CHEMICAL EVOLUTION OF IRRADIATED H_2O:CO_2 ICES: INSIGHTS INTO CHARON'S SURFACE CHEMISTRY

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Abstract

The understanding of the chemical evolution of astrophysical ices under radiation is fundamental to interpret molecular diversity in cold environments of the outer Solar System. In this work, we reanalyzed experimental data of H_2O:CO_2 (1:1) ice irradiated by heavy ions ($^{58}Ni^{13+}$, 52 MeV) and modeled its chemical evolution using the PROCODA code, which solves systems of coupled differential equations to describe molecular formation, consumption, and desorption reactions. The model reproduced the evolution of species such as H_2O_2, CO, and CO_2, in addition to predicting the presence of intermediates like HOCO and H_2CO. The results show good agreement with recent observations of Charon, which reveal relative abundances of H_2O (~69%), CO_2 (~28%), and H_2O_2 (~3%). Modeling suggests that cosmic-ray-induced desorption contributes to maintaining surface CO_2, while H_2O_2 tends to accumulate in the icy mantle. These findings reinforce the relevance of radiolysis processes in the chemistry of trans-Neptunian objects and highlight the usefulness of integrated approaches combining experimentation, simulation, and observation.

Keywords: Astrochemistry; astrophysical ices; Charon; computational modeling; cosmic rays**.**

Field of Knowledge: Exact and Earth Sciences, Astronomy

Introduction

The molecular diversity found in the interstellar medium and in icy bodies of the outer Solar System results from complex interactions between ices, dust, and ionizing radiation. Trans-Neptunian objects (TNOs) such as Charon are particularly interesting in this regard, as their surfaces are dominated by simple ices that are continuously altered by galactic cosmic rays. Recent JWST (James Webb Space Telescope) observations have revealed the presence of H_2O, CO_2, and H_2O_2 on Charon (Protopapa et al., 2024), highlighting the role of radiation-driven chemistry under cryogenic conditions.

Against this background, the present study investigates the chemical evolution of irradiated H_2O:CO_2 ices using the astrochemical code PROCODA. The model is applied to trace reaction pathways, estimate abundances at chemical equilibrium, and evaluate desorption rates. These results are then compared with observational data from Charon, providing insights into the chemical processes that govern the composition of TNO surfaces (Moraes and Pilling, submited).

Fig. 1. The surface of Charon with mixtures of blue and red

source: NASA

Charon, Pluto's largest moon, is one of the most extensively studied trans-Neptunian objects. Discovered in 1978, it measures about 1212 km in diameter roughly half the size of Pluto making the Pluto–Charon system unique in that their barycenter, or common center of mass, lies outside Pluto, effectively classifying it as a binary system.

The surface of Charon is primarily composed of crystalline water ice, with substantial amounts of CO_2 and more recent detections of H_2O_2, as revealed by the James Webb Space Telescope (JWST) in 2024. These findings indicate that the moon's surface is continuously altered by cosmic and solar radiation, driving radiolysis reactions that form new compounds and gradually reshape its chemical composition.

Beyond its chemical makeup, Charon also displays remarkable geological features, such as vast canyons and possible cryovolcanoes, which point to a history of internal activity. Together, its surface chemistry and geology provide critical insights into chemical evolution in the outer Solar System and the mechanisms of ice processing in trans-Neptunian environments.

