PHYSICO-CHEMICAL MODELING OF THE COMA OF COMET C/2004 Q2 (MACHHOLZ). D. C. Boice[1] and S. E. Martinez[2], [1]Southwest Research Institute, Space Science & Engineering Department, 6220 Culebra Road, San Antonio, TX 78238 USA, DBoice@swri.edu, [2]University of Texas at San Antonio, One UTSA Circle, San Antonio, TX 78249, USA, Susan.Martinez@swri.org.

Introduction: Physico-chemical modeling is central to understand the important physical and chemical processes that operate in cometary atmospheres (comae). Photochemistry is a major source of ions and electrons that further initiate key gas-phase reactions, leading to the plethora of molecules and atoms seen in comets. The effects of photoelectrons that react via electron impact reactions are important to the overall ionization. Relevant physico-chemical processes are identified within a global modeling framework to understand observations and *in situ* measurements of comets and to provide valuable insights into the intrinsic properties of their nuclei.

Details of these processes are presented in the collision-dominated, inner coma of comet Machholz (C/2004 Q2); including thermodynamics (e.g., temperature and velocity structure) and photo- and gas-phase chemistry (e.g., composition, gas and electron energetics) throughout this inner region. Prior model results have successfully accounted for the comet Halley water-group composition [1], *in situ* measurements of the PEPE instrument onboard the Deep Space 1 Mission to comet Borrelly [2], S_2 in comet Hyakutake [3], and observations of C_2, C_3, CS, and NS in comet Hale-Bopp [4, 5]. This extensive modeling effort to investigate these important cometary processes is highly relevant to ground-based observations of comets and past, on going, and future spacecraft missions to these primitive objects.

Cometary Processes: Within about 3AU, photochemistry of water is the primary driver of energetics, chemistry, and velocity. Whereas solar visible light mainly heats the nucleus and sublimates volatiles; solar UV initiates photochemistry forming highly reactive ions and radicals that react via gas-phase reactions in the collisionally coupled inner coma. Photo reactions create energetic electrons that cause further ionization via impact reactions. Electron impact processes are very important in high Q comets [4, 6-8].

Since the temperature of the inner coma gas is very low, electron impact ionization from thermal electrons will not significantly contribute to the overall ionization. However, the average excess electron energy for photoionization of, for example, H_2O in the solar radiation field is of order of 12 to 15 eV depending on solar activity. Thus, secondary ionization from photoelectrons can be important, especially in moderate to high production rate comets. In addition, electrons in the solar wind may contribute to the impact ionization of coma gas. A self-consistent description of the electron energetics and associated processes is necessary to accurately investigate the chemistry in the inner coma: Cometocentric profiles of molecules in the inner coma and mapping the chemical pathways that couple them.

Model Results: Model chemistry successfully accounts for composition of many species. [e.g., HCN and H_2O profiles and C_2 consistency with observations of C_2H_2 and C_2H_6]. The formation of CN is predominately due to photo-dissociation and electron impact dissociation of HCN, but other molecules (e.g., CH_3CN) are minor sources. Dust may also act as a source of CN. The formation of a distributed source of CO at distances throughout the inner coma is due to photo and electron impact reactions of H_2CO and CH_3OH. Uncertainties in reaction rates make this linkage somewhat tentative. The chemical model can be used to derive abundances of C_2H_2, C_2H_6, and C_3H_4 from optical observations of C_2 and C_3 at distances far beyond their direct detection and investigate chemical pathways in the reaction network [4].

Future Work: The excitation mechanism for the SH lines is not well understood and can't be entirely explained by fluorescence pumping. We will investigate whether electron impact excitation can explain these spectral features. Extend study to incorporate additional observations of gas and dust to check results, updating the chemical reaction network (especially electron impact reactions) and implementing rigorous error analysis techniques. Bonev et al. [9] conclude that "Evaluating the relative contributions of these pathways requires further modeling of chemistry," indicating that our study should be continued.

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