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Origin, evolution and impact of electrons at comet 67P

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Peter Stephenson, March 2022

Abstract

The comet nucleus is a ball of ice and dust, heated through solar illumination. Near-surface ices sublime under this heating and form the coma, an expanding envelope of neutral gas. These neutral molecules can be ionized through photoionization or by electron-impact, forming a cometary ionosphere. The ionosphere incorporates a variety of electron populations of different temperatures (cold, warm and hot) and origins (cometary or solar wind). My thesis focusses on identifying how these electrons are produced, on assessing how the various populations are formed, and on quantifying the impact the electrons have in the coma.

Rosetta became the first spacecraft to observe a comet from a close and continuous perspective. It escorted comet 67P/Churyumov-Gerasimenko for two years, from August 2014 (at 3.6 au), through perihelion (1.24 au), until Sept 2016 (3.8 au). Instruments onboard Rosetta probed the cometary environment as it evolved from weak activity far from the Sun to highly active around perihelion.

To understand the role of electron-neutral collisions in the coma, I have developed the first three-dimensional collisional model of electrons at a comet. This kinetic test particle model incorporates electrons from the solar wind, photoelectrons, and electrons produced through electron-impact ionization. Electrons in the model move through complex and realistic electric and magnetic fields, inputted from a fully kinetic Particle-in-Cell (PiC) simulation, while subject to a variety of collisional processes.

The test particle model is applied to assess the formation, dynamics and loss of the cold population of electrons. These were observed throughout the Rosetta mission with Rosetta Plasma Consortium (RPC)'s Mutual Impedance Probe (MIP) and Langmuir Probe (LAP), even when the coma was not thought to be collisional. I demonstrate that the combination of realistic fields and the inclusion of collisions can sustain a cold electron population even when the coma is very rarefied. Current estimates of collisionality in the coma are revised and can now explain many of the cold electron observations from the Rosetta missions.

The Alice FUV imaging spectrograph detected emissions from the coma in the far-ultraviolet (FUV, 700 Å-2050 Å). With a multi-instrument approach, I have demonstrated that FUV emissions in the CO₂-rich southern hemisphere of 67P are driven by dissociative excitation of cometary neutrals by electron-impact. In-situ electron measurements with RPC's Ion and Electron Sensor (IES) and neutral gas observations are compared to remote sensing measurements of FUV emissions from the coma. The FUV emissions are generated by accelerated solar wind electrons and are, therefore, aurorae.

The electron-impact ionization frequency is assessed from Rosetta dataset on the one hand and from collisional, test-particle simulations on the other, in order to determine the source of the ionizing electrons in the coma and to identify key drivers behind the ionization frequency they induce.

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Chapter 1

Introduction

Comets, and their transient presence in the sky, have long fascinated astronomers, with the earliest records of observations stretching back over two millennia. The appearance of comets, and particularly Halley's comet, in the sky has been a harbinger of doom across the world from China in the second century BC, to ancient Babylon and through to an appearance in the Bayeux tapestry ([Ridpath and Murtagh, 1985](#)). The transition from an ominous apparition to the focus of astronomical study began in the fifteenth and sixteenth centuries. Comet tails were observed to point away from the Sun by a German astronomer, Peter Apian, in the early sixteenth century, but the paths of comets through the Solar System were, as yet, unknown.

Edmond Halley, in partnership with Isaac Newton and a new theory of gravitation, concluded that comets followed elliptical orbits and predicted the return of the eponymous object that he had observed in 1680. On comet Halley's reappearance in 1759, it was confirmed that (at least some) comets were periodically orbiting members of the Solar System, much like their planetary cousins.

Since these early observations and discoveries, much has changed in our understanding of comets. In addition to improved Earth-based observations, space missions to comets, such as the flyby of comet Halley by Giotto, have allowed in situ measurements of the cometary environment.

Periodic comets, like planets, trace elliptical orbits around the Sun but are much more eccentric. Within the Solar System, they either originate from the Kuiper belt (and scattered disc, 30-50 au) or the more distant Oort cloud, extending up to 100,000 au ([Oort, 1950](#)). These clouds of objects are so distant from the Sun that they remain pristine and un-evolved since the early Solar System. As a result, comets can provide key pieces of information towards understanding the materials that the Solar System was created with.

Comets are split into three main classes: Jupiter family comets (JFCs), Long Period Comets (LPCs) and Halley-type comets (HTCs), distinguished by the orbits of the objects. Jupiter family comets (JFCs) are short period comets (from 2 to 20 years) that are gravitationally influenced

by Jupiter. These began as Kuiper belt objects before entering the inner Solar System and encountering Jupiter at low velocities, where they become gravitationally focussed (Dones et al., 2015).

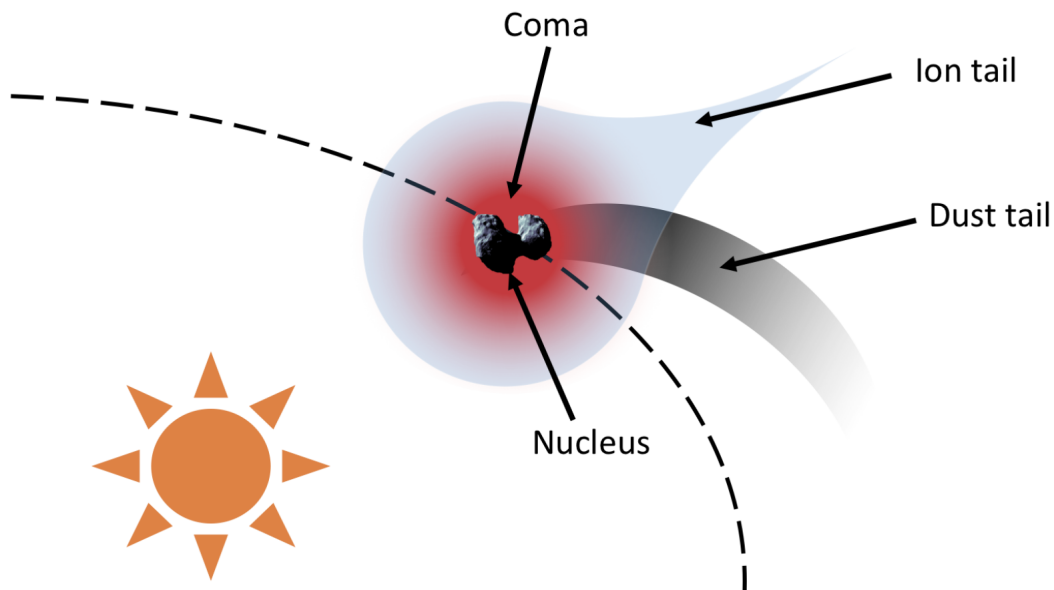


Figure 1.1: The structure of a comet (not to scale). The coma (red) is formed from gases sublimating from the surface, and the tails extend up to a million times the size of the nucleus. Credit: Heritier (2018)

Long period comets (>200 years), such as Hale-Bopp or C/2013 A1 Siding Spring, originate in the Oort cloud (Oort, 1950; Dones et al., 2015). The orbits of the Oort cloud objects are perturbed by galactic tides or passing stars, and brought into the inner Solar System (Dones et al., 2015). Halley-type comets (HTCs), with periods from 20 to 200 years, are also thought to hail from the Oort cloud, although this is still uncertain (Wang and Brasser, 2014; Dones et al., 2015).

What is a comet? A comet is made up of a solid nucleus, a surrounding cloud of neutral gas that has been partially ionized and two tails, which extend anti-sunward from the nucleus (see Figure 1.1). The comet **nucleus** is a mixture of ices, dust and rock, formed in the primordial Solar System. As the nucleus is illuminated and heated by the Sun, near-surface ices sublimate and generate an envelope of expanding neutral gas known as the **coma**. As the neutral gas expands, it drags dust grains out and away from the nucleus. Dust grains decouple from the neutral gas and the gravitational pull of the nucleus weakens further away from the nucleus. Solar radiation pressure then drives the dust particles away from the Sun and into the **dust tail** (Ivanovski et al., 2017; Frattin et al., 2021).

The neutral molecules in the coma can be ionized, either by Extreme-UltraViolet (EUV) photons from the Sun, or by collisions with energetic electrons. These processes generate populations of electrons and ions within the coma, forming a cometary **ionosphere**. The solar wind, a continuous flow of ions and electrons propagating away from the Sun, interacts with the cometary ionosphere and ‘picks-up’ cometary ions. These are pulled downstream into a second tail, which is known as the **ion tail**.

In the early 19th century, some more detailed features of comets started to be discerned in the coma of Halley, such as jets and streamers (e.g. [Bessel, 1836](#)). However, the modern era of cometary science really commenced in 1950. The model of the comet nucleus as a ‘dirty snowball’ ([Whipple, 1950](#)), the identification of the Oort cloud ([Oort, 1950](#)) and the model of tail formation due to its interaction with the solar wind ([Biernmann, 1951](#)) formed a comprehensive description of comets and laid the groundwork for the future of cometary science. The deduction of a solar wind flow from the anti-sunward ion tail by [Biernmann \(1951\)](#) and the prediction of a frozen-in, solar wind magnetic field by [Alfven \(1957\)](#) planted the flag for comets as a key laboratory of plasma physics.

The most defining period in cometary physics was the return of 1P/Halley towards perihelion in 1986, during which six spacecraft visited the comet and made in situ measurements of the coma. The first in situ observations of a comet had actually been made six months prior by the Interplanetary Cometary Explorer (ICE), which flew through the tail of comet 21P/Giacobini-Zinner (GZ) in September 1985 at a distance of 8000 km. The two Vega spacecraft (1 and 2), of the Soviet Union, made closest approaches of 8890 km and 8030 km, respectively. Two Japanese spacecraft, Suisei and Sagikake, made more distant flybys at 150,000 km and 7×10^6 km, while the European Space Agency (ESA) spacecraft, Giotto, passed within 600 km of the nucleus. It returned the first ever pictures of a cometary nucleus. The close perspective of Giotto allowed features to be identified on the surface of the nucleus, such as craters and mountains ([Keller et al., 1988](#)). The picture of nuclei as a ‘dirty snowball’ was revised to an ‘icy dirtball’, as the nucleus was found to be primarily made up of dust with volatiles filling cavities of the nucleus ([Keller, 1989](#)).

The flybys of GZ and Halley heralded a new era of cometary plasma physics and greatly improved the understanding of the comet-solar wind interaction. They provided the testing ground for models describing this interaction, which had been developed over the previous 20 years. A bow shock upstream of an active comet ($Q = 3 \times 10^{28} \text{ s}^{-1}$ for GZ and 10^{30} s^{-1} at Halley during the flybys; [Krakowsky et al., 1986](#); [Cowley et al., 1987](#)) was observed at GZ ([Bame et al., 1986](#); [Smith et al., 1986](#)) and at Halley by Suisei ([Mukai et al., 1986](#)), Vega ([Schwingenschuh et al., 1986](#)) and by Giotto ([Neubauer et al., 1986](#); [Rème et al., 1986](#)), as had been predicted by [Biernmann et al.](#)

(1967). However, the bow shock observed during the Giotto flyby of 26P/Grigg-Skjellerup (GS) was unexpected, as the comet was much less active than either GZ or Halley during the spacecraft encounters (Neubauer et al., 1993; Reme et al., 1993).

The Giotto spacecraft, with its close approach of Halley (596 km), probed deeply into the cometary ionosphere, crossing many plasma boundaries during the flyby. The most surprising structure was the diamagnetic cavity, a magnetic field-free region around the nucleus, which was encountered at 4500 km from the nucleus inbound (4150 km outbound; Neubauer et al., 1986). The variety of instruments on board Giotto and the other spacecraft, which flew by comets, allowed models of the ionosphere, such as that from Ip and Mendis (1976), to be significantly refined. Electrons were found to have a key role in the ionosphere as a source and sink of ions through electron-impact ionization or through recombination with cometary ions (Cravens, 1987; Goldstein et al., 1989; Gan and Cravens, 1990).

After the flybys of GZ, Halley and GS, there have been several more flybys of comets, including 19P/Borrelly by Deep Space 1 and 81P/Wild 2 by Stardust (Boice et al., 2000; Tsou et al., 2004). These encounters have helped to build on the knowledge garnered from the missions to Halley. However, the next major step forward in cometary science would follow the highly-ambitious, ESA/Rosetta mission, which would escort a comet over two years as it orbited the Sun (Glassmeier et al., 2007a). This was the first time a comet had been observed from a close and continuous perspective, allowing the evolution of cometary activity and interaction with the interplanetary environment to be recorded and measured in situ.

Section 1.1 discusses the Rosetta mission and the variety of instruments onboard that were used to enhance our understanding of the cometary ionosphere. Section 1.2 outlines the current state of knowledge of the cometary environment, in the wake of the Rosetta mission. In Section 1.3, I discuss various types of models of the cometary environment and their uses in understanding the behaviour of electrons at a comet. Finally, in Section 1.4, I present the motivation and aims of my thesis.

1.1 The Rosetta mission and instrumentation

The Rosetta mission was one of the cornerstone missions of the ESA Horizon 2000 programme. The mission constituted an orbiter (Rosetta) and a lander (Philae), which could take measurements of the cometary environment and the nucleus. Named after the Rosetta Stone and the Philae Obelisk, it was hoped that the spacecraft would open a window into understanding the formation and identifying the composition of the early Solar System (Budge, 1913; Kamil, 1993).

The original target of the mission was 46P/Wirtanen ([Taylor et al., 2017](#)), but delays to the launch resulted in the selection of a new target comet: 67P/Churyumov-Gerasimenko (67P). Comet 67P was discovered in 1969 by Klim Ivanovich Churyumov and Svetlana Ivanova Gerasimenko ([Churyumov and Gerasimenko, 1972](#)). It is a Jupiter family comet with a period of 6.55 years, perihelion at 1.24 au and aphelion 5.68 au, with dimensions of 4.4 to 5.1 km depending on the orientation ([Sierks et al., 2015](#)).

The Rosetta spacecraft was launched in 2004, undergoing three flybys of Earth and one of Mars, before arcing towards rendezvous with 67P. En route, Rosetta visited asteroids 2867 Steins in 2008 ([Schulz, 2010](#)) and 21 Lutetia in 2010 ([Schulz, 2012](#)), before entering into a hibernation period when it was far from the Sun.

After three years, Rosetta awoke in January 2014 and successfully rendezvoused with 67P on the 6th of August 2014 at 3.6 au. The Philae lander was deployed on the 12th of November 2014, becoming the first man-made object to land on a comet. Rosetta then escorted the comet along its orbit over two years, through perihelion at 1.24 au, until the end of mission at 3.8 au. On the 30th of September 2016, as the power provided by the solar panels dwindled, Rosetta made a final but controlled descent to the surface of 67P. This provided the first vertical profile of cometary ionospheric densities and the first measurements at such proximity to the nucleus ([Heritier et al., 2017b](#)).

During the two-year escort phase, the many instruments onboard Rosetta continuously measured the cometary environment, gathering a unique and extensive dataset. Rosetta provided the first close and continuous observation of a comet as it evolved with heliocentric distance and has led to great developments in the understanding of the cometary environment. The discovery of new cometary molecules and ions and a new appreciation of the interaction of a comet with the solar wind are two of the many steps forward that have been made possible by Rosetta ([Le Roy et al., 2015](#); [Goetz et al., 2016b](#); [Altwegg et al., 2016](#); [Behar et al., 2017](#); [Beth et al., 2020](#)). The science outcomes of Rosetta are discussed in Section 1.2, as they represent many of the latest results in cometary physics.

The Rosetta spacecraft was equipped with a variety of instruments to measure the neutral coma and the plasma environment, as well as the properties of the nucleus ([Glassmeier et al., 2007a](#)). The suite of plasma instruments, proposed under the umbrella of the Rosetta Plasma Consortium (RPC), is described in Section 1.1.1. The RPC instruments are key to understanding the behaviour of electrons at 67P and are used throughout this thesis. In Section 1.1.2, I present the Rosetta Orbiter Spectrometer for Ion and Neutral Analysis (ROSINA), which ‘continuously’ measured, in situ, the properties of the neutral gas and ions in the coma. On board Rosetta, there

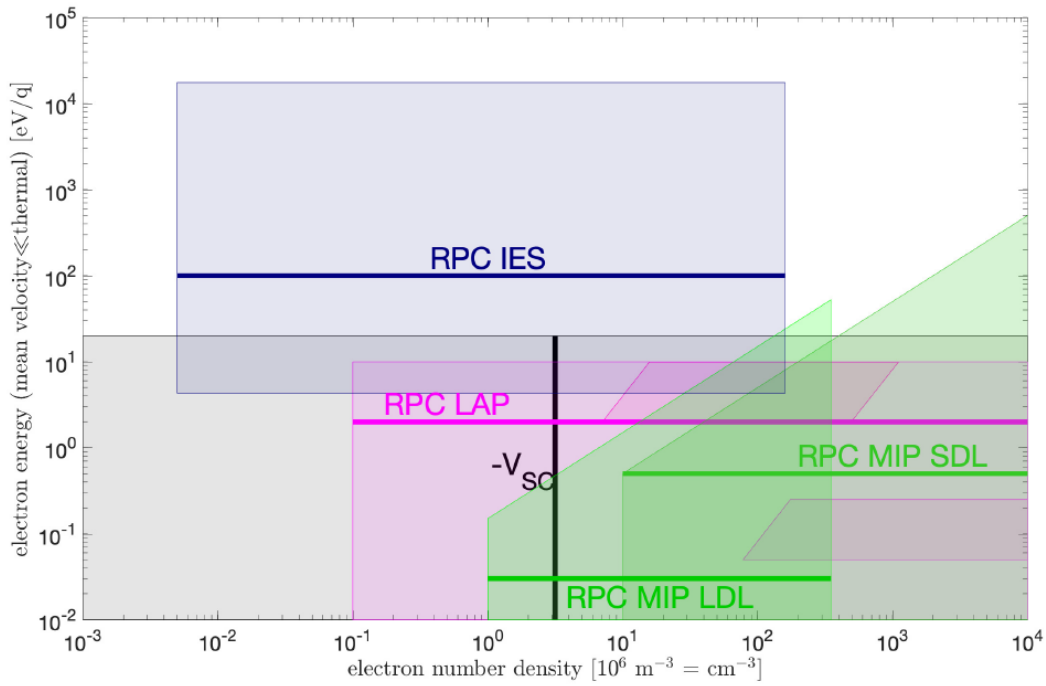


Figure 1.2: Electron density and energy phase space that was probed by the RPC instruments. Credit: [Beth et al. \(2019b\)](#).

were also several detectors making remote observations of the coma, providing context of how the wider cometary environment changed during the mission (Section 1.1.3). The data from all the Rosetta instruments has been consolidated and made publicly available on ESA’s Planetary Science Archive (PSA).

1.1.1 The Rosetta Plasma Consortium - RPC

The Rosetta Plasma Consortium ([Carr et al., 2007](#)) is a group of five distinct instruments capable of measuring in situ plasma properties across a range of conditions (see Figure 1.3). The instruments of the consortium were designed with a wide dynamic range, capable of measuring plasma conditions both in the solar wind and in the dense, collisional coma (see Figure 1.2). As comet 67P travelled from large heliocentric distances towards perihelion, the levels of cometary activity increased substantially. The five plasma instruments are outlined below, along with their measurement capabilities. The telemetry and power of all the RPC sensors were coordinated and provided by the Plasma Interface Unit (RPC/PIU, [Carr et al., 2007](#)), developed in the Department of Physics at Imperial College London.

IES

The Ion and Electron Sensor ([Burch et al., 2007](#)) measured the flux intensity of electrons and ions at the spacecraft as a function of both angle and energy. The instrument was formed from two

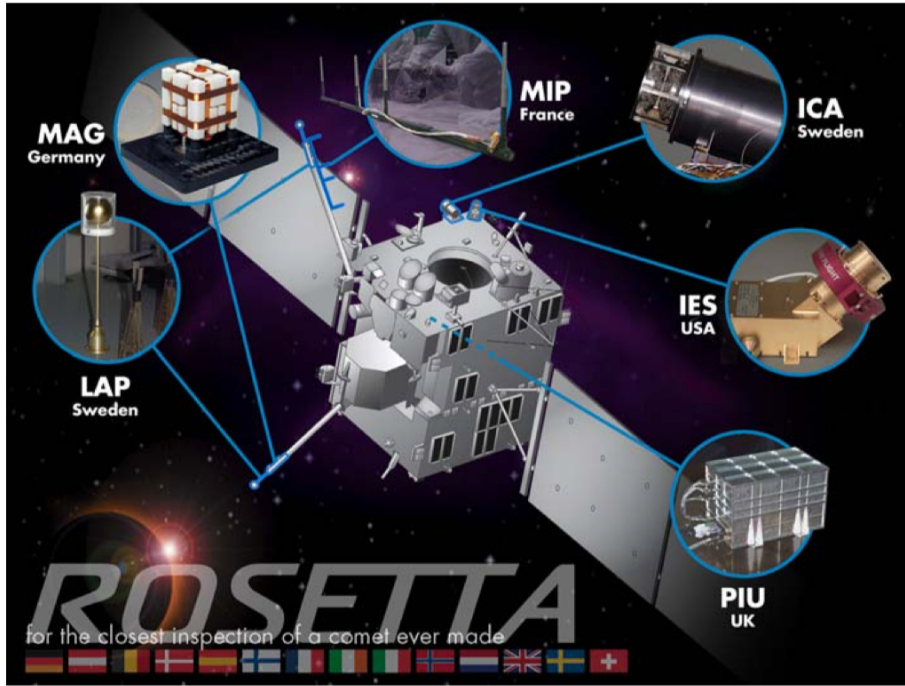


Figure 1.3: The instruments of the Rosetta Plasma Consortium. Credit: Carr et al. (2007).

electrostatic top hat analysers, one for ions and the other for electrons, which sat back to back and shared an entrance aperture. The two analysers allowed the electron and ion distributions to be measured simultaneously.

The charged particles were directed through the instrument by curved plates, across which a potential difference was applied. The voltage was varied to select particle energies from 4.32 eV/ q up to 17.67 keV/ q for both ions and electrons. These energy ranges are for the particles as they enter the detector. However, the particle energies were substantially modified from the ambient plasma, as they travelled through the spacecraft potential before entering the detector.

The energy bins for each mode of operation were distributed approximately logarithmically along the energy scale, with a resolution of $\Delta E/E = 8\%$ for each bin. The electrons were directed towards a micro-channel plate (MCP), where they were detected. A full measurement cycle could take from 128 s to 1024 s as measurements at multiple energies or elevations could not be conducted simultaneously and had to be cycled through.

The electron sensor had a $96^\circ \times 360^\circ$ field of view, with resolution of 6° and 22.5° in the polar and azimuthal directions, respectively. When installed on the spacecraft, parts of the field of view were obstructed by other instruments and the spacecraft body (Clark et al., 2015), which is corrected with a geometric factor (see Section 4.2). The ion sensor covered the same field of view, but the azimuthal resolution was more refined for observations of the solar wind. Generally, the azimuthal resolution was only 45° , but this increased to 5° in the sector most likely to contain the solar wind ions. In April 2015, a number of the anodes (8 to 15) of the electron sensor degraded

and began returning reduced levels of electron flux compared to anodes 0 to 7 (Broiles et al., 2016b).

RPC/IES was able to measure the suprathermal electron flux throughout the Rosetta mission and was used to characterise this population of electrons (Clark et al., 2015; Broiles et al., 2016b,a; Madanian et al., 2016b,a, 2020; Myllys et al., 2019). The energetic electron measurements have also been used to quantify the electron-impact ionization frequency in the coma of 67P over several periods and to demonstrate the substantial contribution of secondary electrons towards the total plasma density (Heritier et al., 2017b, 2018b). Galand et al. (2020) confirmed that energetic electrons are responsible for the atomic far-ultraviolet (FUV) emissions in the northern hemisphere of 67P through dissociative excitation of molecules, when Rosetta was far from perihelion.

The measurements of energetic electrons by RPC/IES are widely used in this thesis. Electron-impact ionization and dissociative excitation frequencies of neutral species are derived from the RPC/IES electron particle measurements and are key components of the studies in Chapters 4 and 5.

RPC/IES was also used to monitor the ion populations and distributions at Rosetta. Solar wind ions were detected in the coma at large heliocentric distances at 1 keV/e, 2 keV/e and 4 keV/e for the H^+ , He^{2+} and the charge-exchanged He^+ populations, respectively (Goldstein et al., 2015). Picked up cometary ions were observed at a few hundred eV/e, before they were fully accelerated in the solar wind flow (Goldstein et al., 2015). Cometary ions were also detected at lower energies (< 20 eV) once they had been accelerated by the spacecraft potential (Mandt et al., 2016; Goldstein et al., 2017). Mandt et al. (2016) used the RPC/IES ion measurements to identify plasma boundaries in the coma (see Section 1.2.2).

MAG

The RPC Magnetometer (RPC/MAG; Glassmeier et al., 2007b) was formed of two triaxial fluxgate magnetometers (Outboard and Inboard) separated by 15 cm along one of the 1.5 m booms on Rosetta. Each sensor could measure the ambient magnetic field vector up to 20 times per second. However, the inboard sensor was used at a lower frequency (up to 1 Hz) to monitor the magnetic field of the spacecraft and the other instruments, such that these effects could be cleaned from the data. The magnetometer operated over field strengths from ± 16384 nT with a resolution of 31 pT.

A fluxgate magnetometer is essentially a transformer around a high permeability, ferromagnetic core. The core is driven into and out of saturation at high frequency, via the drive winding. The core traces out a hysteresis loop, which induces a voltage in the secondary sense winding if there is an external magnetic field. The presence of such a field causes the core to respond asymmetrically

to the driving voltage. The asymmetry generates even harmonics of the driving frequency, f_D , in the sense winding, which are proportional to the strength of the background field. The second harmonic at $2f_D$ is amplified and detected, which can be converted into a field strength with calibration. This gives one component of the magnetic field, so the triaxial fluxgates are arranged orthogonally to return three-dimensional field vectors. The measurement principle is outlined more thoroughly by [Kivelson and Russell \(1995\)](#).

RPC/MAG was used to monitor and assess the evolution of the magnetic field throughout the escort phase and detected evidence of draping around the cometary ionosphere ([Goetz et al., 2017](#); [Volwerk et al., 2019](#)). It was also critical to the detection of a field free region, the diamagnetic cavity, that formed around the nucleus at high outgassing ([Goetz et al., 2016a,b](#), see Section 1.2.2).

MIP

The Mutual Impedance Probe ([Trotignon et al., 2007](#)) was used to assess the density and temperature of electrons at Rosetta. The electron density was determined self-consistently via the electron plasma frequency ($\omega_{pe} = \sqrt{n_e e^2 / m_e \epsilon_0}$), which appeared in the measured impedance spectra as a resonance peak. Further analysis of the spectra can, at times, discern the density and temperature of both warm and cold electron populations ([Gilet et al., 2017, 2020](#); [Wattiaux et al., 2020](#), see Section 1.2.3).

The instrument comprised two transmitting and two receiving antennae, which could be used in two distinct modes: Passive and Active. In passive mode, the transmitters were disabled and the potential difference between the receiving antennae measured. A Fourier transform of the voltage was used to retrieve the plasma frequency.

In active mode, the transmitters swept through frequencies, emitting sinusoidal pulses, and the impedance of the ambient electrons was measured. Within the active mode, measurements were taken in the ‘Short Debye Length’ (SDL) mode or the ‘Long Debye Length’ (LDL) mode. SDL used the receiving antennae of MIP, which were separated from the transmitters by 40 cm. This limited the Debye length ($\lambda_D = \sqrt{\epsilon_0 k_B T_e / n_e e^2}$) to 20 cm ([Trotignon et al., 2007](#)) and was used over a frequency range from 7 kHz to 3.5 MHz. In LDL mode, one of the RPC/LAP probes was utilized as a transmitter, at a distance of 4 m from the MIP receivers. This allowed it to be sensitive to Debye lengths of up to 2 m and was operated over frequencies from 7 kHz to 168 kHz. Between these modes of operation, electron densities from 2 cm^{-3} to $1.5 \times 10^5 \text{ cm}^{-3}$ could theoretically be measured (see Figure 1.2) at a time resolution up to 2.5 s.

While MIP was very reliable in terms of absolute density, it was somewhat limited in the range of densities it could measure, as it usually operated in the SDL mode (lower limit of 200 cm^{-3} for

$T_e = 10$ eV) However, cross-calibration with the plasma density derived from the Langmuir Probe has provided a much more complete set of measurements throughout the mission (Johansson et al., 2021).

A population of cold electrons were observed with RPC/MIP for much of the Rosetta mission from perihelion, all the way through to the end of the mission (Wattiaux et al., 2020; Gilet et al., 2020). The impedance spectra exhibited double peaks, which resulted from the mixture of cold and hot electron populations. These were generally observed in active mode when the transmitters were driving potentials in phase, rather than anti-phase (Gilet et al., 2020). When in anti-phased mode, much flatter impedance spectra were produced by a mixture of cold and hot electrons, preventing the identification of multiple resonance peaks (Wattiaux et al., 2020). This resulted in an asymmetry in the cold electron detections pre vs. post perihelion, as RPC/MIP was usually in anti-phased mode prior to perihelion. Post perihelion, phased mode was generally used, and the cold electron population was frequently identified (Gilet et al., 2020; Wattiaux et al., 2020). RPC/MIP measurements have also been used to examine plasma properties during cavity crossings, where cold electrons were found to be prevalent (Henri et al., 2017; Hajra et al., 2018b).

LAP

The Langmuir Probe (Eriksson et al., 2007) comprised of two spherical probes located at the ends of two 2 m-long booms. LAP measurements were used to calculate a variety of plasma properties including: plasma density, electron temperature, ion flow speed, the spacecraft potential ($V_{S/C}$), and the integrated UV flux. To retrieve these, LAP had two modes of operations: Voltage driven and Current driven. In the first mode, the probe current was measured as the bias potential of the probe swept through values between ± 30 V. In the second mode, a bias current in the range ± 44 nA was applied between the probes and the potential difference measured. The shape of the current response to the applied voltage, and vice versa, contains a wealth of information about the surrounding plasma (see Figure 1.4).

For example, the spacecraft potential can be determined from the photoelectron current. A sunlit probe releases photoelectrons, resulting in a current. When the probe is at a positive potential relative to the plasma, the released photoelectrons are attracted back to the probe, rapidly reducing the current. This feature gives a ‘photoelectron knee’ voltage in the current response, which is related to the spacecraft potential. The measured ‘photoelectron-knee voltage’ has to be corrected to give the spacecraft potential, as the LAP probes do not sit completely outside the influence of the spacecraft (Odelstad et al., 2017).

The spacecraft potential was found to be consistently negative (typically -5V to -20V) from

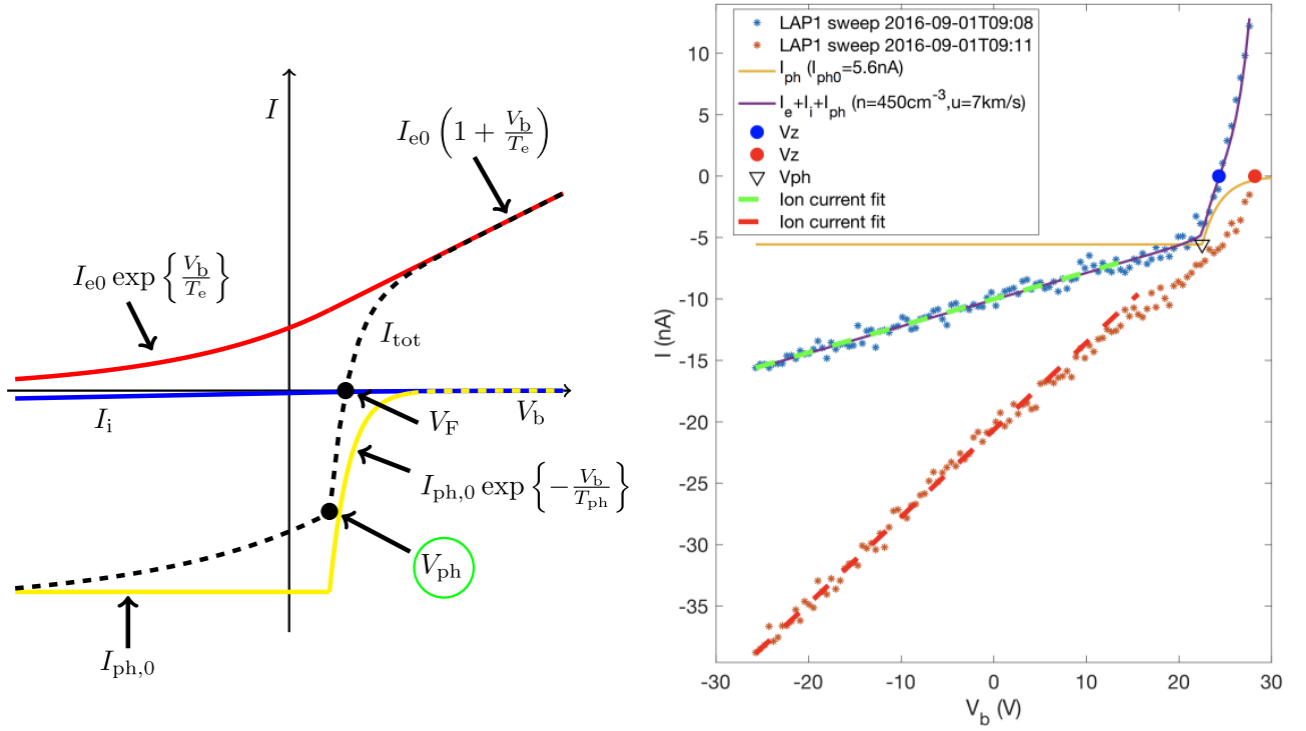


Figure 1.4: (a) Theoretical example of current response to a LAP bias voltage sweep. Credit: Odelstad et al. (2017). (b) Two examples of a LAP bias voltage sweep. Credit: Johansson et al. (2021).

the arrival of Rosetta at 67P until the end of the mission (Odelstad et al., 2015). This was driven by the population of warm electrons (~ 5 -10 eV) continuously observed in the coma (Odelstad et al., 2017). There were times, such as during the excursions, when there were few (energetic) electrons at the spacecraft and the potential reached positive values, but this was uncommon. The spacecraft potential can be used as a measure of the electron density, n_e , using the following relation (Odelstad et al., 2015):

$$n_e = \frac{A}{\sqrt{T_e}} e^{-\frac{|q|V_{S/C}}{k_B T_e}}, \quad (1.1)$$

where A is retrieved from observations and through cross-calibration with RPC/MIP (see Figure 1.5). This relation, alongside the electron temperature, T_e , from MIP when available, allowed measurements of the plasma density over a much larger range (1 to 10^6 cm $^{-3}$) and at higher time resolution than the MIP SDL mode (up to 17 ms, see Figure 1.5; Eriksson et al., 2007; Johansson et al., 2021).

As well as measuring the spacecraft potential and electron density throughout the Rosetta mission, RPC/LAP was also used to identify a cold electron population within the coma of 67P (Eriksson et al., 2017) and their persistent presence within the diamagnetic cavity (Engelhardt et al., 2018). The cross calibration with MIP has also yielded estimates of the ion flow speed (Johansson et al., 2021).

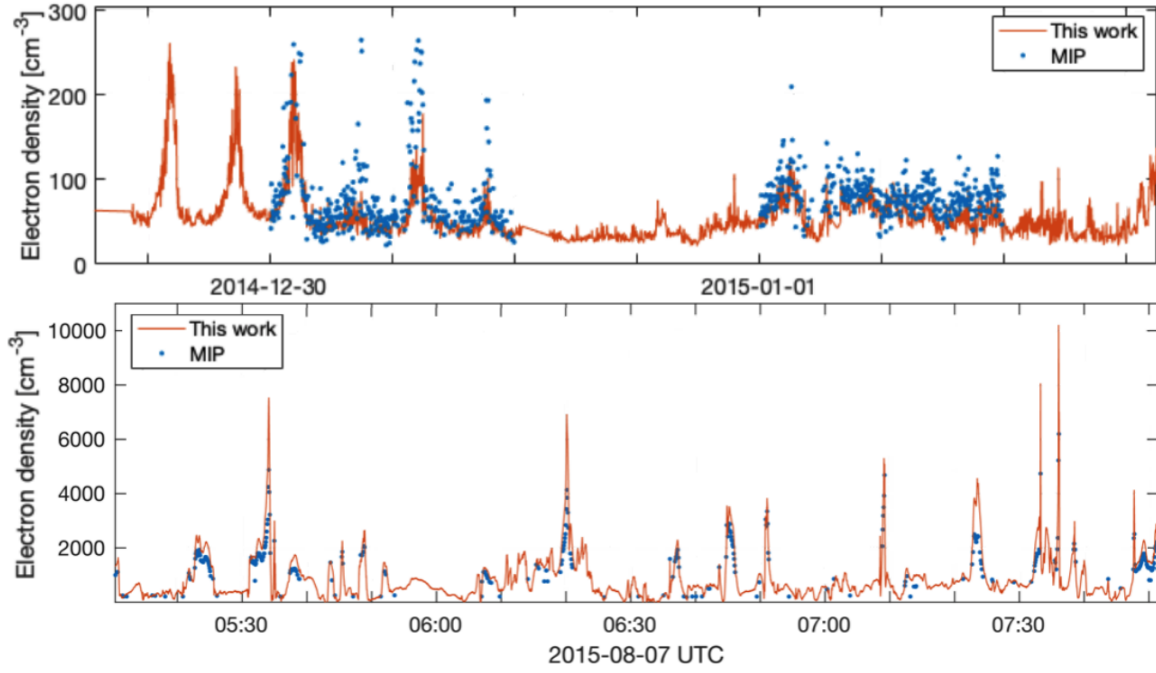


Figure 1.5: Cross calibrated electron densities from RPC/MIP and RPC/LAP over two intervals. Credit: [Johansson et al. \(2021\)](#).

ICA

The Ion Composition Analyser ([Nilsson et al., 2007](#)) measured the 3D distribution of positive ions over a $90^\circ \times 360^\circ$ field of view. ICA could measure ions with energy-charge ratios from 25 eV/e to 40 keV/e, with an angular resolution of $5^\circ \times 22.5^\circ$. The instrument could be biased negatively by 12 V with respect to the spacecraft to accelerate low energy ions into the detector. This, in conjunction with the consistently negative spacecraft potential at ~ -10 V, allowed ICA to detect ions at much lower energies than 25 eV. The spacecraft potential also deflected ions in an energy-dependent way, which perturbed the field of view of each angular bin ([Bergman et al., 2020](#)).

ICA was formed from an angle-selection filter, an electrostatic analyser, a set of magnets and a detector of microchannel plates (MCP). The electrostatic analyser (ESA) uses electric fields between two curved plates to select a specific energy range, with a resolution of $\Delta E/E = 0.07$. If an ion successfully passes through the ESA, it then is deflected by a cylindrical magnetic field. This separates the ions by mass before they reach the MCP. The mass resolution is quite coarse, so can only distinguish between major groups of ions such as those at masses of 1, 2, 4, 8, 16, 32 amu/e ([Nilsson et al., 2015](#)). This allows protons and helium ions to be separated, as well as water group ions and CO_2^+ . ICA has been used to detect and monitor the evolution of the cometary ion populations: both those at low energy and those which have been picked up by the solar wind ([Nilsson et al., 2015, 2017](#)). Moments of the ion distributions show the deflection of the

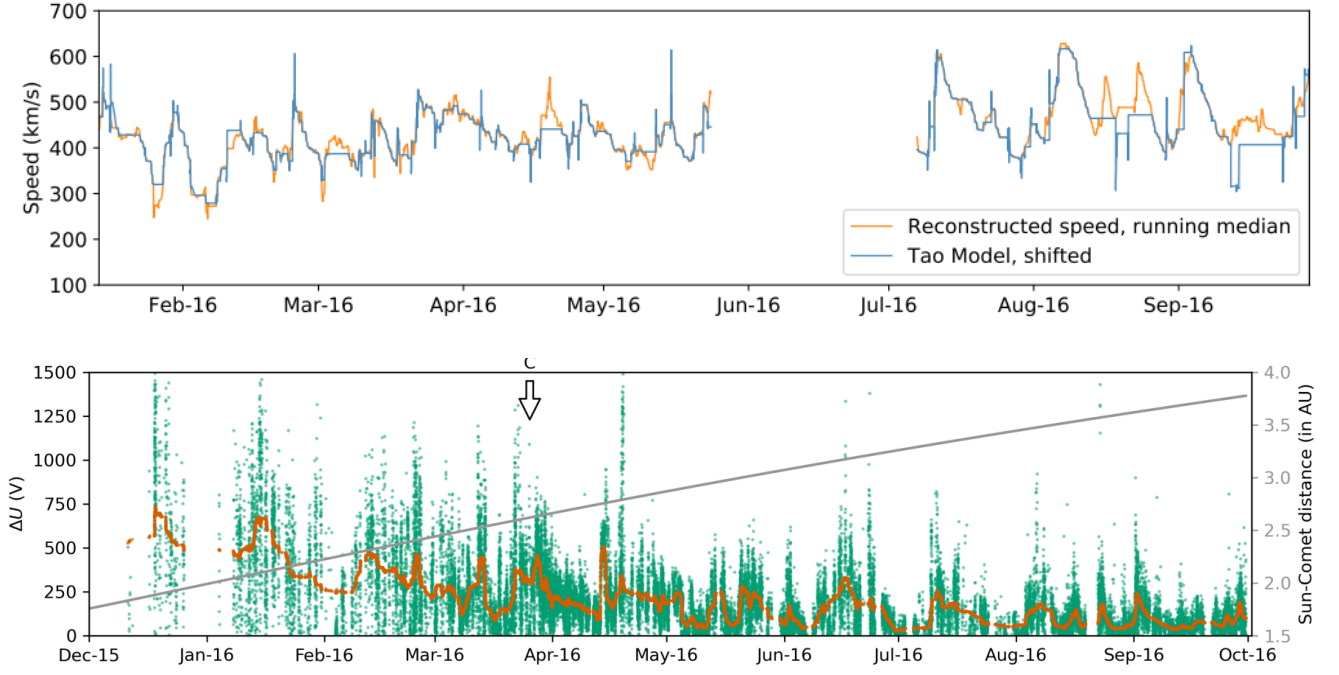


Figure 1.6: (a) Upstream solar wind velocity at 67P, reconstructed from the ICA dataset. (b) Potential difference between the upstream solar wind and Rosetta from ICA. Adapted from Nilsson et al. (2020).

solar wind by the cometary ionosphere (Behar et al., 2016), and give the bulk ion flows in and around the diamagnetic cavity (Bergman et al., 2021). The differences between the solar wind proton and helium ion populations have also been used to reconstruct the upstream solar wind velocity and the potential difference between the solar wind and the spacecraft (see Figure 1.6 Nilsson et al., 2022).

1.1.2 ROSINA

The Rosetta Orbiter Spectrometer for Ion and Neutral Analysis (ROSINA; Balsiger et al., 2007) was made up of three instruments (two mass spectrometers and a pressure sensor) capable of measuring the local gas density and the composition of the neutrals and ions (Balsiger et al., 2007). The neutral Comet Pressure Sensor (COPS) and Double Focusing Mass Spectrometer (DFMS) are described below. The third sensor, the Reflectron Time of Flight Spectrometer (RTOF), was limited by two failures, which occurred during the mission (Gasc et al., 2017b). The capabilities of RTOF were reduced, and hence there is a limited number of publications using its measurements. The instrument has been calibrated and corrected during the different periods of operation (Gasc et al., 2017b) and has been used to measure the composition of the major neutral species in the coma throughout the mission (Hoang et al., 2019).

COPS

The ROSINA Comet Pressure Sensor was made up of two pressure gauges (nude and ram; [Balsiger et al., 2007](#)). These work on the basis of a hot filament ionization gauge ([Redhead, 1966](#)). The neutral gas enters the chamber of the detector, where high energy electrons (150 eV) ionize the gas. The produced ions are then attracted to and detected by the cathode base plate. With calibration, this ion current can be converted into a neutral density. The efficiency of this process depends on the ion species being detected. Therefore, the derived neutral density must be corrected for the gas composition, which is derived from measurements by ROSINA/DFMS. The correction factors for each species are given by [Gasc et al. \(2017a\)](#).

Based on this approach, COPS provided the neutral density throughout the escort phase, from which the local outgassing rate can be estimated ([Hässig et al., 2015](#); [Hansen et al., 2016](#); [Läuter et al., 2018](#)). They observed the increase in outgassing as 67P approached perihelion, and the decrease in activity as it moved towards large heliocentric distances. These measurements revealed the asymmetries in outgassing from the surface, and the sharp increase in outgassing that occurred around perihelion ([Hässig et al., 2015](#); [Hansen et al., 2016](#); [Läuter et al., 2018](#)).