Methodology

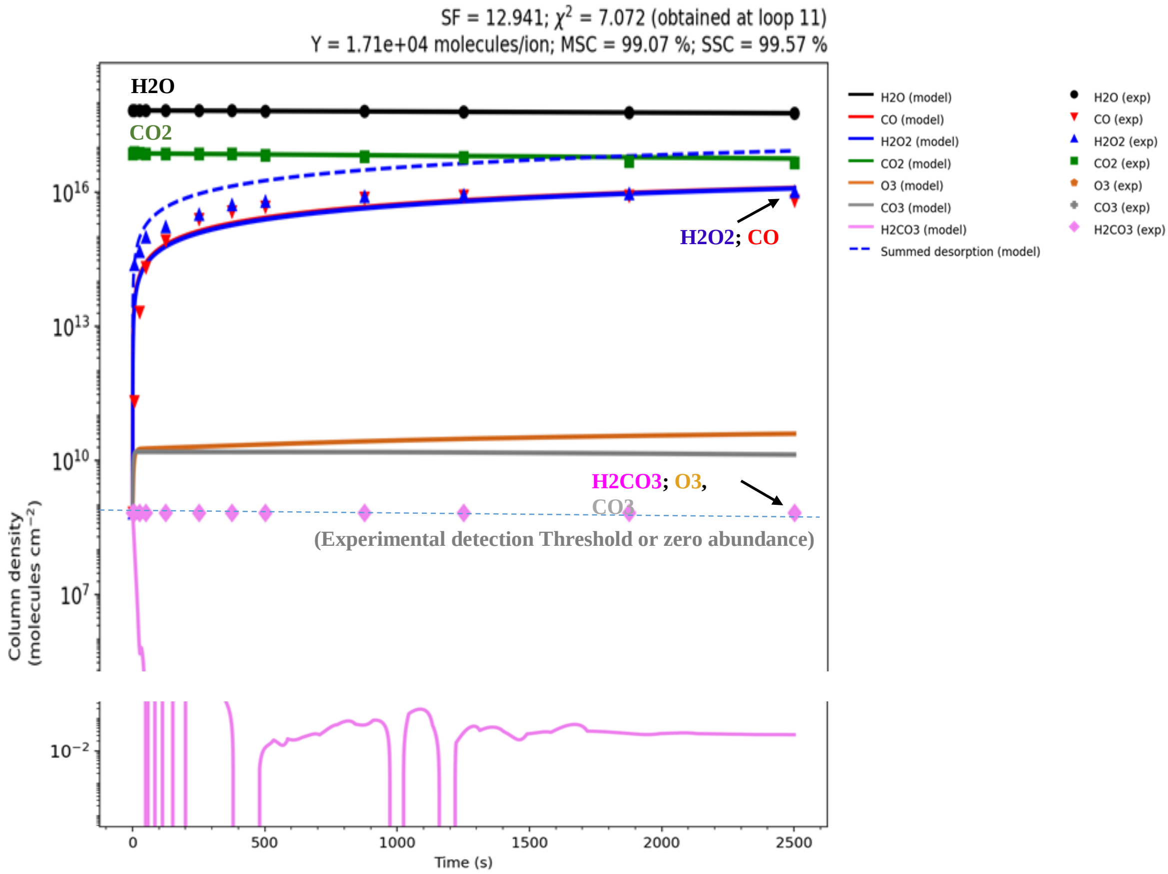
Experimental data from Pilling et al. (2010) were employed, obtained at the GANIL accelerator (France), where $H_2O:CO_2$ (1:1) mixtures were deposited at 13 K onto a CsI substrate and irradiated with $^{58}Ni^{13+}$ (52 MeV) ion beams. In situ monitoring was performed using infrared spectroscopy (FTIR), enabling the determination of column densities for both formed and destroyed species.

These data were subsequently modeled with the PROCODA code (Pilling et al., 2022; Carvalho et al., 2022; da Silveira & Pilling, 2024; Moraes and Pilling, submited), which incorporates 73 chemical species and 1631 elementary reactions. PROCODA calculates effective reaction coefficients (ERCs), simulates radiation-induced desorption, and estimates abundances at chemical equilibrium. This approach makes it possible to extrapolate the formation of species not experimentally detected but considered chemically plausible in irradiated environments.

Results

PROCODA successfully reproduced the experimental evolution of H_2O, CO_2, CO, H_2O_2, CO_3, and O_3, while also predicting the formation of intermediates such as HOCO and H_2CO. At chemical equilibrium, the modeled relative abundances were H_2O (87.3%), CO_2 (8.4%), CO (1.8%), and H_2O_2 (1.8%). The desorption analysis indicated that H_2O is the most mobile species, followed by CO_2, whereas H_2O_2 remains largely trapped within the solid matrix.

Fig. 2. Evolution of column density of chemical species in astrophysical ice. Graph showing the temporal evolution of column density (molecules/cm²) of different chemical species in irradiated astrophysical ice.



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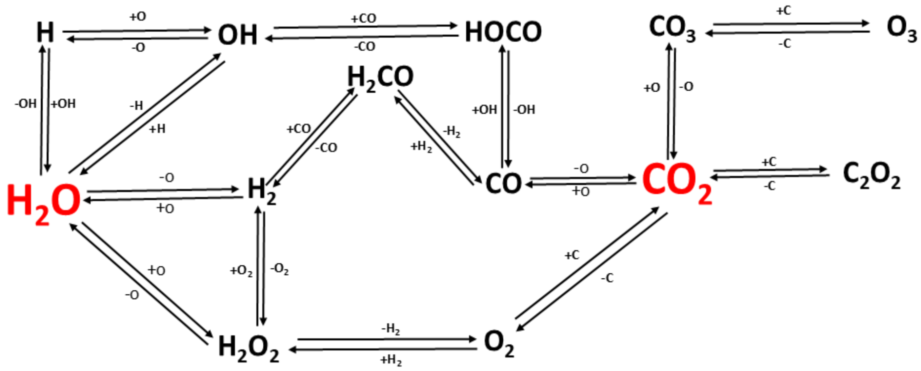
These findings suggest that cosmic radiation is capable of sustaining detectable levels of CO_2 on the surfaces of TNOs even at cryogenic temperatures. Moreover, the accumulation of H_2O_2 emerges as a diagnostic marker of radiolytic processing in astrophysical ices.

