Neutral Gas Composition of Enceladus' Plume – Model Parameter Insights from Cassini-INMS

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Introduction: The Cassini Ion and Neutral Mass Spectrometer (INMS) has made direct measurements of the Enceladus plume neutral gas on over ten flybys during the course of the Cassini mission under varying conditions.

Clear signatures of complex organics up to C_6H_6 were observed during the high-velocity E5 flyby [1]. Later flybys at lower velocities during the E14, E17, and E18 flybys showed remarkable consistency in composition, confirming observations of complex organics. However these measurements also provided strong evidence that the abundances of organics had been previously overestimated due to instrument effects [2]. The E21 flyby provided further insight by utilizing different instrument modes to constrain the limit of such effects primarily with respect to detecting native H_2 [2].

From these combined observations it is clear that the Enceladus plume is comprised of a complex organic composition that is difficult to measure with high accuracy. Though the INMS measurements contain significant ambiguities in the neutral composition that preclude confident detections of species with low abundance relative to H_2O, a large pool of potential species become apparent and limits upon their abundance may be derived. This information provides a blueprint from which one may produce models of the neutral plume gas that are the most representative of contemporary measurements. From these models it is possible to gain insight into the instrument capabilities required of future missions to increase our knowledge of the plume composition and its implications.

Results: The neutral gas composition analysis is performed on Cassini-INMS data by creating a single integrated ('summed') spectrum for each flyby that captures the total signal of each individual mass channel that is directly attributable to the plume. This integrated approach is necessary to account for different sampling frequencies across the mass range (1-100 m/z) as well as for instrument effects that delay the transfer of plume material to the detector. This also results in significantly increasing the signal-to-noise from individual low-count measurements. By investigating mass histories and the integrated spectrum it is possible to determine a list of 'masses of interest' – those masses which show clear signal correlated to the timing of the plume encounter, and 'noise masses' – those which do not show clear indication of signal increase above noise levels during the plume encounter. When analyzing the composition of the integrated spectrum, these 'masses of interest' must be matched within 1 sigma uncertainty levels (generally ± 30%). The 'noise masses' can be used to set a spectrum-wide noise floor which must not be violated when attempting to match the 'masses of interest'.

The E14, E17, and E18 flybys have provided the INMS with its most robust neutral gas composition datasets. These flybys occurred within a short time frame and followed nearly identical trajectories at the slowest encounter velocities (~7.5 km/s) relative to the moon. Their integrated spectra also showed remarkable consistency with each other across the entire mass range. These spectra were therefore combined into a single spectrum to further increase the signal-to-noise and to account for measurement variability between the three flybys. This E14/E17/E18 combined spectrum forms the primary data set for our plume composition analysis. Further refinements on some species were determined by open source measurements during the E21 flyby.

A candidate pool of nearly 200 neutral species reference spectra was compiled from which our INMS plume gas spectra could be compared in order to search for likely present species. The candidate species list was selected to include species detected in comets, other parts of the Saturnian system, and complex hydrocarbons below 200 amu. To qualify as a species which we list below as a 'potential' measurement by the INMS, a species must contribute at least 10% of the necessary signal at one of the 'masses of interest' within a combination of other species such that they together suitably match the INMS signal across all 'masses of interest' and without significantly violating the bounds of the 'noise masses'. Such analysis is intended to be exhaustive within the confines of the candidate pool of species, while maintaining some restriction on the required significance of each species included in a viable 'matched' composition mixture. The 'potential' species listed in the tables below therefore represent the most significant species in matching the INMS data; i.e. species for which there is some evidence from the data of potential presence.

Major species Detected without Ambiguity rel. abundances to H_2O > 0.1%
H_2O
CO_2
CH_4
NH_3
H_2

Table 1: Major species clearly detected by the INMS without ambiguity.

Minor species with Moderate Ambiguity and rel. abundances < 0.2% and > 100 ppm	
CO	N_2
C_2H_2	HCN
C_2H_4	CH_2O
C_2H_6	NO

Table 2: Minor species with moderate abundance and modereate ambiguity. Some combination of at least four of the listed species is required to match the INMS signal measured in the CSN spectra for the "slow" flybys E14, E17, E18, E21.

Potential Species with High Ambiguity and rel. abundances < 100 ppm	
Hydrocarbons	**N-bearing**
C_3H_4	CH_5N
C_3H_6	C_2H_3N
C_3H_8	C_2H_7N
C_4H_8	$C_2H_6N_2$
C_4H_{10}	C_4H_9N
C_5H_{10}	$C_4H_8N_2$
C_5H_{12}	$C_6H_{12}N_4$
C_8H_{18}	
O-bearing	**NO-bearing**
O_2	C_2H_7NO
CH_3OH	$C_2H_5NO_2$
C_2H_2O	$C_3H_7NO_2$
C_2H_4O	
C_2H_6O	
C_3H_6O	
C_3H_8O	**Others…**
$C_2H_4O_2$	Ar
$C_2H_6O_2$	H_2S
$C_4H_{10}O$	PH_3
$C_4H_6O_2$	C_3H_5Cl

Table 3: Potential minor species with low abundance and high ambiguity. In some cases multiple isomers may be represented. Many possible combinations of the listed species may match the INMS signal measured in the CSN spectra for the "slow" flybys, but at least some of these species are necessary to do so.

Discussion: While the INMS observations lead to very interesting results, there is an unfortunate amount of ambiguity in interpreting the data with regard to neutral composition analysis. The INMS instrument and resulting data sets have two significant limitations which lead to this ambiguity – mass resolution and sensitivity. The 1 amu mass resolution of the Cassini-INMS makes it extremely difficult identify individual species within a complex mixture when there are overlapping contributions at similar abundances in many mass channels. This results in several potential species combinations which are effectively identical in matching the measured spectrum. Insufficient sensitivity further exacerbates the problem by resulting in a high noise floor that makes a large range of masses ineffective in the composition analysis. This then precludes many species from being ruled out due to high upper limits. The mass resolution limitation can be seen in the moderate ambiguity of species in Table 2 where only a few different combinations are possible. However, mass resolution and sensitivity combine in contributing to the high ambiguity seen in Table 3 where numerous combinations are possible.

The results shown in Tables 1-3 allow for a wide range of potential compositions, each that adequately match the INMS data. It is currently impossible to unequivocally distinguish between these different potential compositions, which offer a lot of latitude in interpretations of the Enceladus' subsurface and origins. However, the current results can be used via modelling to help determine the requirements of future measurements in order to significantly increase our knowledge of the plume composition and its scientific implications.

More accurate and unambiguous composition measurements of the Enceladus plume would require instruments that could adequately account for the limitations discussed above in a future mission. With a high mass resolution instrument it would be possible to locate mass peaks with high accuracy and to separate individual signal peaks with small mass differences. Increased sensitivity and dynamic range in the signal would also be crucial in determining the most significant species and placing more restricted upper limits on additional species.

References: [1] Waite et al. (2009) Liquid water on Enceladus from observations of ammonia and ^{40}Ar in the plume. *Nature* **460**, 487-490. [2] Waite et al.., (2017) *Science*, submitted.