DFMS

The ROSINA Double Focusing Mass Spectrometer ([Balsiger et al., 2007](#)) measured the molecular and isotopic composition of the volatiles, sublimated from near-surface ices. The detector had two settings for the mass resolution and could be operated in either neutral or ion mode. In high resolution (HR) mode, the mass resolution was $m/\Delta m = 3000$ for 1% peak height. DFMS also had a low resolution (LR) mode with $m/\Delta m = 300$, which could retrieve the spectra more quickly (20 s resolution). In HR mode, a spectrum was measured sequentially around each mass unit, so gathering a full composite spectrum from 12 to $150u/q$ could take 50 min.

In neutral mode, electrodes near the entrance aperture were positively biased to repel cometary ions. The neutral gas molecules entered the detector and were then ionized with energetic electrons. For ion mode, the electrodes were not biased (or slightly positively biased depending on the spacecraft potential) allowing ions to enter the detector. The emission of ionizing electrons was not activated in ion mode. From here, the ions, wherever ionization occurred, followed the same path through the instrument. First, they were accelerated by a potential, which was varied depending on the mass of interest. After this, the ions travelled through an electrostatic analyser, after which a slit filtered them to give a $\Delta E/E = 1\%$ energy range. The ions then entered a magnetic sector, where the ions were split by mass before hitting an MCP detector. The dispersion of the masses

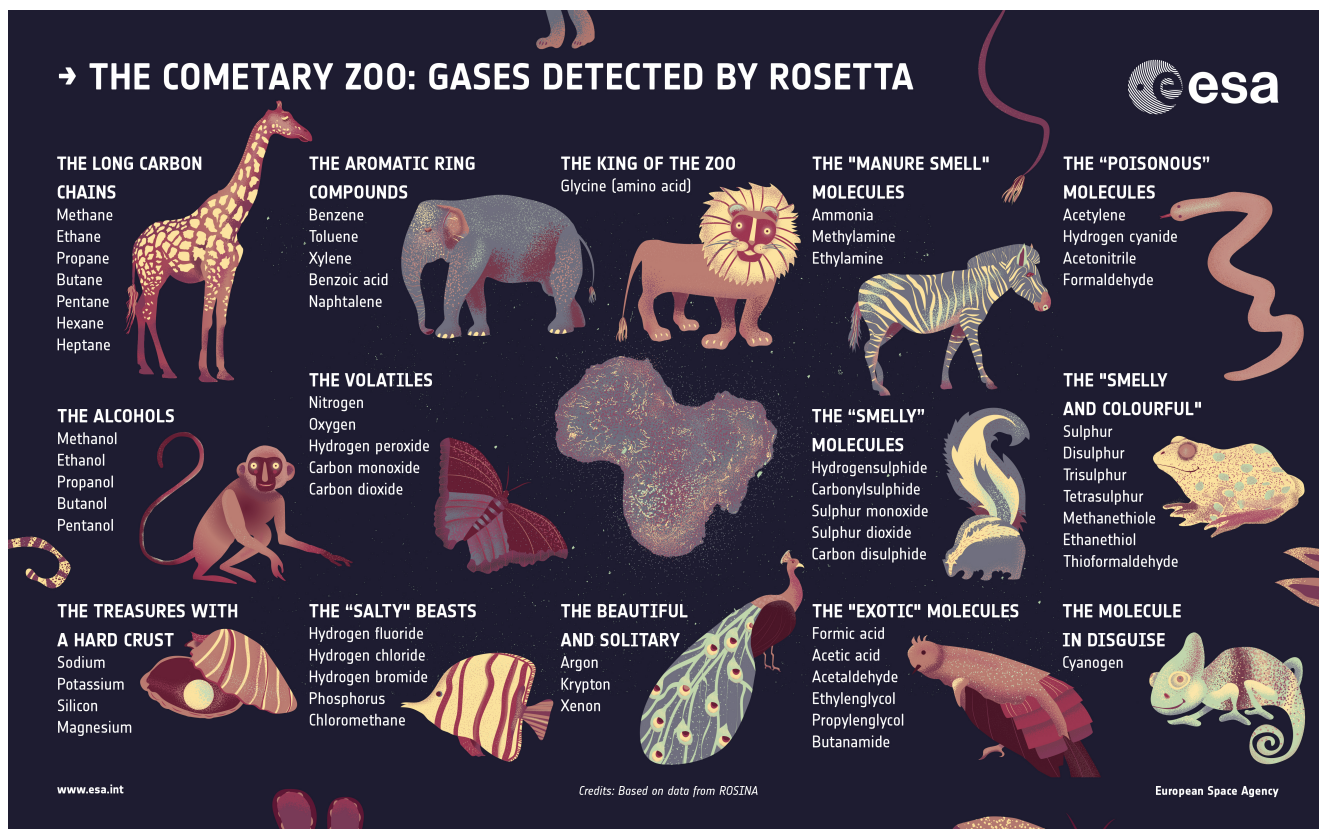


Figure 1.7: The ‘zoo’ of cometary neutrals detected using ROSINA/DFMS at 67P. Credit: [ESA \(2016\)](#).

could be exacerbated by a series of lenses, which were employed in HR mode.

HR was used to distinguish neutrals and ions of very similar mass, such as N_2 and CO isotopes, and was used in the first unambiguous detection of NH_4^+ at a comet ([Fuselier et al., 2015, 2016](#); [Beth et al., 2016](#)). [Heritier et al. \(2017a\)](#) demonstrated the role of chemistry in the coma of 67P, using DFMS ion mode measurements. A full review of the ions present in the coma of 67P is given by [Beth et al. \(2020\)](#), including the discovery of the dication CO_2^{++} . In neutral mode, DFMS has detected a wide variety of volatiles (see [Figure 1.7](#); [Le Roy et al., 2015](#)), including glycine and the first detection of molecular oxygen at a comet ([Bieler et al., 2015a](#); [Altwegg et al., 2016](#)). The hemispherical and seasonal asymmetry in the composition of the coma was observed with DFMS ([Hässig et al., 2015](#); [Gasc et al., 2017a](#)).

1.1.3 Remote sensing instruments

In addition to the in situ measurements taken by RPC ([Section 1.1.1](#)) and ROSINA ([Section 1.1.2](#)), there were a number of instruments that could probe the coma through remote sensing measurements. These instruments operated across different parts of the electromagnetic spectrum. While I only discuss here the three instruments whose data I have exploited in [Chapter 4](#), there were many

used.

Alice performed best when the imaged object was stationary relative to the slit during the period of integration. The integration times were generally 5 or 10 min for each scan, but could be longer. Consecutive spectra can also be co-added to improve the signal-to-noise ratio.

Alice was used to observe emissions from the coma of 67P ([Feldman et al., 2015, 2016, 2018](#); [Noonan et al., 2018, 2021a](#)) and to record the absorption spectrum of the coma during stellar appulses and occultations ([Keeney et al., 2017, 2019](#)). The FUV range of Alice includes many atomic emission lines (e.g., OI, HI, CI, CII) and molecular bands (e.g., CO fourth positive group) produced from neutral species detected at 67P (e.g. H₂O, CO₂, CO...). Analysis of the emissions and atomic line ratios indicated that dissociative excitation by electron-impact (see [Figure 4.1](#)) was a key source of FUV emissions. I have analysed the FUV emission brightnesses quantitatively and thoroughly through a multi-instrument approach applied over the southern hemisphere of 67P (see [Chapter 4](#)).

MIRO

The Microwave Instrument for Rosetta Orbiter (MIRO; [Gulkis et al., 2007](#)) was a mm and sub-mm spectrometer, focusing on two central band frequencies: 190 GHz (1.6 mm) and 562 GHz (0.5 mm). It measured the emissions from the coma over a bandwidth of 180 MHz with 44 kHz resolution.

These two bands allowed MIRO to measure the neutral outflow velocity ([Gulkis et al., 2015](#); [Marshall et al., 2017](#)) and the column density of four species in the coma: H₂O, CO, CH₃OH and NH₃. The frequency resolution was also sufficient to distinguish between the isotopologues of water: H₂¹⁶O, H₂¹⁷O and H₂¹⁸O. The column densities of water were retrieved from analysis of the (110-101) rotational lines of H₂O and H₂¹⁸O at 557 GHz and 548 GHz, respectively. The water isotopologues were particularly useful during high outgassing, as the coma could become optically thick at 557 GHz. CO column densities were similarly retrieved with the (5-4) rotational line at 576 GHz. When viewing the surface of the nucleus, absorption spectra were used to determine the column densities, whereas emission spectra were utilised for limb observations.

The measured column densities were used to derive the production rate and relative abundance of neutral species, including water and CO ([Biver et al., 2015](#); [Lee et al., 2015](#); [Biver et al., 2019](#)). As MIRO was a remote sensing instrument, it gave a better representation of the global outgassing rate as opposed to the in situ measurements from ROSINA (see [1.1.2](#)). It could also probe the day and nightsides of the coma, whereas in situ measurements were restricted by the motion of Rosetta which was typically in the terminator plane.

VIRTIS

The Visual InfraRed Thermal Imaging Spectrometer ([Coradini et al., 2007](#)) on Rosetta had two channels: VIRTIS-M with a high spatial resolution and VIRTIS-H with a high spectral resolution. The two channels operated at similar wavelengths in the infrared and near-infrared ($0.25 - 0.5 \mu\text{m}$ for VIRTIS-M and $1.9 - 5 \mu\text{m}$ for VIRTIS-H) in which rovibrational bands of CO_2 and H_2O were observed ([Fink et al., 2016](#); [Migliorini et al., 2016](#)). The channels M and H had resolutions of $\lambda/\Delta\lambda = 70 - 380$ and $1500 - 3500$, respectively. The cryocooler of VIRTIS-M stopped working in May 2015, so there is no data from this channel after this time ([Bockelée-Morvan et al., 2016](#)).

VIRTIS detected the presence of the following molecules in the coma: H_2O , CO_2 , $^{13}\text{CO}_2$, OCS , CH_4 ; and has been used to measure their column density and relative abundance ([Fink et al., 2016](#); [Bockelée-Morvan et al., 2016](#)). The production rate of each species can subsequently be derived. As with MIRO, VIRTIS gave a more global measurement of outgassing rate than obtained from ROSINA (see [1.1.2](#)).

1.2 Cometary environment

In this section, I introduce our current understanding of the cometary environment after the Rosetta mission. Firstly, I discuss the neutral coma which surrounds the nucleus in [Section 1.2.1](#). In [Section 1.2.2](#), I outline the cometary ionosphere, while [Section 1.2.3](#) focuses on the populations of electrons in the coma and how they form. [Section 1.2.4](#) discusses the interaction of the cometary ionosphere with the solar wind. Finally, in [Section 1.2.5](#), I outline the understanding of FUV emissions from the cometary environment.

1.2.1 Neutral coma

The neutral coma, the gas envelope surrounding a comet, differs greatly from the atmosphere which surrounds a planet, because of the different scale of gravity in the two environments. Whereas the atmosphere of a planet is gravitationally bound to the surface, the coma is constantly flowing away from the nucleus. The escaping gas travels radially at a bulk outflow velocity of $\mathbf{u}_{\text{gas}}$ and must be continuously replenished by further sublimation of near-surface ices in order to maintain the neutral coma. The rate of replenishment is quantified by the outgassing or production rate, Q , which is defined as the total number of gas molecules released from the entire surface per second.

The activity of a cometary nucleus is closely tied to its insolation. This drives variations in outgassing across many timescales. Firstly, outgassing changes periodically with heliocentric

Table 1.1: Neutral molecule loss processes at 67P. r_h is the heliocentric distance in au. Outflow velocity at 67P is typically $\sim 600\text{m s}^{-1}$ (Marshall et al., 2017; Biver et al., 2019), and r is the cometocentric distance.

Process	Loss Frequency [s^{-1}]
Photodissociation of H_2O	$10^{-5}/r_h^2$ (Huebner and Mukherjee, 2015)
Photoionization of H_2O	$10^{-6}/r_h^2$ (Heritier et al., 2018b)
e^- impact dissociation	$< 10^{-6}$ (Feldman et al., 2015)
e^- impact ionization	$< 3 \times 10^{-6}$ (Heritier et al., 2018b)
Transport	$\frac{2u_{gas}}{r}$ (Galand et al., 2016)

distance, r_h , peaking around perihelion (Bondarenko and Medvedev, 2011, although maybe slightly offset) before receding as the comet moves into the outer Solar System (Hansen et al., 2016; Marshall et al., 2017, 2019). At comet 67P, neutral gas was almost exclusively produced from ices at, or near, the surface of the nucleus (Biver et al., 2019). There is evidence of some wet grains in the coma (De Keyser et al., 2017), which leads to sublimation of gas higher in the coma. However, the contribution of these grains to the total outgassing was very limited (Biver et al., 2019). As the flux of outflowing gas is conserved, the neutral density falls as $1/r^2$ with cometocentric distance, r (Haser, 1957). For a spherically symmetric coma, the density of the neutral gas is

$$n(r) = \frac{Q}{4\pi r^2 u_{gas}} \exp \left[-\frac{(r - r_c)k_p}{u_{gas}} \right], \quad (1.2)$$

where u_{gas} is the bulk outflow speed of the neutral gas and k_p is the destruction rate of the neutral species (through e.g., dissociation and ionization). In the regions of 67P probed by Rosetta, the dominant loss mechanism for neutrals was transport (see Table 1.1), so the exponential term in Eq. 1.2 can be neglected.

Over the Rosetta escort phase, comet 67P covered heliocentric distances from 1.24 au to 3.8 au and the production varied by over three orders of magnitude (Hansen et al., 2016; Biver et al., 2019). Close to perihelion, the production rate at 67P peaked at $Q = 4 \times 10^{28} \text{ s}^{-1}$ (see Figure 1.9), but towards the start and end of the Rosetta escort phase the outgassing was far weaker. The beginning of the escort phase at 3.6 au saw outgassing rates less than 10^{26} s^{-1} , with similarly low rates observed in the final stages of the mission at 3.8 au.

The activity levels observed at 67P were generally much smaller than those experienced during the previous cometary missions (see Figure 1.10). The production rate of 1P/Halley reached $Q = 10^{30} \text{ s}^{-1}$ during the numerous flybys in 1986 by Giotto (at 0.89 au), the VEGA spacecraft, Suisei and Sakigake (Gringauz et al., 1986; Krankowsky et al., 1986). The flybys of

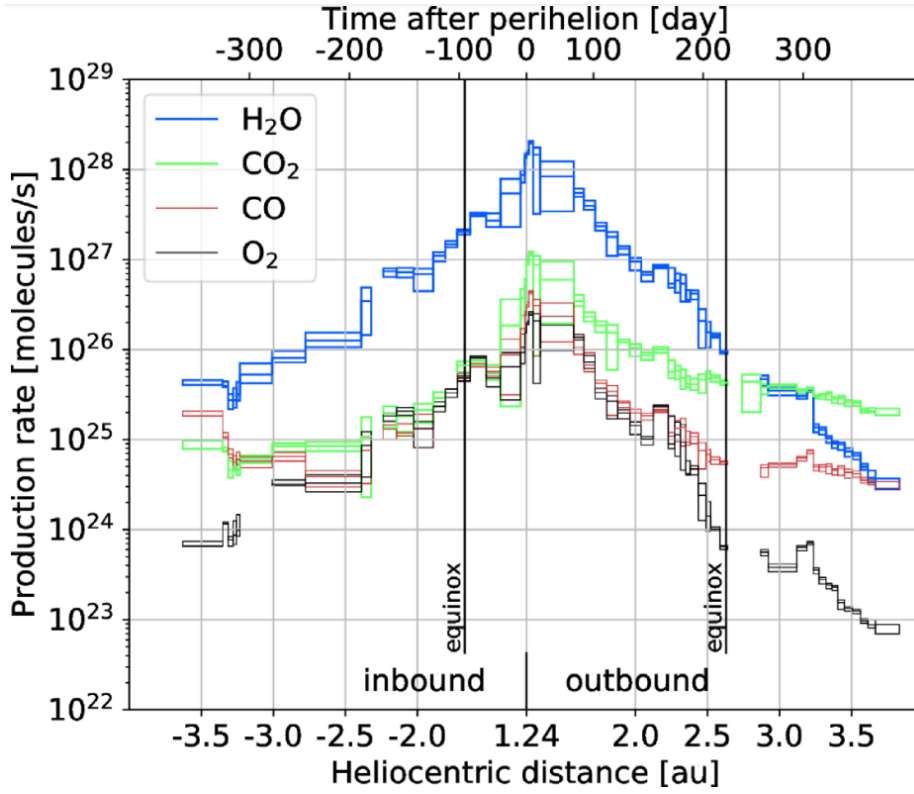


Figure 1.9: Evolution of the local outgassing rate throughout the Rosetta mission for the major species in the coma of 67P: (blue) H_2O , (green) CO_2 , (red) CO and (black) O_2 . Credit: [Läuter et al. \(2018\)](#).

19P/Borelly, 21P/Giacobini-Zinner and 26P/Grigg-Skjellerup by Deep Space 1, ICE and Giotto, respectively, were more similar to the outgassing conditions of 67P when close to perihelion sitting at $Q = 3 \times 10^{28} \text{ s}^{-1}$ ($7 \times 10^{27} \text{ s}^{-1}$ for GS; see Figure 1.10; [Cowley et al., 1987](#); [Richter et al., 2011](#); [Johnstone et al., 1993](#)). The activity of all these comets were dwarfed by the Oort cloud comet, Hale-Bopp (C/1995 O1), which reached peak outgassing of 10^{31} s^{-1} at 0.9 au. The extended escort phase by Rosetta allowed 67P to be observed across a wide range of activity levels and for different levels of collisionality in the coma. The low outgassing levels at 67P seen during long periods of the Rosetta mission led to a less dense, and less collisional coma, than had been probed in any previous cometary missions (see Figure 1.10).

In addition to the long term outgassing trends with heliocentric distance, the insolation of the nucleus resulted in outgassing asymmetries and shorter term fluctuations. While the global production rates are indicative of the wider level of cometary activity, the local outgassing rate varied substantially across the nucleus of 67P ([Hässig et al., 2015](#); [Hansen et al., 2016](#); [Läuter et al., 2018](#)). Typically, local outgassing was stronger near the subsolar point (derived through extrapolation), but the maximum in outgassing was offset by up to 50° ([Hansen et al., 2016](#)). Early in the mission, the northern hemisphere was more strongly outgassing, but the reverse was true post-equinox.

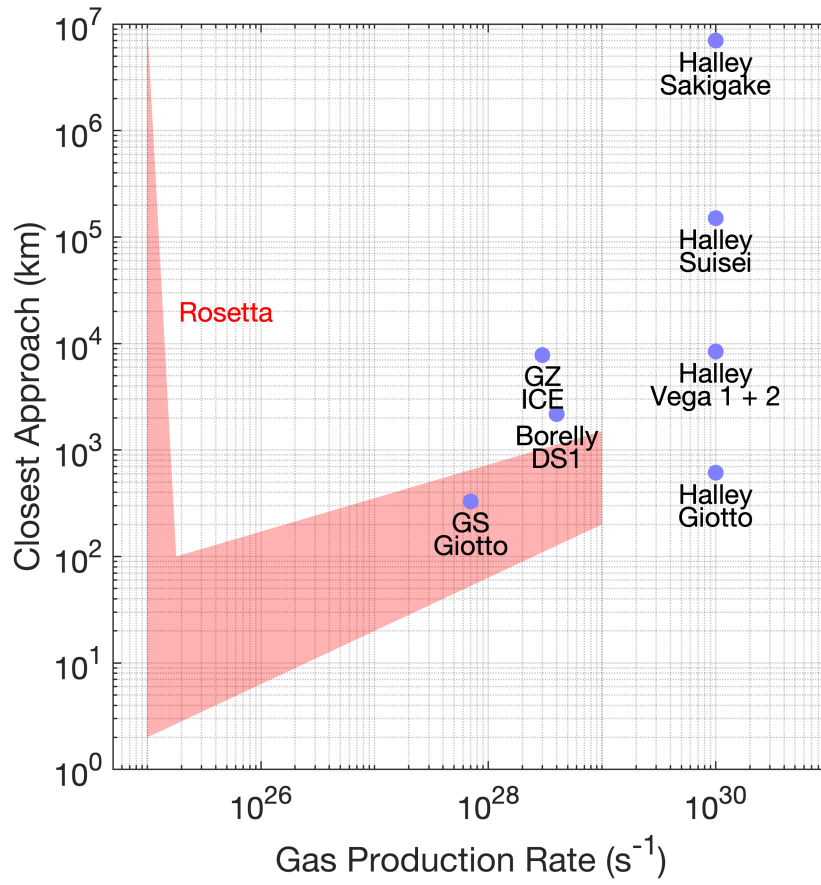


Figure 1.10: Gas production rate and closest approach distance of previous cometary flyby missions. The red shaded area covers the regions probed by the Rosetta mission. GS - Grigg-Skjellerup. GZ - 21P/Giacobini-Zinner. DS1 - Deep Space 1. Credit: [Goetz et al. \(subm\)](#).

The local outgassing from 67P exhibited diurnal fluctuations with a period of 12 hours (Hässig et al., 2015; Lee et al., 2015). The illuminated surface area of the nucleus varied as it rotated, driving the 12 hour periodicity (Bieler et al., 2015b). Longer term seasonal changes in the outgassing of water were also linked to the surface illumination (Bieler et al., 2015b; Fougere et al., 2016a; Marshall et al., 2017).

Beside the local outgassing rate, the neutral density is heavily dependent on the gas outflow speed. Measurements with MIRO (see Section 1.1.3) showed that the outflow velocity decreased with increasing heliocentric distance from 900 m s^{-1} close to perihelion to $\sim 600 \text{ m s}^{-1}$ at 3au (Gulkis et al., 2015; Lee et al., 2015; Marshall et al., 2017; Biver et al., 2019). The neutral gas undergoes some acceleration within the first few km of the nucleus (Heritier et al., 2017a; Marschall et al., 2016), before reaching these terminal and supersonic velocities.

The major neutral species in the coma of 67P were H_2O , CO_2 , CO and O_2 (Bieler et al., 2015a; Mall et al., 2016; Gasc et al., 2017a) but many more have been identified, including the discovery of glycine at a comet (Altwegg et al., 2016). Le Roy et al. (2015) give a more complete list of the observed neutrals at 67P, while Bockelée-Morvan (2011) reviews the composition of comets observed prior to Rosetta. Throughout the Rosetta escort phase, the composition of the outgassed neutrals varied significantly with time, heliocentric distance and latitude (Hässig et al., 2015; Gasc et al., 2017a). Molecular oxygen had not been detected in the cometary environment before Rosetta’s arrival at 67P (Bieler et al., 2015a; Bockelée-Morvan, 2011). However, it was found to be a substantial component of 67P’s coma, reaching mixing ratios up to 10% (Bieler et al., 2015a). Analysis of FUV emissions at Rosetta indicated enhanced O_2 mixing ratios during outbursts, reaching up to 50% relative to water (Keeney et al., 2017, 2019; Noonan et al., 2021b), although such high mixing ratios have not been measured in situ by ROSINA. Many of the minor neutral species are well correlated with the outgassing of either water (e.g. O_2) or CO_2 (e.g. CO and CH_4), suggesting these less abundant species are embedded within water and CO_2 ices (Gasc et al., 2017a).

The composition of the northern and southern hemispheres of 67P were significantly different. In the northern hemisphere, H_2O dominated from the start of the escort phase until 2.5 au post-perihelion, after which it was comparable to the outgassing of CO_2 (Hässig et al., 2015; Läuter et al., 2018). There was an increased abundance of CO_2 , and to a smaller extent CO, in the southern hemisphere at large heliocentric distances (Fougere et al., 2016a; Biver et al., 2019; Läuter et al., 2018), reflecting some inhomogeneity in the nuclear surface. Near perihelion, H_2O was still the dominant species in the southern hemisphere (Heritier et al., 2017a; Läuter et al., 2018). The distinction between the two hemispheres may originate from the contrasting seasons they undergo.

The northern hemisphere summer is a long and mild season around aphelion, leading to little sublimation or surface erosion. Conversely, the southern summer occurs around perihelion. It is a short and intense season, causing substantial erosion of the surface and exposing pristine layers of the nucleus during the Rosetta mission (Keller et al., 2017; Fink et al., 2016; Filacchione et al., 2016).

1.2.2 Cometary ionosphere

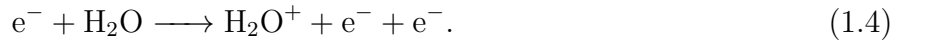
Within the coma, neutral molecules can be ionized, generating populations of cometary electrons and ions. Ionization can be through a number of methods: photoionization, electron-impact or solar wind ion impact. Solar wind charge exchange is also a source and loss mechanism for an ion species, but has no net impact on the plasma density. Photoionization and electron-impact ionization are typically the major sources of ionization.

Photoionization is driven by high energy solar photons in the Extreme UltraViolet (EUV) (Mendis et al., 1985b; Cravens, 1991; Galand et al., 2016; Heritier et al., 2018a) e.g. :



The electrons produced by photoionization inherit almost all the excess energy of the photon, due to their low mass compared to the cometary ion. Photons with wavelengths in the range 0.1 – 100 nm exceed the ionization threshold energy, E_{Th} , of the molecules in the coma (typically 12-15 eV, see Table 1.2) and have a probability of causing ionization. The minimum threshold energy for the major species at 67P (12.07 eV for O_2) corresponds to a wavelength of 102.7 nm, so any longer wavelength photons cannot induce ionization. Photoelectrons have typical energies around 10 eV, though their energy can reach large values (~ 100 eV).

Neutral molecules can also be ionized by the impact of energetic electrons in the coma, which also must have energies exceeding the ionization threshold of a gas molecule e.g.,



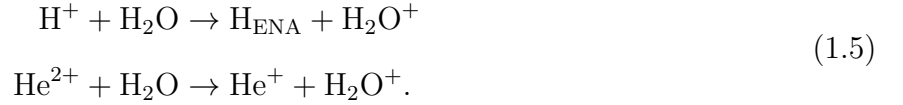
Whereas a photon is wholly absorbed during photoionization, the incident energetic electron retains some energy after an ionization and may cause further ionization in the coma. The electron does become degraded, as it must supply the threshold energy to ionize the neutral (see Table 1.2) as well as sharing some energy with the new secondary electron (Miller et al., 1985; Lummerzheim and Lilensten, 1994).

Table 1.2: ionization threshold energies of the major neutral species at 67P.

Species	Threshold Energy, E_{Th} [eV]	Threshold Wavelength, λ_{Th} [nm]
H ₂ O	12.6	98 (Vigren and Galand, 2013; Itikawa, 2002)
CO ₂	13.77	90 (Cui et al., 2011; Itikawa, 2002)
CO	14.0	90 (Fox, 2011; Vigren and Galand, 2013)
O ₂	12.07	102.7 (Samson and Cairns, 1966)

Solar wind ions can also generate secondary electrons through impact ionization, similarly to electron collisions, but this was only a very minor process at comet 67P (Simon Wedlund et al., 2019a, see Section 5.1.2).

Cometary ions are also produced through charge exchange of solar wind ions with the neutral coma. Solar wind ions ($\sim 92\%$ H⁺ and 8% He²⁺) colliding with neutrals in the coma transfer charge, generating a new, low-energy, cometary ion. The solar wind particle retains the bulk of the energy in the interaction, and may become a differently charged ion or an energetic neutral atom (ENA, ~ 1 keV). In solar wind charge exchange with water, two of the reactions that may take place are:



While charge exchange is an important source of cometary ions within the coma (Simon Wedlund et al., 2019a), these processes do not produce electrons and therefore have no net impact on the total plasma density. Although it does not generate cometary electrons, emission of soft X-Rays in the cometary environment has been attributed to charge exchange reactions between heavy solar wind ions (e.g., O⁶⁺) and cometary neutrals (Lisse et al., 1996; Lisse et al., 1997; Wegmann et al., 1998; Dennerl, 2010).

Electron-impact on cometary neutrals was an important source of ionization at Halley during the Giotto flyby at 0.89 au (Cravens et al., 1987; Boice et al., 1986; Körösmezey et al., 1987). Outside the bow shock (see Section 1.2.4), photoionization was the primary source of cometary electrons; but closer to the nucleus, electron-impact ionization had a substantial contribution to the ionization frequency. The electrons in the undisturbed solar wind are usually not energetic enough to cause significant ionization. However, once heated by the bow shock, electrons were sufficiently energized to give ionization frequencies comparable to the photoionization frequency (Cravens et al., 1987). Models of the energetic auroral electrons and photoelectrons in the coma of Halley indicated electron-impact ionization was the major source of electrons in the inner coma (Bhardwaj et al., 1996; Bhardwaj, 2003). At highly outgassing comets, like Halley, solar flux is

largely absorbed high in the coma, so only high energy photons can penetrate into the inner coma. These high energy photons produce energetic secondary electrons (~ 100 eV), which can cause multiple ionizations and lead to a large ionization frequency.

At comet 67P, electron-neutral collisions were found to be a key source of ionization within the coma (Galand et al., 2016; Heritier et al., 2017b, 2018b) when far from perihelion. Electron-impact was at times more efficient than photoionization (Heritier et al., 2018b), and was prevalent down to the surface of the nucleus (Heritier et al., 2017b). The origin of these energetic, ionizing electrons is not well understood at comet 67P. Potential processes, at least away from perihelion, are reviewed in Section 1.2.3. Hajra et al. (2020) compared the total electron content (the electron density integrated radially over cometocentric distance) to the photoionization rate from solar flux. They found that the correlation between the electron density and photoionization frequency was best at low heliocentric distances ($1.5 < r_h < 2$ au), but much weaker when 67P was far from perihelion. This poor correlation when far from the Sun may be caused by a strong contribution from electron-impact ionization (see Chapter 5; Heritier et al., 2017b, 2018b). However, the strength of electron impact ionization has not been assessed across the whole Rosetta mission. **This is one of the focuses of my thesis.**

The production of electrons and ions by ionization within the coma are balanced by various loss processes. For electrons, these are transport and electron-ion recombination, which vary in relative importance depending on the activity of the comet and the cometocentric distance (Gombosi, 2015; Galand et al., 2016; Beth et al., 2019a). For a given ion species, additional loss processes include chemistry and charge exchange (Heritier et al., 2017a; Simon Wedlund et al., 2019b), which produce different ions but do not cause a net change in the plasma density.

The production, source and loss of each species, j , are encapsulated by the continuity equation

$$\frac{\partial n_j}{\partial t} + \nabla \cdot (n_j \mathbf{u}_j) = P_j - L_j, \quad (1.6)$$

where n_j is the number density of the species and $\mathbf{u}_j$ its bulk velocity. P_j and L_j are its production and chemical loss rates, incorporating all the ionization mechanisms, electron-ion recombination and ion-neutral reactions.

At both 1P/Halley and comet 67P, the ion density profiles were shown to follow a $1/r$ dependence with cometocentric distance, r (Balsiger et al., 1986; Galand et al., 2016; Heritier et al., 2017b). At Halley, the r^{-1} dependence between 600 km and 4800 km was attributed to a combination of photoionization and electron-ion recombination (Cravens, 1987; Gombosi et al., 1996). The neutral coma of Halley was very dense during the 1986 flybys, so the inner coma was in photochemical

equilibrium. This is when the production and chemical loss rates for an ion species are balanced locally, and both occur at a much faster rate (smaller timescale) than any transport of the species. This was valid in the inner coma of Halley (Cravens, 1987), but was not the case at the more weakly outgassing 67P.

When 67P was far from perihelion, the lower production rate and neutral density led to less frequent collisions, reducing the rate at which electrons and ions recombined. Instead, the ions existed for long enough without a potential recombination that they were instead transported effectively away from the nucleus (Gombosi, 2015; Galand et al., 2016; Beth et al., 2019a). In this scenario, the resulting ion density follows $1/r$ at large cometocentric distances. When transport dominates over chemical loss, the plasma density is given by

$$n_i(r) = \frac{Q\nu^{ioni}}{4\pi u_{gas}u_{ion}} \frac{r - r_c}{r^2} \quad (1.7)$$

given a constant ionization frequency, ν^{ioni} , throughout the coma and a plasma bulk outflow speed, u_{ion} (Galand et al., 2016; Heritier et al., 2017b). The plasma density deviates from the $1/r$ dependence at low cometocentric distances, because of the finite size of the nucleus (radius r_c). The cometary plasma density is an accumulation of the ionization over many layers of the coma. Close to the nucleus, few layers have contributed to this total plasma production, which causes a peak in the electron density at $r = 2r_c$ (Galand et al., 2016; Heritier et al., 2017b). This predicted peak was observed for the first time in the final descent of Rosetta to the surface of the comet in September 2016 (Heritier et al., 2017b).

As water makes up the overall bulk of the cometary neutrals at 67P (Rubin et al., 2015; Bockelée-Morvan et al., 2016; Biver et al., 2019), many of the major cometary ions are water based. However, chemistry can have a major impact on the ion composition in dense comae. In a pure water coma, the primary ion produced within the coma is H_2O^+ (Ip and Mendis, 1976; Heritier et al., 2017a), but this is quickly converted to H_3O^+ via proton transfer. In dense regions of the coma, H_3O^+ is dominant over H_2O^+ as protonation occurs on short timescales (Heritier et al., 2017a), but farther from the nucleus H_2O^+ prevails (up to a region where the coma is photodissociated). At large distances, collisions are rare and chemistry is inefficient.

When the coma is more varied, including many neutral species, the chemistry within the coma can become highly complex. A huge variety of ions have been discerned in the comae of Halley (Balsiger et al., 1986; Eberhardt et al., 1994; Geiss et al., 1991; Marconi et al., 1990) and 67P (Fuselier et al., 2016; Beth et al., 2016, 2018), through a combination of measurements and ionospheric models. Sophisticated chemistry models help the interpretation of ion spectra with

low mass resolution from IMS on Giotto (Haider and Bhardwaj, 2005; Rubin et al., 2009) and ROSINA/DFMS on Rosetta (Fuselier et al., 2015, 2016; Beth et al., 2016; Heritier et al., 2017a) and help in assessing the origin of the ions. Neutrals with high proton affinity, such as NH_3 , can become the dominant ions (NH_4^+) in the coma (Beth et al., 2016; Heritier et al., 2017a), despite being minor neutral species ($< 1\%$; Hässig et al., 2015; Le Roy et al., 2015). While the ionosphere of 67P was chemically vibrant around perihelion, the complexity of the ion population was greatly reduced at large heliocentric distances (Heritier et al., 2017a). At low activity, the weakly collisional coma of 67P limited the number of reactions that could take place before ions left the cometary environment.

1.2.3 Electron populations at a comet

After the flotilla of cometary missions in 1986, the understanding of the electron populations at highly outgassing comets greatly advanced. Electron properties were examined across many regions of the coma with Giotto (Rème et al., 1986), and electron spectra were retrieved during the VEGA-2 flyby of Halley (Gringauz et al., 1986). During flybys of highly outgassing comets like Halley and 21P/Giacobini-Zinner, several distinct electron populations were observed (Meyer-Vernet et al., 1986; Zwickl et al., 1986; Bame et al., 1986). These are distinguished as a **cold** (< 1 eV), a **warm** ($10 \sim 15$ eV) and a **hot** ($\gtrsim 20$ eV) population of electrons. Similar populations have also been observed at 67P despite much weaker outgassing conditions (Clark et al., 2015; Broiles et al., 2016b; Eriksson et al., 2017; Engelhardt et al., 2018; Gilet, 2019; Gilet et al., 2020). The warm and hot populations are variably defined in the literature, but the above energy ranges are used throughout this thesis.

The warm and hot populations of electrons are often collectively referred to as the **suprathermal electrons**, as they are not thermalised in the coma of 67P (Clark et al., 2015; Broiles et al., 2016b,a; Myllys et al., 2019). The suprathermal electrons are better described using two kappa distributions rather than a Maxwellian (Pierrard and Lazar, 2010). However, even the kappa distributions do not fit the electron spectra retrieved by RPC/IES on many occasions. They are more applicable close to the perihelion of 67P, but at large heliocentric distances $\sim 80\%$ of electron spectra could not be fit using kappa distributions (Myllys et al., 2019).

The **warm electron population** is made up of newly-born cometary electrons, produced either through photoionization or by electron-impact at around 10 eV (Galand et al., 2016; Heritier et al., 2018b). These newly-born electrons are ubiquitous in the coma (Odelstad et al., 2017; Gilet, 2019) but the size and properties of this population are highly variable (Heritier et al.,

2018b; Myllys et al., 2019). Warm electrons make up the bulk of the electrons at large heliocentric distances at Rosetta (Gilet, 2019), reaching densities up to 1000 cm^{-3} (Myllys et al., 2019). This greatly exceeds the density of the solar wind, so the warm population must be largely of cometary origin (Madanian et al., 2016b).

Warm electrons have much higher speeds and pressures than ions in the inner coma, due to their much smaller mass. In the absence of fields, the electron pressure would quickly drive electrons out of the inner coma, leaving a charge imbalance. As quasi-neutrality must be satisfied ($n_e \approx n_i$), an electric field arises which opposes the charge separation, which is known as an ambipolar, or polarisation, electric field. The charge separation occurs approximately radially away from the nucleus, generating a roughly spherical potential well. Three-dimensional kinetic simulations of the cometary environment confirm that such an ambipolar field forms a potential well around the nucleus of a weakly outgassing comet (Deca et al., 2017; Divin et al., 2020).

The ambipolar field is one of the terms in the Generalised Ohm's Law (GOL, Eq. 1.8), which is derived from the electron and ion momentum equations. Typically, the largest component of the electric field is the motional field. This is associated with the reference frame of the plasma flow, which the magnetic field is frozen into. When ions decouple from the magnetic field, currents in the plasma drive a Hall electric field. The Ohmic term is associated with collisional processes, which can be approximated through a resistivity, η . Collisions are infrequent at a weakly outgassing comet, so the Ohmic term is small. The electron inertial term is usually smaller than the others and is often neglected. The contributions of these terms at a weakly outgassing comet are separated by Deca et al. (2019).

$$\mathbf{E} = \underbrace{-\mathbf{u} \times \mathbf{B}}_{\text{Motional Field}} + \underbrace{\frac{1}{n_e e} \mathbf{J} \times \mathbf{B}}_{\text{Hall Field}} - \underbrace{\frac{1}{n_e e} \nabla p_e}_{\text{Ambipolar Field}} + \underbrace{\eta \mathbf{J}}_{\text{Ohmic Term}} + \underbrace{\frac{m_e}{n_e e^2} \left\{ \frac{\partial \mathbf{J}}{\partial t} + \nabla \cdot [\mathbf{J} \mathbf{u} + \mathbf{u} \mathbf{J}] \right\}}_{\text{Electron Inertia}} \quad (1.8)$$

The **hot electron population** ($\gtrsim 20 \text{ eV}$) is responsible for electron-impact ionization in the coma. At Halley and GZ, there was a weak bow shock upstream of the comet (Mach no., $M \sim 2$), which led to heating of the electrons downstream of the shock (Rème et al., 1986; Thomsen et al., 1986; Gan and Cravens, 1990), forming part of the hot population. In the artificial comet of the AMPTE mission (Hall et al., 1986; Bingham et al., 1988) and at comet Hyakutake, hot electrons were accelerated by wave particle interactions, heating electrons up to $\sim 100 \text{ eV}$ (Shapiro et al., 1999).

Within the coma of 67P, the hot electrons are likely of solar wind origin (Broiles et al., 2016b;

Myllys et al., 2019). Broiles et al. (2016b) suggested that this ~ 40 eV population, with density $n_e = 0.01 \text{ cm}^{-3}$, was made up of solar wind halo electrons. Myllys et al. (2019) revised up the density of the hot population ($n_e = 0.1 - 100 \text{ cm}^{-3}$) and suggested that they were instead the bulk solar wind electrons that had undergone acceleration in the cometary environment, likely driven by the ambipolar field. Kinetic simulations show that this potential well reaches 60 eV for an outgassing rate of $Q = 10^{25} \text{ s}^{-1}$ (Deca et al., 2017; Divin et al., 2020). Nilsson et al. (2022) used solar wind ion properties to reconstruct the potential difference between the upstream solar wind and the Rosetta spacecraft, finding voltages of several hundred electron volts throughout 2016 (see Figure 1.6).

Goldstein et al. (2019) demonstrated that lower hybrid waves were, at times, responsible for the acceleration of electrons to energies in excess of 1 keV at Rosetta, forming a superhot population. Electrons with similar energies were measured during the VEGA flyby of Halley, but not by Giotto (Gringauz et al., 1988). These waves are driven by the two stream-instability between solar wind and cometary ions (Shapiro et al., 1999; Goldstein et al., 2019), and have been observed at other times at Rosetta without the accompanying energetic electrons (André et al., 2017). The relative importance of such wave particle interactions towards energizing, compared to global acceleration processes, the wider electron population is not well established. Analysis of far-ultraviolet aurorae in the northern hemisphere of 67P indicates that the suprathermal electrons are accelerated by more global processes, rather than locally (Galand et al., 2020). **I aim to identify the key heating processes at 67P in this thesis.**

A **cold electron population** is formed by cooling the warm, newly-born electrons through collisions with the neutral gas at 0.01 eV (Cravens, 1987; Gan and Cravens, 1990; Gulkis et al., 2015). At high outgassing rates ($Q = 10^{28} - 10^{30} \text{ s}^{-1}$), cold electrons were prevalent close to the nucleus (Meyer-Vernet et al., 1986). Modelling of these environments demonstrated that the electrons were cooled by collisions with the neutral gas (Gan and Cravens, 1990; Körösmezey et al., 1987; Cravens and Korosmezey, 1986).

At 67P, the cold electron population (< 1 eV, Figure 1.11) was expected around perihelion, when outgassing was at its highest. However, cold electrons were also observed near the start and end of the Rosetta mission (see Figure 1.11; Eriksson et al., 2017; Engelhardt et al., 2018; Gilet et al., 2020; Wattieaux et al., 2020), when the outgassing rate was 2-3 orders of magnitude smaller than the peak production (Läuter et al., 2018; Biver et al., 2019).

The diamagnetic cavity (a magnetic field-free region around that can form around the nucleus) is closely tied to the cold and energetic electron populations. The cavity boundary was shown to be closely related to the electron exobase (Henri et al., 2017) and 96% of cavity crossings

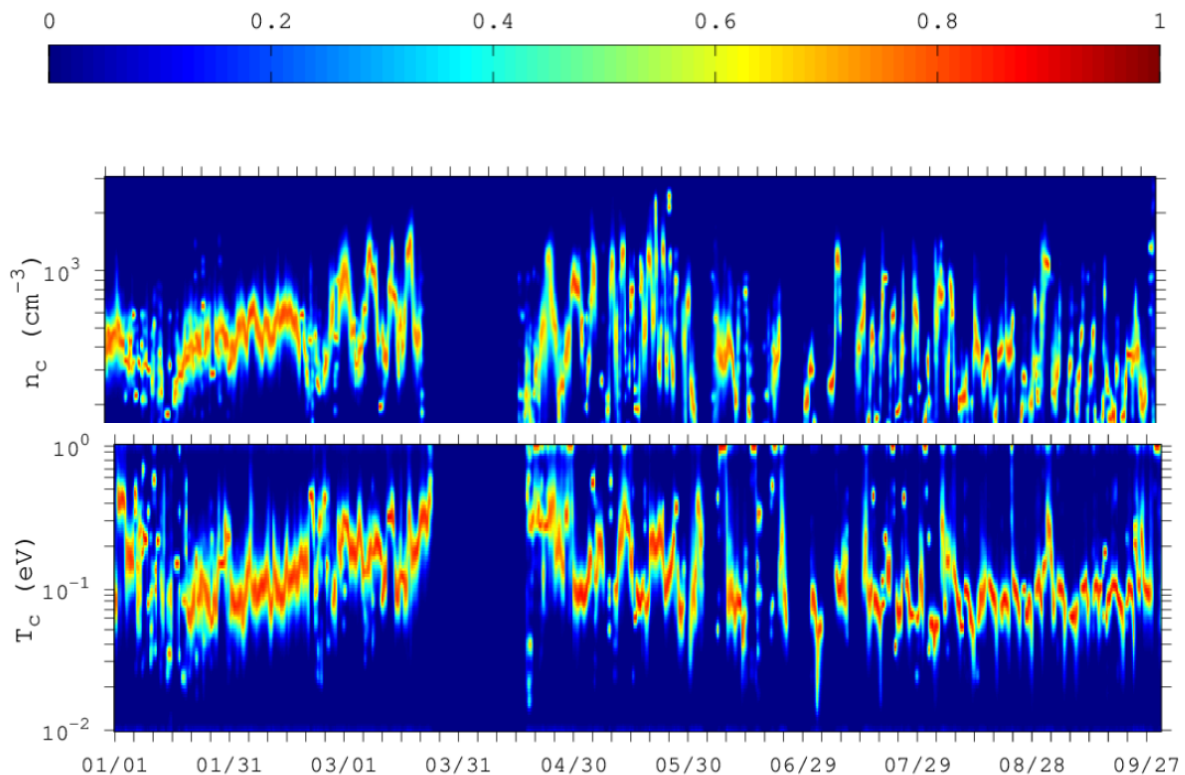


Figure 1.11: (top) Density and (bottom) temperature of the cold electron population at Rosetta retrieved using RPC/MIP throughout 2016. Adapted from [Wattieaux et al. \(2020\)](#).

contained cold electrons ([Odelstad et al., 2018](#)). The cavity was also depleted of suprathermal electrons, suggesting that suprathermal electrons are strongly driven by or originate in the solar wind ([Nemeth et al., 2016](#); [Madanian et al., 2020](#)).