In Figure 3, some of the main species derived from their parent molecules are shown, along with their reaction pathways. Among them, the hydroxyl radical (OH) stands out as one of the most important oxidants in the interstellar medium (ISM), where it plays a crucial role in the synthesis of water and other molecules. This radical is frequently detected in molecular clouds and star-forming regions, being produced primarily through the photodissociation of H_2O and through reactions involving atomic oxygen (O) (Van Dishoeck et al., 2013). In this study, its formation is represented by reaction O + H_2O → OH + OH, which appears with high abundance in the simulations.

Fig. 3. Some chemical species and their reaction pathways originated from parent species (in red), thus presenting some of the most important ones within this study; the remaining 1631 reactions will be presented in the supplementary material.



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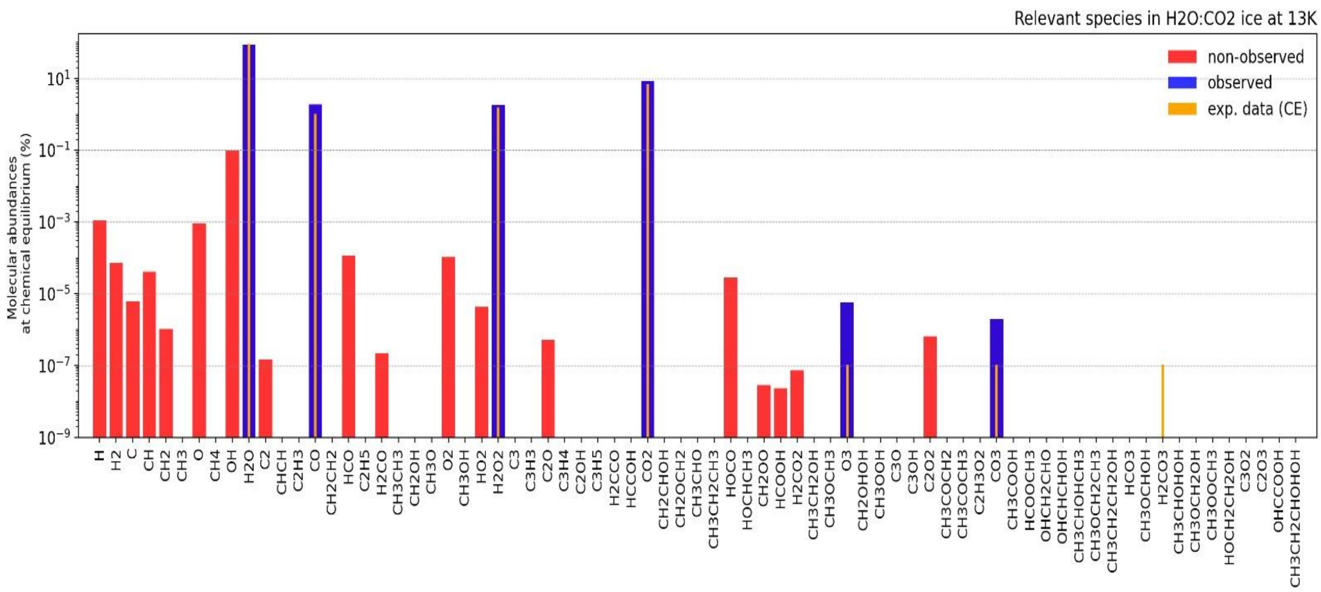
Hydrogen peroxide (H_2O_2) is another key species, acting as a major contributor to oxygen production in the ISM, with several detections reported in molecular clouds and icy surfaces (Cuppen et al., 2010). Ethylenedione (C_2O_2), although a transient compound, can serve as an intermediate in the formation of more complex organic molecules, likely produced from CO dissociation and, more prominently, through interactions with cosmic rays, as shown by reaction $C_2O_2 \rightarrow C + CO_2$. Carbon trioxide ($CO_3$), in contrast, is an unstable oxide formed in reactions between CO_2 and atomic oxygen (O). The formyloxyl radical (HOCO) functions as a central intermediate in the production of formic acid (HCOOH), which has been detected in interstellar clouds and holds astrobiological significance.

Formaldehyde (H_2CO) is also commonly found in the ISM, having been identified in nearly all analyzed comets (Eistrup et al., 2019) as well as in the protoplanetary disk surrounding LKCa 15 (Thi et al., 2004).

