentation products. Simply detecting these products will not lead to unambiguous identication of the precursor molecules. Fragmentation due to ionization acts in addition to impact fragmentation, and together the two make it very challenging to know the native chemical composition of an exosphere. We present a hardware solution to this problem—an inlet that will reduce the fragmentation of molecules that impact at relevant high velocities.

Inlet Design: We are developing a new design for an inlet that will reduce fragmentation of the incoming molecules. The inlet, intended to replace the conventional spherical antechamber, still provides the advantages of ram-enhanced pressure and improved sensitivity. The reduction in fragmentation can be achieved using the shape of the inlet, which will be detailed in the presentation. Considering that fragmentation occurs as a unimolecular dissociation reaction driven by vibrational energy, collisions with walls of the inlet dissipate energy on a timescale that is fast compared with the vibrational dissociation time. Translational energies as low as 5 eV are sufficient to activate chemical transfromations [3] indicating that the dissipation of the translational energy is necessary to keep the molecule intact. Typical kinetic energies of impact range from a few eV for low molecular weight molecules at low encounter velocities to more than 100 eV for larger molecules and higher flyby velocities.

Preliminary calculations indicate that impact-induced fragmentation will be reduced by 2-3 orders of magnitude for all flyby velocities compared with conventional closed sources. This reduction is sufficient to allow essentially all volatile and semi-volatile organic compounds to be analyzed without chemical modification or fragmentation. In addition, experiments are currently underway to characterize the performance of this inlet using beams of high-velocity neutral molecules in the range of several km/s.

References:

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