The **electron exobase** bounds the region in which electrons are collisionally coupled to the neutral gas. Assuming the electrons flow radially away from the nucleus, this can be defined where the scale height of the neutral gas ($H = [\frac{1}{n_n} \frac{dn_n}{dr}]^{-1} = r$) equals the mean free path of an electron $\lambda = [n_n \sigma_{\text{mom}}]^{-1}$, where σ_{mom} is the electron-neutral momentum transfer cross section ([Mandt et al., 2016](#); [Eriksson et al., 2017](#); [Engelhardt et al., 2018](#)). If the derived exobase sits below the surface of the nucleus, there should be no region of the coma where electrons are collisional, and a cold electron population would not form. Under this radial outflow assumption, a cold population could only form for outgassing rates $Q \geq 5 \times 10^{26} \text{ s}^{-1}$, which correspond to heliocentric distances of $< 2.3 \text{ au}$ for 67P ([Engelhardt et al., 2018](#)). However, cold electrons were regularly observed at 67P at much larger heliocentric distances ($> 3 \text{ au}$), near the start and end of the escort phase ([Engelhardt et al., 2018](#); [Wattieaux et al., 2020](#); [Gilet et al., 2020](#)). At all heliocentric distances, Rosetta was very rarely close to the electron exobase and frequently observed cold electrons at cometocentric distances 10-100 times larger than the exobase (see Figure 1.12; [Engelhardt et al., 2018](#); [Gilet et al., 2020](#)). Consequently, the picture of radially outflowing electrons, which collide

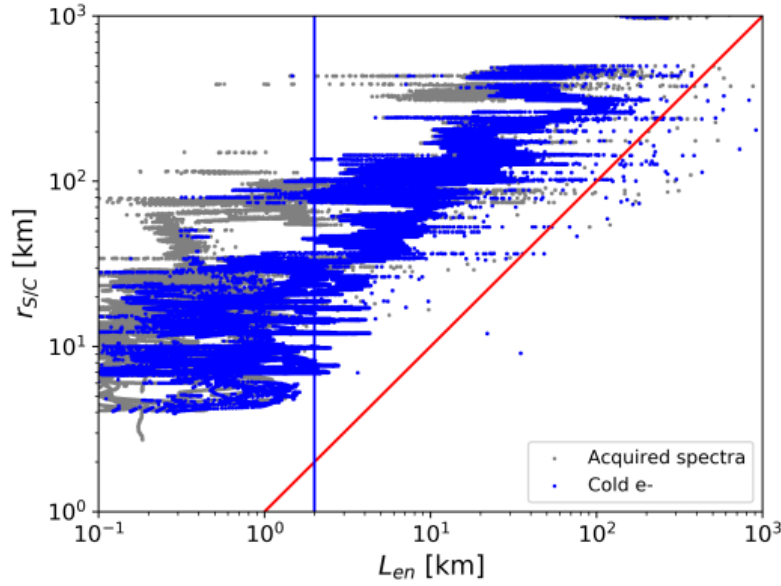


Figure 1.12: Cometocentric distance of Rosetta, $r_{S/C}$, during detections of the cold electron population against the theoretical electron exobase, L_{en} , location. Credit: [Gilet et al. \(2020\)](#).

with the neutral gas, is insufficient to capture the cooling of electrons at comets.

In reality, electrons do not flow radially away from the nucleus under weak outgassing conditions. Models which assume the radial outflow of ions reproduce the plasma density very well ([Galand et al., 2016](#); [Heritier et al., 2017b, 2018b](#)), but it is not clear the electrons follow the same paths despite being tied to the ions through quasineutrality. Collisionless kinetic simulations show that cometary electrons can become trapped in the inner coma by an ambipolar potential well ([Deca et al., 2019](#); [Sishtla et al., 2019](#)), which could extend the time spent and distance travelled in dense regions of the neutral coma. This could lead to increased collisionality with the neutral coma, but the efficiency of the trapping process has not been established. It is not clear whether trapping combined with electron-neutral collisions is sufficient to generate a cold population of electrons even at very low outgassing rates. **The mechanism by which electrons are cooled in a weakly outgassing coma is one of the key areas that my research hopes to address.**

1.2.4 Interaction between a comet and the solar wind

The solar wind is the main external driver of structures and dynamics in the cometary ionosphere. Comprising protons (92%) and α -particles (8%), the solar wind typically has a density of 5 cm^{-3} and a bulk antisunward velocity of 400 km s^{-1} at 1 au, which is supersonic and super-Alfvénic ([Cravens, 1997b](#)). The solar wind carries with it the interplanetary magnetic field (IMF), $\mathbf{B}_{IMF}$, and has an associated convective electric field, $\mathbf{E} = -\mathbf{u}_{SW} \times \mathbf{B}_{IMF}$, arising from the bulk flow (see Eq. 1.8). As the solar wind arrives at a comet, the convective electric field accelerates the

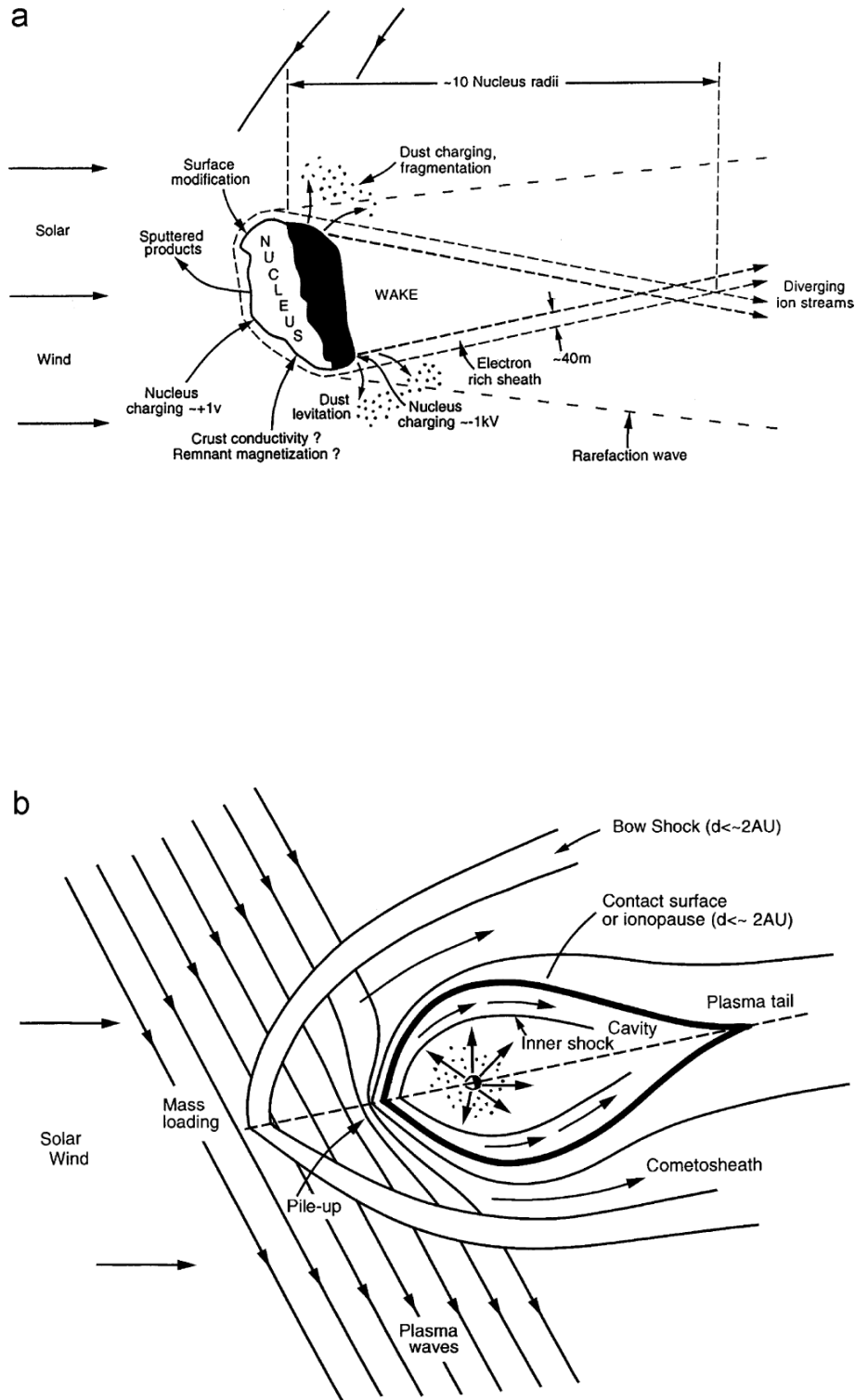


Figure 1.13: Schematic of two different comet-solar wind interaction regimes. Top: At aphelion, the comet has minimal activity. The ionosphere presents little or no barrier to the solar wind, which penetrates to the comet surface. A small wake is formed downstream of the nucleus. Bottom: At perihelion, the neutral coma is dense, and the ionosphere presents a substantial obstacle to the solar wind. Collisions are frequent. The solar wind is slowed and deflected by mass loading, resulting in the formation of a bowshock. A diamagnetic cavity forms, which solar wind electrons and ions cannot penetrate. The solar wind drapes around the cometary ionosphere. At intermediate levels of activity, the cometary ionosphere presents some barrier to the solar wind, but is only weakly collisional. Electrons and ions behave kinetically within the cometary environment. Many of the electron processes at weakly collisional comets are poorly understood. Credit: [Coates and Jones \(2009\)](#).

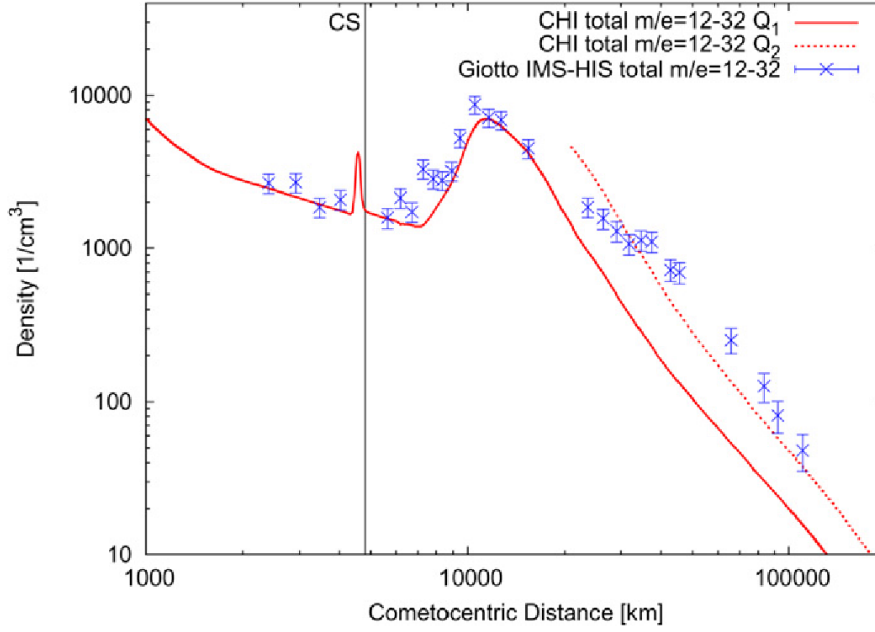


Figure 1.14: Comparison of modelled ion densities with those observed using the ion mass spectrometer (IMS; [Balsiger et al., 1986](#)) on Giotto during the flyby of Halley. An inner shock gives a peak in ion density just inside the contact surface of the diamagnetic cavity (CS). Credit: [Rubin et al. \(2009\)](#).

slow, heavy cometary ions ([Coates, 2004](#)) to the bulk solar wind velocity. The pickup and addition of cometary ions into the solar wind results in mass-loading ([Mendis et al., 1985a](#); [Szegö et al., 2000](#)), which slows and deflects the flow of the solar wind ([Nilsson et al., 2015](#)). As the solar wind slows, the frozen-in magnetic field piles up and the field strength increases ([Neubauer et al., 1986](#); [Goetz et al., 2017](#)). The slowing of the solar wind flow and resulting pile-up are more effective in the denser regions of the cometary ionosphere. The differences in the magnetic field convection throughout the coma causes the field lines to drape around the ionosphere ([Reidler et al., 1986](#); [Volwerk et al., 2019](#)).

Under weakly outgassing conditions, the solar wind is not substantially decelerated, but there is still significant deflection of the flow direction ([Nilsson et al., 2015](#); [Broiles et al., 2015](#); [Behar et al., 2016](#)). The interaction between a weak cometary ionosphere and the solar wind is very three-dimensional and highly kinetic, requiring models to shine light on the interactions. A number of kinetic effects arise in the weakly outgassing and weakly collisional regime, which impact the comet solar-wind interaction. During mass loading, the solar wind and cometary electrons decouple from their ion counterparts ([Deca et al., 2017](#)). The cometary electrons, instead, couple more strongly with the solar wind ions, and are quickly picked up and transported downstream, while the solar wind electrons more closely follow cometary ions as they are picked up ([Deca et al., 2017, 2019](#)).

Nilsson et al. (2018) predict the presence of a polarization electric field that arises from the large gyroradius of cometary ions as they are picked up. If the ion gyroradius is larger than the scale of the cometary ionosphere, then the cometary ions and electrons become spatially separated, driving the polarization field (Gunell et al., 2019).

Closer to the nucleus, an ambipolar electric field is driven by the cometary electron pressure gradient (Cravens, 1997a). Cometary ions and electrons are produced with very different temperatures (0.1 eV vs. 10 eV) and pressures, driving an ambipolar potential well to form around the nucleus (see Section 2.5.3 Deca et al., 2017, 2019). This process can cause the acceleration of solar wind electrons as they enter the inner coma, and trap cometary electrons within the potential well (Deca et al., 2017; Divin et al., 2020; Sishtla et al., 2019). The acceleration of solar wind electrons by this process may be a significant source of energetic electrons in the coma, and a key source of electron-impact ionization. However, this has not yet been quantitatively assessed with a self-consistent set of electric and magnetic fields.

At high outgassing conditions, the solar wind-comet interaction is much more structured, with many boundaries appearing in the ionosphere (see Figure 1.13; Mandt et al., 2016). At very active comets, the cometary ionosphere present a strong enough obstacle to produce a bow shock, where the solar wind is decelerated to subsonic speeds and substantial heating of the plasma occurs (Biermann et al., 1967; Wallis, 1971). The bow shock at a comet is generally quite weak (Mach no., $M = 2$) as the mass loading by the cometary ions is an extensive process. The solar wind ion gyroradii are large in the cometary environment, much larger than the comet nucleus, so consideration of kinetic effects can be very important (Clark et al., 2015). Bow shocks have been observed at many highly outgassing comets including Halley (at 1.15×10^6 km; Neubauer et al., 1986; Coates et al., 1987), 26P/GS (at 2.5×10^4 km; Neubauer et al., 1993) and 19P/Borrelly (at 1.5×10^5 km; Richter et al., 2011).

The outgassing from 67P (up to $Q = 4 \times 10^{28} \text{s}^{-1}$; Hansen et al., 2016) was generally much weaker than at the above comets during the Rosetta mission, and Rosetta was usually at much lower cometocentric distances. When 67P was close to perihelion, the bow shock was predicted to be between 1500 km and 3000 km from the nucleus using hybrid and magnetohydrodynamic (MHD) simulations (see Section 1.3; Hansen et al., 2007; Koenders et al., 2013, 2015). However, no bowshock was observed during an excursion by Rosetta to 1500 km in Oct 2015 (Goetz et al., 2017). Evidence of a partially formed or infant bowshock at 67P has been proposed by Gunell et al. (2018).

Closer to the nucleus, the cumulation of the solar wind mass loading can form a region which the solar wind ions do not enter. The solar wind ion cavity was detected at Rosetta from mid-April

2015 to Dec 2015, as solar wind ions were absent from RPC/ICA and RPC/IES (see Section 1.1.1) measurements during this period (Nilsson et al., 2017). In intermediate outgassing conditions, the ions are excluded from the ion cavity, largely due to kinetic effects (Behar et al., 2017). The slowing of the magnetic field convection (mediated by solar wind electrons) in the coma, causes the solar wind ions to be efficiently scattered anti-sunward (Behar et al., 2017). Although the solar wind ions are excluded from the ion cavity, solar wind electrons are free to penetrate deeper into the coma, carrying the interplanetary magnetic field (IMF) with them.

With sufficient outgassing, another boundary can form closer to the nucleus, which also excludes the entrance of solar wind electrons. The diamagnetic cavity lies within the solar wind ion cavity and is a magnetic field free region, as no solar wind plasma can carry the IMF into the region and the comet nucleus is unmagnetised (Auster et al., 2015; Heinisch et al., 2019).

A diamagnetic cavity was observed during the Halley flyby by Giotto, with the cavity boundary (sometimes ‘contact surface’) located at 4500 km and 4150 km on the inbound and outbound legs. The boundary was proposed to result from the balance between magnetic pressure (from the solar wind) and ion-neutral drag (on the ionospheric side; Cravens and Korosmezey, 1986; Cravens, 1987). The outflowing cometary ions stagnate at the cavity boundary (Puhl-Quinn and Cravens, 1995) causing a build-up of ions. This is balanced by transport of ions along the boundary edge and an increase in electron-ion recombination (Goldstein et al., 1989). Near the cavity boundary at Halley, a discontinuity in the plasma speeds (Balsiger et al., 1986) and an increase in the plasma density was observed (Goldstein et al., 1989). MHD modelling of the cavity by Rubin et al. (2009) produced an inner shock near the boundary (see Figure 1.14), where the supersonic cometary ions are slowed. Puhl-Quinn and Cravens (1995) show the flow of currents along the cavity boundary, which are largely driven by electron motion as the ions undergo efficient Coulomb collisions at the contact surface.

At 67P, Rosetta detected the presence of the diamagnetic cavity much further away from the cometary nucleus than expected from previous models for pressure balance with ion neutral drag (Goetz et al., 2016b,a). The cavity crossing were typically of two types: single extended crossings and clusters of short crossings. The clustered crossings were interpreted as instabilities in the surface of the cavity (Rubin et al., 2012; Henri et al., 2017). The contact surface was also shown to be unstable at Halley (Neubauer, 1987) and subject to instabilities such as Kelvin-Helmholtz (Ershkovich and Mendis, 1986; Ershkovich and Flammer, 1988).

Timar et al. (2017) predicted the location of cavity boundary from ion-neutral drag at 67P during the Rosetta mission, but based on the assumption of photochemical equilibrium in the coma. While valid at Halley (Cravens, 1986), the coma of 67P was never in photochemical equilibrium

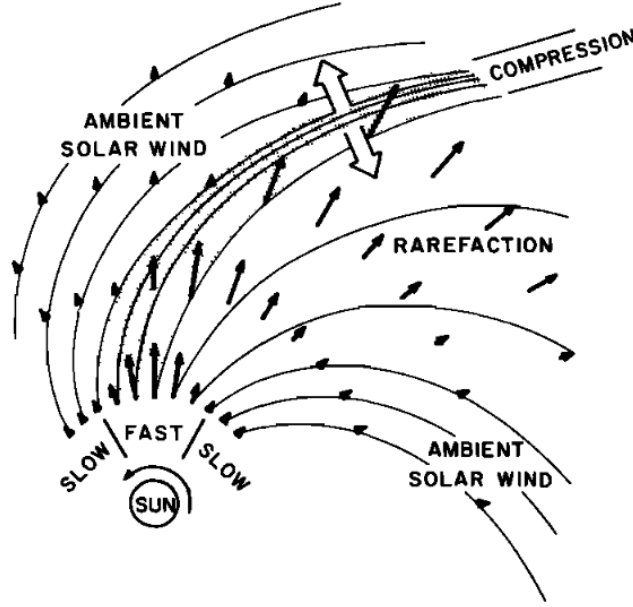


Figure 1.15: Schematic of a corotating interaction region. Fast solar wind flowing radially out from the Sun catches a slower solar wind stream, forming a region of compression. Credit: [Pizzo \(1978\)](#)

([Beth et al., 2019a](#)). Therefore, the very good correlation between the modelled contact surface location and observed cavity crossings is puzzling. [Henri et al. \(2017\)](#) noted that the location of the cavity crossings was well-organised by the electron exobase, indicating that electrons and electron-neutral collisions may play a crucial role in the formation of the cavity boundary.

Transient solar wind events As well as being key in forming the structure of the cometary ionosphere, the solar wind is a significant driver of the plasma dynamics at comet 67P.

Throughout the escort phase, many solar events and solar wind structures arrived at 67P. These included interplanetary coronal mass ejections (ICMEs [Edberg et al., 2016a](#)), Corotating Interaction Regions (CIRs [Edberg et al., 2016b](#); [Hajra et al., 2018a](#)) and solar flares ([Johansson et al., 2017](#); [Edberg et al., 2019](#)). An ICME constitutes a large expulsion of plasma and magnetic flux from the Sun, which is more energetic than the background solar wind. These have a finite angular extent.

Fast solar wind, originating from coronal holes, can catch and interact with slower solar wind that was ejected from the Sun at an earlier time, forming a CIR (see Figure 1.15). A CIR typically sees increases in magnetic field strength, plasma density and temperature (see Figure 1.16; [Pizzo, 1978](#); [Edberg et al., 2016b](#)). The interaction region rotates with the Sun (at periods of ~ 28 days), persisting for several solar rotations. At 67P, CIRs were observed over at least four solar rotations from Oct-Dec 2014 ([Edberg et al., 2016b](#)) and from Jun-Sep 2016 ([Hajra et al., 2018a](#); [Heritier](#)

et al., 2018b). Remote measurements of various comets show that ICMEs can modify the tail structure (Jones and Brandt, 2004) and induce disconnection events in the comet tail (Vourlidas et al., 2007; Kuchar et al., 2008). The evolution of ICMEs with heliocentric distance has also been examined using measurements from Rosetta, in conjunction with data taken at Earth and Mars (Witasse et al., 2017).

At comet 67P, the arrival of ICMEs and CIRs saw increases in the plasma density and a boost to the suprathermal electron population (Edberg et al., 2016a,b; Hajra et al., 2018a; Heritier et al., 2018b; Galand et al., 2020). The driver of the enhanced plasma density was not clear, however. Initial suggestions included an increase in charge exchange and a compression of the ionosphere due to the enhancement of the solar wind (Edberg et al., 2016b). However, it has since been demonstrated that although these processes do occur, they are much less significant than the increase in ionizing electrons (Hajra et al., 2018a; Heritier et al., 2018b). This can result in an increase in plasma density by a factor of 5-10, primarily driven by the boosted electron-impact ionization frequency (see Figure 1.16). Additionally, increased emissions in the FUV were observed during CME impacts at comet 67P (see Section 1.2.5; Feldman et al., 2015; Noonan et al., 2018).

1.2.5 FUV emissions in the coma of 67P

Spectroscopy in the far-ultraviolet (FUV, 700 Å to 2050 Å) can be used to probe many properties of ionospheres and atmospheres, such as neutral composition. O₂ was identified as a major species in the atmospheres of both Europa and Ganymede through UV spectroscopy (Hall et al., 1995, 1998; Feldman et al., 2000; Molyneux et al., 2018). Water production rates of comets have also been inferred using the International Ultraviolet Explorer (IUE) onboard the Hubble Space Telescope (HST) by Festou and Feldman (1987). Prior to Rosetta, the application to comets had been limited to those of sufficient brightness to be observed from Earth-orbit: generally active comets within 1.5 au (Stern et al., 2007). The spatial resolution was limited to tens of kilometres at best (Feldman et al., 2015), as observations were from such large distances. Rosetta, with an orbit within 300 km of the nucleus' surface, was able to resolve spatial variation down to several hundred metres. The Alice FUV imaging spectrograph (see Section 1.1.3; Stern et al., 2007) observed emissions from the near nucleus coma at large heliocentric distances for the first time.

The FUV range is particularly useful in the observation of comets due to the plethora of atomic lines and molecular bands of the predominant neutral species found in comae. The key emission features detected at 67P are listed in Table 1.3.

There are four major sources of FUV photons at comet 67P. These are:

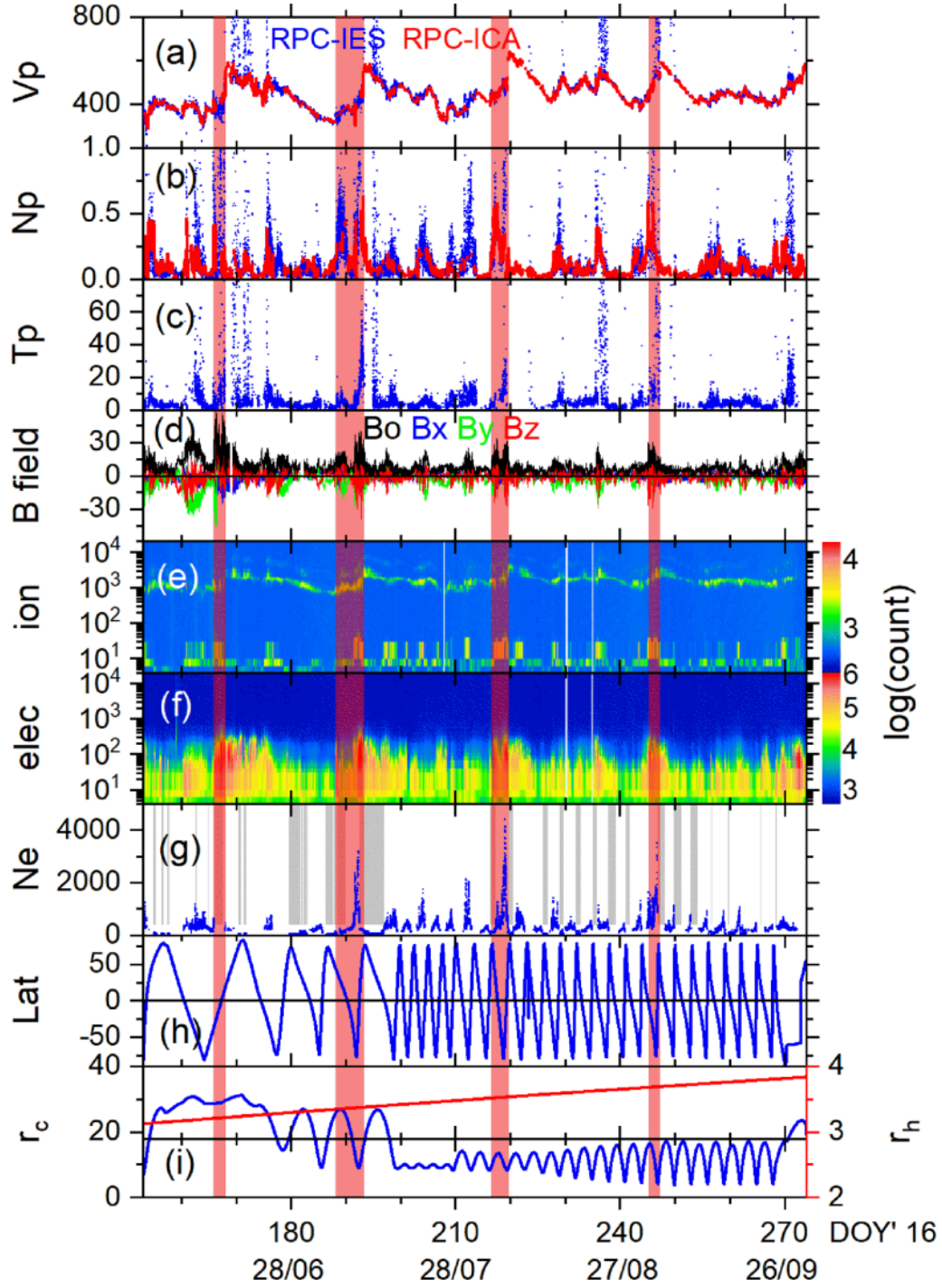


Figure 1.16: Measurements from the Rosetta Plasma Consortium (see Section 1.1.1) in Summer 2016. The appearances of four CIRs during this time are highlighted in red. (a) Solar wind proton speed from RPC-IES (blue) and RPC-ICA (red). (b) Proton density from RPC-IES and ICA. (c) Proton temperature from RPC-IES (d) Magnetic field strength from RPC-MAG in CESQ. (e) Ion and (f) electron spectrograms from RPC-IES. (g) Electron density from RPC-MIP. (h) Spacecraft latitude and (i) cometocentric distance, heliocentric distance. From Hajra et al. (2018a).

Table 1.3: The key emission features observed at 67P in the FUV.

Excited Species	Emission Feature	Wavelength [Å]
H	Ly- $\alpha, \beta, \dots$	1216, 1026, ...
O	OI	1027, 1152, 1304, 1356
C	CI	1561, 1657
C	CII	1335
CO	Fourth Positive Group	1400-1800
CO	Cameron bands	> 1800 (esp. 1868, 1928, 1993)

Solar flux The solar spectrum has peaks at several atomic emission lines in the FUV (see Figure 1.17). The tail of the solar continuum is seen at long wavelengths (> 1400 Å).

Resonant Scattering and Fluorescence Atoms, dissociated by photoabsorption or electron-impact, or molecules can absorb and re-emit photons with wavelengths of atomic lines and molecular bands (Lupu et al., 2007; Liu and Dalgarno, 1996).

Electron-impact dissociative excitation Energetic electrons (> 15 eV) within the coma (e.g. Broiles et al., 2016a) can collide with neutrals in the coma and cause dissociation of the molecule. Excited atomic fragments (indicated *) produced in this process (e.g. reactions. 1.9; Makarov et al., 2004) de-excite and release FUV emissions (Feldman et al., 2015).



Interplanetary Radiation The radiation present throughout the interplanetary medium can contribute significantly to the observed Ly- α and Ly- β (Feldman et al., 2015).

The observed emissions at a given wavelength may be produced by several or all of the processes mentioned above and originate from multiple neutral species in the coma. These sources can be disentangled by examining the ratios between the brightness of emission lines. For example, the ratio Ly- α /Ly- β from the interplanetary background or from resonant fluorescence in the coma is ~ 300 (Feldman et al., 2015). However, the impact of energetic electrons on H_2O in the coma gives Ly- α /Ly- β = 7 (assuming 100 eV electrons; Makarov et al., 2004).

The observation of significant emissions of OI1356 at comet 67P was unexpected as during previous cometary flybys, such as that of C/1995 Hale-Bopp, OI1304 was dominant over OI1356 (McPhate et al., 1999). OI1356 arises from a forbidden transition ($^5\text{S}^\circ - ^3\text{P}$) and so is not produced through resonance. As such, Feldman et al. (2015) suggested that the impact of energetic electrons

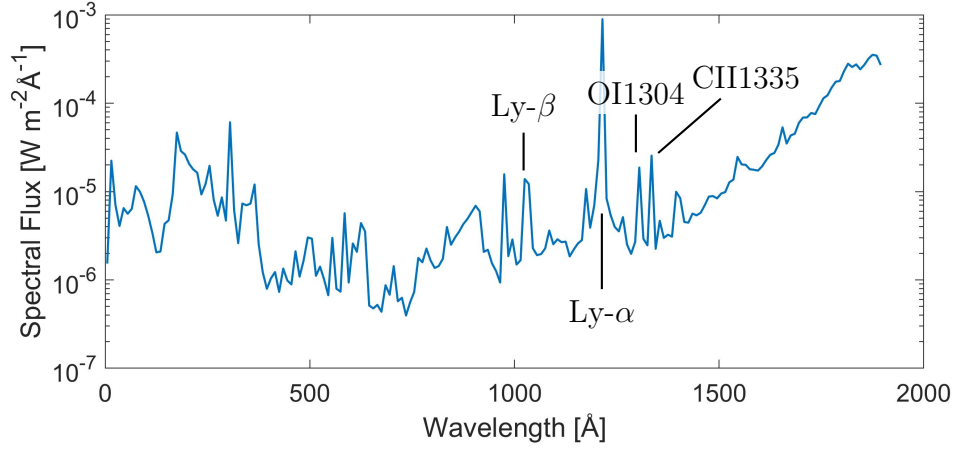


Figure 1.17: The Solar spectrum measured by TIMED-SEE at 1au on 30th Jan 2015. (Woods et al., 2005) Peaks are seen at Ly- α , Ly- β , OI1304 and CII1335.

could be a major source of emissions from the coma of 67P.

Emissions of CII1657, CII1561 and CII1335 in a ratio of 2:1:1 as seen in October 2014 are typical of electron-impact on CO₂ (Ajello, 1971b; Mumma et al., 1972). Analysis of the widths of the Cameron bands observed in the southern hemisphere were also indicative of electron-impact on CO₂ (Feldman et al., 2018). Feldman et al. (2015) proposed a basic model of electron-induced emission to reproduce the observed Ly- β brightness. This model was limited as it was dependent on the total electron density. Only the energetic electron populations can induce FUV emissions due to the high threshold energies (> 10 eV, see Table 4.1), so the model was not accurately deriving the emission excitation frequencies.

Feldman et al. (2015) used synthetic emission spectra generated in a laboratory from the impact of 100eV electrons on a gas. These were fitted to the observed Alice spectra by normalising to certain emission bands, such as Ly- β for water. The ratios of emission lines were used to derive the mixing ratio of CO₂ with respect to H₂O, which were found to be in reasonable agreement with values derived from VIRTIS-H (Bockelée-Morvan et al., 2015) and ROSINA/DFMS (Hässig et al., 2015).

Feldman et al. (2018) provided a more complete picture of the typical spectra observed at 67P away from perihelion. They highlighted the transition of the spectra from being dominated by water emissions in the northern hemisphere pre-perihelion (Figure 1.18a) to cases in which CO₂ is clearly present in the southern hemisphere (see Figure 1.18b). This transition reflects the substantial difference in composition between the northern and southern hemisphere (see Section 1.2.1; Hässig et al., 2015; Gasc et al., 2017a). Post-perihelion there are many spectra that display a ‘picket-fence’, which is typical of strong emissions of the CO Fourth Positive Group (CO4PG, from 1400-1800 Å).

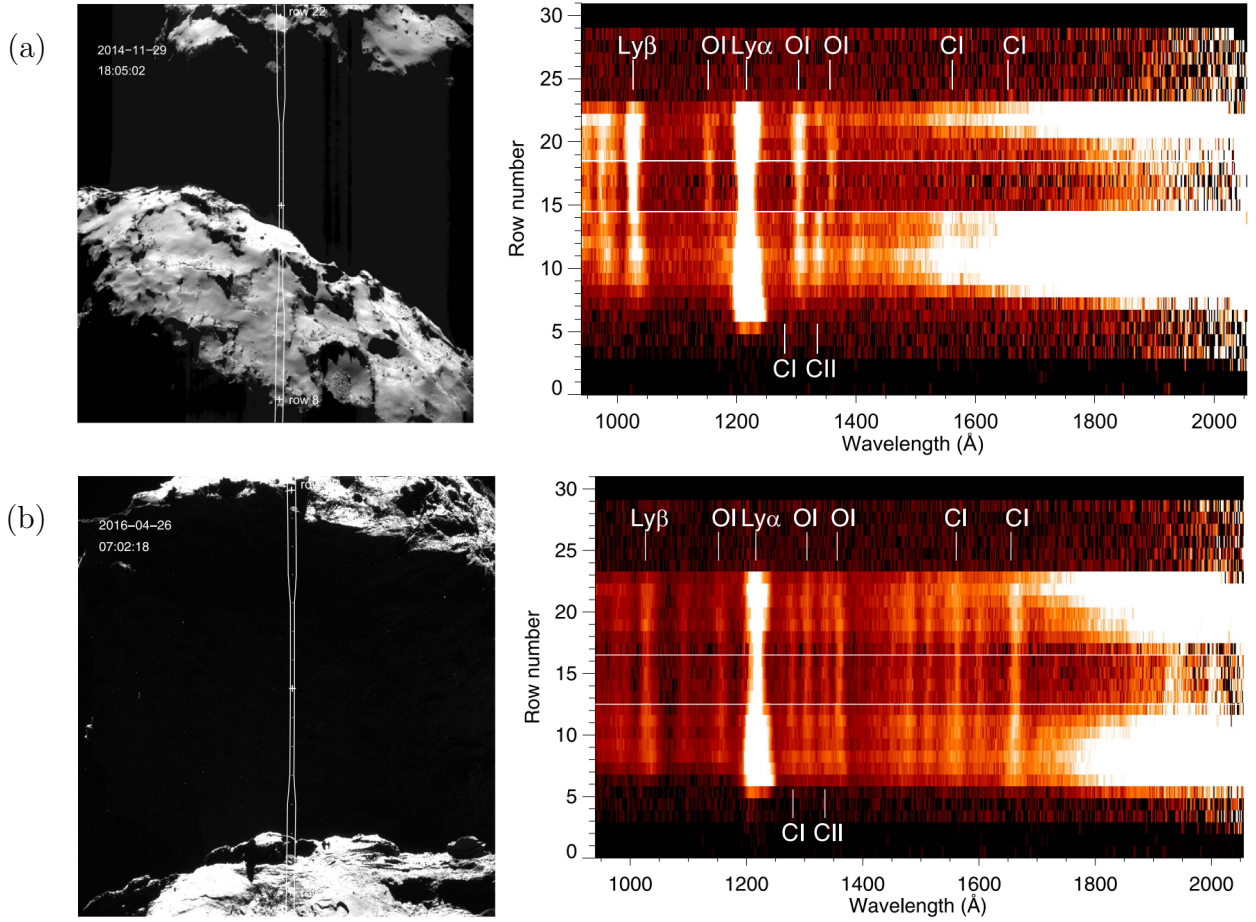


Figure 1.18: (a): Alice spectrum from over the northern hemisphere on 29th Nov 2014. Bright oxygen and hydrogen lines. (b): Alice spectrum from over the southern hemisphere on 26th April 2016. Picket fence of CO Fourth Positive Group and bright atomic carbon lines observed. Pollution of the spectra by solar flux is seen at long wavelengths, where the nucleus was illuminated. Credit: [Feldman et al. \(2018\)](#).

There have also been several studies of emissions during extreme events at 67P. [Feldman et al. \(2016\)](#) looked at outbursts of gas from the coma through observations of the limb near perihelion. The outbursts saw greatly increased in emissions of OI1356 and CI1657, which were attributed to spikes in O₂ and CO₂. Through spectral analysis, a mixing ratio of O₂/H₂O ≥ 0.5 was derived ([Feldman et al., 2016](#)), greatly exceeding the values measured by ROSINA/DFMS ([Bieler et al., 2015a](#)). Similar analysis applied to other outbursts of gas and dust also returned high mixing ratios of O₂/H₂O = 0.14 – 0.3 ([Noonan et al., 2021a,b](#)). [Noonan et al. \(2021a\)](#) used Alice raster scans to create maps of the FUV emissions from the coma of 67P, during increased levels of activity in Nov 2015. They also used emission line ratios to derive large densities of CO₂ relative to H₂O during the transient outburst events, which may have been induced by cliff collapses and geological failures ([Steckloff et al., 2016](#); [Vincent et al., 2016](#); [Noonan et al., 2021b](#)).

[Chaufray et al. \(2017\)](#) demonstrated that emissions of HI-Ly- β are correlated with the water column density measured with VIRTIS (see Section 1.1.3). Emission rates derived from the correlation were compared to an estimate calculated with an energetic electron population, characterized by a Maxwellian with a temperature of 17 eV and density 20 cm⁻³. This assumed electron population does not capture the large fluctuations seen in the suprathermal electron flux by 2-3 orders of magnitude (see Figure 5.1a) or the non-thermal nature of energetic electrons at 67P ([Broiles et al., 2016b,a](#); [Myllys et al., 2019](#)). Far from perihelion, [Chaufray et al. \(2017\)](#) found that the suprathermal electron flux did not show any clear variation with cometocentric distance, in contrast to the bulk electron density which follows a 1/*r* dependence ([Galand et al., 2016](#); [Heritier et al., 2017b](#)).

[Noonan et al. \(2018\)](#) qualitatively evaluated the impact of a CME on FUV emissions on the 5th/6th October 2015 at 1.4au. The large increase in OI1356, by a factor of 15, indicates a substantial increase in suprathermal electrons at the comet, as is seen by [Edberg et al. \(2016a\)](#). They compared the observed emissions to hot and warm electron densities derived from the moments of kappa distributions. During the CME impact, the diamagnetic cavity is compressed. As the cavity is strongly depleted in suprathermal electrons ([Nemeth et al., 2016](#); [Madanian et al., 2020](#)), the compression of the cavity and increase in suprathermal electron flux allow more energetic electrons to reach dense regions of the neutral coma, which results in increased emission line brightnesses.

The analysis of emissions in the FUV is a useful diagnostic tool at the coma, but there has been little quantitative analysis of the emissions. [Raghuram et al. \(2016\)](#) modelled Cameron band and OI1356 emissions from the coma at 1.29 au ($Q = 10^{28} \text{ s}^{-1}$) and 3 au ($Q = 5 \times 10^{25} \text{ s}^{-1}$), with a spherically symmetric coma model. The neutral composition applied was typical of the

northern hemisphere of 67P, with 80% water. They modelled electron fluxes in the coma, through the production, transport and degradation of photoelectrons along one dimension. However, this does not account for any acceleration processes in the coma, which may be a key driver of the suprathermal electron population (Deca et al., 2017, 2019). Additionally, the model cannot reliably be compared to a given set of observed FUV emissions, due to the variable electron flux, neutral density and composition throughout the mission. Raghuram and Bhardwaj (2020) applied a photochemical model to the FUV emission lines (including OI1304 and OI1356) at high outgassing rates ($Q > 10^{27} \text{ s}^{-1}$). However, the model includes photodissociation emissions from several processes that involve spin-forbidden transitions, such as OI1304 and OI1356 emission from photodissociation of H_2O . These processes do not occur. The application of the model to large heliocentric distances (1.99 au) does not accurately reproduce the observed FUV line brightnesses.

Galand et al. (2020) performed the first forward modelling of emissions from the coma of 67P via a multi-instrument analysis. They considered both nadir and limb viewing geometries over the northern hemisphere of 67P away from perihelion. The model, driven by in situ RPC measurements and column densities from MIRO, VIRTIS or ROSINA, agrees well with Alice observations. The model reproduces the limb observed variations well, suggesting that the changes in the energetic electrons are large scale rather than localised fluctuations.

There has not yet been any forward modelling of FUV emissions in the southern hemisphere of 67P, which saw substantial carbon line emissions. Therefore, it is not clear whether dissociative excitation by electron-impact is sufficient to explain the observed emission brightnesses. It also has not been established whether the southern hemisphere emissions are induced by cometary electrons or by solar wind electrons, which have undergone acceleration in the cometary environment. **This is one of the areas I aim to address in this thesis.**

1.3 Models of the cometary plasma environment - Energy budget

Many models of cometary plasma have been developed for Halley-type comets and for comet 67P. These models are generally one of three types: magnetohydrodynamic (MHD, Section 1.3.1), hybrid (Section 1.3.2) or fully kinetic models (Section 1.3.3). In this section, I discuss the scopes of these models and some key results. While Giotto and Rosetta provided only single-point measurements at a given time, models help to contextualize the data points into the wider environment, whether in just one dimension or in three.

1.3.1 MHD

MHD models describe the plasma as one or more fluid (e.g., solar wind ions, cometary ions, electrons) populations, with well-defined boundary conditions for the magnetic field which is tied to the plasma. Quasineutrality is assumed, and electrons behave as a massless, charge-neutralizing fluid. MHD models are best applied when the scale of the system, and structures of interest are much larger than kinetic scales: such as the ion-inertial length or the ion gyroradius. The electric field is calculated using the electron momentum equation or Generalized Ohm's law (see Eq. 1.8). Often some terms, such as electron inertia, are neglected as they are small. This gives different types of MHD models, such as Hall-MHD, which includes the Hall field.

MHD models have successfully been applied to comet Halley, reproducing many of the plasma structures observed by Giotto (Gombosi et al., 1996; Rubin et al., 2009, 2014a). Cravens (1989) used a one dimensional MHD model to examine plasma dynamics within the diamagnetic cavity and the presence of substantial electron-ion recombination at the cavity boundary. Gombosi et al. (1996) modelled the extensive cometary environment of Halley in three dimensions, including the formation of the bow shock and the diamagnetic cavity in the inner coma. They captured the mass loading of the solar wind, as well as the formation of currents at the cavity boundary. However, they could not calculate the electron temperature in the single fluid model, instead opting to use empirical temperature profiles derived from Giotto measurements and kinetic models (Körösmezey et al., 1987; Cravens, 1989; Gan and Cravens, 1990; Eberhardt and Krankowsky, 1995). The electron impact ionization frequency was also imposed, using results from the kinetic model of Cravens et al. (1987).