Fig. 4. Abundances at chemical equilibrium: relevant chemical species at equilibrium. Red bars indicate species not observed, blue bars those detected observationally, and yellow bars, overlaid on the blue, represent experimental data.



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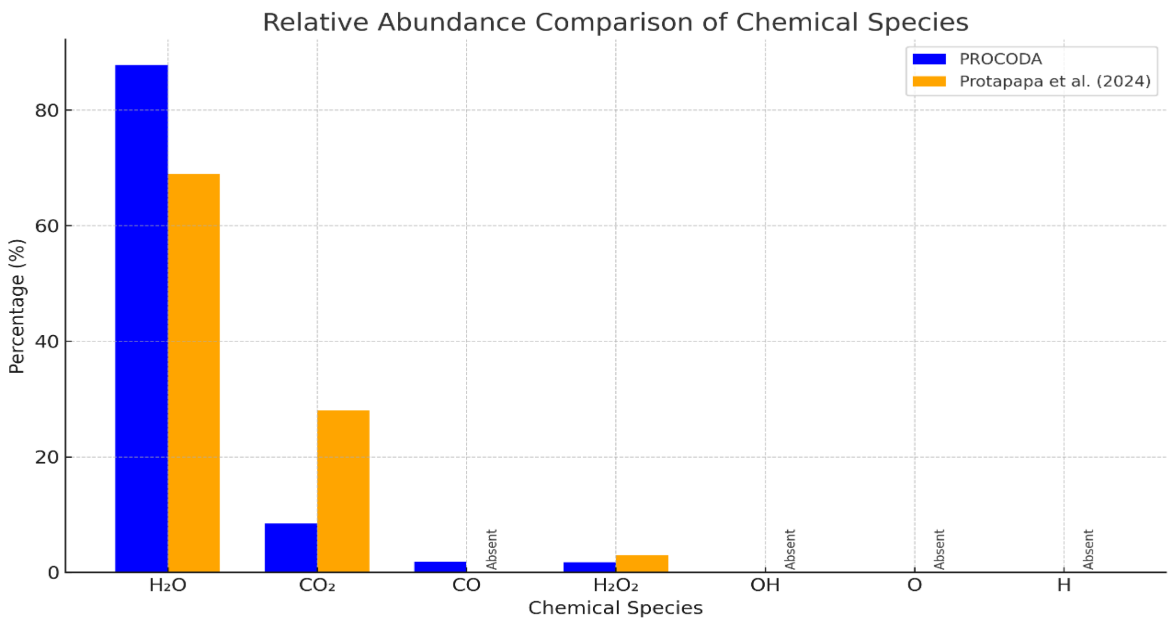
In Figure 4, the red bars represent species not experimentally detected, while the blue bars correspond to species observed experimentally and reproduced by PROCODA. The actual experimental data are shown in yellow, overlaid on the blue bars. The agreement between model and experiment is highly satisfactory, indicating that additional species may also form within the same ice. This highlights the presence of an “invisible chemistry” in these environments currently hidden by observational limitations but likely to become accessible with future advances in more sensitive instrumentation (Moraes and Pilling, submited).

Discussion

The strong agreement between the modeled results and JWST data for Charon (H_2O ~69%, CO_2 ~28%, and H_2O_2 ~3%) underscores the reliability of PROCODA for studying outer Solar System environments. The model indicates that the elevated fraction of CO_2 may result from both initial trapping and ongoing radiation-driven reprocessing, with partial release through non-thermal desorption. In contrast, the low volatility of H_2O_2 favors its retention within the ice matrix, consistent with its detection in relatively small amounts.

Fig. 5. Comparison of the relative abundance of chemical species between the PROCODA model and observational data from Protopapa et al. (2024). The graph shows the relative percentages of H_2O, CO_2, CO, H_2O_2, OH, O, and H molecules simulated by the PROCODA computational model (blue bars) and those reported in Protopapa et al. (2024) (orange bars). Species absent in the observational study were indicated with the annotation “Absent.”



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In addition, PROCODA predicts the presence of species not yet observed, including OH, HCO, and HOCO, which could serve as promising targets for future observations using more sensitive instrumentation. Although present only in low concentrations, these reactive intermediates may play critical roles in the synthesis of more complex organic molecules on icy surfaces.

Conclusion

This study highlights the importance of chemical modeling of irradiated $H_2O:CO_2$ ices for interpreting observations of Charon and other TNOs. The results demonstrate that radiolysis not only generates H_2O_2 but also sustains CO_2 on cold, irradiated surfaces, consistent with recent JWST findings. Overall, the integration of laboratory experiments, computational simulations, and astronomical observations is essential for uncovering the "invisible chemistry" that shapes trans-Neptunian environments.

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