Multi-fluid models were then developed, such as those of Benna and Mahaffy (2007) and Rubin et al. (2009), which separate the ion and electron fluids. In multi-fluid models, the ion populations from the solar wind and from the comet may be modelled individually, with source and loss terms in the continuity, momentum and pressure equations accounting for their interactions. Rubin et al. (2009) applied a multi-fluid approach to Halley, in conjunction with an ion-chemistry model. Again, a fixed electron temperature profile and a pre-set suprathermal electron population were used. An inner shock formed inside the diamagnetic cavity, with an associated spike in plasma density. Rubin et al. (2014a) modelled the electron temperature, with cooling driven by collisions with the neutral gas and other fluids. They reproduced temperature profiles similar to those measured by Eberhardt and Krankowsky (1995) and imposed in Gombosi et al. (1996). In MHD models, the electrons are treated as only a single fluid, so the suprathermal electron population cannot be simulated with this approach. Suprathermal electrons only appear in the model as a

source of ionization and of electron heating, where the associated rates are taken from [Cravens et al. \(1987\)](#) and [Gan and Cravens \(1990\)](#), respectively. In addition, the cooling of electrons is applied to the whole electron population in a fluid approach. In the inner coma of Halley, the cold, thermalized population makes up the bulk of the electrons, so this assumption is valid. If the cold electrons are no longer the bulk electron population, then energy degradation has to be treated in a kinetic manner.

Several efforts have been made to model the large scale environment of 67P using multi-fluid MHD. However, in a relatively small and weakly outgassing coma, the kinetic effects of both ions and electrons become important. Multi-fluid models also use temperature dependent electron-impact ionization frequencies, derived by [Cravens et al. \(1987\)](#), which are less applicable to weakly outgassing conditions. [Rubin et al. \(2014b\)](#) compare hybrid and MHD models applied to 67P at low outgassing ($Q = 8 \times 10^{25} \text{ s}^{-1}$), finding that pickup ions were quickly lost in the multi-fluid MHD simulations. The multi-fluid models are significantly better at capturing the environment than single fluid approaches ([Hansen et al., 2007](#); [Rubin et al., 2014b](#)), at least capturing some gyration of cometary ions.

In a weakly outgassing regime, the comet-solar wind interaction is highly kinetic, so the validity of MHD models is limited. [Huang et al. \(2016, 2018\)](#) examined the coma close to perihelion, looking at the formation of the cavity at $Q = 8 \times 10^{27} \text{ s}^{-1}$. [Huang et al. \(2018\)](#) incorporated electron pressure and Hall terms into the MHD equations, which led to substantial reconnection near the cavity boundary. However, the ion gyroradius was comparable to the size of the cavity in these simulations, so the fluid-like behaviour may not be valid in the inner coma.

MHD models are much less computationally intensive than hybrid or fully-kinetic models. This allows 3D simulations to be run over huge domains, spanning from beyond the bow shock to the inner coma and into tail. This also has a lot of potential to be used for time dependent simulations, such as tail disconnection during CMEs ([Jia et al., 2009](#)). Electrons are only treated as a single, thermalized fluid, which is not reflective of the electrons observed at 67P. Rosetta measured electrons in multiple populations (see Section 1.2.3), and the bulk of the electron were in suprathermal populations ([Clark et al., 2015](#); [Broiles et al., 2016a,b](#)). The cold electrons were not dominant at 67P ([Gilet et al., 2020](#); [Wattiaux et al., 2020](#)), so the formation of this population cannot be captured with an MHD model. They also cannot account for kinetic effects, which are prevalent within a weakly outgassing coma ([Behar et al., 2017](#); [Deca et al., 2017](#); [Sishtla et al., 2019](#)) and may be a key driver of the electron cooling processes.

1.3.2 Hybrid

Hybrid models treat ions as kinetic particles, but approximate electrons as a charge-neutralising fluid. As in MHD models, quasineutrality is assumed and the electric field is derived from the GOL (Eq. 1.8). The kinetic treatment of ions allows for the inclusion of different energy populations of ions, ion scattering, gyroradius effects and differing source regions for ions at a given location. [Puhl-Quinn and Cravens \(1995\)](#) demonstrated the importance of kinetic effects in the formation of the diamagnetic cavity boundary at Halley with a 1D hybrid model. Cometary ions are magnetically reflected at the outer cavity boundary and undergo collisions with both the neutral coma and other outflowing ions. This results in a stagnation of the ion flow at the boundary, where ions can either be transported or recombine with the cold electron population ([Goldstein et al., 1989](#)). Ion kinetics were important at Halley during the Giotto flyby at an outgassing rate near $Q = 10^{30} \text{ s}^{-1}$ ([Krankowsky et al., 1986](#)) [Koenders et al. \(2013\)](#) modelled the interaction of 67P with the solar wind, predicting the formation of a bow shock at 2000 km for $Q = 5 \times 10^{27} \text{ s}^{-1}$. The pick-up of cometary ions is much better captured by hybrid models than in MHD codes, allowing cometary ions to be accelerated over large scales compared to the coma. [Rubin et al. \(2014b\)](#) demonstrated hybrid models also far outperform multi-fluid MHD codes, when modelling ion pickup.

Hybrid codes allowed for deeper examination of charge-exchange processes and their importance in mass loading of the solar wind at 67P ([Simon Wedlund et al., 2017, 2019b](#)). Charge exchange collisions generated more ions than photoionization in the cometary environment. [Simon Wedlund et al. \(2017\)](#) found that electron-impact ionization was also a major ion source, but used ionization frequencies based on a Maxwellian distribution and assumed a constant electron temperature across the domain. Hybrid models have also been used to examine energy transfer between fields and charged particles at a weakly outgassing comet ([Lindkvist et al., 2018](#)). They showed that mass loading of the solar wind transfers energy from particles to EM fields through pile-up, while energy stored in the fields is transferred to cometary ions as they are picked up. [Lindkvist et al. \(2018\)](#) also found that electrons are not a major driver of energy transfer within the coma, but the model does not include the kinetic effects of electrons.

While hybrid simulations improve upon MHD models by allowing for ion kinetics, they have all the same limitations in terms of the electron behaviour. They are unable to distinguish multiple electron populations, cannot accurately depict the energy degradation or energisation of suprathermal electrons. Electrons must be treated kinetically to account for energy dependent collision processes and the substantial non-thermal electron populations in the coma of 67P. In

addition to electron heating in the coma, these reasons mean hybrid models cannot accurately represent the electron population at 67P.

1.3.3 Kinetic

In order to fully capture the behaviour of electrons at a weakly outgassing comet they must be treated kinetically. Models which include kinetic electrons either solve the Boltzmann equation or use a Particle-in-Cell (PiC) approach. Quasineutrality is not assumed in PiC models and the fields are derived from the particle dynamics rather than from a Generalised Ohm's Law (Deca et al., 2019).

Gan and Cravens (1990) used a two-stream approach to solve the Boltzmann equation along parabolic magnetic field lines at Halley, including inelastic electron collisions with neutrals. This method allows the flow of electrons along the field line in both directions (up and down the field), while retaining two dimensions in velocity space (two average pitch angles for the up and down directions). Electron-impact ionization and electron-ion recombination were strongly dependent on the electron dynamics and heavily influenced the structure of the cometary plasma.

At Halley, the bulk of the electrons formed a cold population which can be modelled as a fluid and only the suprathermal electrons were modelled kinetically. Gan and Cravens (1990) estimated a potential drop of up to 10V in the coma of Halley, which acts to accelerate the solar wind electrons and enhances the suprathermal electron densities.

At 67P, the bulk of the electrons were split into several populations, including the suprathermal populations (Broiles et al., 2016b,a; Gilet et al., 2020). The cold population does not form the bulk of the electrons (Gilet et al., 2020), so cannot be treated through a fluid approach. Madanian et al. (2016b) applied a two-stream model to 67P, like that used by Gan and Cravens (1990), to examine the suprathermal electron population. An estimated ambipolar electric field was applied at the ends of the magnetic field lines, rather than calculated self consistently. The parallel field confined photoelectrons and accelerated solar wind electrons into the inner coma, while electron-impact collisions drove electron cooling. With only a one-dimensional model, the full dynamics of the electrons are not captured. In addition, a quantitative assessment of the heating and trapping by the ambipolar potential well requires a set of self-consistently calculated fields.

Deca et al. (2017) produced a fully-kinetic but collisionless model of the 3D cometary environment. The PiC model self-consistently calculated electric and magnetic fields with both cometary and solar wind electron and ion populations. The cometary electrons are generated purely through photoionization. As electrons are treated kinetically, the time-interval between steps must be short

enough such that the electron gyromotion is resolved. This can be computationally intensive, so it is common that PiC models use an increased electron mass ($m_e = m_p/100 = 1.67 \times 10^{-29}$ kg). Heavier electrons lengthen the gyroperiod ($T_{gyro} = 2\pi m_e/qB$), allowing for longer timesteps. The increased electron mass retains a separation in scales between the electron and ion motions but does have other consequences, such as a reduced electron gyroradius.

Deca et al. (2017) found that the electron populations from each source spatially decoupled from their ion counterparts, following very different paths through the solar wind. Quasineutrality was satisfied by the solar wind electrons pairing with cometary ions and vice versa. An ambipolar potential well formed around the nucleus (Deca et al., 2017, 2019; Divin et al., 2020) leading to trapping of photoelectrons and acceleration of the solar wind (Deca et al., 2017; Sishtla et al., 2019).

Electrons are more efficiently trapped within the potential well when they have a small parallel velocity and undergo more oscillations before leaving the region (Sishtla et al., 2019). The parallel potential well at a weakly outgassing comet ($Q = 10^{25} \text{ s}^{-1}$) exceeded 60 eV, with electron temperatures and densities well correlated with the potential. The acceleration of solar wind electrons in the potential well may be a significant source of ionizing electrons, which were prevalent at 67P (Heritier et al., 2017b, 2018b). The trapping of electrons within the potential well may also increase the efficiency of cooling processes. Neither of these processes have been addressed quantitatively.

Although the GOL (Eq. 1.8) is not used in the PiC model, Deca et al. (2019) separated the self-consistently calculated fields into the terms of the GOL. The ambipolar and Hall fields both have strong components close to the nucleus, playing substantial roles in shaping the trajectories of the charged particles.

The 3D kinetic simulations have so far neglected collisional processes, which are critical to describe the different electron populations. For instance, they cannot assess the role of electron-impact ionization in the generation of warm electrons. Neither can they quantify the efficiency of electron degradation in combination with the potential well. It is not clear whether this process is sufficient to generate a population of cold electrons in the coma. The one dimensional models better simulate the collisional processes, but lose the 3D nature of the comet-solar wind interaction and the plasma dynamics while lacking self-consistent fields. No simulation is currently able to simulate all three electron populations in the complex 3D electromagnetic environment, which is required to capture the electron cooling and ionization at a weakly outgassing comet.

1.4 Aims and originality of the thesis

Motivation The Rosetta mission provided the most extensive dataset of observations and measurements of the cometary environment. It also allowed in situ measurements of a comet at far weaker outgassing rates than any previous cometary mission and gathered data for far longer. It captured the evolution of cometary activity and its interaction with the space environment as the heliocentric distance varied. While our understanding has greatly improved in the wake of Rosetta, the data from Rosetta have not yet been fully exploited and there are still major outstanding questions to be answered.

One area that is poorly understood is the role of electron-neutral collisions in weakly outgassing comets and their effect combined with the complex fields surrounding the comet. The weakly outgassing coma provides a unique environment in which the interface between collisionless and highly collisional plasmas can be explored.

Firstly, electron-impact ionization has been shown to be important during short time-intervals during the Rosetta mission ([Galand et al., 2016](#); [Heritier et al., 2017b, 2018b](#)), but the process has not been assessed throughout the escort phase. The origin and drivers of the ionizing electrons are still unclear. The variation of electron-impact ionization throughout the coma and its response to external solar wind conditions are poorly constrained. As electron-impact ionization is one of, if not the major source of plasma at a weakly outgassing comet, it is crucial to understanding the cometary ionosphere as a whole.

Secondly, cold electrons were observed throughout the Rosetta mission ([Engelhardt et al., 2018](#); [Gilet et al., 2020](#); [Wattiaux et al., 2020](#)), even when none of the coma was thought to be collisional. The origin of these cold electrons and the process by which they are cooled has not been established. It is thought that trapping by an ambipolar field may increase the collisionality of the coma ([Deca et al., 2017, 2019](#)), but there has not been a quantitative assessment of this process.

Finally, collisions of energetic electrons on neutrals can also be detected remotely, such as through emission of FUV photons resulting from dissociative excitation of cometary neutrals. Analysis of atomic emission line ratios suggests that energetic electrons are responsible for FUV emissions in the coma. However, no forward modelling of this process has been done yet for the carbon-dioxide rich, southern hemisphere of comet 67P. Does dissociative excitation by electron impact fully account for the observed FUV emissions? And are the electrons responsible for causing dissociative excitation accelerated on local or global scales?

Aims

The goals of my thesis are:

- To develop the first three-dimensional, collisional model of electrons at a weakly outgassing comet. This model uses realistic and self-consistently calculated sets of electric and magnetic fields as an input. The model incorporates the 3D electron dynamics and electron-neutral collisions to simulate the full electron population, from cold to hot.
- To understand the interplay between the fields and collisions at a weakly outgassing comet, and quantify whether the combination of trapping and collisions can generate a cold electron population.
- To examine the role of electron-neutral collisions in generating FUV emissions from the coma. I aim to use a multi-instrument model to compare electron-induced emissions to the observed FUV emission brightness.
- To analyse the energetic electron population measured with RPC/IES and to assess the evolution of this population throughout the Rosetta mission.
- To understand the role of electron-impact ionization within the coma, and assess the source of the ionizing electrons.
- To develop a dataset of the electron-impact ionization frequency throughout the Rosetta mission. I aim to compare this to a variety of other datasets from Rosetta to determine what are the key drivers of electron-impact ionization.

1.5 Thesis outline

Chapter 2 presents the first three-dimensional, collisional model of electrons at a comet. The inputs, workings, outputs and parameters are outlined. The model is validated against analytical drifts, the continuous-slowing-down approximation and against kinetic, collisionless simulations. The roles of electron trapping and electron-neutral collisions are assessed for a weakly outgassing coma.

Chapter 3 utilizes the test particle model to examine the cold electron population that was observed throughout the Rosetta mission. A cold population of electrons is sustained within the coma, even at low outgassing rates. The impact of electron dynamics on the collisionality of the coma is assessed, and the location of the collisional boundary (electron exobase) is revisited in light of this.

In **chapter 4**, a multi-instrument analysis is applied to the FUV emissions from the coma to determine whether they are driven by electron-neutral collisions. This study employs numerous instruments from the Rosetta mission to drive the data-based model. The observed and modelled emission brightnesses show excellent agreement, and the model is used to determine which neutral species are the key sources for each emission line. Electron induced emissions from the coma during several corotating interaction regions are modelled and closely follow the observed brightnesses. The correlation between the in situ measurements of electrons and remotely sensed FUV emissions gives insight to the scales over which electrons are accelerated.

Chapter 5 examines the source of electrons within the coma across the Rosetta mission. Section 5.1 is based on the analysis of in situ Rosetta observations. A database of the electron-impact ionization frequency is created for the whole escort phase. This is compared to the photoionization frequency and other measurements of the coma, particularly from RPC (see Section 1.1.1) and ROSINA (Section 1.1.2), to demonstrate the importance of electron-impact ionization in the coma. This analysis is also used to determine some key drivers of the ionization frequency and the source of ionizing electrons. In Section 5.2, the test particle model is exploited to examine the source of the ionizing electrons in the coma. Finally, in Section 5.3, some controversy is addressed regarding the recent measurements of cometary ion velocities and the implications these measurements have on the suprathermal electron population. This discussion incorporates the data-analysis of the electron-impact ionization frequency, test particle modelling and the multi-instrument analysis.

Chapter 2

A collisional test particle model of electrons

In this chapter, I discuss the collisional test particle model of electrons in a cometary environment, which I have developed. This is the first three-dimensional collisional model of electrons at a comet.

Section 2.1 summarizes the key processes that occur in the test particle simulations and the domain of the simulations. The description of the test particle model is then further broken down into four parts. Section 2.2 discusses the propagation of single test particles through the simulation domain. Following this, Section 2.3 presents the mechanics of the electron-neutral collisions for elastic and inelastic processes, as well as the relevant cross-sections for each. The conversion from single particle trajectories to macroscopic quantities (moments) is presented in Section 2.4. In Section 2.5, the initialization of the model and the boundary conditions are explained to complete the model description. This includes the neutral coma model, the set of electromagnetic fields, the choice of grids for photoelectron production and the initial conditions of electrons injected into the simulations. To conclude this chapter, I validate the model under collisionless and collisional conditions with a complex set of electromagnetic fields in Section 2.6.

2.1 Model Overview

Figure 2.1 illustrates the key processes involved in the test particle model. The first generation (G_1) of electron test particles, comprising either solar wind or photoelectrons, is created in the simulation domain. The initial positions and velocities of the macroparticles are dependent on the source of the primary electrons. Once created, the test particles are pushed through the simulation as they respond to the stationary electric and magnetic fields, until they are terminated. As

the particles move through the domain, they may undergo collisions with the neutral gas in the simulation. Depending on the type of collision, the particle is degraded in energy or scattered. Additionally, if electron-impact ionization occurs, the properties of a new electron are recorded, which will form part of the following generation (G_{n+1}). Once all the particle trajectories of a generation have been calculated, the next generation of electrons are injected into the domain, using the stored properties from the previous generation. The new generation is simulated in the same way as the first with propagation, collisions, ionization and termination. This cycle is repeated until a maximum number of generations are complete, or no electrons are produced in a generation.

2.1.1 Simulation Domain

The x axis points along the Sun-comet line towards the nucleus, while the y -axis is parallel to the interplanetary magnetic field. The z -axis completes a right-handed set. At the large heliocentric distances (> 2 au) considered in this thesis, the Parker angle is approximately 90° , so it is reasonable to assume that x and y are orthogonal.

The simulation domain extends 2200 km in each direction, with the comet nucleus centred in the y and z directions. The origin is defined at the centre of the nucleus, so the y and z boundaries lie at ± 1100 km. Along x , the domain is shifted in order to capture more of the electron behaviour downstream of the nucleus, giving boundaries at -770 km and 1430 km. The size of the domain is limited to the region where the electric and magnetic fields, which are sourced from a PiC simulation (see Section 2.5.3), are provided. This greatly exceeds the scale of domain required to capture the collisional region of the coma.

2.2 Single particle trajectories

2.2.1 Description of the Model

A test particle model is built from many single particle trajectories, each independent of the other, under the assumption that the test particles do not significantly alter the environment they pass through. As such, it is a stationary simulation, with no temporal changes of the background field. Each ‘particle’ in the simulation is more accurately a *macroparticle*, which represents a flow of identical electrons following the same trajectory. The macroparticles are assigned a weight, W , which quantifies the number of electrons per second which follow this path. Particles from different populations or created in different regions of the coma may have different weights.

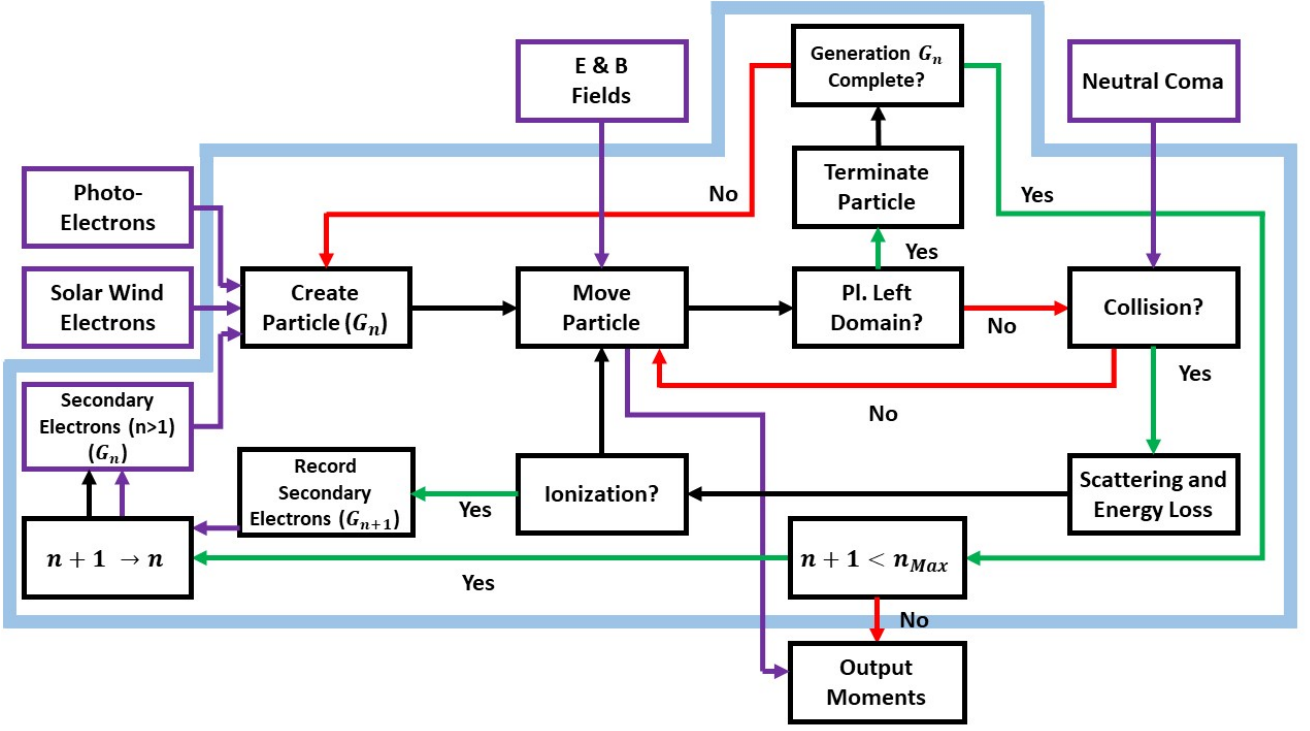


Figure 2.1: Schematic of processes included in the test particle model. Inputs to the simulation are outlined by purple boxes. The secondary electron properties act as inputs for n th generation of electrons when $n > 1$, although they are an output of the previous generation, G_{n-1} . The blue border separates the processes occurring within a simulation from the inputs, outputs and parameters of the model. Extracted from [Stephenson et al. \(2022\)](#).

The trajectory of a single macroparticle is built in three phases: the creation, its propagation through the coma and its termination. A macroparticle must be created with a weight, an initial position and a velocity. The choice of these properties is dependent on the electron population and is outlined for photoelectrons, solar wind electrons and secondary electrons in Sections 2.5.4, 2.5.5 and 2.3.2, respectively.

Once a particle is created, it is pushed through the simulation domain as it responds to the electric and magnetic fields, which are a stationary input to the simulation (see Section 2.5.3). The velocity of the particle is updated using the Boris integrator ([Boris, 1970](#); [Carnielli, 2019](#)).

The numerical integrator separates the Lorentz force into two boosts, resulting from the electric field, sandwiching a rotation of the velocity, caused by the magnetic field. The velocity, $\mathbf{v}_i$, at the beginning of the step is transformed into the final velocity, $\mathbf{v}_{i+1}$, through the series of operations

hereafter:

$$\mathbf{v}_- = \mathbf{v}_i + \frac{e\mathbf{E}dt}{2m_e} \quad (2.1)$$

$$\mathbf{t}_{rot} = \tan\left(\frac{e dt |\mathbf{B}|}{2m_e}\right) \times \hat{\mathbf{b}} \quad (2.2)$$

$$\mathbf{s}_{rot} = \frac{2\mathbf{t}_{rot}}{1 + t_{rot}^2} \quad (2.3)$$

$$\mathbf{v}' = \mathbf{v}_- + \mathbf{v}_- \times \mathbf{t}_{rot} \quad (2.4)$$

$$\mathbf{v}_+ = \mathbf{v}_- + \mathbf{v}' \times \mathbf{s}_{rot} \quad (2.5)$$

$$\mathbf{v}_{i+1} = \mathbf{v}_+ + \frac{e\mathbf{E}dt}{2m_e} \quad (2.6)$$

$$(2.7)$$

where e is the charge of an electron. The particle position is then updated using

$$x_{i+3/2} = x_{i+1/2} + v_{i+1} \times dt. \quad (2.8)$$

As the particle travels through the coma, it may undergo collisions with neutral gas molecules, causing it to lose energy or to be scattered (see Section 2.3). The electron may also ionize the impacted neutral gas molecule during a collision, generating secondary electrons within the coma (see Section 2.3.2). After a collision, the energy and velocity direction are updated to reflect the type of collision. The particle continues to travel until it leaves the simulation domain, where it is terminated. The particle can leave the domain either by colliding with the nucleus surface or by exiting the outer boundaries.

2.2.2 Timestep selection

In order to resolve the particle trajectories, there are a number of conditions on the timestep that must be satisfied. The Boris integrator requires that a constant time interval be used, to ensure that it behaves well and accurately models the particle motion. The following conditions must also be fulfilled:

- $dt < dt_{gyro} = T_{gyro}/N_{Cycle}$.

The electrons gyrate around the magnetic field lines with a frequency $\omega_{gyro} = qB/m_e$. It is necessary that the timestep is small compared to the gyroperiod, $T_{gyro} = \frac{2\pi m_e}{qB}$, so the gyromotion is resolved. N_{Cycle} is a parameter, taken to be $N_{Cycle} = 20$, which dictates the minimum number of points per gyration. [Carnielli \(2019\)](#) shows that the choice of $N_{Cycle} = 20$ is the most efficient

choice to accurately capture the particle motion.

- $dt < dt_{EB} = \frac{dx_{EB}}{2|\mathbf{v}|}$.

It is crucial that the particle does not tunnel past points of the electromagnetic field. If the particle passes through grid cells without responding to the closest field data, the trajectory is not accurately captured. As such, the maximum timestep must ensure that the particle does not travel further than the field resolution, dx_{EB} . The factor of two gives some leeway on the condition.

- $dt < dt_{\text{Grid}} = \frac{\min(dx_i, dy_j, dz_k)}{2|\mathbf{v}|}$.

Similarly, when calculating the moments of the particle distributions (see Section 2.4), it is important that a particle has a step in each cell of the moment grid that it passes through. The dimensions of the current grid cell, (i, j, k) , are dx_i, dy_j, dz_k .

- $dt < dt_{Eng} = \frac{dE_l}{2e|\mathbf{E} \cdot \mathbf{v}|}$.

As the moment grid is separated along the energy dimension as well as spatially, particles should not tunnel through cells in energy space. As such, the work done by the electric field, $e\mathbf{E} \cdot d\mathbf{x}$, in a single step must be smaller than the energy resolution of the grid, dE_l . Again, the factor of two is used to ensure the condition is fulfilled.

- $dt < dt_{prob} = -\frac{\log(1-p_{\max})}{n(\mathbf{x}) \times \sigma_{Tot} \times |\mathbf{v}|}$,

where σ_{Tot} is the total collision probability (see Section 2.3) and $n(\mathbf{x})$ is the neutral density at the particle. This ensures that a particle is unlikely to undergo a collision in a single step, and therefore is very unlikely to have multiple collisions per step. The parameter, $p_{\max} = 0.01$, is the maximum probability of a collision allowed in a step, which means there is a 0.01% chance of multiple collisions in a step.

The most suitable timestep for the simulation would be the largest possible while satisfying the above conditions, allowing simulations to run efficiently and accurately. To determine this property, I ran a test particle simulation which calculated the minimum timestep, t_{min} , to satisfy each condition for every step of every particle in the simulation:

$$t_{min} = \min(dt_{gyro}, dt_{EB}, dt_{\text{Grid}}, dt_{Eng}, dt_{prob}). \quad (2.9)$$

For collisional simulations using the realistic electron mass, the overwhelming majority of time intervals were above $dt = 10^{-6} \text{ s}^{-1}$ (which has been used as the constant timestep). For a heavier electron ($m_e = m_p/100$), which is used in comparison to the PiC models, the velocities are smaller so a larger timestep of $dt = 10^{-5} \text{ s}^{-1}$ satisfies the set of conditions above.

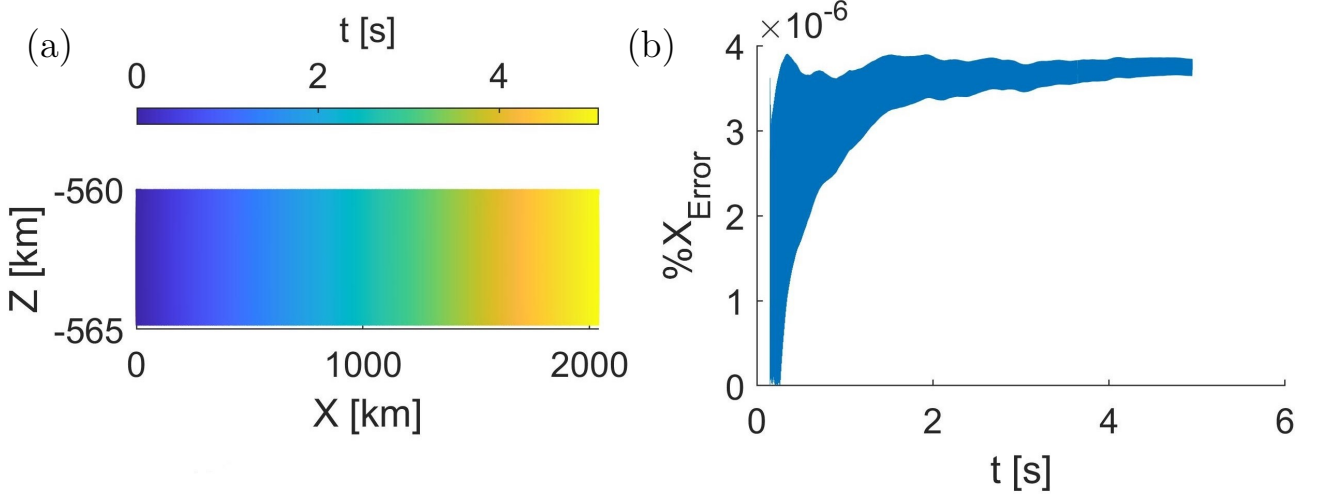


Figure 2.2: (a) Trajectory of an electron undergoing $\mathbf{E} \times \mathbf{B}$ drift in the xz -plane. (b) Percentage deviation of the test particle from its expected location along $+x$, the direction of the $\mathbf{E} \times \mathbf{B}$ drift. Extracted from [Stephenson et al. \(2022\)](#).

2.2.3 Validation of Particle Drifts

To validate the calculation of trajectories within the domain, several test cases are considered, for which the analytical solutions are known. Three standard particle drifts are tested in the collisionless case: $\mathbf{E} \times \mathbf{B}$ drift, curvature drift and grad-B drift.

$\mathbf{E} \times \mathbf{B}$ Drift

Uniform and orthogonal electric and magnetic fields are used to test the replication of the $\mathbf{E} \times \mathbf{B}$ drift. I used typical quiet solar wind conditions of $\mathbf{B} = 6 \text{ nT } \hat{\mathbf{y}}$ and $\mathbf{E} = -2.4 \times 10^{-3} \text{ V m}^{-1} \hat{\mathbf{z}}$, which are the same field strengths seen at the upstream boundary of the PiC simulations (see Table 2.4; [Deca et al., 2019](#)). This choice of fields results in a theoretical uniform drift velocity of:

$$\mathbf{v}_{\mathbf{E} \times \mathbf{B}} = \frac{\mathbf{E} \times \mathbf{B}}{B^2} = 400 \text{ km s}^{-1} \hat{\mathbf{x}}. \quad (2.10)$$

Under these conditions electrons undergo no change of velocity along $\hat{\mathbf{y}}$, so the initial electron velocities have been set to $v_y = 0 \text{ m s}^{-1}$. This ensures the electrons remain in the simulation domain for sufficient time to observe a substantial drift. Figure 2.2a depicts the motion of an electron in the xz -plane, which is initiated at 25 eV. However, electrons have been tested across a range of electron energies (0.1 to 300 eV), corresponding to the energies of interest in the simulations. The gyroaveraged velocity of the electron agrees with the expected drift velocity (Eq. 2.10), with variations of the order of 2 m s^{-1} (1 in 2×10^6). To determine whether these small variations impact the electron position, I compared the gyrocentre to its expected position,

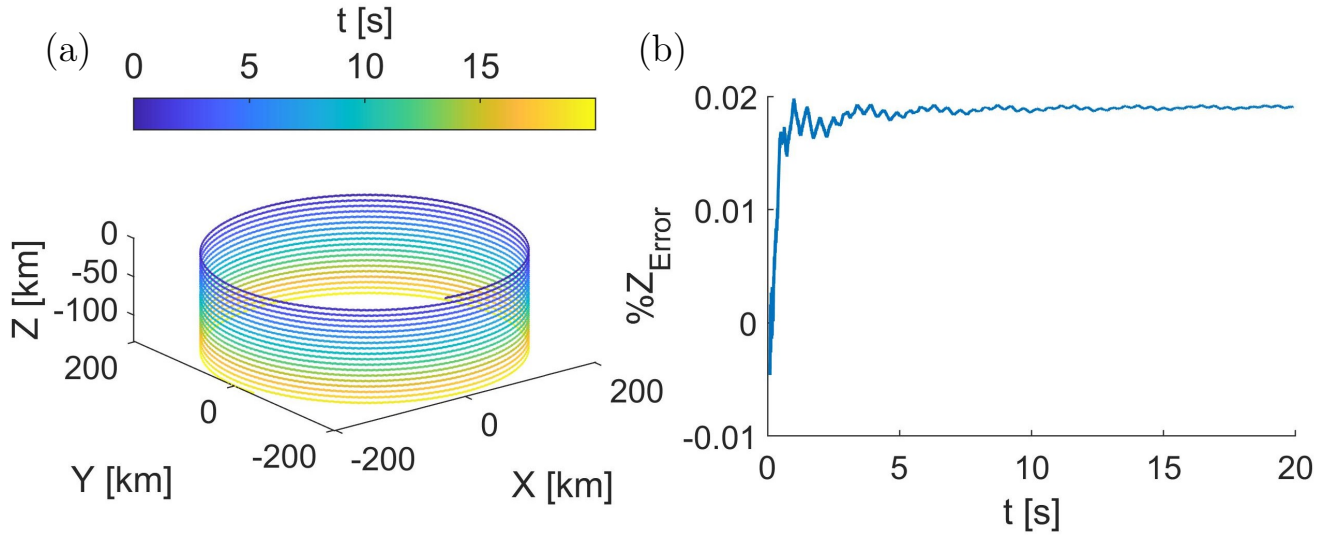


Figure 2.3: (a) Trajectory of an electron undergoing curvature drift in a cylindrical field. Its initial position is (0, -201.6, 0) (b) Difference of the particle position from the expected value along the direction of the curvature drift (+z here). Credit: [Stephenson et al. \(2022\)](#).

$x_{\text{exp}}(t) = x_0 + v_{\mathbf{E} \times \mathbf{B}} t$. In the test particle simulation, the electron gyrocentre deviated from its expected position by less than $4 \times 10^{-6} \%$ across the 2000 km domain (see Figure 2.2b). As such, the $\mathbf{E} \times \mathbf{B}$ drift is accurately reproduced in the simulation.

Curvature Drift

A curvature drift arises from the additional centripetal force required to maintain circular motion on a curved field line. For the validation of this drift, the electric field is set to zero throughout the domain and a cylindrical magnetic field of $B = 6 \text{ nT}$ $\hat{\varphi}$ is imposed, where $\hat{\varphi}$ is the cylindrical polar vector. The strength of the magnetic field is uniform, which eliminates any grad-B drift. This does mean the magnetic field is not physical, but this is used purely to validate the numerical treatment of the curvature drift. The expected drift velocity is ([Cravens, 1997a](#)):

$$\mathbf{v}_{\text{curv}} = \frac{v_{\parallel}^2}{\omega_{\text{gyro}} R_{\text{curv}}^2} (\mathbf{R}_{\text{curv}} \times \hat{\mathbf{b}}), \quad (2.11)$$

where $\omega_{\text{gyro}} = qB/m_e$ is the electron gyrofrequency and $\mathbf{R}_{\text{curv}}$ is the radius of curvature of the magnetic field line. $\mathbf{R}_{\text{curv}} = \boldsymbol{\rho}$, the polar radial vector (in the cylindrical coordinate system) for the prescribed set of magnetic fields. Figure 2.3a shows the motion of an electron undergoing curvature drift. The electron has an initial energy of 4.5 eV of which 4.02 eV is parallel to the magnetic field. The electron moves with a gyrofrequency of 1054 rad s^{-1} and has an average radius of curvature is 201.6 km, i.e., the electron is 201.6 km from the axis of the cylindrical field. Therefore, the expected velocity of the curvature drift is $-6676 \text{ m s}^{-1} \hat{\mathbf{z}}$, causing the helical motion seen in

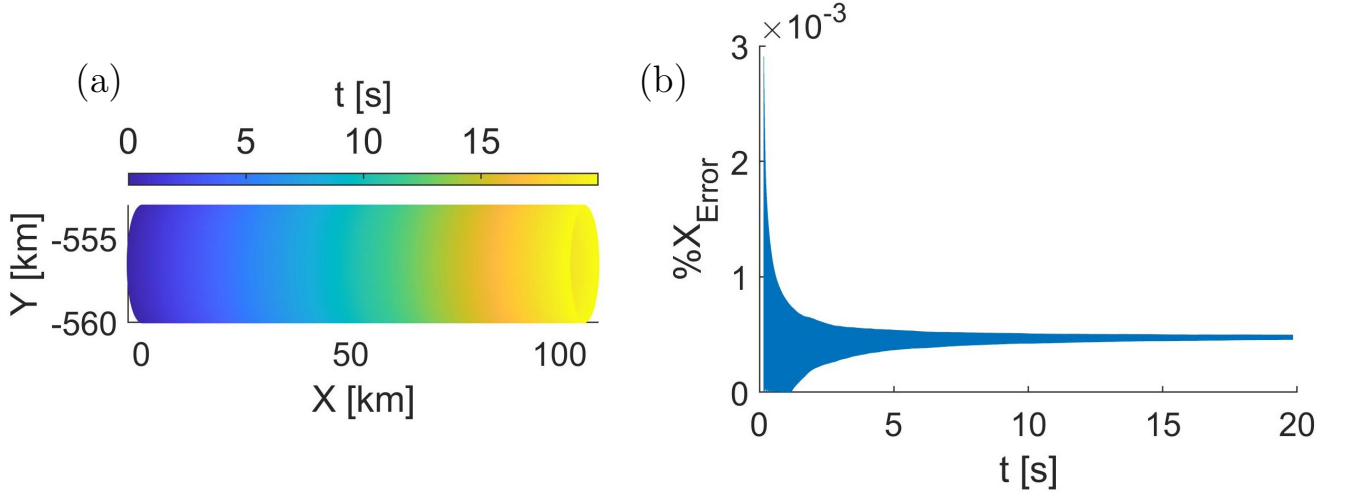


Figure 2.4: (a) Trajectory of an electron undergoing grad-B drift (b) Percentage deviation of particle position from the expected value along $+x$, the direction of the gradient drift. Reproduced from [Stephenson et al. \(2022\)](#).

Figure 2.3a. The gyroaveraged test particle velocity is centred on the expected drift velocity, but varies by up to 25 m s^{-1} from the average value. This variation is very small compared to the electron speed (order of 10^6 m s^{-1}) and also small compared to the magnitude of the drift velocity. The expected position of the electron along the z axis is given by $z_{\text{exp}}(t) = z_0 + v_{\text{curv}} \mathbf{B} t$. Over a 20-second lifetime in the simulation (similar to those in the cometary simulations), the difference between the test particle and expected z positions is less than 0.02%. Hence, the curvature drift is accurately captured by the test particle simulation.

Grad-B Drift

When an electron gyrates in a magnetic field of non-uniform strength, its gyroradius varies within a gyration giving rise to a gradient drift. The analytical expression for the grad-B drift velocity, $\mathbf{v}_{\nabla B}$, is ([Cravens, 1997a](#)):

$$\mathbf{v}_{\nabla B} = \frac{mv_{\perp}^2}{2qB} \frac{\mathbf{B} \times \nabla B}{B^2}. \quad (2.12)$$

To test this drift, the magnetic field is aligned along $+z$ with the field gradient in the $+y$ direction: $\mathbf{B} = B(y)\hat{\mathbf{z}}$. The electric field is set to zero throughout the domain. The particle is created in a region with a background field strength of $B_0 = 4.85 \text{ nT}$ and the field gradient is $\nabla \mathbf{B} = -5 \times 10^{-3} \text{ nT km}^{-1} \hat{\mathbf{y}}$. The electron has an initial energy of 25 eV, all of which is perpendicular to the magnetic field. The lack of parallel energy confines the particle motion to the xy plane (see Fig 2.4a), allowing the electron to remain in the simulation for long enough to exhibit the drift over a large distance.

The simulated electron closely follows the expected drift velocity, with a magnitude of 5276 m s^{-1} ,

deviating by less than 20 m s^{-1} from the theoretical drift. This is small in comparison to the magnitude of both the drift velocity and the electron velocity. The variations also have negligible impact on the electron position, as the error in the gyrocentre location tends to $5 \times 10^{-4} \%$ (see Fig. 2.4b) over a 20 second period. Consequently, the grad-B drift is properly reproduced using the test particle model and the collisionless trajectories are validated.

2.3 Electron-neutral collisions in the model

Collisions of electrons with neutral species, in the test particle model, are separated into three types: elastic, non-ionizing inelastic (excitation, dissociation) and electron-impact ionization collisions. The impact of each set of collision processes on an electron and their distinct features are discussed in the following sections (Sections 2.3.1 to 2.3.3). However, the processes to determine whether a collision occurs, and which type of collision it is, are common to all the processes.

Given an initial flux of electrons, $\Gamma_e(E)$, at energy E , through a medium with number density, n , of water, the change in flux due to collisions along the path length, ds , is:

$$d\Gamma_e(E) = -n \times \sigma_{Tot}(E) \times \Gamma_e(E) \times ds, \quad (2.13)$$

where $\sigma_{Tot}(E)$ is the total collision cross section of electron impact on water. Only water is included as it is the sole species in the modelled coma (see Section 2.5.2).

If colliding particles are removed from the initial flux, the remaining electron flux after a distance, s , along their trajectories is given by:

$$\Gamma_e(s = 0, E) - \Gamma_e(s, E) = \Gamma_e(s = 0, E) [1 - \exp\{-n \sigma_{Tot}(E) s\}]. \quad (2.14)$$

Normalising this to the initial flux, the probability of a single collision process, i , occurring in a timestep of length, dt , is given by:

$$P_{\text{coll}, i}(dt) = 1 - \exp[-n(\mathbf{x}) \sigma_i(E) v dt], \quad (2.15)$$

where the distance travelled by the particle is $ds = v dt$. The column density traced by the particle in the step $n(\mathbf{x})v dt$, is formed from the neutral density at the particle position, $n(\mathbf{x})$, and the speed of the electron, v . As the model currently only includes water in the neutral coma, the neutral density is that of water and all the collisional processes considered are those of electrons on water. The addition of further species, such as CO_2 , would be a simple generalisation of this

model and could be applied in the future.

In the model, the total collision probability in a step is given by:

$$P_{\text{coll}}(dt) = \sum_i P_{\text{coll},i} \quad (2.16)$$

$$\approx 1 - \exp \left[- n(\mathbf{x}) \sigma_{Tot}(E) v dt \right]. \quad (2.17)$$

where the summation is over all the relevant collision processes, i . This includes elastic, excitation, dissociation and ionization processes. This discounts the possibility of multiple collisions in a given step. However, this is a reasonable approximation of the more rigorous expression (Eq. 2.17), as the constraints on the timestep (see Section 2.2.2) ensure the likelihood of multiple collisions is small ($P < 0.01\%$).

This approach ensures the expected energy loss and number of collisions are replicated in the model, although the total probability that a collision occurs in a given step is slightly overestimated. A random number, R_{coll} , is sampled from a uniform distribution between 0 and 1. A collision occurs if $R_{\text{coll}} < P_{\text{coll}}$ and the type of collision, l , which occurs is given by:

$$\sum_{i=1}^{l-1} P_{\text{coll},i} < R_{\text{coll}} \leq \sum_{i=1}^l P_{\text{coll},i} \quad (2.18)$$

Once the type of collision has been determined, the properties of the electron are changed to reflect the collision process as described in Section 2.3.1 (non-ionising inelastic collisions), Section 2.3.2 (ionization) and Section 2.3.3 (elastic scattering). The cross sections, $\sigma(E)$, for each collision process are summarized in Figure 2.5. The importance of each process towards electron cooling can be assessed by the loss function, $L(E)$, which is given by:

$$L(E) = \sum_j \sigma_j(E) E_{\text{loss},j}, \quad (2.19)$$

where $\sigma_j(E)$ is the collision cross section of the j th process at the electron energy. The loss function for each process is shown in Figure 2.6.

2.3.1 Inelastic (non-ionizing) collisions

Inelastic collisions cause the incident electron to lose energy. An electron can cause an inelastic excitation of a neutral molecule if it has an energy exceeding the threshold energy, E_{Th} , of the process. The energy loss associated with the collision is approximated by the threshold energy of

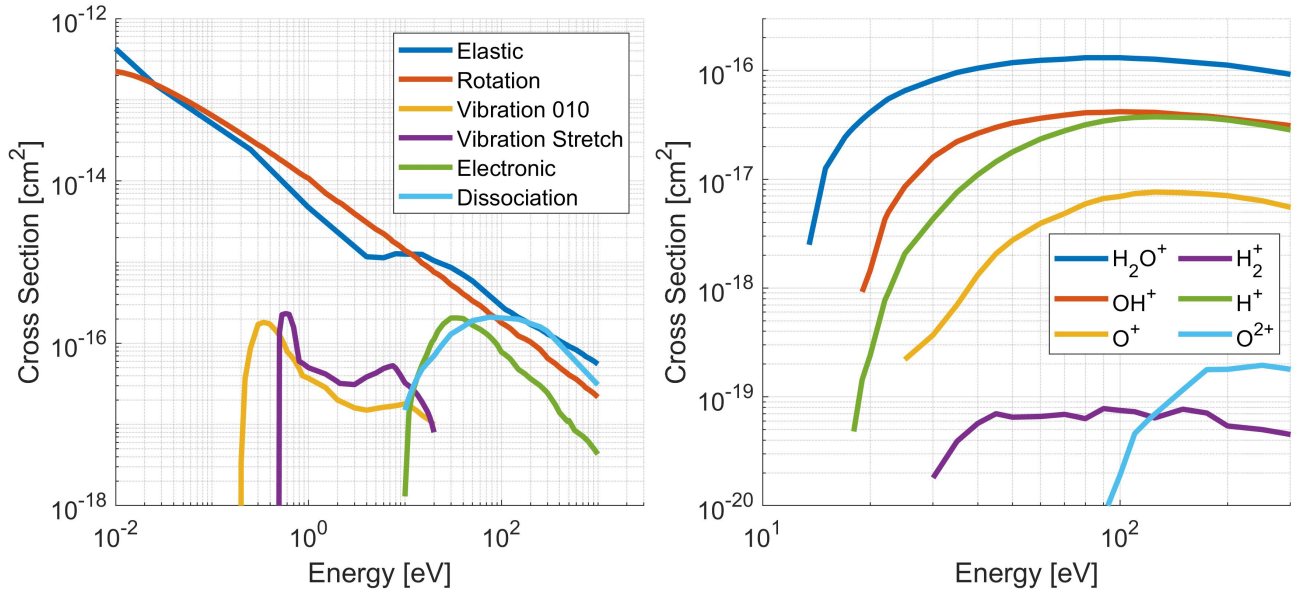


Figure 2.5: (a) Cross sections of elastic scattering and inelastic collisions of electrons on water. The elastic scattering cross section has been derived from measurements by [Faure et al. \(2004\)](#) and [Cho et al. \(2004\)](#) (see Section 2.3.3). The inelastic cross sections are taken from [Itikawa and Mason \(2005\)](#). (b) Cross sections of electron-impact ionization of water ([Itikawa and Mason, 2005](#)).

the process. As water is a triatomic molecule, the threshold energies of all the possible excitations span several orders of magnitude. A rotational excitation (e.g. $J = 0 \rightarrow 1$) results in a loss of 0.004 eV, while dissociation of the water molecule or electronic transitions have threshold energies on the order of 10 eV ([Itikawa and Mason, 2005](#); [Chutjian et al., 1975](#)).

Most inelastic collisions have highly forward peaked cross-sections, meaning that they contribute little to any angular redistribution of the electron velocity. However, the low energy collisions, such as the rotational mode, do contribute to the scattering. In the model, all the scattering has been incorporated into one elastic process (see Section 2.3.3), including that from the weakly inelastic processes. As such, inelastic collisions only cause energy loss and the direction of the electron velocity is unchanged.

All the relevant inelastic electron-water collision processes are included in the model. The cross sections and threshold energies are summarized by [Itikawa and Mason \(2005\)](#), except the threshold energy of the electronic transition, which is provided by [Chutjian et al. \(1975\)](#). The vibrational excitations are split into a bending mode (010) and a set of stretching modes (100 & 001).

2.3.2 Electron-impact ionization and generation of secondary electrons

Electron impact ionization results in the loss of energy of an incident electron and the production of secondary electron(s). Much like the inelastic collisions, ionization processes are forward peaked and so scattering has been neglected. Six ionization processes are included, with cross sections

Table 2.1: Inelastic non-ionizing collision processes and the corresponding threshold energies, E_{Th} for electron impact on water (Itikawa and Mason, 2005; Chutjian et al., 1975).

Inelastic Process	Threshold Energy [eV]
Rotational ($J = 0 \rightarrow 1$)	0.004
Vibrational bending (010)	0.198
Vibrational stretching (100 & 001)	0.453
Electronic	10
Dissociation	7

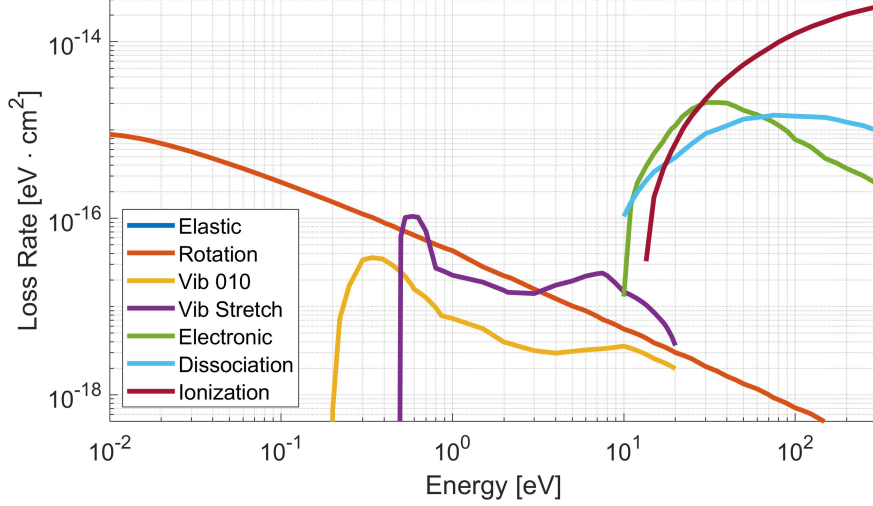


Figure 2.6: Loss rate of the inelastic and ionization processes, associated with electron impact on water, included in the test particle model. The ionization loss rate is derived assuming that the outgoing electrons from an ionization site share the remaining energy equally.

provided by Itikawa and Mason (2005). The ion products and threshold energies of each process are listed in Table 2.2 while the shape of the cross sections are shown in Figure 2.5b.

In electron-impact ionization, the incident electron provides the threshold energy required to release an electron from the impacted atom. The remaining energy of the incident electron is then distributed between the two (or three) electrons, leaving the ionization site. In the model, the remaining energy is equally partitioned between the outgoing electrons. For single ionization, there are two outgoing electrons, each with energy $E_{out} = (E_{in} - E_{Th})/2$. As such, the incident electron has lost $E_{loss} = (E_{in} + E_{Th})/2$ through ionization. For double ionization (forming O^{2+}), the three electrons each leave with $E_{out} = (E_{in} - E_{Th})/3$. This is a simple, but reasonable, first approximation of the energy partition. Moving forward, the division of energy could be sampled from a distribution such as given by Miller et al. (1985). However, when testing extreme cases of the energy distribution (50% or 90% of the kinetic energy is retained by the incident electron) there was no major impact on the electron energies in the coma.

The newly-born secondary electrons have velocities distributed isotropically. The initial

direction is defined by spherical polar angles (θ_v, ϕ_v) , using random numbers R_θ and R_ϕ :

$$\theta_v = \arccos(2R_\theta - 1) \quad (2.20)$$

$$\phi_v = 2\pi R_\phi. \quad (2.21)$$

while the magnitude is set by their initial energy. The random numbers, $R_{\theta,\phi}$, are sampled from uniform distributions between 0 and 1. The isotropic distribution of electrons is also a simplification, but could be refined using data from [Opal et al. \(1972\)](#). However, [Lummerzheim and Liliensten \(1994\)](#) found that the angular distribution of secondaries had little impact on ionospheric simulations.

For a singly ionizing collision, the weight of the produced secondary electrons is the same as that of the incident electron. To improve the statistics for the secondary electron, the weight is distributed between $N_{ioni} = 10$ macroparticles, each of which is created with an independent velocity direction but with the same energy. After seven generations, the simulation is halted. However, for $N_{ioni} = 10$, the number of secondary electron macroparticles declines between each generation and the weight of each macroparticle is greatly reduced. Therefore, after seven generations the additional electron weight of each macroparticle is a factor 10^7 smaller and so can be neglected. After five generations, none of the simulations had more than 5×10^4 remaining macroparticles, which had weights 10^5 times smaller than the primary particles. As $\sim 5 \times 10^5$ primary macroparticles are used in the simulations ($> 3 \times 10^6$ for solar wind simulations), the weight of the remaining particles is less than a single of the primary electrons.

Table 2.2: Ionization products and the associated threshold energy, E_{Th} , for the ionization of water ([Itikawa and Mason, 2005](#)).

Ion Product	Threshold Energy [eV]
H ₂ O ⁺	12.62
OH ⁺	18.1
O ⁺	19.0
H ₂ ⁺	20.7
H ⁺	16.95
O ²⁺	54.1

2.3.3 Elastic scattering

Elastic scattering reorients the velocity of the electron with no energy loss. There are some collision processes that cause a small energy loss and a change in the electron direction, such as the rotational excitation ($E_{Th} = 0.004$ eV). As the energy loss is small, we separate the scattering and

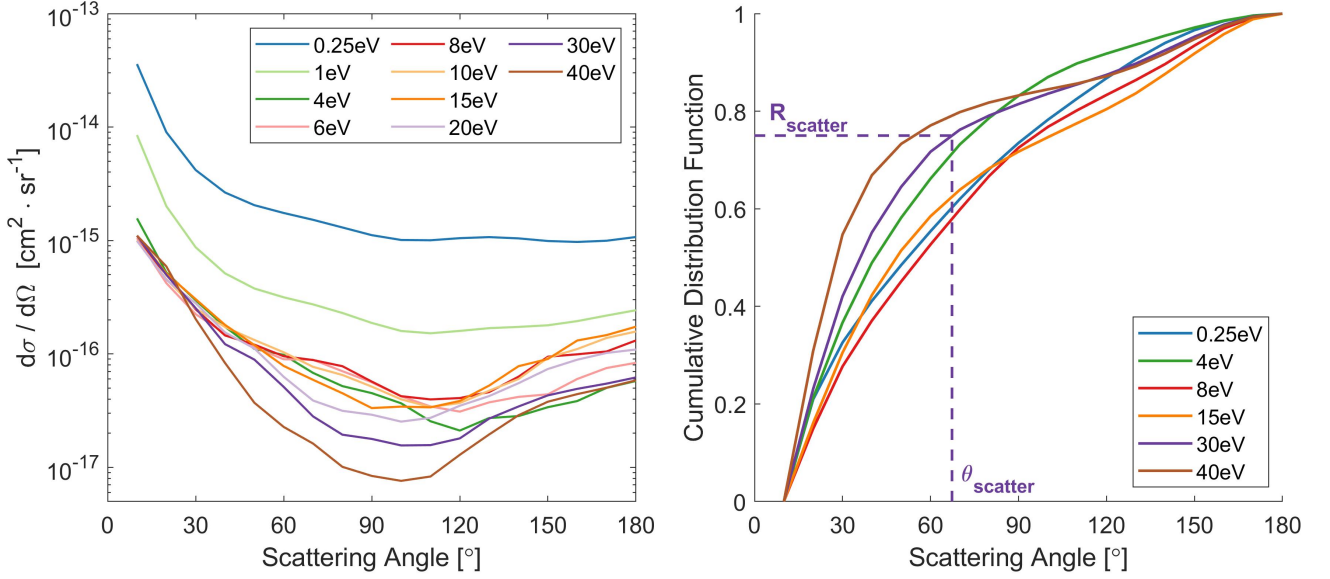


Figure 2.7: (a) Differential scattering cross-section for electron collisions on water from [Cho et al. \(2004\)](#) and [Faure et al. \(2004\)](#). (b) Cumulative distribution functions for a selection of particle energies as a function of scattering angle. The purple dashed line demonstrates how the scattering angle, θ_{scatter} , is derived using a random number, R_{scatter} , for a 30 eV electron.

energy loss into different mechanisms. The energy loss is encapsulated in Section 2.3.1. The elastic scattering presented here includes scattering from purely elastic collisions (no rotational modes excited, $E_{Th} = 0$ eV) and from vibrationally elastic collisions (only very low energy, rotational modes are excited, $E_{Th} \ll 0.1$ eV). These account for the bulk of the angular redistribution, as collisions with higher threshold energies have lower cross sections (see Figure 2.5a) and are more forward peaked.

Differential scattering cross sections from [Faure et al. \(2004\)](#) and [Cho et al. \(2004\)](#) cover energies from 0.25 eV up to 50 eV between 10° and 180° . These incorporate scattering by both rotationally and vibrationally elastic collisions. Any scattering by angles smaller than 10° is neglected, as this is approximately equivalent to no rotation of the velocity. [Cho et al. \(2004\)](#) only provides differential cross sections down to 20° at 4, 6 and 8 eV, so I have extrapolated to 10° by multiplying the cross section at 20° by 2.2. This is consistent with the ratio between the two angles for energies up to 30 eV.

The total elastic scattering cross section (blue, Figure 2.5a) is computed from the differential cross sections between 0.25 and 50 eV. The computed cross section is given by

$$\sigma^{el}(E) = 2\pi \int_{10^\circ}^{180^\circ} \frac{d\sigma}{d\Omega}(E, \theta) \cdot \sin \theta d\theta \quad (2.22)$$

where $\frac{d\sigma}{d\Omega}$ is the differential cross section for the elastic and rotational collisions (see Figure 2.7).

This is not the same as the rotationally elastic cross section provided in [Itikawa and Mason](#)

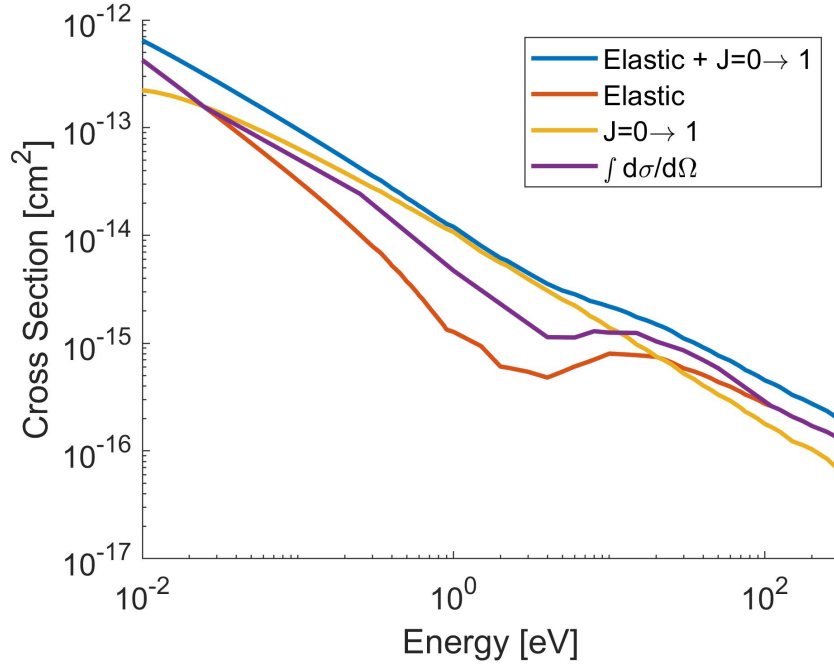


Figure 2.8: Comparison of the derived scattering cross section (purple) to the rotationally elastic ($E_{Th} = 0$ eV, orange) and vibrationally elastic ($J = 0 \rightarrow 1$, $E_{Th} = 0.004$ eV, yellow) cross sections of electron impact on water.

(2005). It additionally includes the scattering cross section from rotational transitions ($J = 0 \rightarrow 1$) but excludes the cross section of particles scattered by less than 10° . The computed cross section (purple, Figure 2.8) sits between the rotationally elastic ($E_{Th} = 0$ eV, red) collision cross section and the sum of the rotationally and vibrationally elastic ($E_{Th} = 0.004$ eV, blue) collisions between 0.25 and 50 eV. This is expected as collisions resulting in a rotational transition are forward peaked (see Figure 2.7a).

Below 0.25 eV and above 50 eV, there are no data for the differential scattering cross section, but the contribution from the rotational transition becomes small compared to the purely elastic collisions. The scattering cross section used in the model is set equal to the elastic scattering cross section in Itikawa and Mason (2005) below 0.03 eV and above 100 eV, as beyond these energies the cross section of the rotational transition (yellow, 2.8) is small compared to the rotationally elastic mode (red). In the intermediate regions (e.g., 0.03 to 0.25 eV), the scattering cross section is calculated using a power law.

The total scattering cross section is used to determine whether an electron is scattered through Eq.s 2.15 and 2.18. If scattering occurs, the degree of angular scattering is then determined. The differential cross section is converted into a cumulative distribution function (cdf), $F(\theta)$ for each energy using:

$$F(\theta) = \frac{2\pi \sum_{X=el,rot} \int_{10^\circ}^{\theta} \frac{d\sigma^{el,X}}{d\Omega}(E, \vartheta) \cdot \sin \vartheta d\vartheta}{\sigma^{el}(E)} \quad (2.23)$$

At 0 eV the elastic scattering is taken as isotropic and above 50 eV the shape of the cdf remains constant at the 50 eV values. The cumulative distribution function is interpolated to the energy of the colliding particle and then a random number R_{scatter} is used to determine the scattering angle as shown in Figure 2.7b.

Once the scattering angle has been determined, the velocity of the incident electron is updated. Firstly, the velocity is transformed into the zero momentum frame (ZMF). As the electron mass is much smaller than the mass of the neutral atoms, the ZMF moves approximately at the outflow velocity of the neutral gas (see Section 2.5.2). Using a more thorough approach, the ZMF velocity varies by $\pm 50 \text{ m s}^{-1}$ for electrons up to 10 eV, depending on the orientation of the neutral and electron velocities. The electron velocity in the ZMF, $\mathbf{v}'$, is given by:

$$\mathbf{v}' = \mathbf{v} - \mathbf{v}_{ZMF} = \mathbf{v} - \mathbf{u}_{gas} \hat{\mathbf{r}}. \quad (2.24)$$

The electron velocity in the ZMF is then rotated through the scattering angle θ'_{scatter} as obtained in Figure 2.7b, to give the new electron velocity $\mathbf{v}'_+$. This is done by increasing the spherical polar angle i.e. $\theta'_{v+} = \theta'_v + \theta'_{\text{scatter}}$, where θ'_v and θ'_{v+} are the polar angles of $\mathbf{v}'$ and $\mathbf{v}'_+$, respectively. To complete the scattering, the new electron velocity, $\mathbf{v}'_+$, is rotated around the original velocity in the ZMF by a random azimuthal angle, ϕ'_{scatter} :

$$\mathbf{v}'_{\text{rot}} = \mathbf{v}'_+ \cos \phi'_{\text{scatter}} + (\hat{\mathbf{v}}' \times \mathbf{v}'_+) \sin \phi'_{\text{scatter}} + \hat{\mathbf{v}}' (\hat{\mathbf{v}}' \cdot \mathbf{v}'_+) (1 - \cos \phi'_{\text{scatter}}). \quad (2.25)$$

The final scattered velocity is then retrieved by re-adding the ZMF velocity.

2.3.4 Validation with the continuous slowing down approximation

To validate the implementation of energy degradation in the test particle model, I have compared the collisional energy loss seen in the model to the continuous slowing down approximation (CSDA). The CSDA is applicable when the energy loss associated with each collision, E_{loss} , is much smaller than the energy of the colliding particle. Instead of modelling the energy loss as an intermittent, stochastic process, it can be viewed as a continuous loss of energy. Removing the probabilistic nature of collisions is far more computationally efficient. The CSDA has been applied in models of proton aurora at Earth (Edgar et al., 1973, 1975), and to proton and electron energy deposition in the atmosphere of Jupiter (Gérard and Singh, 1982; Singhal et al., 1992; Rego et al., 1994). In these cases, the proton energies exceed 1 keV, so the energy loss per collision ($\sim 10 \text{ eV}$) is indeed small compared to the particle energy. Although this approximation is not generally valid for the

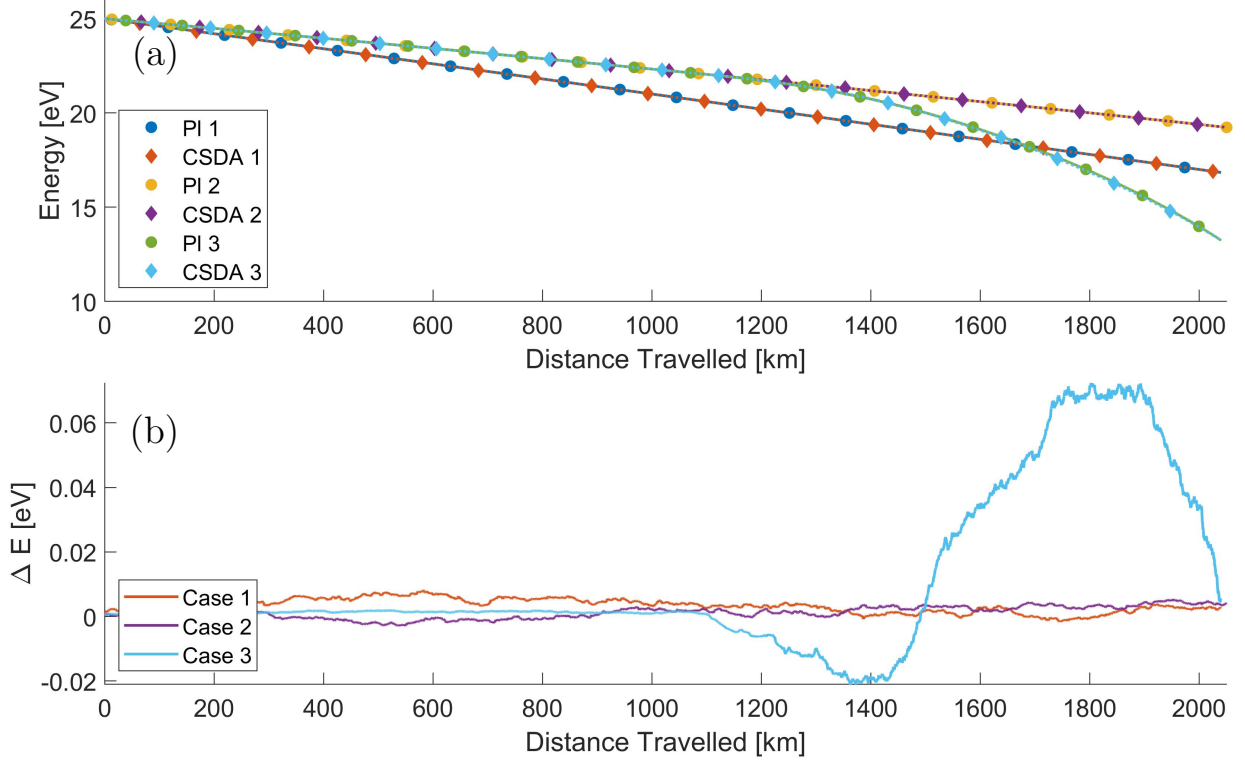


Figure 2.9: (a) Electron energy variation for three test cases for both the test particle model (circles) and CSDA approximation (diamonds). (b) Difference in the test particle energy compared to the CSDA approximation throughout its trajectory for each of the test cases (see Table 2.3). Credit: [Stephenson et al. \(2022\)](#).

case of electrons in the cometary environment, it is useful to compare with a limited version of the test particle model to verify the collisional algorithm.

For a single species, the CSDA gives the rate of energy change with distance as

$$\frac{dE}{dx} = -n(x)L(E) \quad , \quad (2.26)$$

where $n(x)$ is the neutral number density and $L(E)$ is the loss function (see Eq. 2.19). For inelastic excitations of H_2O , which are the processes considered here for the validation, the energy loss is the same as the threshold energy of the collision ($E_{\text{loss},j} = E_{\text{Th},j}$).

The particle energy, using the CSDA, is calculated by integrating the energy loss along the trajectory of the particle. In the test cases presented here, the energy loss per collision is much smaller than the particle energy.

For the validation, the dynamics of the electrons has been significantly simplified. The electric and magnetic fields are set to zero and the macroparticles are created at the same energy with their velocities along $+x$. The neutral density is set as constant throughout the domain ($n_{\text{H}_2\text{O}} = 10^{10} \text{ cm}^{-3}$) for all the tests.

Table 2.3: Summary of the test cases used to validate the collisional cooling processes.

Test case	Energy dependent cross section	Rotational colls ($E_{Th} = 0.004$ eV)	Vibrational colls ($E_{Th} = 0.198, 0.453$ eV)
1	✗	✓	✗
2	✓	✓	✗
3	✓	✓	✓

Three cases are considered here, which include increasingly complex collision processes. These are summarised in Table 2.3. The first case incorporates one process with a constant cross section of $\sigma = 5 \times 10^{-16}$ cm² and a threshold energy of $E_{Th} = 0.004$ eV. The second case is similar, but allows for a variable cross section with energy. Only the rotational transition ($J = 0 \rightarrow 1$, see Fig 2.5a) is included, which has the same threshold energy as in Case 1 ($E_{Th} = 0.004$ eV). The third and final case includes the rotational transition ($J = 0 \rightarrow 1$) and the two vibrational excitations (bending and stretching modes), all with variable cross sections (see Figure 2.5). The threshold energy of the vibrational modes are two orders of magnitude larger ($E_{Th} = 0.198$ and 0.453 eV) than for the rotational excitation. As the energy loss per collision is much larger in this case, it is near the limitations of the CSDA which requires $\Delta E \ll E$. This is acceptable for use in validation of the collisional processes in the test particle model, but the CSDA is not generally applicable to electron degradation in the cometary environment.

In the test particle model, collisions are a stochastic process. For direct comparison to the CSDA, the average energy of 5000 macroparticles is taken across a 2000 km range. The average electron energy from the test particle model is displayed in Figure 2.9a, alongside the expected energy derived using the CSDA. Figure 2.9b shows the residual between the test particle model and CSDA approaches for each of the test cases. Here, the results are presented for electrons initially at 25 eV, although other energies have been tested with similar results.

For the first two cases, the energy loss in the test particle model agrees very closely with the CSDA over the full 2000 km range. In these cases, the threshold energy of the collisions is very low, which satisfies the assumptions of the CSDA. The discrepancy in the energy is less than 0.01 eV for both cases, with the total energy loss reaching up to 8 eV. Therefore, the test particle model is clearly reproducing the expected number of electron collisions and correctly degrading the electron energy.

In case 3, the energy loss associated with the vibrational modes is more comparable to the particle energy, compared to the cases with only rotational excitations. In the first 1000 km, the difference in energy between the test particle model and CSDA is negligible. In this region, the electron energy exceeds 20 eV, so the cross sections of the vibrational excitations are small (see

Fig. 2.5a). The energy loss is driven by the rotational mode. Beyond 100 km, the electron loses energy more quickly and the particle energy deviates more significantly (up to 0.065 eV) from the CSDA, as the vibrational modes begin to contribute significantly (Fig. 2.6). However, the difference in approaches is still very small compared to the energy, E , and energy loss of the electron (deviations of $< 0.5\%$).

Therefore, the test particle model accurately reproduces the expected energy loss as derived using the CSDA, when the CSDA is valid. Generally, it is not viable to use the CSDA in the test particle model as the energy loss per collision is often comparable to the energy of the electron (e.g. a 10 eV electron losing 7 eV by causing dissociation of a water molecule). In light of this, it is imperative that a probabilistic implementation of the collisional processes is used in the cometary environment.

2.4 Moments of the distributions

From the calculation of many macroparticle trajectories, it is possible to calculate the energy distribution function (edf) in four dimensions (three spatial and one energy) and compute moments of the electron population in three spatial dimensions. At each time, t_α , throughout its trajectory, the particle contributes to the macroscopic quantities of the cell it resides in. The size of the contribution depends on the weight of the macroparticle, W_p (see Sections 2.3.2, 2.5.4 and 2.5.5), the length of the timestep dt_α (see Section 2.2.2) and, in some cases, the velocity of the particle $\mathbf{v}_\alpha$. The output values of the statistical quantities are known once all the macroparticles, p , have been simulated, each adding their contribution to the relevant totals.

The energy distribution function (edf) is the number of electrons per unit volume per unit energy [$\text{cm}^{-3} \text{ eV}^{-1}$]. The edf, $f(x_i, y_j, z_k, E_l)$, in a cell, (i, j, k, l) , is given by:

$$f(x_i, y_j, z_k, E_l) = \sum_{p, \alpha} \frac{W_p \times dt_\alpha}{V_{i,j,k} \times dE_l}, \quad (2.27)$$

where $V_{i,j,k} = dx_i \times dy_j \times dz_k$ is the spatial volume of the cell (see Section 2.5.1) and dE_l is the size of the energy bin.

The electron density, $n_e(x_i, y_j, z_k)$, is derived by integrating the edf over the energy space

$$n_e(x_i, y_j, z_k) = \sum_l f(x_i, y_j, z_k, E_l) dE_l = \sum_{p, \alpha} \frac{W_p \times dt_\alpha}{V_{i,j,k}}. \quad (2.28)$$

The bulk velocity, $\mathbf{u}$, of the electrons is:

$$u_s(x_i, y_j, z_k) = \frac{1}{n_e(x_i, y_j, z_k) V_{i,j,k}} \sum_{p,\alpha} W_p \times dt_\alpha \times v_{s,\alpha}. \quad (2.29)$$

where $s = x, y, z$ is the component of the bulk velocity, u_s , and macroparticle velocity, $v_{s,\alpha}$. The square velocity, $\overline{v_s^2}$, is calculated as

$$\overline{v_s^2}(x_i, y_j, z_k) = \frac{1}{n_e(x_i, y_j, z_k) V_{i,j,k}} \sum_{p,\alpha} W_p \times dt_\alpha \times v_{s,\alpha}^2 \quad (2.30)$$

This is used to determine the temperature of the electron distribution, T_e using:

$$\frac{3k_B T_e}{2} = \frac{m_e}{2} \left(\sum_s \overline{v_s^2}(x_i, y_j, z_k) - |\mathbf{u}|^2 \right) \quad (2.31)$$

To ensure the moment results are statistically significant we require that at least 20 particles pass through a given cell to include it in our results. The photoelectron simulations use over 5×10^5 primary macroparticles, while solar wind simulations use over 3×10^6 .

2.5 Initialisation of the model

2.5.1 Grid

Statistical quantities derived from the model (see Section 2.4) are calculated on a three-dimensional Cartesian grid, with its origin at the nucleus. This grid is different to the grid of the magnetic and electric fields, but the resolution is limited by that of the fields (see Table 2.4). The resolution of the moment grid should not be much smaller than the field resolution and structures smaller than this scale may be an artefact, rather than physical. As well as the spatial grid, electrons are separated by energy for properties such as the edf.

The spatial grid is defined using two distinct methods, depending on the purpose. Firstly, a constant grid size is used for validation or direct comparisons to the PiC simulation, which has the same resolution as the fields. Alternatively, a variable cell size is employed. A finer spacing is imposed close to the nucleus, and a coarser grid further away. This is favourable when examining collisional processes, which primarily impact the inner coma. The 10 closest cells to the nucleus have a constant size of 4 km in each dimension. Beyond this, the cell size along each dimension grows exponentially with the distance from the nucleus along that axis, i.e. $dx_i = dx_i(x_i)$, where dx_i is the side length of a cell with midpoint x_i . This variation is also applied in the y and z

directions to give $dy_j = dy_j(y_j)$ and $dz_k = dz_k(z_k)$. The exponential growth continues up to a maximum distance of 1000 km from the nucleus, at which point the grid stops. In some cases, it is preferable to only consider a subset of the domain, so the upper limits of the grid may be reduced to ~ 300 km. The production of photoelectrons is calculated on a separate spatial grid to the output statistical quantities. The grid has the same structure, with variable cell size, but the range of the grid is limited to ± 300 km as $r_{max} = 300$ km for photoelectron production (see Section 2.5.4).

The energy grid is set up similarly to the spatial grid. A constant resolution of 0.5 eV is applied up to 5 eV, beyond which the size of the energy bins increases exponentially. The maximum energy of the grid is set at 300 eV, which is significantly larger than the energy of any electrons seen in the model. Therefore, the contribution from higher energy electrons towards any statistical properties can be neglected.

2.5.2 Neutral coma

The neutral coma fulfils two main functions in this model: to derive the photoelectron production profile, and to degrade electrons in energy through collisions. Currently, a pure water coma with uniform outgassing is assumed for simplicity. This is not wholly reflective of the outgassing at comet 67P, which showed significant spatial variation in the outgassing rate across the surface of the nucleus (Fougere et al., 2016a,b; Biver et al., 2019). This approximation also neglects the presence of CO₂, which became abundant in the southern hemisphere of 67P post-perihelion (Hässig et al., 2015; Gasc et al., 2017a; Läuter et al., 2018). There is scope to develop the model of the neutral coma with asymmetric outgassing (e.g. Hansen et al., 2016) or to incorporate additional species in the future.

As H₂O is outgassed from the comet surface through sublimation of water ice (as opposed to having an extended source), the neutral number density is given by the Haser model (Haser, 1957):

$$n_{\text{H}_2\text{O}}(r) = \frac{Q}{4\pi u_{\text{gas}} r^2}, \quad (2.32)$$

where Q is the global outgassing rate of H₂O, u_{gas} is the radial outflow speed of the neutral gas and r is the cometocentric distance. It is assumed that the outflow speed is constant ($u_{\text{gas}} = 1 \text{ km s}^{-1}$). This neglects variation due to the expansion of the neutral gas, but this was only important within the first few kilometres of the nucleus (Heritier et al., 2017b).

In this thesis, I use three sets of outgassing conditions: $Q = 10^{26} \text{ s}^{-1}$, $Q = 3 \times 10^{26} \text{ s}^{-1}$ and $Q = 1.5 \times 10^{27} \text{ s}^{-1}$. The full sets of simulation parameters are given in Table 2.4. In this chapter, I

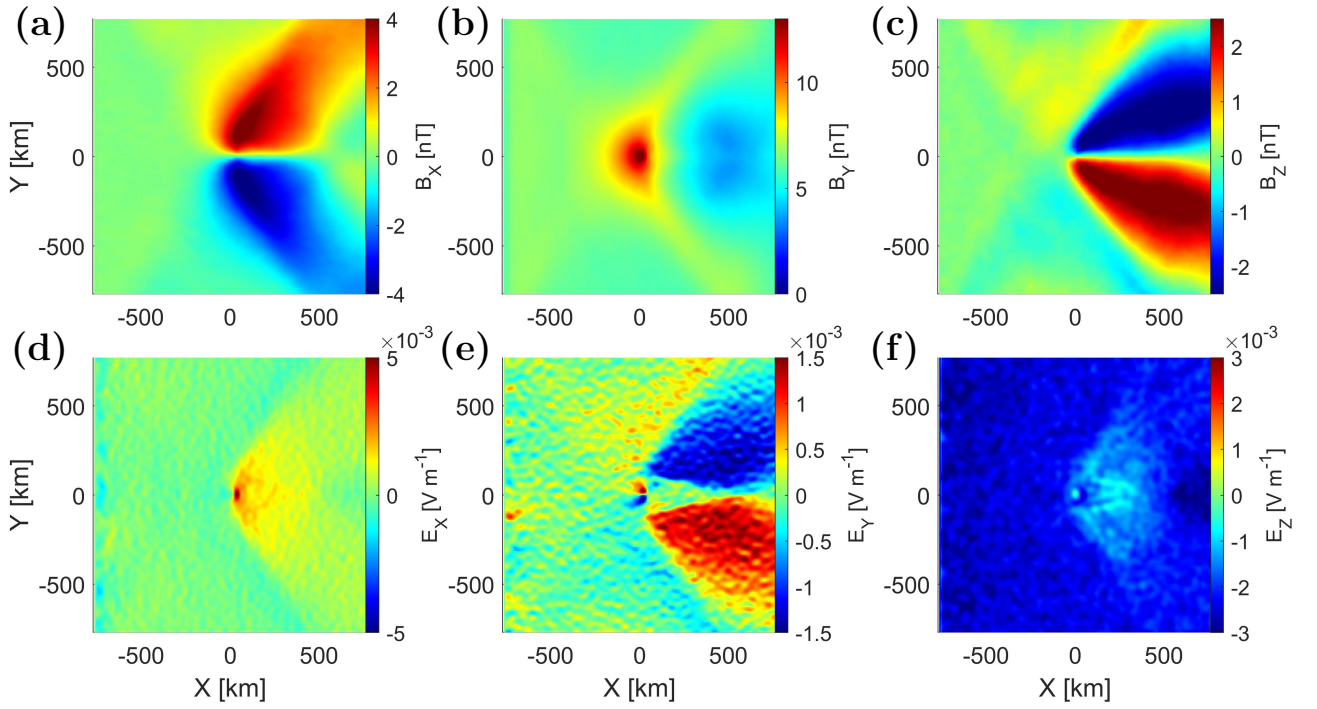


Figure 2.10: Electric and magnetic fields from a fully kinetic, self-consistent, collisionless PiC simulation at $Q = 10^{26} \text{ s}^{-1}$ (see Table 2.4 Deca et al., 2017, 2019). (a)-(c): components of the magnetic field in the xy plane with the nucleus at the origin. (d)-(f): components of the electric field in the same plane.

focus mainly on the simulation at $Q = 10^{26} \text{ s}^{-1}$, but the other two cases have also been validated. All three simulations are used in Chapter 3 to examine the cooling of electrons. The first and third cases are used in Chapter 5 to explore the origin of electrons in the coma.

Table 2.4: Parameters of the test particle simulations.

Parameter		Simulation 1	Simulation 2	Simulation 3
Q	$[\text{s}^{-1}]$	10^{26}	3×10^{26}	1.5×10^{27}
n_{SW}	$[\text{cm}^{-3}]$	1	1	1
T_{SW}	$[\text{eV}]$	10	30	10
$u_{SW,x}$	$[\text{km s}^{-1}]$	400	400	400
$\nu_{h\nu}^{ioni}$	$[\text{s}^{-1}]$	1.32×10^{-7}	1.32×10^{-7}	1.32×10^{-7}
$T_{h\nu}$	$[\text{eV}]$	10	30	10
u_{gas}	$[\text{km s}^{-1}]$	1	1	1
$B_{SW,y}$	$[\text{nT}]$	6	6	6
dx_{EB}	$[\text{km}]$	7.66	10	10

2.5.3 Electric and magnetic fields

The electric and magnetic fields used in the test particle model are time-averaged fields self-consistently calculated in a fully kinetic, collisionless PiC simulation (Deca et al., 2017, 2019). The field components in the xy plane are shown in Figure 2.10, for an outgassing rate of $Q = 10^{26} \text{ s}^{-1}$.

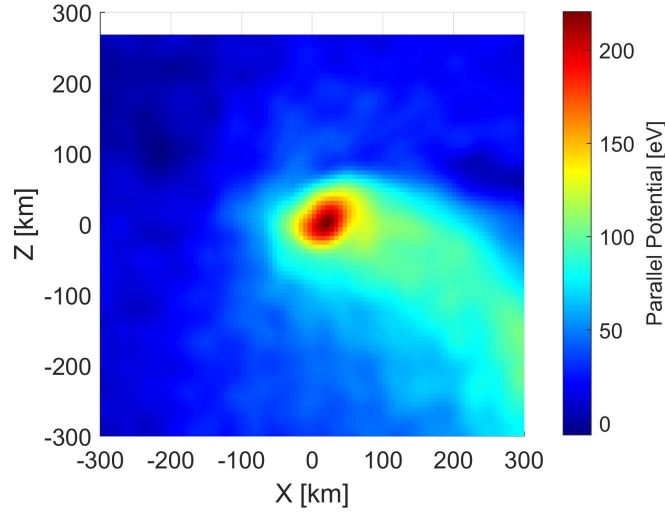


Figure 2.11: Depth of the ambipolar potential well parallel to the magnetic field. Computed using fields from a PiC simulation at an outgassing rate of $Q = 10^{26} \text{ s}^{-1}$ (see Figure 2.10).

The fields are a stationary input to the model. By construction, there is no feedback on the fields from particles simulated in the test particle model. Therefore, it is important that the bulk properties of the simulated electrons are similar between the PiC and test particle simulations, to ensure the fields are consistent. To this end, the properties of the neutral coma and solar wind used in the test particle model are the same as those used to generate the set of fields in the PiC simulation (see Table 2.4). Other simulation parameters, such as the photoionization rate, are also kept the same to minimize any differences. The validation of the fields in both collisionless and collisional cases is presented in Section 2.6.

The fields from the PiC simulation are given on a grid including 288 points in each dimension spanning a domain of $2200 \text{ km} \times 2200 \text{ km} \times 2200 \text{ km}$. At the upstream boundary, the pristine solar wind conditions are $\mathbf{B} = 6 \text{ nT } \hat{\mathbf{y}}$ and $\mathbf{E} = -2.4 \times 10^{-3} \text{ V m}^{-1} \hat{\mathbf{z}}$. This gives a bulk solar wind speed of $u_{SW} = 400 \text{ km s}^{-1}$, which is driven by the $\mathbf{E} \times \mathbf{B}$ drift. Closer to the nucleus, cometary ions and electrons present a barrier to the solar wind, causing a pile-up of the magnetic field (see Figure 2.10b). The cometary plasma also contributes towards additional components of the electric field in the inner coma, such as the Hall and ambipolar fields. The ambipolar field, which is generated by an electron pressure gradient, sets up a potential well around the nucleus. The depth of the potential well, calculated parallel to the magnetic field lines, peaks close to the nucleus at $\approx 200 \text{ eV}$ at $Q = 10^{26} \text{ s}^{-1}$ (Figure 2.11). This potential well is a key driver of electron trapping in the coma and can accelerate solar wind electrons (see Section 2.5.5).

2.5.4 Photoelectrons

Photoelectrons are produced through photoionization of the neutral coma by extreme ultraviolet photons. When the coma is optically thin, a constant photoionization frequency is used throughout the across the simulation domain. This can be verified with the Beer-Lambert law

$$I(\mathbf{x}, \lambda) = I_0(\lambda) \times e^{-\tau(\mathbf{x}, \lambda)} = I_0 \exp \left[\sigma^{\text{abs}}(\lambda) \times \int_{-\infty}^x n(\mathbf{x}') dx' \right], \quad (2.33)$$

where the integral gives the column density from the Sun to the position of interest. I is the solar photon flux, $\tau(\mathbf{x}, \lambda)$ is the optical depth, and σ^{abs} is the wavelength-dependent absorption cross section. For an outgassing rate of $Q = 10^{26} \text{ s}^{-1}$, the optical depth is small ($\tau \ll 1$) throughout the coma (Heritier et al., 2018a) so any attenuation can be neglected. Therefore, we use a constant photoionization frequency throughout the coma. At $Q = 1.5 \times 10^{27} \text{ s}^{-1}$, the solar flux is attenuated by less than 10% in the inner coma (10 km) so using a constant photoionization frequency is a reasonable approximation.

For consistency with the PiC simulations, we use a photoionization frequency of $\nu_{h\nu}^{\text{ioni}} = 1.32 \times 10^{-7} \text{ s}^{-1}$, which corresponds to a heliocentric distance of 2.3 au (Huebner and Mukherjee, 2015). At 2.3 au, comet 67P was outgassing water at a rate of $\sim 3 \times 10^{26} \text{ s}^{-1}$, which is a similar to those used in the PiC simulations (Biver et al., 2019).

The weight of each photoelectron macroparticle produced within a cell is given by

$$W_p = \frac{1}{N_p} \int_{\text{Cell}} \nu_{h\nu}^{\text{ioni}} n(\mathbf{x}) d^3\mathbf{x}, \quad (2.34)$$

where N_p is the number of macroparticles produced within the photoelectron cell (see Section 2.5.1). The macroparticles are then created at random locations within the cell. The dimensions of the cells are small enough that the production rate of photoelectrons follows a $1/r^2$ dependence with cometocentric distance. In the case of an optically thin coma, the spatial variation is inherited directly from the neutral coma. If the coma were optically thick, the solar flux would become attenuated close to the nucleus in dense regions of the coma, and consequently decrease photoelectron production in the inner coma.

The photoelectron energy distribution is approximated by a 10 eV Maxwellian (Cravens, 1987; Galand et al., 2016), which is consistent with the PiC simulations (Deca et al., 2019, 2017). The velocities of the photoelectron macroparticles are generated using the Box-Mueller transformation (Box and Muller, 1958). Two uniform random variables $U_{1,2}$, in the interval $[0, 1]$, transform into

two independent, normally-distributed, random numbers, $R_{v,1}$ and $R_{v,2}$, through:

$$R_{v,1} = \sqrt{-2 \log(U_1)} \times \cos(2\pi U_2) \quad (2.35)$$

$$R_{v,2} = \sqrt{-2 \log(U_1)} \times \sin(2\pi U_2). \quad (2.36)$$

The same algorithm is applied to a second pair of numbers, $U_{3,4}$, to generate R_3 . The normally distributed random numbers are converted to components of the photoelectron velocity using

$$v_x = \varsigma_v \times R_{v,1}, \quad v_y = \varsigma_v \times R_{v,2}, \quad v_z = \varsigma_v \times R_{v,3}, \quad (2.37)$$

where $\varsigma_v = \sqrt{\frac{k_B T_{h\nu}}{m_e}}$ is the width of the velocity distribution and $T_{h\nu}$ is the photoelectron temperature.

Validation of photoelectron production

The spatial distribution and weighting of photoelectron macroparticles is validated by comparison to the case of radially outflowing electrons. Electrons are produced with a uniform outflow velocity, which is the same as the outflow velocity of the neutral gas, u_{gas} . Plasma loss is assumed to be only through transport, and there is no acceleration of the bulk plasma flow as it moves radially away from the nucleus. This can be solved analytically in the case where the optical depth of the coma is small (Galand et al., 2016). Under these conditions and with a uniform photoionization frequency, the electron density is given by:

$$n_e(r) = \frac{Q\nu_{h\nu}^{ioni}}{4\pi u_{gas}^2} \frac{(r - r_c)}{r^2}. \quad (2.38)$$

The test particle simulation is set up to mirror the radial outflow conditions. All macroparticles are created with an initial velocity of $\mathbf{v} = u_{gas}\hat{\mathbf{r}}$, which is dependent on the initial position. The electric and magnetic fields are set to zero, so there is no evolution of the particle velocity with time.

The electron densities computed analytically and with the test particle model are shown in Figures 2.12a and b, respectively. The test particle electron density is within 15% of the theoretical value throughout the domain, and varies around the expected value. The higher levels of variation are due to fairly low numbers of macroparticles produced close to the nucleus, which are weighted more heavily. With improved statistics, the density deviations would be significantly reduced. As the electron density has the same radial variation and magnitude as expected, the initialization of the photoelectrons is implemented correctly.

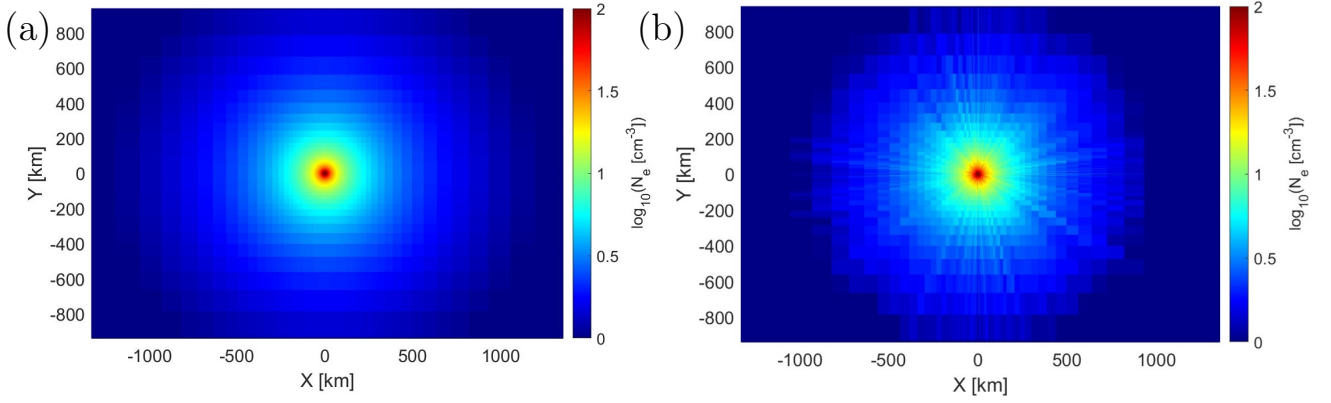


Figure 2.12: Electron density in the xy plane for radially outflowing electrons using (a) the analytical expression (Eq. 2.38) and (b) the test particle model. Lines of higher density are associated with the paths of electrons from the innermost region of the coma, where the electrons are more heavily weighted. Credit: [Stephenson et al. \(2022\)](#).

Trajectory of a photoelectron

Figure 2.13 gives an example trajectory of a photoelectron through the realistic electric and magnetic fields (see Fig. 2.10 [Deca et al., 2019](#)), produced within the coma at $(-49.5, -2.7, -72.6)$ km. It is produced at 20.56 eV (blue, Figure 2.13b), with 12.3 eV of the initial energy perpendicular to the magnetic field (orange). The electron is initially directed towards the inner coma, and falls into the ambipolar potential well ([Deca et al., 2017](#)). The electron's parallel energy (yellow, Figure 2.13b) increases to 12 eV, before falling to 0 eV as it tries to leave the inner coma and the potential well. This trapping continues for several oscillations, during which the parallel energy reaches a maximum of 24 eV. The perpendicular energy (orange) varies within a gyration as the electron $\mathbf{E} \times \mathbf{B}$ drifts, causing it to appear as an orange band (Figure 2.13b).

The particle energy and the fields at the particle have been used to calculate theoretical drift velocities (using Eqs. 2.10, 2.11 and 2.12), at each point along the electron trajectory. The sum of the calculated drifts closely agree with the gyroaveraged particle velocity, perpendicular to the magnetic field. The gyroaveraged motion perpendicular to $\mathbf{B}$, is mostly driven by an $\mathbf{E} \times \mathbf{B}$ drift (up to a speed of $6 \times 10^5 \text{ m s}^{-1}$), with a smaller contribution from the curvature drift (up to $6 \times 10^4 \text{ m s}^{-1}$) seen in the inner coma. The curvature drift is caused by draping of magnetic field lines around the cometary ionosphere. After $t = 1.2$ s, the electron follows the theoretical $\mathbf{E} \times \mathbf{B}$ drift as it flows into the tail.

The electron collides twice as it is trapped in the inner coma by the ambipolar potential well, seen as sharp changes in the perpendicular energy (orange) in Figure 2.13b. The electron is elastically scattered by 122° at $t = 0.54$ s. In the scattering, the perpendicular energy increases from 12.6 eV to 20.22 eV, while the parallel energy undergoes a corresponding decrease (15.04 eV

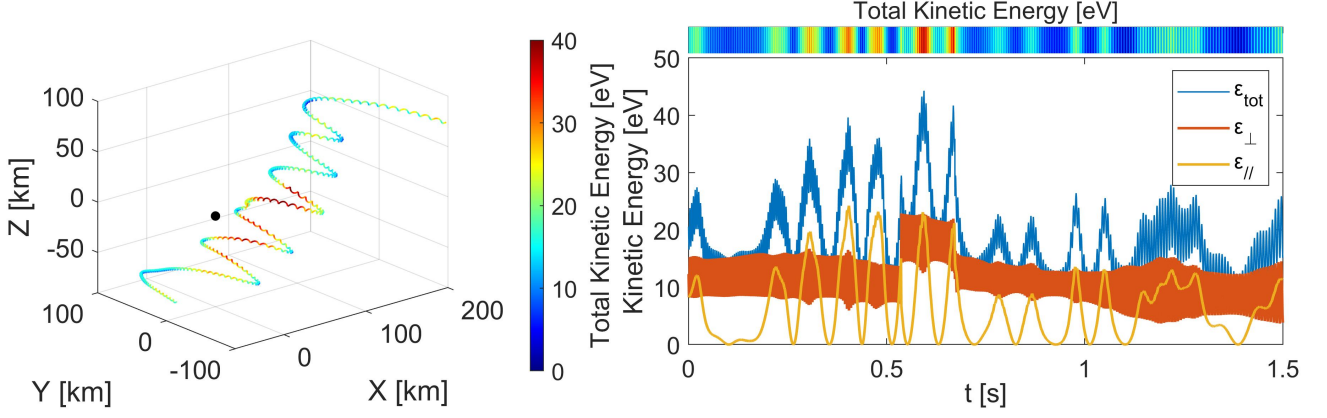


Figure 2.13: (a) Trajectory of a photoelectron through the cometary environment, colour-coded by the particle energy. (b) The total (blue), perpendicular (red) and parallel (yellow) energy of the photoelectron, as it moves through the coma and collides with neutrals. The colorbar above (b) corresponds to the energy variation of the particle and the colormap of the trajectory in (a).

to 7.42 eV). The electron causes an electronic excitation ($E_{Th} = 10$ eV) at $t = 0.67$ s, causing a reduction in energy from 35.9 eV to 25.9 eV, which is proportionally split between the perpendicular and parallel directions.

2.5.5 Solar wind electrons

The solar wind is the second source of primary electrons in the coma. The electrons enter the simulation at the boundaries of the domain, where the solar wind is assumed to be undisturbed. The electrons are approximated by a 10 eV Maxwellian distribution shifted to the bulk flow velocity ($\mathbf{u}_{SW} = 400 \text{ km s}^{-1} \hat{\mathbf{x}}$), in all three of the simulations (see Table 2.4). The velocity distribution function (vdf) of the solar wind electrons is

$$f_{SW}(\mathbf{x}, \mathbf{v}) = n_{SW}(\mathbf{x}) \left(\frac{m_e}{2\pi k_B T_{SW}} \right)^{\frac{3}{2}} \exp \left(- \frac{m_e |\mathbf{v} - \mathbf{u}_{SW}|^2}{2k_B T_{SW}} \right), \quad (2.39)$$

where T_{SW} is the solar wind electron temperature.

The thermal speed of the solar wind electrons, $v_{th} = \sqrt{\frac{2k_B T_{SW}}{m_e}} = 1870 \text{ km s}^{-1}$, greatly exceeds the bulk SW speed, so a significant number of electrons will enter the simulation domain from the boundaries in the y and z directions as well as from the upstream x boundary.

Particles entering the domain at the downstream boundary are dragged further downstream by the $\mathbf{E} \times \mathbf{B}$ drift. Using simulations of only downstream particles, I have validated that no electrons generated at the downstream boundary pass within 500 km of the nucleus and can therefore be neglected. The conditions of the electrons are also less well constrained than at the other boundaries, as the pristine solar wind is disturbed by the comet.

The y and z velocities of newly born solar wind electrons are sampled from the vdf using the Box-Mueller algorithm (see Eq. 2.35; Box and Muller, 1958), with $\varsigma_v = \sqrt{\frac{k_B T_{SW}}{m_e}}$. The x velocity is shifted to correct for the bulk flow of the solar wind plasma:

$$v_x = u_{SW,x} + \varsigma_v \times R_{v,1}. \quad (2.40)$$

A macroparticle must have a velocity into the domain in the direction along which it enters the simulation. The weight of each solar wind macroparticle, W_p , is given by

$$W_p = \frac{A_{Face} \times n_{SW,in} \times v_{\perp}}{N_{Face}} \quad (2.41)$$

where N_{Face} is the number of macroparticles created at each face of the domain and A_{Face} is the area of the face through which it enters the domain. $v_{\perp}$ is the velocity of the macroparticle perpendicular to that face, and must point into the simulation box. $n_{SW,in}$ is the zeroth-order moment (number density) of particles entering the simulation domain at the given face. For example, at the upstream boundary, $\mathbf{x}_{up}$,

$$n_{SW,in} = \int_{v_z=-\infty}^{\infty} \int_{v_y=-\infty}^{\infty} \int_{v_x=0}^{\infty} f_{SW}(\mathbf{x}_{up}, \mathbf{v}) \, dv_x dv_y dv_z, \quad (2.42)$$

which gives $n_{SW,in} = 0.61 \text{ cm}^{-3}$ for the realistic electron mass.

Validation in quiet solar wind conditions

To validate the production scheme for solar wind electrons, quiet solar wind conditions are considered. The electric and magnetic fields are uniform throughout the simulation domain. The interplanetary magnetic field is set to $\mathbf{B} = 6 \text{ nT } \hat{\mathbf{y}}$ and the accompanying electric field is $\mathbf{E} = -2.4 \times 10^{-3} \text{ Vm}^{-1} \hat{\mathbf{z}}$. The parameters of the solar wind are given by $n_{SW} = 1 \text{ cm}^{-3}$, $v_{SW} = 400 \text{ km s}^{-1} \hat{\mathbf{x}}$ and $T_{SW} = 10 \text{ eV}$ (see Table 2.4). The solar wind bulk velocity is the same as the velocity of the $\mathbf{E} \times \mathbf{B}$ drift, which is driven by the fields. As only the production scheme is being tested here, no collisions are included in this simulation and no neutral coma is required.

The electron density is very close to $n_{SW} = 1 \text{ cm}^{-3}$ throughout the simulation domain (see Fig. 2.14a), with an increase by up to 3% near the upstream boundary of the domain. This variation is small compared to the variation of the electron density between cycles of the PiC simulation, so can be neglected. The bulk velocity (not shown) and electron temperature (see Figure 2.14b) are centred on their expected values of $v_{SW} = 400 \text{ km s}^{-1} \hat{\mathbf{x}}$ and $T_{SW} = 10 \text{ eV}$,

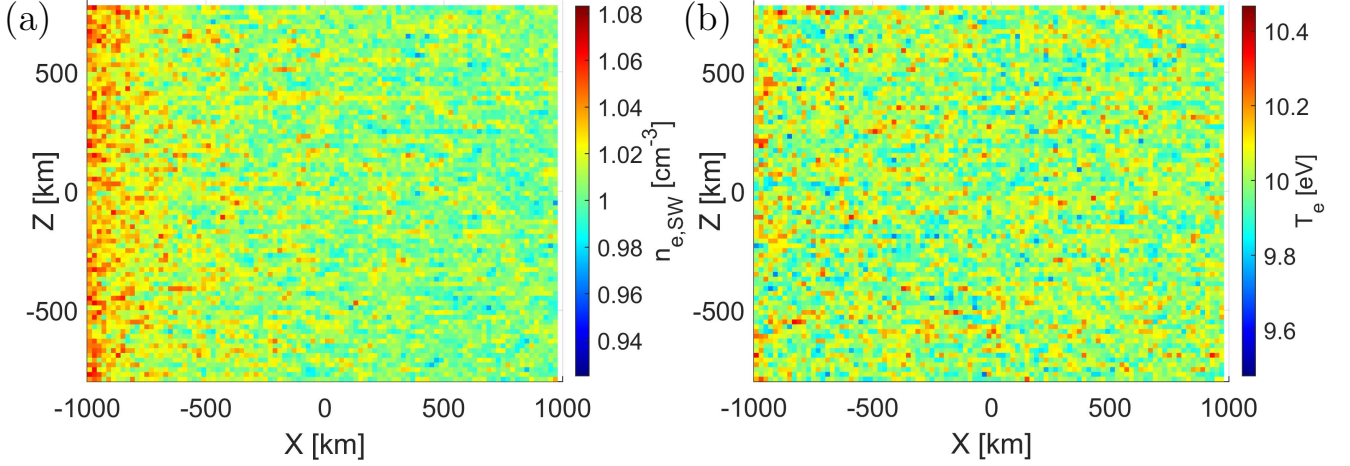


Figure 2.14: Properties of solar wind electrons under quiet solar wind conditions. (a) Electron density in the xz plane. (b) Solar wind electron temperature calculated from Eq. 2.31 in the xz plane. Reproduced from Stephenson et al. (2022).

respectively, and do not vary substantially ($< 2\%$) across the simulation domain. Therefore, the weighting and initialization of the solar wind electrons is validated.

Trajectory of a solar wind electron

Figure 2.15 shows an example of a solar wind electron that falls into the ambipolar potential well and causes ionization. The secondary electron is also shown, but the trajectory has been shifted by 200 km along y to improve visibility. The solar wind electron enters the domain with 27.6 eV and is accelerated to 110 eV as it enters the inner coma. This is mostly seen as an increase in the perpendicular energy (from 25 eV to 100 eV).

Some energy gain is caused by the curvature drift, which has a substantial component anti-parallel to the electric field ($\mathbf{v}_{curv} \cdot \hat{\mathbf{E}} \sim -2 \times 10^4 \text{ m s}^{-1}$). The magnetic field strength also increases substantially from 6 nT to 13.6 nT along the trajectory. Under adiabatic conditions, the perpendicular energy scales linearly with field strength, and energy is transferred from parallel to perpendicular with increasing field strength. In the test particle simulations, the electron motion is not adiabatic, given the presence of an ambipolar potential well, but the increasing field strength converts energy from parallel to perpendicular. This limits the parallel energy of the electron and ensures that it is confined by the ambipolar field.

During the trapping, the solar wind electron passes within 3 km of the nucleus and causes electron-impact ionization. The incident electron loses 61 eV, and generates a secondary electron with an initial energy of 43.14 eV. The secondary electron is also confined by the ambipolar electric field, and causes ionization (producing a tertiary electron). The secondary electrons behave

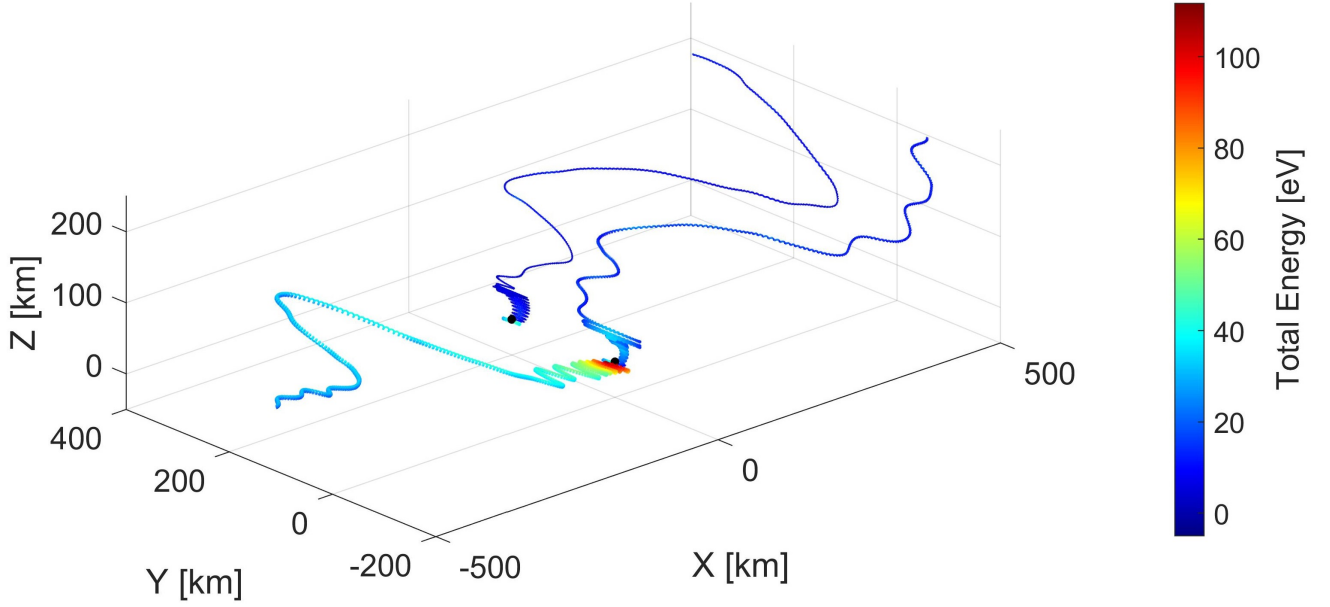


Figure 2.15: Trajectory of a solar wind electron through the cometary environment, color-coded by the particle energy. The solar wind electron undergoes collisions in the inner coma, one of which ionizes a neutral atom. The secondary electron trajectory is also plotted, but shifted by 200 km in the $+\hat{y}$ direction for clarity. Reproduced from [Stephenson et al. \(2022\)](#).

similarly to photoelectrons within the coma (see Section 2.5.4).

2.6 Validation with PiC fields and the impact of the electron-ion mass ratio

In order to validate the test particle approach, the outputs of the model are compared to the results of the PiC simulations, under collisionless conditions. However, the electron mass in the PiC simulations is artificially increased, to reduce the computational demand. As the electron mass directly impacts the electron path length, through the gyroradius, it is important to use the true physical electron mass for collisional simulations. Large scale, fully kinetic, three-dimensional PiC simulations using a physical ion-electron mass ratio are beyond even state-of-the-art computational facilities. Therefore, artificially reduced ion-electron mass ratios are used in such models, even if the impact of using such reduced mass ratios is not assessed. The test particle model can explore the use of a physical electron mass, as it is much less computationally demanding than the PiC model. The comparison between collisional simulations with different electron masses can assess the impact of a reduced ratio and provide insight into how collisional processes may be adjusted when applied in a collisional PiC simulation.

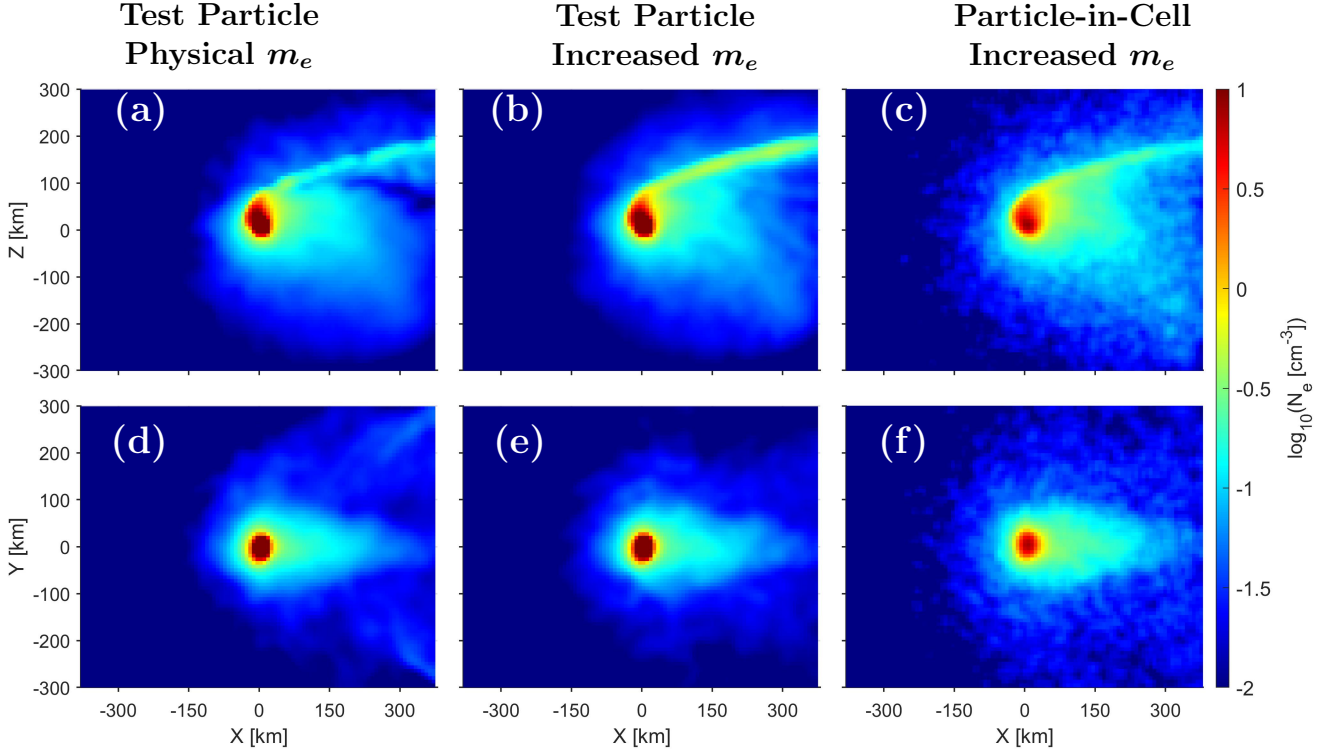


Figure 2.16: Density of photoelectrons in the xz (a-c) and xy (d-f) planes for slices through the nucleus. (a) and (d) are from test particle simulations using the physical electron mass. (b) and (e) are also collisionless test particle simulations, but using an artificially increased electron mass $m_e = m_p/100$. Finally, (c) and (f) depict densities from the PiC model which uses the increased electron mass. The electron densities in the PiC simulation have been smoothed using a $3 \times 3 \times 3$ sliding window. Adapted from [Stephenson et al. \(2022\)](#).

2.6.1 Validation in the collisionless case

To understand the impact of the electron mass on a collisionless simulation, we consider three simulations in the following discussion. The first is a collisionless test particle simulation using the physical electron mass ($m_e = 9.11 \times 10^{-31}$ kg). The second is also a test particle simulation, but using the artificially increased electron mass ($m_e = m_p/100$), as used in a PiC simulation. The final case is the PiC simulation with $m_e = m_p/100$. The fields used as an input in the test particle simulations are calculated from the PiC simulation to which the test particle simulations are compared (see Section 2.5.3).

Photoelectrons The production of photoelectrons in the PiC simulation is capped close to the nucleus ($r < 11$ km), in order to reduce the computation time. For the validation of the test particle model, we apply this same cap to the production of photoelectrons. However, outside of the validation case the production rate is not capped in the test particle model, as this most closely resembles the physical case.

When the same artificially increased electron mass is used, the test particle (Figs. 2.16b and e)

and PiC (Figs. 2.16c and f) simulations produce electron clouds with similar shapes and magnitudes across the wider coma.

In both simulations, a wide high density region extends up to 400 km downstream from the inner coma in the xy plane (Figs. 2.16e and f). This near-tail region is also present when the realistic electron mass is used (Fig. 2.16d), and exhibits the same properties as in the higher mass cases. The electron densities in this tailward region are within 15% of the PiC electron densities for both test particle simulations.

A narrower tailward branch is seen extending from the inner coma in the xz plane, moving towards $+z$ as it moves downstream. This structure has the same width in z when the increased mass is used in the test particle simulation. Up to 100 km downstream of the nucleus, the electron density in the test particle model (Figure 2.16b) is 25% larger than the density in the PiC simulation (Figure 2.16c). However, beyond 100 km downstream the width of the shapes of the near-tail regions diverge. The electrons are more tightly confined along y in the test particle simulation than for the PiC model. As such, the densities are larger in the test particle simulation by 80%, but the total number of electrons in the region is similar when the width of the tail is accounted for. The difference between stationary and dynamic fields in the simulations may drive the disparity in the extent of the tail.

The shape of the inner coma is consistent between the PiC and increased mass test particle simulations, but the magnitude of the electron density is 3.5 times larger for the test particle model. Some of this difference can be attributed to a difference in the photoelectron production scheme close to the nucleus: the PiC simulation uses a larger cometary radius than the test particle model (1.7 km), so fewer electrons are produced in the inner coma. When cometary radius is increased in the test particle model, the difference in electron density is reduced to a factor of 2 close to the nucleus. The efficient trapping by the ambipolar field and the high production rates close to the nucleus mean that the electron densities are very sensitive to the plasma production in this region. Going forward, this should be refined in future kinetic simulations of cometary plasma, whether fully-kinetic or hybrid.

When using the physical electron mass in the test particle simulation, the electron density (see Figures 2.16a and d) is not significantly perturbed from the high mass case across the wider coma. There is some deviation in the near-tail region seen in the xz plane (Figure 2.16a), where the electron density is reduced by 30% relative to the PiC simulation. This structure has a narrower profile in z but extends further in the y direction than for the simulation with increased electron mass. Additionally, a low density region below the tailward branch is seen in the xz plane. This is attributed to the thinned profile of the near-tail region in the xz plane, which arises from

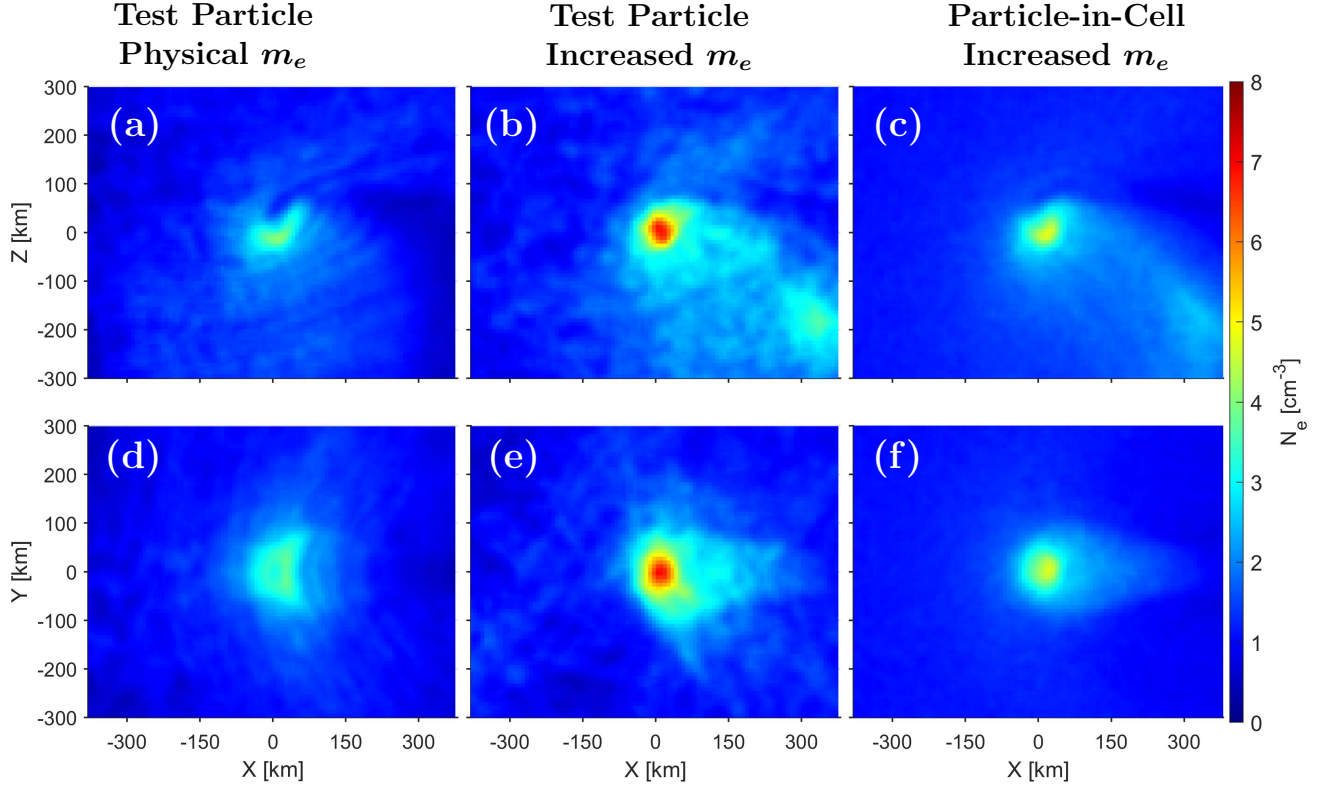


Figure 2.17: Density of solar wind electrons in the xz (a-c) and xy (d-f) planes for slices through the nucleus. (a) and (d) are from collisionless test particle simulations using the physical electron mass. (b) and (e) are also collisionless test particle simulations, but using an artificially increased electron mass $m_e = m_p/100$. Finally, (c) and (f) depict densities from the PiC model which uses the increased electron mass. The electron densities have been smoothed with a $3 \times 3 \times 3$ sliding window. Adapted from [Stephenson et al. \(2022\)](#).

differences in the electron transport. The low density region also correlates closely to the shallowest region of the potential well (see Figure 2.11), suggesting that many electrons do not have sufficient energy to reach that part of the coma.

To summarize, the PiC and test particle simulations are largely in agreement throughout the wider coma, when the same electron mass is used. The higher density seen close to the nucleus in the test particle model is primarily caused by distinctions in the production schemes, but there is also a contribution from the stationary nature of the fields (as opposed to temporally evolving fields in the PiC). The different natures of the fields may also be responsible for dissimilarities in the tailward structures, when using the artificially increased electron mass. When the physical mass is used, there are no major changes from the high mass case. The structure of the tailward region is somewhat altered, due to changes in the electron transport from the inner coma. This is a consequence of the different velocity scales occupied by the heavy and light electrons. The impact of electron mass on the simulations is further discussed in Section 2.6.2.

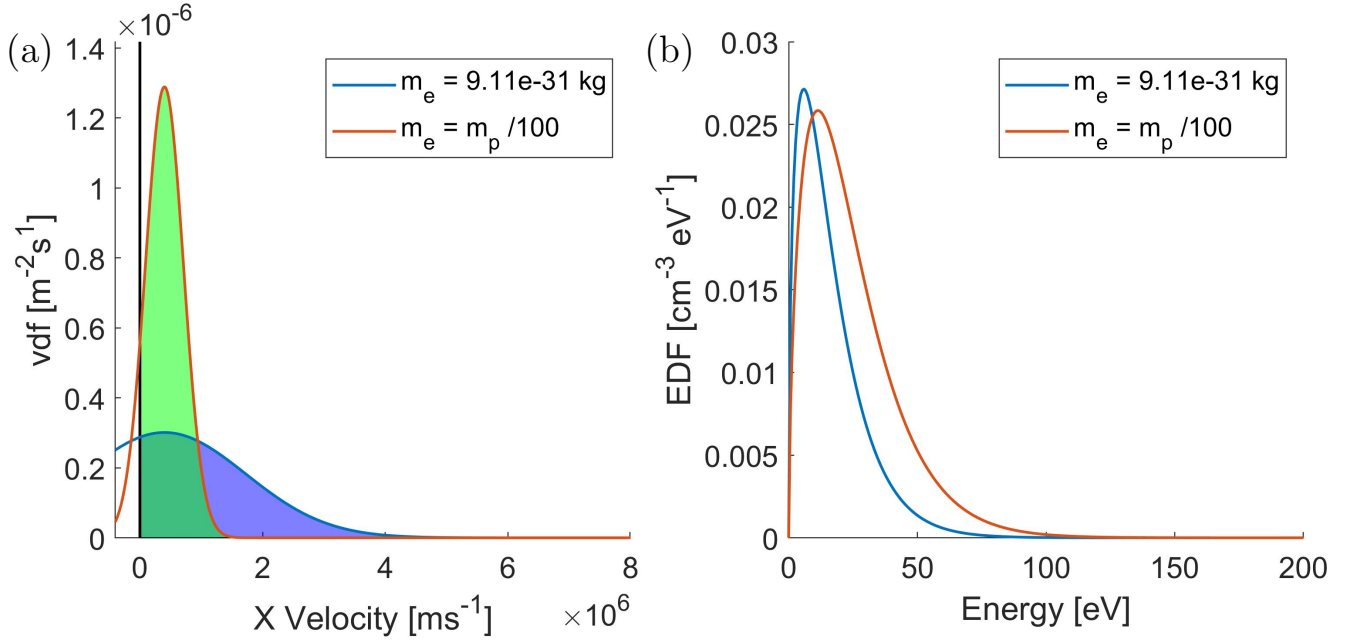


Figure 2.18: (a) Distribution of 10 eV solar wind electron velocities along x for a realistic (blue) and increased (orange) electron mass, for a bulk velocity of $v_{SW} = 400 \text{ kms}^{-1} \hat{x}$. The shaded areas indicate the electrons which enter the domain at the upstream boundary. (b) Distribution of electron energies entering the simulation at the upstream boundary for physical and increased electron masses.

Solar Wind Electrons The solar wind population is validated by comparing two collisionless test particle simulations, with a physical (Figures 2.17a and d) and an increased electron mass (Figures 2.17b and e), to the PiC solar wind electrons (Figures 2.17c and f).

When the same artificially increased electron mass is used, the test particle and PiC simulations produce electron clouds of very similar shape (see Figures 2.17b, c, e and f). In both cases, there is a high density of electrons around the nucleus. This results from the ambipolar field, which funnels electrons towards the deepest part of the potential well (see Figure 2.11). The high density region extends downstream from the inner coma and towards $-x$ through transport of the electrons. The near tail also correlates closely with the regions where the potential well is strongest. A region of enhanced density is present in the near tail at (300,0,-200) km in both the test particle and PiC simulations. However, despite these similarities, the electron density is 40% larger in the test particle simulation around the inner coma. The density peaks at 7 cm^{-3} in the test particle model, whereas in the PiC simulation the maximum electron density is only 5 cm^{-3} . The higher density arises from the lack of evolution in the fields by construct of the test particle simulation.

When the physical electron mass is used (Figures 2.17a and d) the electron density clearly diverges from the high mass cases. The maximum electron density peaks around 4.5 cm^{-3} , similar to the PiC simulation. However, the high density region is not spherical, forming a banana-like

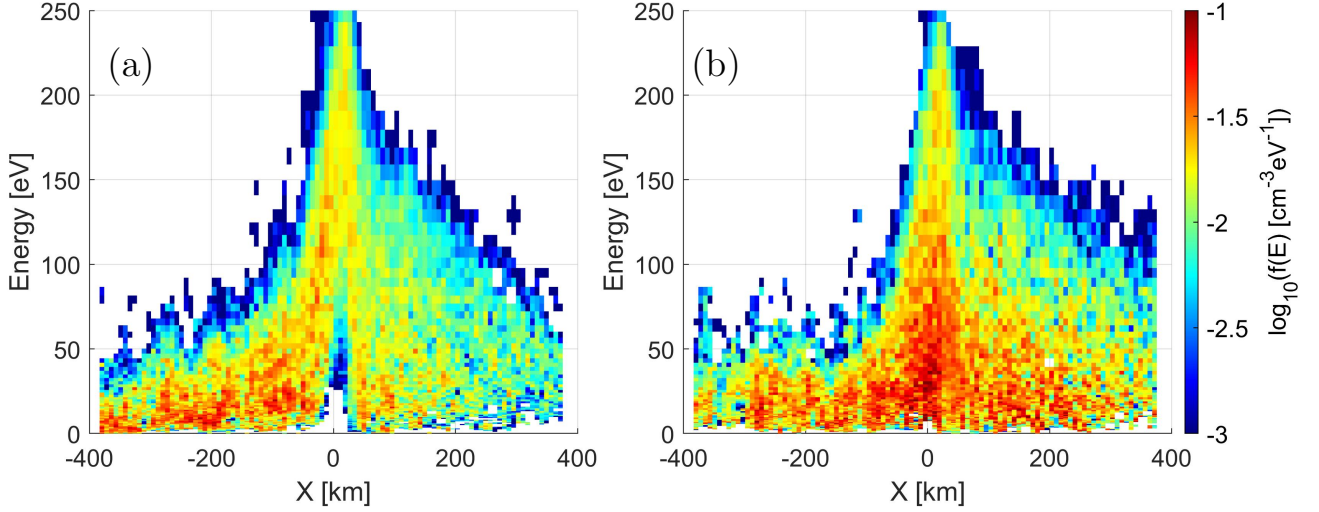


Figure 2.19: Energy distribution function of solar wind electrons for a slice along x through the nucleus for two different electron masses: (a) $m_e = 9.11 \times 10^{-31}$ kg (b) $m_e = 1.67 \times 10^{-29}$ kg. Both simulations are collisionless. Reproduced from [Stephenson et al. \(2022\)](#).

profile in the xz plane. The electron cloud extending downstream of the nucleus is less well-defined, although it spans the same space in xz . The tailward region seen in the xy plane (see Figure 2.17d) is also much weaker in the physical mass case. For both electron masses, there is a region of depleted electrons at $z = 50$ km extending downstream. This is associated with the region where the potential well is at its shallowest, so electrons are deflected away by the ambipolar field.

The major driver of the disparities, between the physical and artificial electron mass simulations, is the boundary conditions at the upstream boundary. For a realistic electron mass, fewer electrons enter the simulation from upstream and the solar wind electrons have less energy at all boundaries. This effect is driven by the shift in scales between the bulk solar wind velocity and the thermal solar wind speed. This is further discussed in Section 2.6.2.

Despite some notable differences, the physical electron mass test particle simulation and the PiC simulation, with an artificially increased electron mass, generally agree well on large scales and have generally consistent electron densities. Therefore, the electric and magnetic fields from the PiC simulation are a good set of fields while being largely consistent with the densities calculated in the test particle simulations

2.6.2 Mass ratio effects

The use of an artificially reduced electron-ion mass ratio ($m_p/m_e = 100$) is common in fully kinetic PiC models. This reduces the computational demands of the simulations, while retaining a separation in scales between the electrons and ions. The artificially reduced mass ratio is equivalent to the use of an increased electron mass. There has been some investigation into the effect of

artificially boosting the electron mass in kinetic simulations (e.g. [Jun and Quan-Ming, 2007](#); [Hong et al., 2012](#)), but not in the three-dimensional case.

To examine the impact of the mass ratio, two 3D collisionless test particle simulations are considered: one using the physical electron mass ($m_e = 9.11 \times 10^{-31}$ kg; Figure 2.19a), and the other using the heavier electrons as seen in the PiC model ($m_e = 1.67 \times 10^{-29}$ kg; Figure 2.19b). In both cases, solar wind electrons are modelled in the presence of the cometary fields, from the PiC simulation (see Section 2.5.3). The differences between the simulations originate from two sources: the boundary conditions and the particle dynamics in the simulation.

The upstream solar wind boundary conditions are largely responsible for the differences in magnitude and shape that are seen in the solar wind density (see Figure 2.17). At the upstream boundary, only solar wind electrons with a positive x velocity enter the simulation domain. The electrons in the quiet solar wind are sampled from a 10 eV Maxwellian distribution with a bulk velocity of $400 \text{ km s}^{-1} \hat{x}$. Figure 2.18a shows the distributions of x velocities for the physical and increased electron masses. In the high mass case, the width of the distribution is reduced by a factor of ≈ 4.3 to give a thermal velocity of $v_{th} = \sqrt{(2k_B T_e / m_e)} = 438 \text{ km} \cdot \text{s}^{-1}$. This is comparable to the bulk velocity of the solar wind so 91% of the high mass electrons have a velocity into the simulation domain (area highlighted in green, corresponds to $v_x > 0$ in Figure 2.18a). Conversely, for the physical mass electrons, the thermal velocity ($1874 \text{ km} \cdot \text{s}^{-1}$) greatly exceeds the bulk flow speed. In this case there are far more electrons moving upstream at the boundary at a given instant and only 61% of the electrons enter the domain. This means that the contribution from the upstream boundary is reduced when using realistic electrons. This accounts for the weakened near-tail structure in the xy plane, which is primarily populated by solar wind electrons from upstream.

In addition to the reduction in the solar wind density at the upstream boundary, there is also a disparity between the energy distributions. The kinetic energy associated with the bulk flow of the solar wind is much larger for the artificially increased electron mass (0.46 eV vs. 8.35 eV). The peak in the electron energy distribution (see Figure 2.18b) is shifted to higher energies and has more electrons in the 50 to 100 eV range. The bulk flow energy is seen as the minima of energy variation in Figure 2.20.

Once in the simulations, the particle dynamics are also impacted by the electron mass. Figure 2.19 shows the energy distribution function along the Sun-comet line (with the nucleus at $x = 0 \text{ km}$) for the physical and artificially increased electron masses. Towards the upstream boundary ($x = -400 \text{ km}$), both simulations show similar energy distributions and span the same energy range. The electrons are still in pristine solar wind conditions at this point and have not

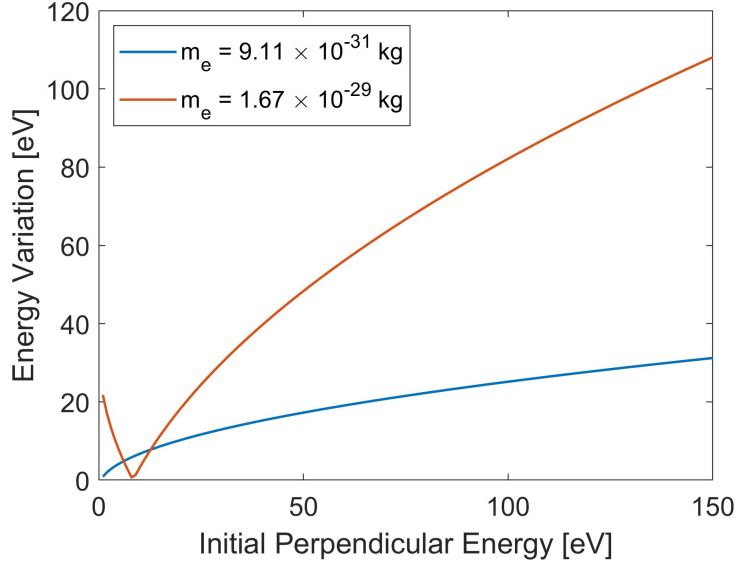


Figure 2.20: Variation of electron energy during a gyration under quiet solar wind conditions ($\mathbf{B} = 6 \text{ nT } \hat{\mathbf{y}}$ and $\mathbf{E} = -2.4 \times 10^{-3} \text{ Vm}^{-1} \hat{\mathbf{z}}$) for a range of initial perpendicular energies. Above 8.35 eV, the energy variation is a loss in energy for the increased electron mass (i.e. falls from 100 eV to 17.9 eV), but below 8.35 eV the electron gains energy through its gyration (i.e. 1 eV rises to 22.8 eV). For the physical electron mass, the boundary is at 0.46 eV. Credit: [Stephenson et al. \(2022\)](#).

been substantially perturbed from the 10 eV Maxwellian upstream. Moving close to the nucleus, the electrons fall into the deep potential well and are accelerated up to ~ 250 eV at a maximum. This is caused by the depth of the ambipolar potential, which reaches ~ 200 eV in the inner coma (see Figure 2.11). For both electron masses, the maximum energy reached is very similar. However, there is a clear deviation at low energies between the two cases. For a physical electron mass, very few solar wind electrons are observed below 70 eV. Conversely, these electrons are abundant when an artificially increased electron mass is used.

As the same maximum energy is achieved in the two simulations, the low energy differences cannot be attributed solely to the fields. The key distinction between the cases is the scale of the electron gyroradius. When electrons gyrate in the presence of non-parallel electric and magnetic fields, the electron energy varies throughout a single gyration (e.g. Figure 2.13). The convective electric field is the major driver of the energy variation and sets up an $\mathbf{E} \times \mathbf{B}$ drift. As the gyroradius ($r_{gyro} = mv_{\perp}/qB$) is larger for a heavier electron (by a factor of $\sqrt{m_{heavy}/m_{real}} = 4.3$ for the same perpendicular energy), the electron travels further along the electric field and has more work done on it. Therefore, the scale of the energy variations will be larger.

To test the impact of the gyration effect, I consider the simplest case of quiet solar wind conditions, using $\mathbf{B} = 6 \text{ nT } \hat{\mathbf{y}}$ and $\mathbf{E} = -2.4 \times 10^{-3} \text{ V m}^{-1} \hat{\mathbf{z}}$ (same upstream solar wind conditions used in the test particle simulations; Table 2.4). Test particles are produced with a range of initial

energies, with their velocities aligned with $\hat{\mathbf{x}}$ ($\mathbf{v}_{\text{init}} = v_{\text{init}}\hat{\mathbf{x}}$). Figure 2.20 shows the energy range in a single gyration as a function of perpendicular energies, for both the physical and artificially increased mass cases. An electron with realistic mass and an initial perpendicular energy of 100 eV varies by 25 eV within a gyration. However, under the same conditions, the artificially heavier electron's energy varies by 82.1 eV. Electrons with increased mass between 50 and 100 eV lose between 72 and 97% of their initial energy within a single gyration, before returning to their initial energy.

During $\mathbf{E} \times \mathbf{B}$ drift, the heavier electrons cover a much larger region of the energy space than the realistic electrons. The electrons contribute to the distribution functions at each point in their trajectories, so a nominally 100 eV electron may contribute to the edf at 15 eV half a gyration later. For the lighter, realistic electrons, the smaller gyroradius constrains the energy variation and prevents any contribution to the lowest energies e.g. < 70 eV close to the nucleus. This explains the absence of low energy solar wind electrons close to the nucleus for the physical electron mass in the collisionless simulations.

2.6.3 Validation of the fields in collisional simulations

Having validated that the test particle and PiC simulations are consistent in the collisionless case (see Section 2.6.1), it is then important to ensure the fields remain valid when collisional processes are introduced. Firstly, I discuss the impact of electron-neutral collisions on the properties of electrons in the coma. After this, I examine how these changes would impact the fields in a self-consistent collisional model.

Impact of collisions on the electron populations

This section is not an exhaustive review of the impact of collisions in the coma, but more to give an impression of how electron-neutral collisions affect the electrons modelled in the test particle simulations. The wider effects of collisions in terms of electron cooling and as a source of ionization are more thoroughly discussed in Chapters 3 and 5. Here, I compare the photoelectron population from a collisionless and collisional test particle simulation at $Q = 10^{26} \text{ s}^{-1}$, using the physical electron mass in both simulations (the other parameters are listed in Table 2.4).

Figure 2.21 shows the edf of photoelectrons and their secondaries for a slice through the nucleus along y (approximately along the magnetic field lines) for the collisionless and collisional simulations. The electron distributions exhibit the same shape away from the inner coma, where electron-neutral collisions are infrequent. However, there are notable differences in the inner coma

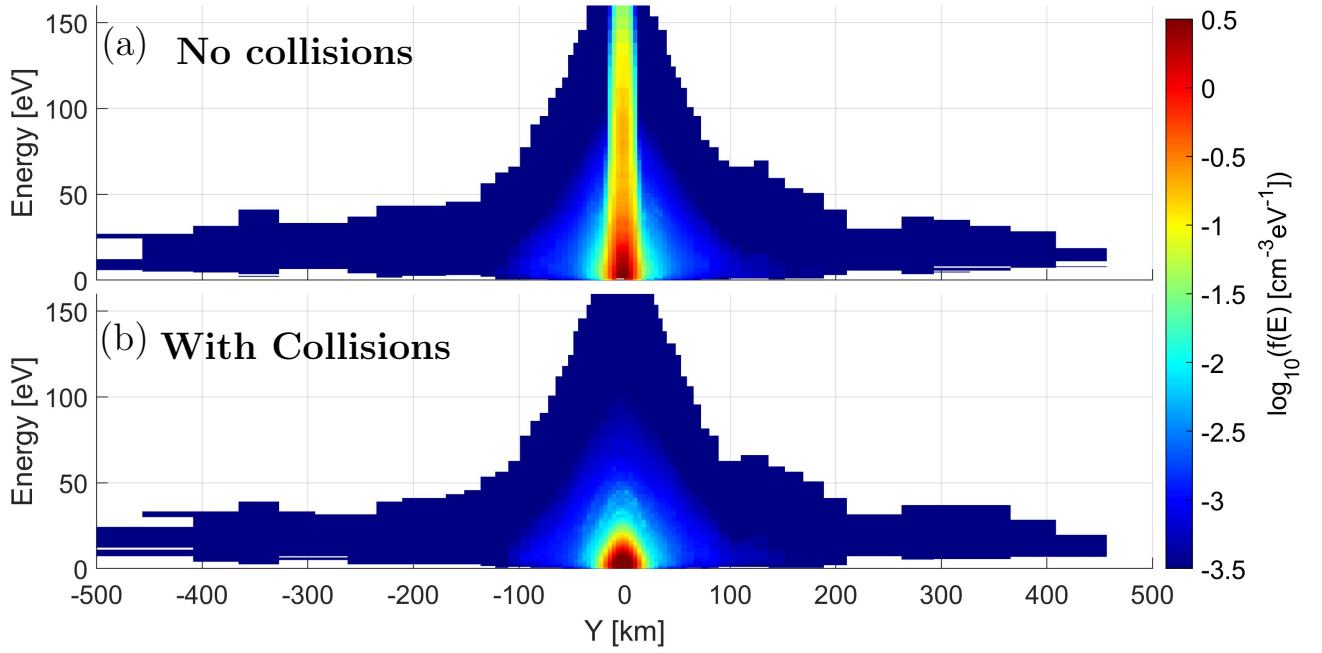


Figure 2.21: Energy distribution functions of cometary photoelectrons and their secondaries along the y axis going through the nucleus (0,0,0) (a) the non-collisional case and (b) the collisional simulation. Credit: [Stephenson et al. \(2022\)](#).

($y < 25$ km). In the collisionless simulation, electrons reach energies in excess of 160 eV close to the nucleus. These are photoelectrons produced far from the nucleus at up to $r = 300$ km. They have fallen into the deep ambipolar potential well (see Figure 2.11) and behave very similarly to solar wind electrons (see Figure 2.15). When collisions are introduced, the same acceleration processes occur, but the high energy tail is efficiently quenched through electron-neutral collision processes. The cooling of the high energy electrons is primarily caused by electron-impact ionization collisions, because of the large cross sections and loss rates of ionization at $E \sim 100$ eV (see Figures 2.5 and 2.6). The high energy tail (> 100 eV) is weaker by three orders of magnitude when collisions are included, but lowest energy electrons (< 8 eV) increase in density by a factor of 3.

Between 20 and 40 km from the nucleus, there is a smaller reduction in high energy electrons (between 20 and 80 eV) by 30% and a slight increase in the low energy population (< 10 eV). Beyond 40 km, the impact of electron-neutral collisions is not apparent for the slice along y , but the effects of collisions can still be seen in some distant regions of the coma. The effects of collisions are more pronounced in regions connected to the inner coma through transport, such as where low temperatures are seen in the tail (see Figure 2.22, Section 3.2.4).

With collisions, the electron temperature falls as low as 2 eV within 10 km of the nucleus, where the coma is dense and collisions are more frequent. The tailward region also sees reduced temperatures (4 eV), which are substantially lower than seen in the collisionless simulation. The

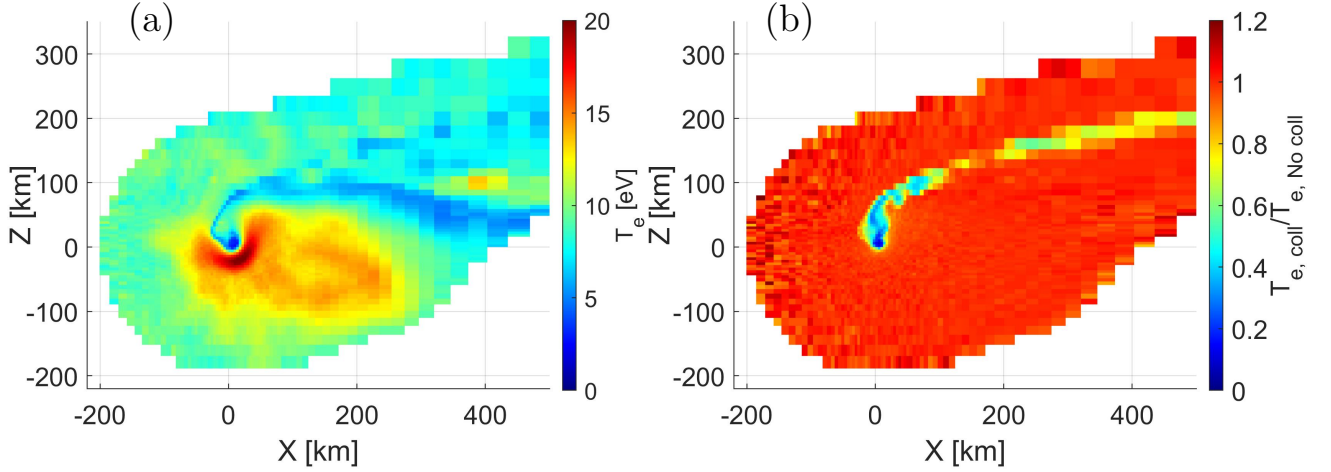


Figure 2.22: (a) Photoelectron temperature in the xz plane from a collisional simulation. (b) Ratio of electron temperatures from a collisional and non-collisional simulation. Credit: [Stephenson et al. \(2022\)](#).

low temperature region at (300, 0, 50) km is seen in both the collisionless and collisional cases ($T_{e, \text{coll}}/T_{e, \text{nocoll}} \approx 1$), as it is associated with a maximum in the potential well. The high tailward region passing through (300, 0, 150) km is substantially cooled in the collisional simulation ($T_{e, \text{coll}}/T_{e, \text{nocoll}} \approx 0.5$), because electrons are transported from the collisional inner coma into this region. In the collisionless simulation, the accelerated electrons drift towards the tail, giving electron temperatures up to 17 eV in the same region. When collisions are included, the highest energy electrons are cooled (Figure 2.21) before they move tailward, resulting in temperatures of ~ 6 eV.

For $z < -20$ km, the electrons are largely unchanged by the introduction of collisional processes (see Figure 2.22b), as the coma is rarefied and not magnetically connected to collisional regions. The high electron temperature (~ 19 eV) seen below the coolest region of the coma is driven by acceleration in the ambipolar potential well. This is mostly a result of a large parallel temperature, which is caused by the acceleration of photoelectrons along the field lines from the edge of the potential well.

Despite differences in temperature in the inner coma, the collisionless and collisional simulations show similar behaviour on large scales. The electron densities have a similar shape and are of the same order of magnitude throughout the coma (see Figures 2.16 a and d for the collisionless case). Outside the inner coma ($r > 40$ km), the plasma density is within 5% of the non-collisional case. In the inner coma, the density does deviate by up to 40% in inner coma. The increase is caused partially by the tighter confinement of cooled electrons in the potential well and partially by the addition of secondary electrons to the total electron density. The trapping of cooled electrons by

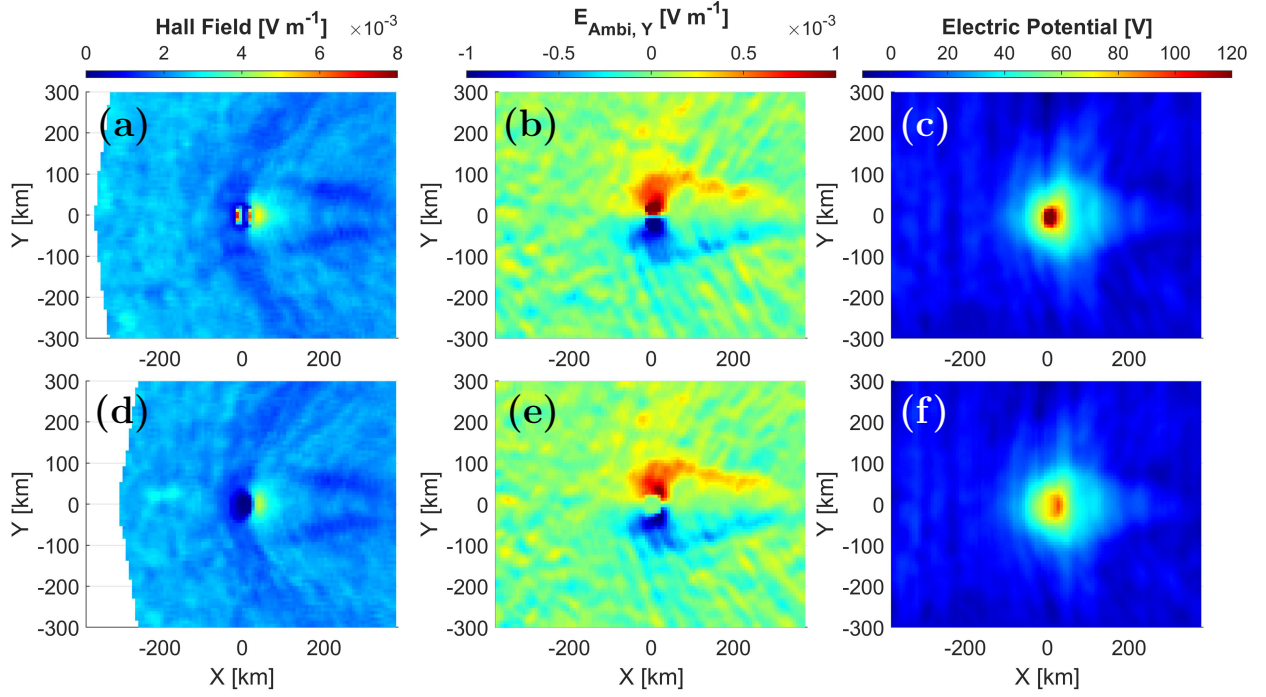


Figure 2.23: Electric field components and ambipolar potential well computed from (a-c) collisionless and (d-f) collisional test particle simulations at $Q = 10^{26} \text{ s}^{-1}$ for both cometary electrons (photoelectrons and secondaries) and solar wind electrons. (a,d) Electron Hall field magnitude (see Eq. 2.44), (b,e) y component of the ambipolar field (Eq. 2.43), and (c,f) ambipolar potential well.

the ambipolar fields also results in 40% lower electron densities between $\pm 10 \text{ km}$ and $\pm 60 \text{ km}$ along y , for regions magnetically connected to the inner coma.

Feedback of collisions on the fields

The electric and magnetic fields used in the test particle simulation are calculated in a collisionless PiC model. To examine whether the fields remain valid for the collisional simulations, I have compared collisionless and collisional test particle simulations of cometary (both photo and secondary) electrons and solar wind electrons, with the simulation parameters given in Table 2.4. Here, I present the fields for the lowest and highest outgassing cases ($Q = 10^{26} \text{ s}^{-1}$ and $Q = 1.5 \times 10^{27} \text{ s}^{-1}$).

The large scale structures of the density, bulk velocity and temperature are in good agreement throughout the wider coma (see Section 2.6.3). Two processes contribute to the increased density in the inner coma, compared to the collisionless case. Firstly, electron-impact ionization boosts the production of electrons near the nucleus. Secondly, electrons are more efficiently trapped in the inner coma in the collisional case, once they have been cooled through collisions with the neutral gas. The collisional cooling also leads to a reduction in the bulk velocity and temperature of the electron population as electrons become more coupled to the neutral coma.

These changes to the electron population would have a feedback on the electric and magnetic fields in a self-consistent simulation. In lieu of the self-consistent approach, it is useful to assess the changes in the fields that would be driven by the differences in the electron behaviour. As only the electron population is simulated, it is not possible to compute the total electric and magnetic fields from the outputs of the test particle model. However, it is possible to calculate some components of the electric field using the Generalized Ohm's Law (Eq. 1.8).

The magnetic field in the coma originates upstream in the solar wind, as the comet nucleus is not magnetized (Heinisch et al., 2019). The increased magnetic field strength seen close to the nucleus (see Figure 2.10b) is caused by the pile-up and draping of the magnetic field lines around the cometary ionosphere (Koenders et al., 2016; Goetz et al., 2017). During pile-up, the strength of the magnetic field saturates, so the change in the magnitude of the magnetic field is not expected to be significant. Given this and the similar electron populations throughout the wider coma, the magnetic field is not anticipated to be substantially different from the collisionless case.

Taken in isolation, the increased electron density close to the nucleus would violate quasineutrality. However, this would be mitigated by the increased production of cometary ions close to the nucleus, through electron-impact ionization. Any remaining imbalance between the electron and ion populations would be restored through an increased transport of cooled electrons away from the inner coma.

Assuming that quasineutrality is satisfied, we can compute components of the field using the Generalized Ohm's Law, namely the ambipolar and Hall fields (see Figures 2.23 and 2.24). The ambipolar field strength is computed from the gradient in the electron pressure,

$$\mathbf{E}_{Ambi} = -\frac{1}{n_e e} \nabla p_e = -\frac{1}{n_e e} \nabla (n_e k_B T_e), \quad (2.43)$$

where the electron density and temperature are outputs of the test particle electron model (see Section 2.4). Similarly, the Hall field is given by:

$$\mathbf{E}_{Hall} = \frac{1}{n_e e} \mathbf{J} \times \mathbf{B} = [\mathbf{u}_i - \mathbf{u}_e] \times \mathbf{B} \quad (2.44)$$

$$\mathbf{E}_{Hall,e} = -\mathbf{u}_e \times \mathbf{B} \quad (2.45)$$

where the electron bulk velocity, $\mathbf{u}_e$, is also outputted from the simulation. Note that the computed Hall field, $\mathbf{E}_{Hall,e}$ is only accounting for the electron contribution to the field, neglecting the ions. Generally, electrons have much higher speeds than the ions, but the bulk velocities are largely driven by the field conditions and are of comparable magnitude. The ion properties are not derived

in the test particle model, so only the electron contribution of the Hall field has been considered. This is indicative of regions where the bulk velocity is substantially altered by the introduction of collisional processes. The magnetic field used to compute the Hall field is assumed to be the same as calculated in the collisionless PiC simulation, as it is unlikely to change substantially due to collisions.

$Q = 10^{26} \text{ s}^{-1}$ Figure 2.24 shows the components of the field for the simulation at $Q = 10^{26} \text{ s}^{-1}$. Outside the inner coma ($r > 30 \text{ km}$), the ambipolar and Hall fields are not substantially altered from the collisionless case. The ratios in field strength (collisional/collisionless) between the simulations is close to 1 for both the ambipolar (0.9 ± 0.26) and Hall (1.00 ± 0.07) fields. This region of the coma is not strongly impacted by collisions, except where it is linked to the inner coma through transport (see Chapter 3). However, close to the nucleus ($r < 30 \text{ km}$) both the ambipolar and Hall fields are substantially weakened by the introduction of collisions by factor of 0.28 ± 0.33 and Hall 0.41 ± 0.38 , respectively. The ambipolar field is weakened as the temperature is reduced in the inner coma, as a result of electron neutral collisions (see Figure 2.22).

It is difficult to directly assess the impact of the potentially reduced electron Hall field in this region, but it is likely to slightly alter trajectories in the inner coma. There would be some feedback on the magnetic field as a consequence of the reduced currents. However, the Hall field shown here is only driven by the electron current, neglecting any contribution from the ions. The ions would also need to be accounted for to reasonably estimate the change in magnetic field, arising from the reduction in current.

The ambipolar field is responsible for the construction of the potential well that traps electrons in the inner coma. As such, it is important to determine how the weakened ambipolar field in the inner coma would alter the electron trapping, and any implication on the efficiency of the electron cooling. When collisions are included, the depth of potential well (see Figure 2.23c and f) reduced by a factor of 0.85 close to nucleus. Despite the reduction in the ambipolar field strength in the collisional region, the potential well is not significantly shallower. The potential barrier is constructed over a large spatial range ($y \pm 150 \text{ km}$), which extends well beyond the region of the coma that is highly collisional. Consequently, the trapping of electrons is not significantly diminished by the inclusion of collisions, although there would be some level of negative feedback in a self-consistent simulation.

$Q = 1.5 \times 10^{27} \text{ s}^{-1}$ Figure 2.24 shows the components of the field for the simulation at $Q = 1.5 \times 10^{27} \text{ s}^{-1}$. The behaviour of the fields is very similar to the case at lower outgassing.

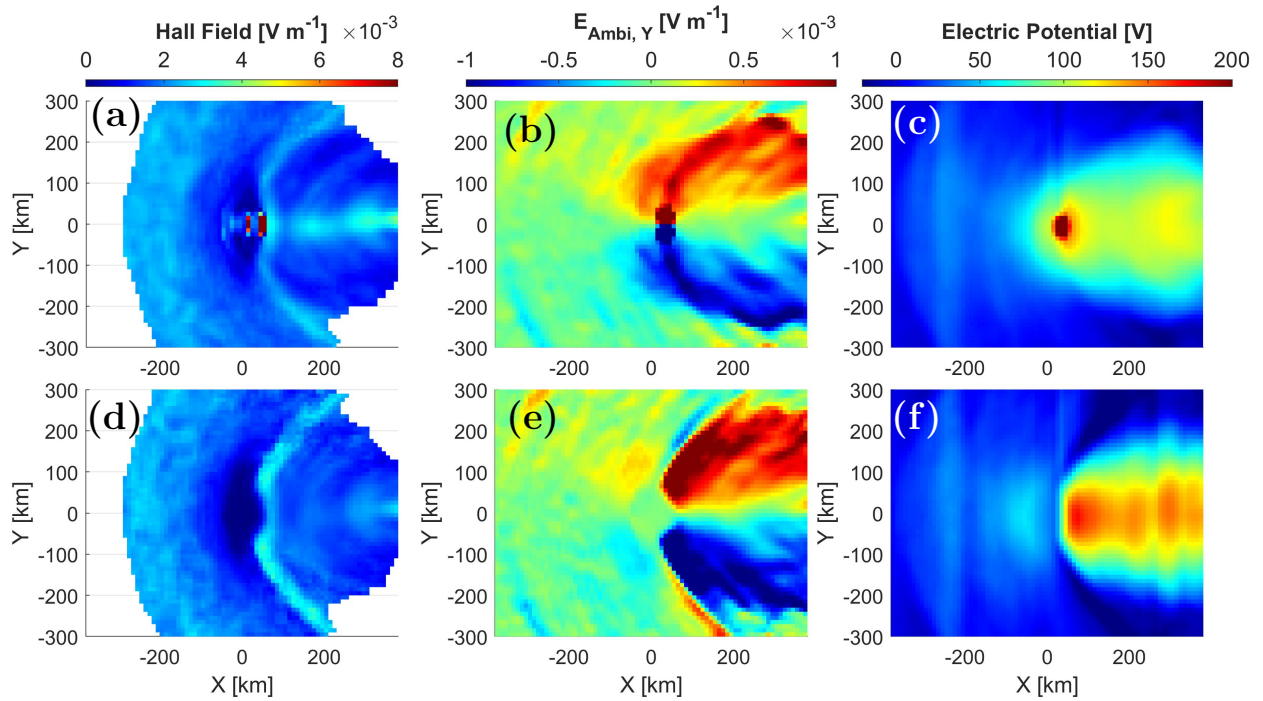


Figure 2.24: Electric field components and ambipolar potential well computed from (a-c) collisionless and (d-f) collisional test particle simulations at $Q = 1.5 \times 10^{27} \text{ s}^{-1}$ for both cometary (photoelectrons and secondaries) and solar wind electrons. (a,d) Electron Hall field magnitude (see Eq. 2.44), (b,e) y component of the ambipolar field (Eq. 2.43), and (c,f) ambipolar potential well. The fields are calculated using only the electron population from the test particle simulations, and do not have any contribution from ions.

In innermost coma ($r < 50 \text{ km}$), the coma is highly collisional and both the Hall and ambipolar fields become small for the collisional case. Farther from the nucleus ($r > 100 \text{ km}$), the fields have similar shapes and magnitudes for the collisionless and collisional simulations.

The electron Hall field is largely unaffected by collisional processes away from the inner coma. The Hall field is negligible in the inner coma ($r < 50 \text{ km}$), as the bulk electron velocity is small when collisions are frequent. Downstream of the collisional region, the Hall fields are enhanced by up to 40%, because of the increased electron density from electron-impact ionization (see Section 5.2).

The ambipolar field (Figures 2.24b and e) shows the same structures and field magnitudes outside the inner coma ($r > 60 \text{ km}$), but is effectively repressed by collisions around the nucleus. As seen for the lower outgassing case, the potential well is much more resistant to collisions, as the depth of the well is set up over hundreds of kilometres. The potential well depth is reduced by 50% within 50 km of the nucleus, but outside this region the potential well has a similar structure and depth. The strengthened ambipolar field, seen downstream of the nucleus, leads to a deeper potential well around $(200, 0, 0) \text{ km}$ by 20%.

While there are some differences in the fields, especially in the inner coma, the wider coma

is consistent between the collisionless and collisional simulations. While the ambipolar field is effectively quenched in the densest region of the coma, the potential well is more resistant to the impacts of collisions and can still effectively trap cometary electrons within the inner coma.

To conclude, collisions do have an impact on the fields, but only in a region close to the nucleus. Although the ambipolar field is weakened by collisions, it is not likely to have a major impact on the efficiency of electron trapping, or significantly reduce the collisionality of the coma. The fields derived in the collisional case are in good agreement with those from the collisionless case, across the wider coma. Given these findings, the fields from the PiC simulation are consistent enough with the output of the collisional simulations to demonstrate the efficiency of electron trapping and the impact of trapping for collisional effects.

Chapter Summary

- I have developed a new test particle model of electrons in the cometary environment. This is the first collisional 3D model of electrons at a comet. I have outlined the calculation of single particle trajectories and statistical properties for a large electron population.
- I have validated particle trajectories by comparison to analytically calculated drifts in simple cases. The collisional algorithm is tested against the continuous slowing down approximation. Production schemes for photo and solar wind electrons are validated in steady conditions.
- The test particle model is further tested by comparison with collisionless PiC simulations, for both cometary and solar wind populations. The validity of the electric and magnetic field on both collisionless and collisional simulations has been discussed.
- The impact of using a reduced ion-electron mass ratio ($m_e = m_p/100$) in fully-kinetic simulations is examined, with the test particle model.

Chapter 3

Cooling of electrons at a weakly outgassing comet

In this chapter, I examine the formation of a cold electron population within a weakly outgassing coma using the collisional test particle model, which is presented in Chapter 2. Cold electrons were observed around comet 67P throughout the Rosetta mission, even when none of the coma was thought to be collisional ($Q < 5 \times 10^{26} \text{ s}^{-1}$; Eriksson et al., 2017; Engelhardt et al., 2018; Gilet et al., 2020). However, previous models have not incorporated both the collisional cooling processes and the complex dynamics of electrons within the cometary environment. The test particle model I have developed is the first model that includes both of these key kinetic processes.

Section 3.1 outlines the test particle simulations used in this chapter and how these are used to calculate properties of the cold electron population. In Section 3.2, I present the formation of cold electrons in weakly outgassing comae. I consider an example of a collisionally cooled electron, as well as the presence and origin of the cold electron population. The impact of electron dynamics on the collisionality of the coma is presented in Section 3.3. Given that electron trapping plays a major role in the cooling of electrons, I revisit the definition of the electron exobase and introduce the concept of an electron-cooling exobase in Section 3.4.

3.1 Methods

The cooling of warm electrons through collisions with the neutral coma is modelled using test particle simulations. The collisional test particle model is presented in full in Chapter 2 and the parameters of the test particle simulations used are outlined in Table 2.4. I consider three outgassing rates: $Q = 10^{26} \text{ s}^{-1}$, $Q = 3 \times 10^{26} \text{ s}^{-1}$ and $Q = 1.5 \times 10^{27} \text{ s}^{-1}$. While the outgassing rate differs between the simulations, the ionization frequency, interplanetary magnetic field and solar

wind density remain the same. Therefore, the different outgassing rates do not necessarily translate to a shift in heliocentric distance. The simulations at $Q = 10^{26} \text{ s}^{-1}$ and $Q = 1.5 \times 10^{27} \text{ s}^{-1}$ have temperatures of 10 eV for both the newly-born photoelectron and solar wind electron populations. At $Q = 3 \times 10^{26} \text{ s}^{-1}$, the electrons from both sources are initialized with a temperature of 30 eV. In this chapter, the electron densities shown correspond to the sum of the densities from photoelectrons, solar wind electrons and electrons produced from electron-impact ionization.

Despite using the same input parameters as outlined in Table 2.4, there are some differences between the test particle and PiC simulations. Firstly, the PiC simulation does not include any collisional processes. The introduction of collisional processes weakens the ambipolar field close to the nucleus, but the overall strength of the potential well is not greatly effected (see Section 2.6.3). Secondly, the test particle model uses a realistic electron mass ($m_e = 9.11 \times 10^{-31} \text{ kg}$), as opposed to the reduced ion-electron mass ratio in the PiC ($m_e = m_p/100$). The test particle model is less computationally constrained and therefore can use the realistic electron mass, which was not possible in the PiC model. While there is a perturbation associated with the change in electron mass, the test particle electron densities are not significantly altered from those calculated with the PiC simulation (see Section 2.6.1). The use of the realistic electron mass also gives a gyroradius of the correct scale, which is important for deriving the path length traced by the particle. This is crucial for determining the probability of a collision and consequently the cooling of the electrons.

If a heavier electron mass were used (as is the case in PiC simulations), the gyroradius of the electron could be scaled to correct this difference in path length. For a given perpendicular energy, the gyroradius scales as $r_{gyro} \propto \sqrt{m_e}$. However, this scaling only applies to the electron motion perpendicular to the magnetic field. The path length traced by the electron parallel to the field line would not scale in the same way, so the correction in three dimensions is not simple. Therefore, the ability to use a realistic electron mass is greatly beneficial to the accurate modelling of the collisional cooling.

Cold electron density. Cold electrons are defined as those with an energy $E < 1 \text{ eV}$. This was the maximum temperature of the cold electron population during the Rosetta mission (Wattieaux et al., 2020). The density of cold electrons is calculated from the electron energy distribution function, $f(x, y, z, E)$, that is one of the outputs of the test particle model (see Eq. 2.27). The

cold electron density, $n_{e,cold}$ is given by:

$$n_{e,cold}(\mathbf{x}) = \int_0^{1\text{ eV}} f(\mathbf{x}, E) dE \quad (3.1)$$

Cold electron production. The density of electrons reflects a combination of production at the location and transport into or out of the area. To distinguish the production and transport of cold electrons in the coma, I consider the production of cold electrons through collisions, $P_{e,cold}$ [$\text{cm}^{-3}\text{s}^{-1}$]. This production is distinct from the generation of cold electrons through ionization. No new electrons are being generated. It is defined as the number of electrons per unit volume and time that become cold as a result of an inelastic collision in a region. This is given by:

$$P_{e,cold} = n(\mathbf{x}) \sum_j \int_{E_{th,j}}^{E_{loss,j}+E_{cold}} J(E) \sigma_j(E) dE, \quad (3.2)$$

where $\sigma_j(E)$ is the collision cross section for the process, j , at energy E and $J(E)$ is the electron particle flux. The summation is over all the inelastic electron-impact collisions on water and the integration is from the threshold energy $E_{Th,j}$, to the maximum energy that would leave an electron with $E < E_{cold}$ for a given collision process. For inelastic excitations, the energy loss $E_{loss,j}$ is the same as the threshold energy. However, for ionization, the energy of the incident electron, E_{in} is shared evenly with the secondary electron(s) produced, once the threshold energy is provided. For single ionization, this results in an energy loss of $E_{loss,j} = E_{Th} + \frac{E_{in}-E_{Th}}{2} = \frac{E_{Th}+E_{in}}{2}$. The electron particle flux, $J(E)$ [$\text{cm}^{-2}\text{s}^{-1}\text{eV}^{-1}$], is given by:

$$J(E) = f(\mathbf{x}, E) \sqrt{\frac{2E}{m_e}} \quad (3.3)$$

Electron depth. A useful measure of the collisionality of the coma, or a given electron trajectory, is the electron depth. This is defined as

$$\tau_e = \sum_j \int_{\text{path}} n(\mathbf{x}) \sigma_j(E) ds, \quad (3.4)$$

where the integral is over the path the electron follows through the cometary environment. The summation is over all the relevant neutral collision processes the electron undergoes, which are outlined in Section 2.3. In this study, I am interested in energy degradation through collisions, so only collisions with $E_{Th} > 0.15$ eV (see Tables 2.1 and 1.2) are included for the calculation of τ_e .

This excludes the elastic and rotational excitation collisions. If the electron depth $\tau_e \gg 1$, then the electron is likely to undergo many collisions with the neutral coma and will be efficiently cooled.

Electron exobase The electron exobase is the boundary where electrons go from collisional to non-collisional in the coma. This is estimated to lie where the mean free path, λ , is equal to the scale height of the system (here r). Under radial outflow of electrons, this is approximated by (Mandt et al., 2016; Henri et al., 2017; Eriksson et al., 2017):

$$\begin{aligned} r = \lambda, \quad \text{where } \lambda &= n_{S/C} \sigma_{mom} r_{S/C}^2 \\ &= \frac{Q \sigma_{mom}}{4\pi u_{gas}} \end{aligned} \quad (3.5)$$

σ_{mom} is the electron-neutral momentum transfer cross section, which is $\sigma_{mom} = 5 \times 10^{-16} \text{ cm}^2$ at 5 eV (Mandt et al., 2016). However, electrons undergo substantial trapping within the ambipolar potential well, so the path travelled through the coma is not well estimated by the scale height of the system.

3.2 Formation of a cold electron population

In this section, I consider the formation of a cold electron population in a weakly outgassing comet. The test particle simulations are used to demonstrate how a newly born electron can be trapped by the ambipolar potential well, and how that leads to increased energy degradation through collisions of electrons with neutrals. I also show that a cold electron population can be sustained at the low outgassing rates (down to $Q = 10^{26} \text{ s}^{-1}$) considered here.

3.2.1 Trajectory of a cold electron

Figure 3.1 shows the gyroaveraged trajectory of a cometary electron through the coma (at $Q = 3 \times 10^{26} \text{ s}^{-1}$), as it undergoes collisions and becomes cold. The particle is born at 35.3 eV (see Figure 3.1c) at a cometocentric distance of 20 km, with most of the distance along y ($y_{init} = -19.3 \text{ km}$). The cometary electron motion is initially mostly gyration around the magnetic field, as it has a perpendicular energy of 28.5 eV (yellow, Figure 3.1c).

It bounces back and forth along the magnetic field line, as it does not have enough parallel energy (red, Figure 3.1c) to overcome the ambipolar potential well. The electron quickly builds up a substantial electron depth ($\tau_e > 2$) over the first 0.25 s of its motion through the coma. If the elastic and rotational excitations are included in the τ_e calculation, the electron depth exceeds

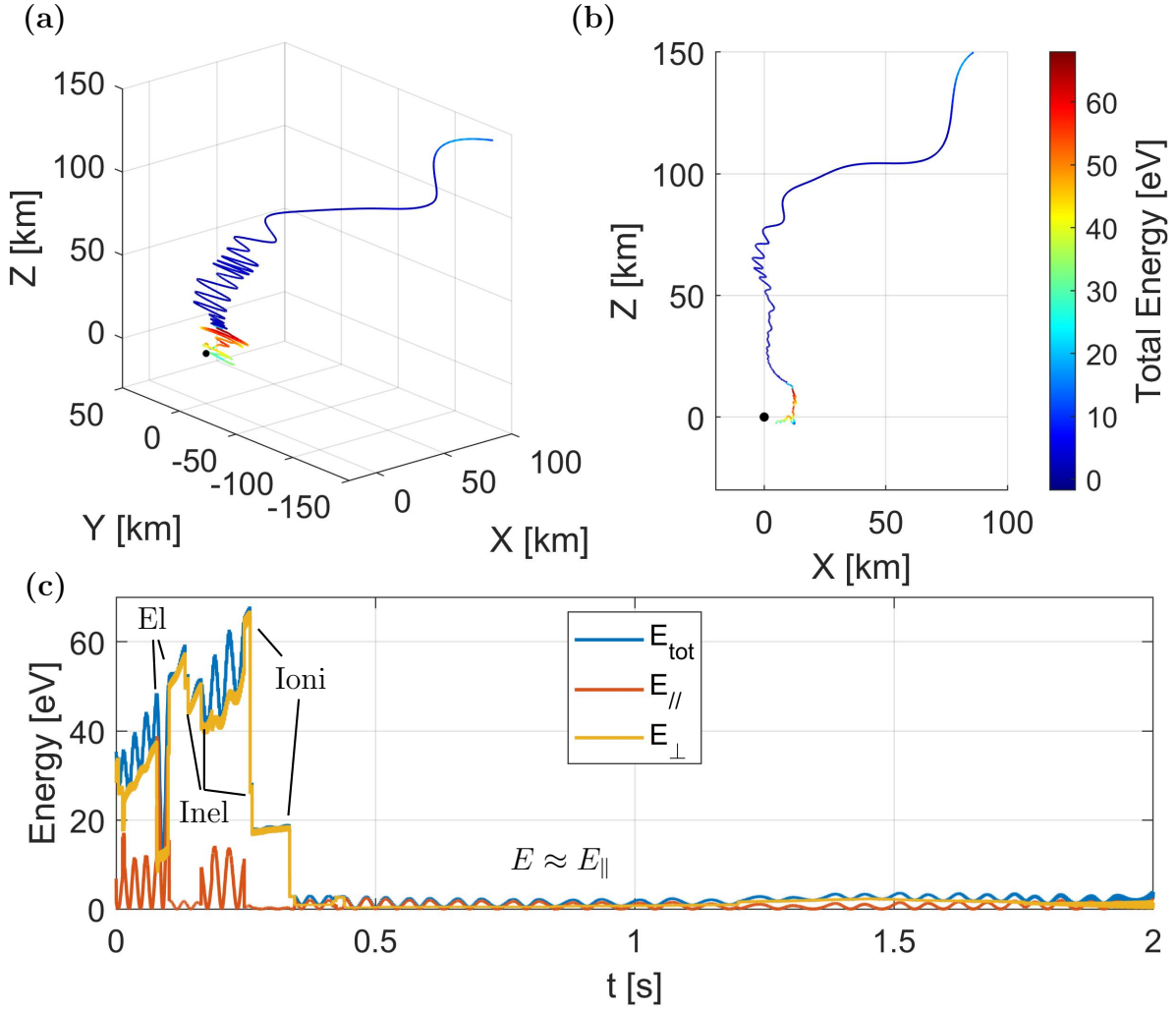


Figure 3.1: (a,b) Trajectory of a cometary electron that is collisionally cooled at an outgassing rate of $Q = 3 \times 10^{26} \text{ s}^{-1}$. (c) Energy variation of the cometary electron as it moves through the coma. The major collisions undergone by the electron are highlighted. El - elastic. Inel - inelastic collisions e.g., dissociation or electronic transitions. Ioni - electron-impact ionization.

$\tau_e > 5$ over this period and reaches 15 over the full lifetime of the electron in the coma.

During the oscillations in the potential well, the electron undergoes a number of elastic collisions, which rotate the electron velocity (see Section 2.3.3). This transfers energy between the perpendicular and parallel directions. At $t = 0.1$ s, the drop in the perpendicular energy from 36.9 eV to 9.4 eV and the subsequent increase to 49.8 eV are both caused by elastic collisions. Despite the elastic collisions, the electron spends little time with a large parallel energy. This ensures it is tightly confined parallel to the magnetic field, and is restricted to very dense regions of the neutral coma. Electrons with high parallel energies can reach regions further away from the nucleus where the coma is less dense, and pass through the inner coma more quickly for each oscillation in the potential well. This limits the number of gyrations the electron makes in the dense coma and therefore limits the electron depth it traces out.

As well as the elastic collisions, this electron undergoes six inelastic collisions during the first 0.35 s it spends in the coma. The electron causes dissociation of a water molecule ($E_{Th} = 7$ eV, see Table 2.1) on three occasions. These have relatively minor effects on the particle, causing reductions in the perpendicular energy, which was dominant on each occasion. The strongest energy loss, around $t = 0.26$ s, is driven by the ionization of a water molecule (forming H_2O^+ , $E_{Th} = 12.62$ eV) shortly followed by an electronic transition ($E_{Th} = 10$ eV). This pair of collisions occurs at a cometocentric distance of 17.5 km and reduces the particle energy from 65.5 eV to 17.6 eV. After these collisions, the electron had a parallel energy of less than 0.3 eV, preventing much motion along the field line. At $t = 0.33$ s, the electron again causes an ionization and falls to an energy of only 2.55 eV.

After several gyrations, the electron is scattered by a neutral molecule and the energy becomes primarily parallel to the field. As the electron moves towards higher potentials, this parallel energy is reduced and the electron spends extended periods of time below 1 eV. Although, the electron regains energy in the centre of the well (up to a maximum of 3 eV), it is cold over large periods of its motion and undergoes further inelastic collisions (vibrational and rotational excitations) which further reduce the electron energy. The electron remains at very low energies for a long time (~ 1.7 s), as it is transported downstream from the inner coma towards $+z$ and into the tailward region. This electron has been cooled through collisions with neutrals, and forms part of the cold electron population for large parts of its path through the coma.

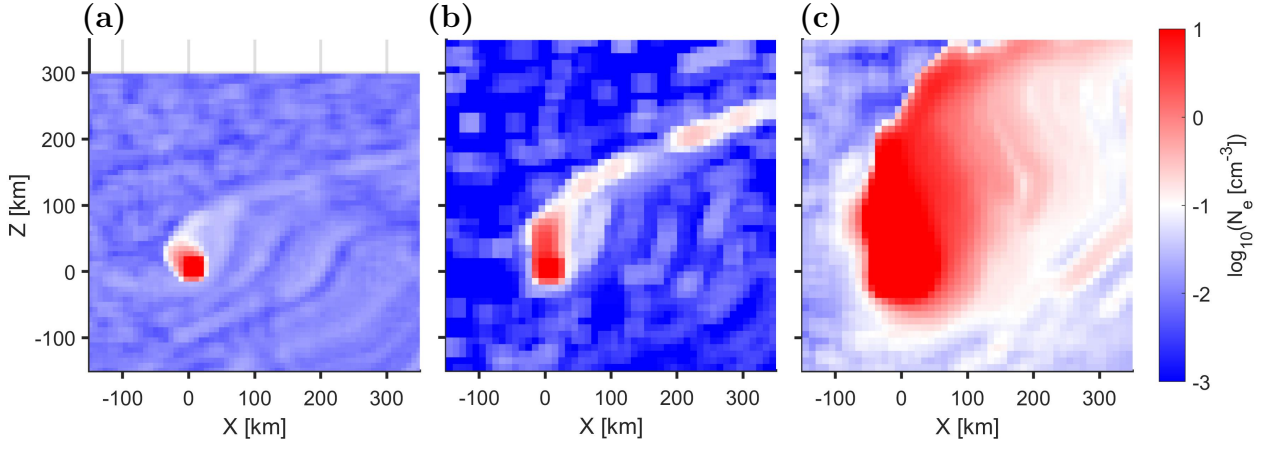


Figure 3.2: Cold electron density in the $x - z$ plane at outgassing rates of (a) 10^{26} s^{-1} , (b) $3 \times 10^{26} \text{ s}^{-1}$ and (c) $1.5 \times 10^{27} \text{ s}^{-1}$. In (a) the moments are only recorded between $z = \pm 300 \text{ km}$, so the region is left blank.

3.2.2 Cold electron density

Figure 3.2 shows the cold electron density ($< 1 \text{ eV}$) for all three outgassing conditions (see Table 2.4) in the xz -plane. Even at the lowest outgassing rate ($Q = 10^{26} \text{ s}^{-1}$), a cold electron population is seen close to the nucleus, reaching a maximum density of 10 cm^{-3} . The density of the cold electrons decreases sharply with distance from the nucleus, falling to 1 cm^{-3} at 30 km and 0.1 cm^{-3} by 50 km (see Figure 3.3a). A tail of cold electrons extending towards $+x$ and $+z$ can be seen, with a density of 0.03 cm^{-3} . There are also some cold electrons present in the wider coma, which can be seen in the wider domain in the low outgassing case. These are uniform with cometocentric distance and have a density similar to the cold electron tail.

The two regions of cold electrons have distinct origins. Those close to the nucleus and in the tail are mostly of cometary origin, whereas the spatially uniform background is largely made up of solar wind electrons. There is a contribution of cooled solar wind electrons (15%) to the dense inner coma region, but cometary electrons are much more efficiently trapped by the potential well. The cold electrons appearing far from the nucleus are likely to be driven by the particle gyration and the convective electric field. As discussed in Section 2.6.2, the electrons vary in energy throughout as they gyrate. As they are sampled from a 10 eV Maxwellian, some solar wind electrons are low enough in energy to reach below 1 eV in parts of their gyration. These electrons have not undergone substantial collisional cooling and only appear cold temporarily.

At $Q = 3 \times 10^{26} \text{ s}^{-1}$, the cold electron population is more developed (Figure 3.2b). The densest region, peaking at 35 cm^{-3} , extends 70 km from the nucleus, although very asymmetrically. The cold electrons are found preferentially at $+z$, with very few found on the opposite side of the nucleus. The tailward structure is very similar to the one seen at lower outgassing, but broader and

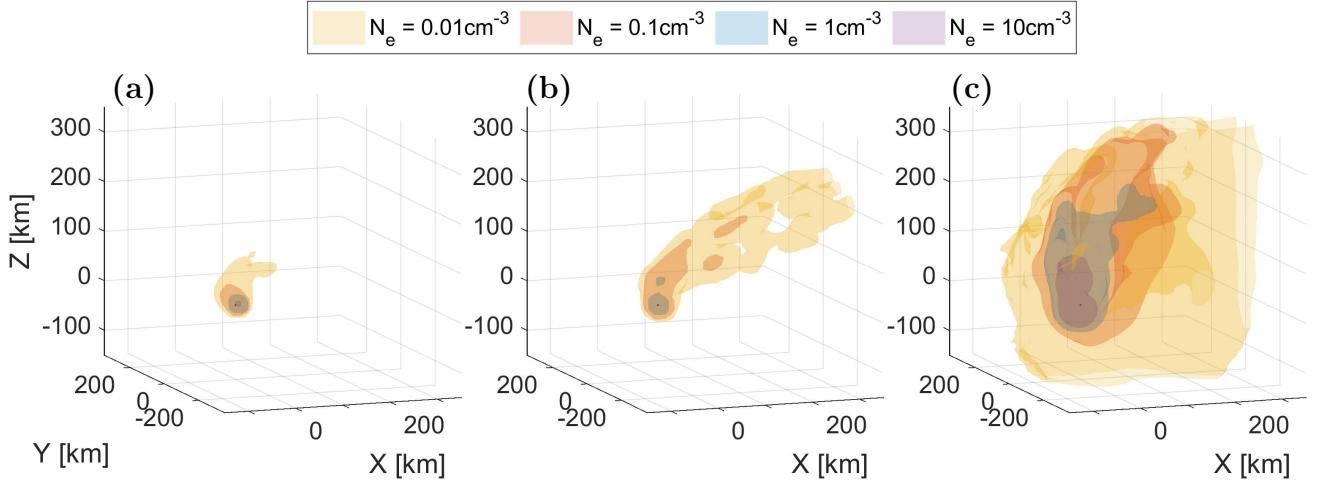


Figure 3.3: Surfaces of constant cold electron density (< 1 eV) at outgassing rates of (a) 10^{26} s^{-1} , (b) $3 \times 10^{26} \text{ s}^{-1}$ and (c) $1.5 \times 10^{27} \text{ s}^{-1}$. Only the cometary electron populations are included.

at higher density (0.1 cm^{-3}). The 3D shape of the tailward region is shown in Figure 3.3b. The tail is also much more extended along x than at $Q = 10^{26} \text{ s}^{-1}$ and has a greater width (300 km vs. 100 km, see Figure 3.3). There are fewer cold electrons present in the wider solar wind than in the lower outgassing case. The solar wind and cometary electrons were produced with temperatures of 30 eV for this simulation, as opposed to 10 eV in the low and high outgassing cases. As a result, the energy variation during the electron gyration rarely brings electrons below the threshold of 1 eV.

At a higher outgassing rate ($Q = 1.5 \times 10^{27} \text{ s}^{-1}$), the cold electron cloud is much larger and denser than in either of the low outgassing cases (Figure 3.2c). Rather than being confined to a relatively small region at low cometocentric distance, a dense cold electron population extends up to 300 km from the nucleus. The cold electrons reach 220 cm^{-3} within the inner coma, and they sustain a density of 50 cm^{-3} at 100 km from the nucleus along $+z$. The wide profile of the cold electron population at $Q = 1.5 \times 10^{27} \text{ s}^{-1}$ (see Figure 3.3c) contrasts with the tail-like structure seen at lower outgassing (Figures 3.3a and b).

The background cold population from uncooled solar wind electrons at $Q = 1.5 \times 10^{27} \text{ s}^{-1}$ has the same density as for $Q = 10^{26} \text{ s}^{-1}$ far from the nucleus. However, this background is very minor compared to the cold electron density driven by collisions. Close to the nucleus, some solar wind electrons undergo collisions and become cold enough to become trapped in the potential well and undergo substantial energy degradation. The cooled solar wind electrons make up 17% of the cold

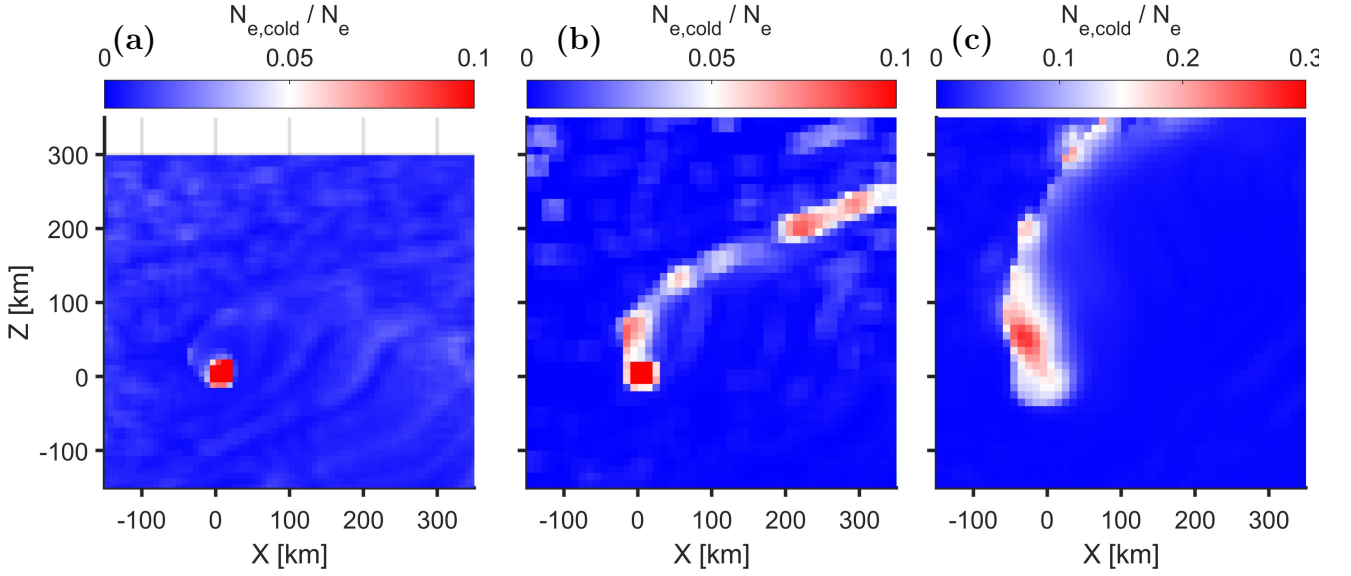


Figure 3.4: Fraction of electron density which constitutes cold electrons in the coma at outgassing rates of (a) 10^{26} s^{-1} , (b) $3 \times 10^{26} \text{ s}^{-1}$ and (c) $1.5 \times 10^{27} \text{ s}^{-1}$. In (a) the moments are only recorded between $z = \pm 300 \text{ km}$, so the region is left blank.

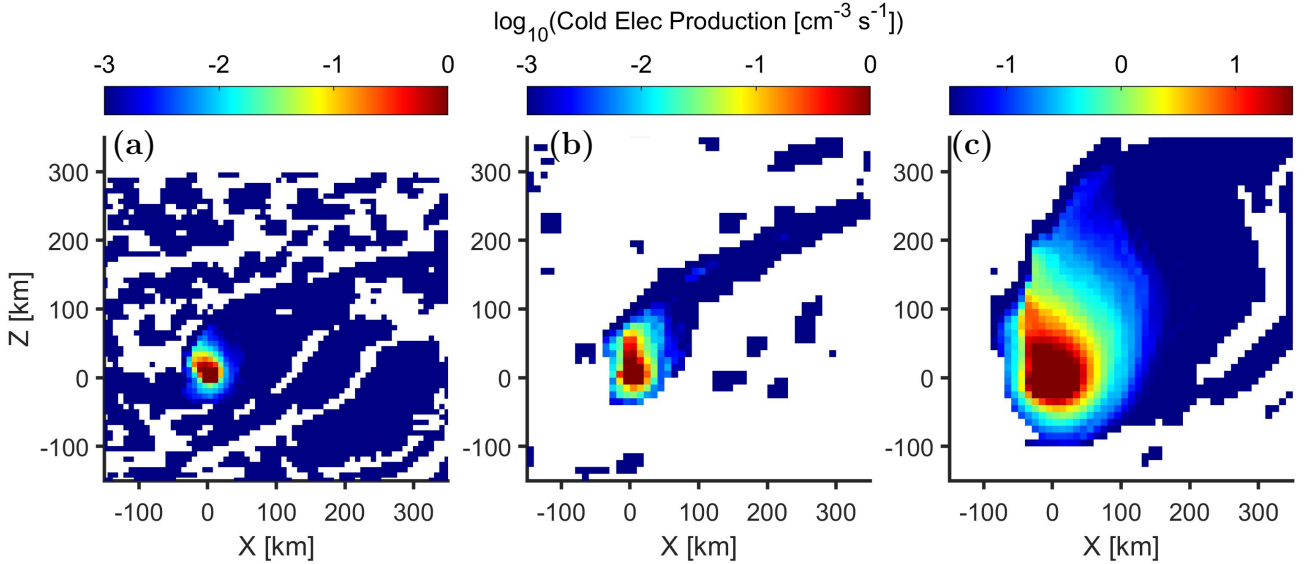


Figure 3.5: Cold electron production rate at outgassing rates of (a) 10^{26} s^{-1} , (b) $3 \times 10^{26} \text{ s}^{-1}$ and (c) $1.5 \times 10^{27} \text{ s}^{-1}$. Values calculated using Eq. 3.2. Regions set as white where the cold electron density was less than (a, b) 0.01 cm^{-3} (c) 0.1 cm^{-3} . The reduction in cold electrons produced far from the coma in (b) compared with (a) results from the higher solar wind electron temperature (30 eV vs. 10 eV).

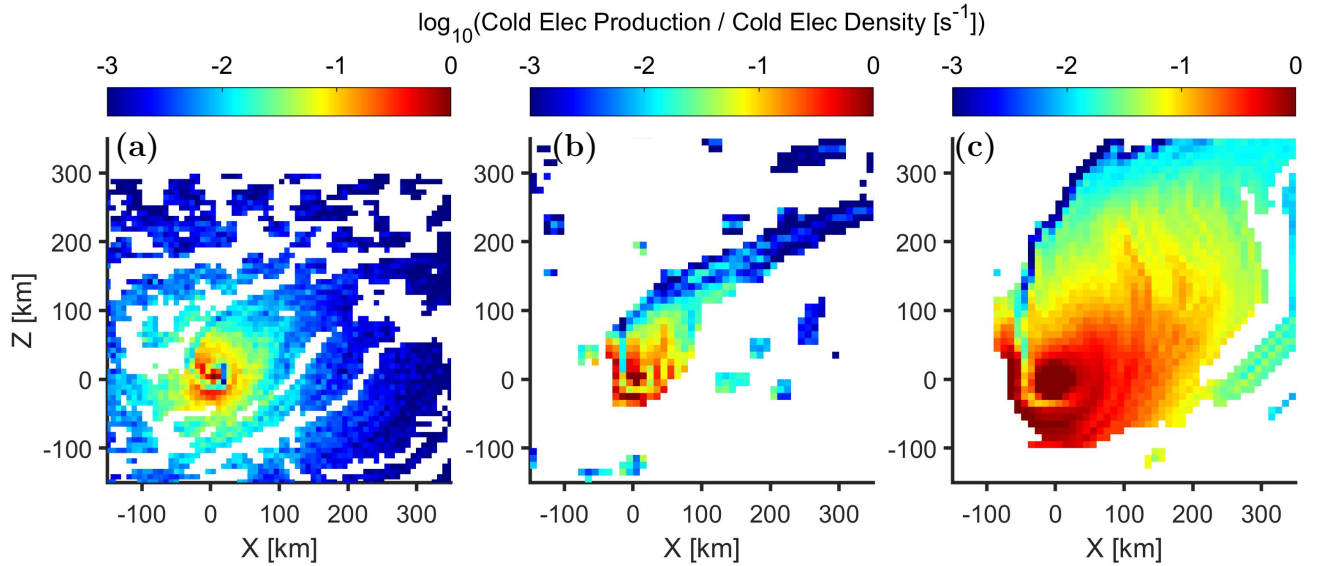


Figure 3.6: Ratio between the production rate and density of cold electrons at outgassing rates of (a) 10^{26} s^{-1} , (b) $3 \times 10^{26} \text{ s}^{-1}$ and (c) $1.5 \times 10^{27} \text{ s}^{-1}$. White regions occur where the cold electron density was less than (a, b) 0.01 cm^{-3} (c) 0.1 cm^{-3} .

electrons close to the nucleus, with the rest produced through ionization of the coma.

3.2.3 Fraction of cold electrons

The fraction of electrons which are cold (see Figure 3.4) increases with the outgassing rate. At the lowest outgassing, only a very small region around the nucleus has a significant fraction of cold electrons (10%, Figure 3.4). In the wider coma and towards the tail, a minimal fraction of the electrons ($< 3\%$) have energies below 1 eV. At the more active comets, the cold electrons are substantial components of the total electron population, both around the nucleus and downstream in the tailward region. At low cometocentric distances, the cold electron fraction reaches 13% and 25% for $Q = 3 \times 10^{26} \text{ s}^{-1}$ and $Q = 1.5 \times 10^{27} \text{ s}^{-1}$, respectively. This demonstrates that the increasing cold electron density with outgassing (see Figure 3.2) is not simply reflective of more electron production within the coma. As the activity of the nucleus increases, electrons are more likely to undergo collisions with the neutral coma and become degraded in energy.

3.2.4 Source of cold electrons

The density and fraction of cold electrons show where cold electrons are in the coma, but do not provide information on where they are produced. The cold electron density is formed through a balance between production and transport. In Figure 3.5, I have plotted the cold electron

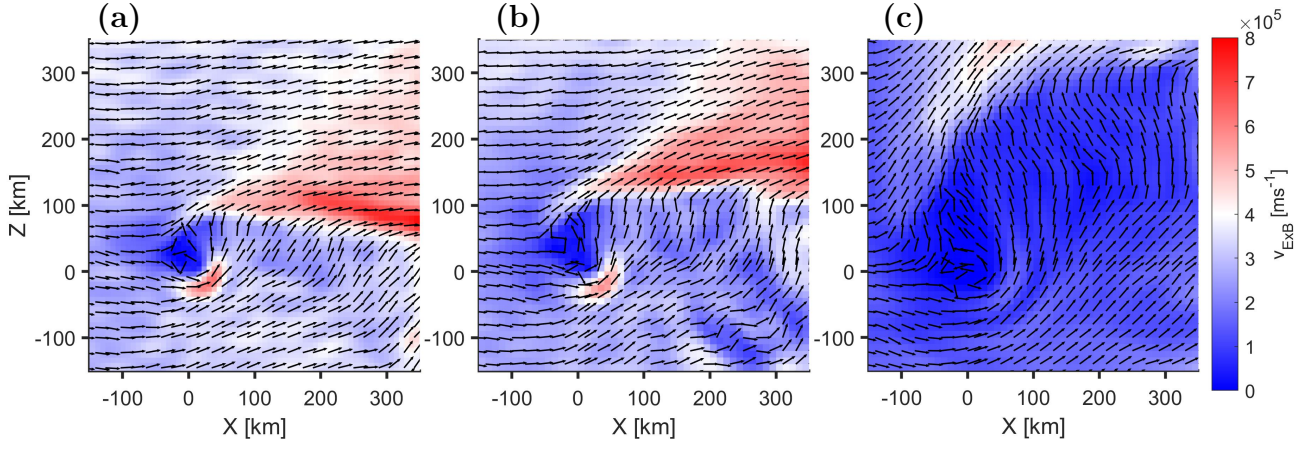


Figure 3.7: $\mathbf{E} \times \mathbf{B}$ drift velocity in the xz -plane at outgassing rates of (a) 10^{26} s^{-1} , (b) $3 \times 10^{26} \text{ s}^{-1}$ and (c) $1.5 \times 10^{27} \text{ s}^{-1}$. The arrows indicate the direction of the velocity vector projected onto the plane.

production derived from Eq. 3.2. The region of maximum electron production in all three cases is focussed around the nucleus. For electrons to become cold, they must undergo inelastic collisions with the neutral gas, so the production of cold electrons is heavily weighted towards regions of high neutral density. The $\pm z$ asymmetry, that is seen in the cold electron density, is repeated in the cold electron production, with more cold electrons produced towards $+z$. Electrons are transported from the inner coma towards $+z$, due to drifts such as the $\mathbf{E} \times \mathbf{B}$ drift (see Figure 3.7). In this part of the coma, there are more electrons which can undergo collisions and then become cold. Farther into the tailward region ($> 100 \text{ km}$, Figures 3.5a & b; $> 200 \text{ km}$ Figures 3.5c), very few cold electrons are produced as the neutral coma is rarefied and collisions of electrons on neutrals are infrequent.

Figure 3.6 shows the ratio between the cold electron production rate (Figure 3.5) and the density of cold electrons in the coma (Figure 3.2). This further clarifies the relative importance of production and transport in each region. The red inner coma produces cold electrons at high rates compared to the density of cold electrons in the region. In the tailward regions, the ratio between production and density is two orders of magnitude smaller. These tails have high cold electron densities, given their production rates, suggesting that cold electrons are transported into these regions.

In weakly outgassing comae, collisions with the neutral gas are infrequent and the gyroaveraged motion of the electrons can be attributed to drifts associated with the fields. Grad- $\mathbf{B}$ drift (Eq. 2.12) is not significant throughout the coma and can be ignored. Curvature drift (Eq. 2.11) is dependent on the parallel energy of the electron, so can be neglected for low energy electrons. Therefore, the cold population is primarily subject to the $\mathbf{E} \times \mathbf{B}$ drift (Eq. 2.10). Figure 3.7 shows

the $\mathbf{E} \times \mathbf{B}$ drift in the xz plane. The transport of electrons through the coma is a three-dimensional process, so the slice at $y = 0$ km does not fully capture the path that electrons will follow. However, it is clear that the dense tailward structure (Figure 3.2) closely follows the direction of the $\mathbf{E} \times \mathbf{B}$ drift when outside the inner coma. Very close to the nucleus, the structure of the drift is very complex. Here the magnetic field piles up and drapes around the cometary ionosphere, while the ambipolar and Hall fields become substantial (Deca et al., 2019).

Cold electrons are produced close to the nucleus by cooling warm cometary electrons through collisions with the neutral gas. The warm electrons are efficiently trapped in the inner coma by the ambipolar potential well. The cold electrons in the inner coma are then transported into the tailward region, primarily by the $\mathbf{E} \times \mathbf{B}$ drift. Once into the tailward region, they flow downstream into the solar wind.

3.3 Cooling: trapping vs radial flow

Current estimates of the electron exobase (see Eq. 3.5) and simple models of electron cooling assume that electrons flow radially away from the nucleus. In the previous section, I have demonstrated that the motion of electrons in the complex electric and magnetic fields is crucial in generating cold electrons. The fields, particularly the combination of the magnetic fields and the ambipolar potential well, cause electrons to become trapped within the inner coma and trace out a long path through the cometary environment. In this section, I quantify the impact of trapping on the collisionality of cometary electrons and compare it to the often-assumed case of radial outflow.

The electron depth (see Eq. 3.4) was calculated for each electron macroparticle in the test particle simulations. I included all inelastic excitations and ionization collisions which have threshold energies exceeding 0.15 eV. This excludes only elastic ($E_{Th} = 0$ eV) and rotational excitations ($E_{Th} = 0.004$ eV). These collisions have very large cross sections, while causing relatively little energy degradation (see Figures 2.5 and 2.6).

Figure 3.8 shows the distribution of electron depths for each outgassing rate, when using the self-consistently calculated fields (histograms). The electrons are differentiated by the cometocentric distance at which the electron was produced through ionization (whether by photoionization or electron-impact ionization). They are sorted into 10 km radial bins from the surface of the comet to 300 km. The solar wind electrons have been excluded from this analysis, as they are not accounted for in the case of radial outflow. They are also a small component of the cold electron population ($< 15\%$). The distribution of electron depths calculated under radial outflow of photoelectrons is also given at each outgassing rate (black). Under radial outflow, the photoelectrons are sampled

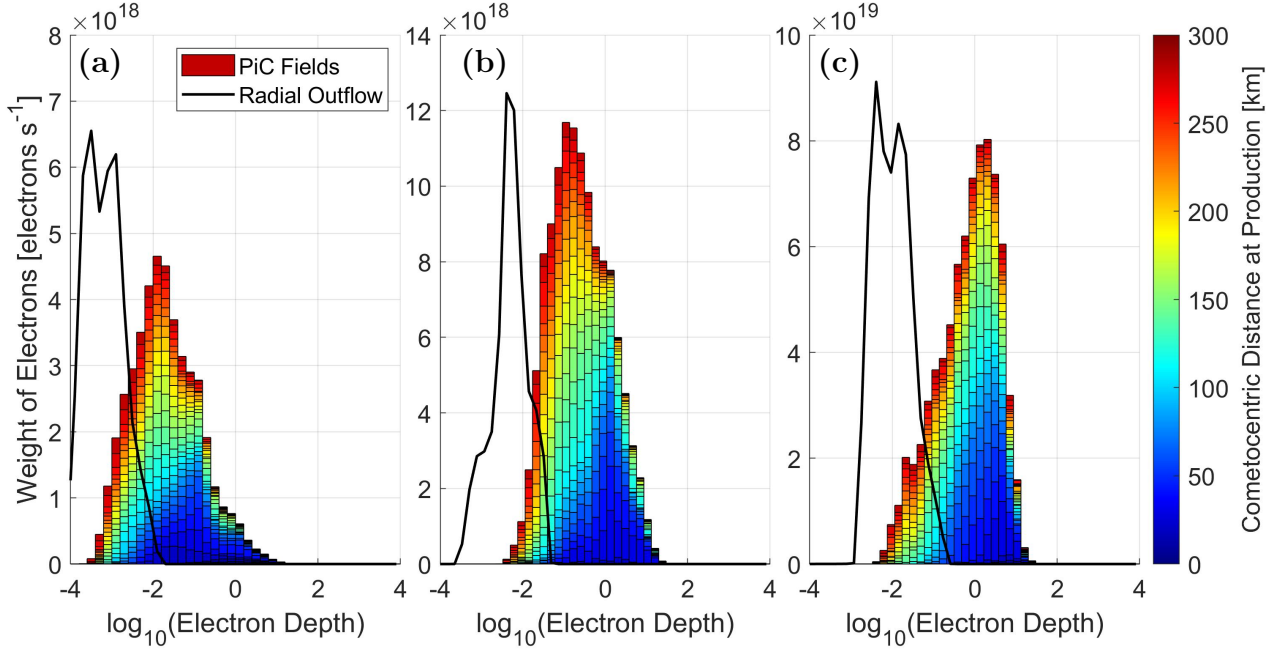


Figure 3.8: Electron depth distributions of cometary electrons (photoelectrons and secondary electrons) at outgassing rates of (a) 10^{26} s^{-1} , (b) $3 \times 10^{26} \text{ s}^{-1}$ and (c) $1.5 \times 10^{27} \text{ s}^{-1}$. The colour of the bars indicates the cometocentric distance at which the electron was initially produced in the coma. The black lines correspond to the radial outflow case, with electrons produced through photoionization.

from a Maxwellian energy distribution, but the macroparticle velocity is imposed as the neutral outflow velocity and the fields are set to zero throughout the domain.

For radially outflowing electrons, 98% of the electrons have depths ranging from 1.3×10^{-3} to 0.1 at the highest outgassing rate ($Q = 1.5 \times 10^{27} \text{ s}^{-1}$). In this case, none of the electrons exceed the threshold for a collisional coma ($\tau_e = 1$), so the photoelectrons are unlikely to be degraded in energy. The radial outflow case is estimated to be less collisional than the approximation by Mandt et al. (2016) as only inelastic collisions are included here rather than the momentum transfer cross section ($\sigma_{mom} = 5 \times 10^{-16} \text{ cm}^2$). Under the weaker outgassing conditions, the coma is even less collisional and the electron depths do not reach 3×10^{-2} . Radial outflow of electrons does not lead to a collisional coma under any of the considered outgassing conditions.

However, when using the realistic set of electric and magnetic fields, the electron depth distributions are substantially shifted towards more collisionality. The median electron depths are between a factor of 25 (at $Q = 10^{26} \text{ s}^{-1}$) and 91 (at $Q = 1.5 \times 10^{27} \text{ s}^{-1}$) larger when the fields are accounted for (see Table 3.1). The lower quartiles of the distribution are shifted by a factor of 17 to 50 (increasing with outgassing rate), but the upper quartiles are boosted by a factor of 50 to 120. The electrons which give the lowest electron depths are those that quickly leave the coma and exit the domain. These do not fall into the potential well around the nucleus, and instead enter

Table 3.1: Properties of the electron depth distributions for radial outflow and with realistic electric and magnetic fields.

Outgassing rate [s ⁻¹]	Median τ_e radial outflow	Median τ_e PiC fields	Collisional electron percentage [%]	Average e^- cooling exobase radius [km]
10^{26}	4.9×10^{-4}	0.013	2.5	10-20
3×10^{26}	4.0×10^{-3}	0.18	20	50-60
1.5×10^{27}	7.5×10^{-3}	0.68	41	190-200

the solar wind. The increased path length for the electrons which quickly leave the coma is largely driven by the gyration around the field lines, compared with the linear trajectory of radial outflow. Moving to intermediate and larger electron depths, the electrons are subject to trapping in the ambipolar potential well. This causes them to trace long paths through the coma, and they are funnelled into regions of high neutral density where the potential well is deepest. Consequently, the electron motion is even further removed from the case of radial outflow and the disparity in electron depths is enhanced.

Electrons depths increase with outgassing rate, as was expected. The median electron depth increases from 1.3×10^{-2} to 0.68 between the lowest and highest outgassing cases. The percentage of collisional electrons in the coma ($\tau_e > 1$) also increases with the outgassing rate. At $Q = 10^{26} \text{ s}^{-1}$, only 2.5% of the cometary electrons produced underwent a large electron depth, resulting in a very weakly collisional coma. This is reflected in the small cold electron population observed in Figures 3.2a and 3.3a and the low fraction of cold electrons across the wider coma (see Figure 3.4a). At $Q = 3 \times 10^{26} \text{ s}^{-1}$, 20% of the cometary electrons are collisional and the fraction of cold electrons is much higher ($n_{\text{cold}}/n_e > 5 \%$) in the extended tailward region (Figure 3.2b). The cometary cold electron population is also prevalent much further away from the nucleus (see Figure 3.3b). When the outgassing rate is increased to $Q = 1.5 \times 10^{26} \text{ s}^{-1}$, the median electron depth increases to 0.68 and 41% of the produced cometary electrons are likely to undergo collisions. The larger collisional fraction complements the higher fraction of cold electrons seen in Figure 3.4c.

The distribution of electron depths is skewed further to the right as the outgassing rate rises. At $Q = 1.5 \times 10^{27} \text{ s}^{-1}$, the distribution has almost no tail at high electron depths. The cut-off occurs at $\tau_e = 10$. At such large electron depths, the electron has likely undergone many inelastic collisions with the neutral coma and become significantly degraded in energy. As the electrons lose energy, they fall below the threshold energies of many of the collisional processes (see Tables 2.1 and 2.2). When this occurs, the electron depth no longer accumulates for that process. As electrons approach $\tau_e = 10$, they may fall below the threshold energies for even vibrational collisions. They still undergo inelastic, rotational collisions ($E_{Th} = 0.004 \text{ eV}$) when below 0.2 eV and can become increasingly cooled, but this is not included in the calculated electron depth.

Electrons produced close to the nucleus (blue, Figure 3.8) undergo larger electron depths than those produced at a large cometocentric distance (red). At one extreme, the electrons produced in the inner coma are efficiently trapped by the ambipolar potential well and build up large electron depths. At the other extreme, in the tail, which is associated with low electron depths, photoelectrons are produced far from the nucleus and leave the coma quickly into the solar wind. There are substantial overlaps between cometocentric distances, with some electrons produced close to the nucleus (< 20 km) leaving the domain with smaller electron depths than others produced beyond 280 km. When using realistic fields, there is substantial variation in the trajectories for electrons produced at the same cometocentric distance. The electric and magnetic environment in all three cases is very asymmetric (see Figure 2.10), so there are significant differences between regions at the same cometocentric distance. In addition, the initial particle velocity and the probabilistic nature of collisions can result in a wide variety of trajectories through the coma, even for electrons ionized at the same location.

The overlap between cometocentric distances is also seen in the radial outflow case, although to a lesser extent than when using realistic fields. The particles produced at each cometocentric distance follow identical trajectories through the coma, removing one source of variation. However, the photoelectrons are sampled from a Maxwellian distributions. The total inelastic collision cross section ($E_{Th} > 0.15$ eV) varies with energy from a minimum of 4.7×10^{-17} cm² at 3 eV to a maximum of 5.3×10^{-16} cm² at 60 eV. Therefore, the electron depths from a given cometocentric distance have a range of just over an order of magnitude, under radial outflow. As the column density traced by an electron moving radially from its initial radius, r , is $N_{col,r \rightarrow \infty} = \frac{Q}{4\pi u_{gas} r}$, the electron depth distribution overlaps with electrons emitted ten times closer to or further from the nucleus.

The electric and magnetic fields substantially increase the collisionality of the coma, compared to the case of radial outflow. Many of the electrons produced within the coma are collisional at outgassing rates of $Q = 3 \times 10^{26}$ s⁻¹ and $Q = 1.5 \times 10^{27}$ s⁻¹.

3.4 Impact of trapping on the electron exobase

As the distribution of electron depths is significantly altered from the case of radial outflow, I now consider the position of the electron exobase. This is defined as the boundary below which electrons are collisional, although the boundary is not sharp. Figure 3.9 shows the fraction of cometary electrons which experience an electron depth $\tau_e > 1$ against the cometocentric distance at which the electrons are initially produced, at each outgassing rate. The electron depth only

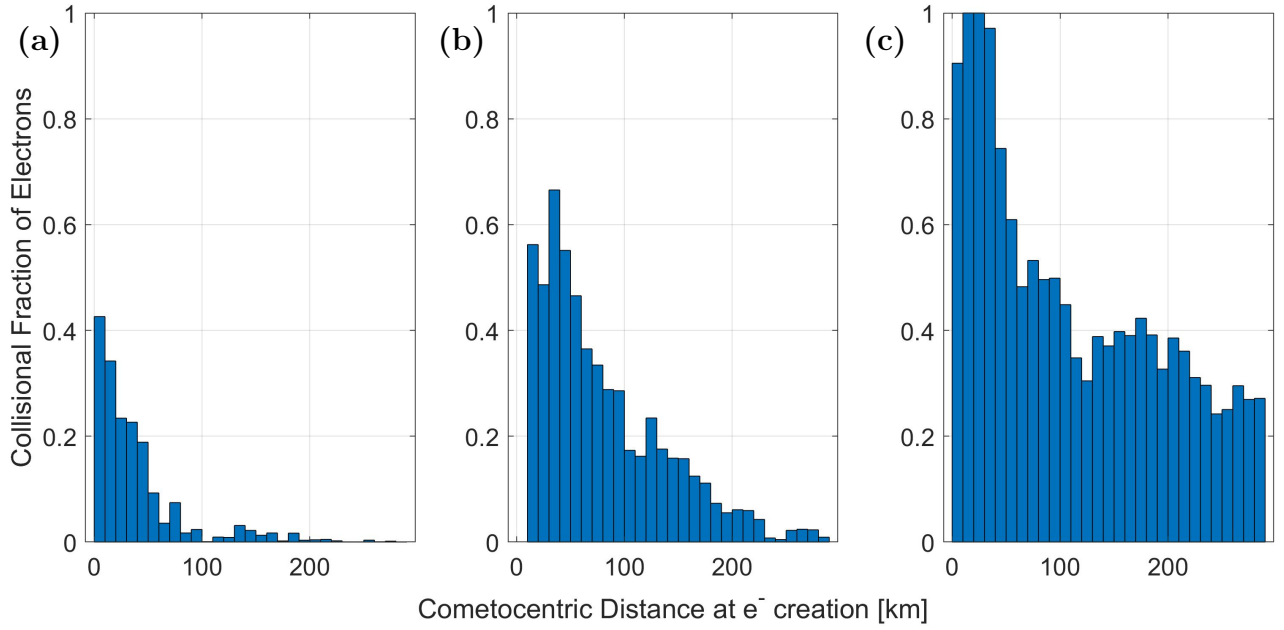


Figure 3.9: Fraction of electrons with an electron depth $\tau_e > 1$, among all electrons initially produced at a given cometocentric distance (in 10 km bins) through photoionization or electron-impact ionization. (a) $Q = 10^{26} \text{ s}^{-1}$, (b) $Q = 3 \times 10^{26} \text{ s}^{-1}$ and (c) $Q = 1.5 \times 10^{27} \text{ s}^{-1}$.

includes collisions which cause substantial energy loss ($E_{Th} > 0.15 \text{ eV}$), so the boundary should be considered as an ‘electron cooling exobase’. This is distinguished from the electron exobase which also accounts for elastic collision processes.

As discussed in Section 3.3, the electrons produced farther from the nucleus are less likely to undergo collisions with the neutral gas. The fraction of collisional electrons also decreases with increasing cometocentric distance under all three outgassing conditions. Although only 2.5% of all the electrons were collisional at $Q = 10^{26} \text{ s}^{-1}$, this fraction increase to 40% when considering the electrons produced within 20 km of the nucleus. Despite the small collisional fraction of electrons across the whole coma, the region near the nucleus can still be considered collisional. At higher outgassing rates, the collisional fraction is larger within 20 km of the nucleus (60% and $\sim 100\%$ for $Q = 3 \times 10^{26} \text{ s}^{-1}$ and $Q = 1.5 \times 10^{27} \text{ s}^{-1}$, respectively). A large fraction of the electrons is collisional at larger cometocentric distances.

Given the wide variety of particle trajectories possible with the complex fields, not all electrons are required to undergo collisions, for a region to be collisional. I suggest that the region is collisional if 30-40% of the electrons are likely to undergo collisions and become degraded in energy. This places the average cooling exobase at a cometocentric distance of 10-20 km for $Q = 10^{26} \text{ s}^{-1}$, 50-60 km for $Q = 3 \times 10^{26} \text{ s}^{-1}$ and in the region of 200 km for $Q = 1.5 \times 10^{27} \text{ s}^{-1}$ (see Figure 3.9). These values are also consistent with the regions of high cold electron density seen in Figure 3.2. In all of the above cases, no electron exobase (meaning no collisional region) is predicted in the

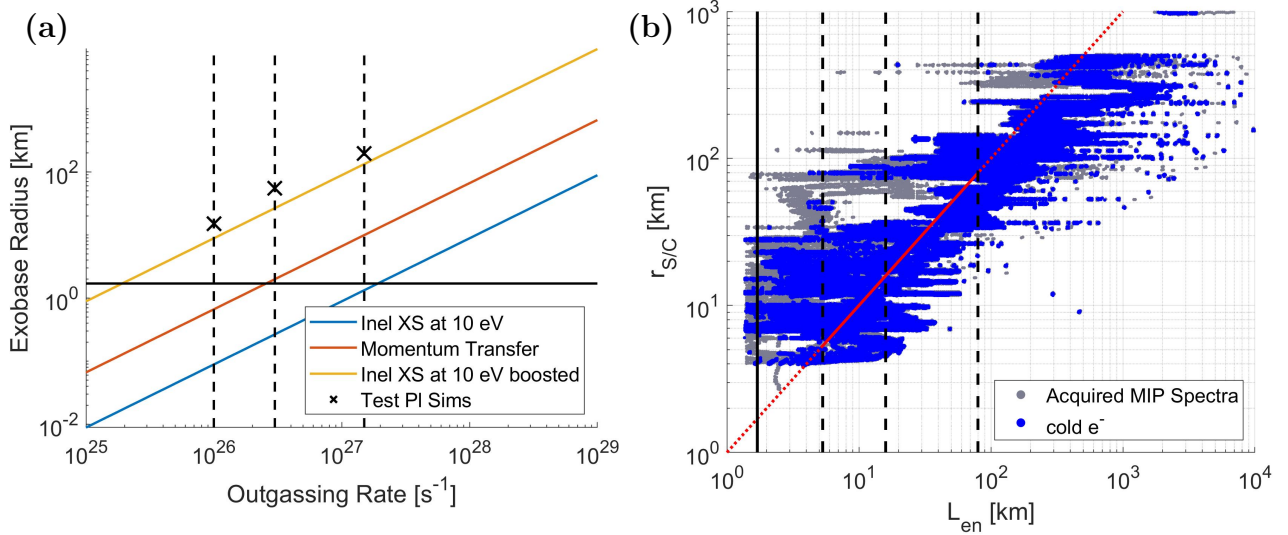


Figure 3.10: (a) Estimated positions of the electron cooling exobase from Eq. 3.5 using $u_{gas} = 1 \text{ km s}^{-1}$ and (blue) the inelastic collision cross section at 10 eV for $E_{Th} > 0.15 \text{ eV}$, (red) the electron-neutral momentum transfer cross section (Mandt et al., 2016) and (yellow) the inelastic cross section boosted by a factor of 100 (Eq.3.6). The horizontal black line is the radius of the nucleus. Vertical dashed lines indicate the outgassing rates used in the test particle simulations. Crosses - estimated position of the electron cooling exobase in the test particle simulations. (b) Cometocentric distance of Rosetta against the new estimate of the electron cooling exobase distance, L_{en} , for the cold electron detections (blue) by RPC/MIP (Gilet et al., 2020). Grey points are the acquired RPC/MIP spectra without cold electron detections (Gilet et al., 2020). The red line indicates where the exobase is at the spacecraft location. Points to the left of the red line are not expected to be collisional. The dotted red line is used outside the range of outgassing rates modelled here, as the approximation of the cooling exobase position may not be valid. Vertical dashed lines correspond to outgassing rates of the test particle simulations, with $u_{gas} = 1 \text{ km s}^{-1}$ (see Section 3.1 and Eq. 3.6), while the solid black line indicates the nucleus surface.

coma, when assuming radial outflow of electrons. While the cooling exobase is placed here at a specific, uniform cometocentric distance, the boundary between the collisional and non-collisional regions of the coma would be highly asymmetric. At a distance of 150 km for $Q = 1.5 \times 10^{27} \text{ s}^{-1}$, an electron may still be deep in the ambipolar potential well or in a region of weak potential and free to enter the solar wind.

It is clear that when the dynamics of electrons are accounted for, even weakly outgassing comae have collisional regions for electrons and can sustain a cold electron population. Figure 3.10a illustrates estimates of the electron cooling exobase using Equation 3.5 (based on radial outflow) compared to the test particle simulations. Mandt et al. (2016) used the electron-neutral momentum transfer cross-section at 5 eV ($\sigma_{mom} = 5 \times 10^{-16} \text{ cm}^2$) to estimate the exobase position (red, Figure 3.9). In this chapter, I have used the inelastic collision cross section (for $E_{Th} > 0.15 \text{ eV}$) to estimate the exobase position, as these are the collisional processes which cause substantial energy loss. The estimated cooling exobase location using the inelastic cross section for a 10 eV

electron ($\sigma_{inel} = 6.7 \times 10^{-17} \text{ cm}^2$) is shown by the blue line. For both cross sections, the estimated exobase radius is greatly underestimated compared to the exobase derived from the test particle simulations (black crosses).

The collisional tail of electron depths were enhanced by 2 orders of magnitude when using realistic fields compared to the radial outflow case. The scale height of the neutral coma is not a good estimate of the path traced through the coma, when fields are accounted for. If the expected path length traced by an electron is increased by a factor of 100 to approximate the motion of the electrons in the fields, the new cooling exobase position is given by:

$$\begin{aligned} r_{exobase} &= 100 \times n_{S/C} \sigma_{inel} r_{S/C}^2 \\ &= \frac{100 Q \sigma_{inel}}{4\pi u_{gas}} \end{aligned} \quad (3.6)$$

The estimated cooling exobase position (yellow, Figure 3.10a) agrees well with the test particle results (black crosses).

The increased electron exobase estimate is also in much better agreement with the cold electrons observed by Engelhardt et al. (2018) and Gilet et al. (2020), compared to the estimate by Mandt et al. (2016). Figure 3.10b shows the location of cold electron detections using RPC/MIP electron density measurements throughout the escort phase, compared to the new estimated values of the cooling exobase location. With the previous approach, the spacecraft was estimated to almost never be below the electron exobase despite frequent cold electron measurements (Gilet et al., 2020). With the new estimate of the electron cooling exobase, the spacecraft was often below the estimated exobase (bottom right) and detected many cold electrons when it was. There were few MIP spectra taken below the estimated cooling exobase that did not contain cold electrons, for the range of outgassing rates modelled here (vertical dashed lines).

There were still many cold electron detections above the new electron cooling exobase estimate, even over the modelled outgassing rates. There are a number of potential causes of this. Firstly, the exobase here is defined by the fraction of collisional electrons produced at a given cometocentric distance. This does not exclude the transport of cold electrons out of the collisional region and in fact many cold electrons are seen outside the exobase in the test particle models (see Figures 3.2 and 3.3), where transport is dominating as a source of cold electrons (see Fig 3.6). These detections could be in the tailward region, where cold electrons are preferentially transported. Secondly, the simulations are only driven under one set of solar wind conditions. Variation of the solar wind density and magnetic field strength could significantly modify the size and depth of the potential well, which would then impact the trapping and cooling of electrons. Finally, the

model does not include any consideration of asymmetric outgassing from the nucleus. The effect of asymmetry on the field structure and the collisionality of the coma has not yet been explored.

The new estimate of the exobase certainly breaks down at high outgassing rates, when the collisional processes become too strong and electron motions are not so dependent on the fields. Extensive cooling of electrons in the coma may also reduce the depth of the potential well and moderate the efficiency of trapping in the inner coma. Therefore, Eq. 3.6 is best applied between outgassing rates of $Q = \text{times}10^{26} \rightarrow 1.5 \times 10^{27} \text{ s}^{-1}$ and care should be taken outside this range.

The new estimate of the electron cooling exobase, based on the collisional test particle simulations, is in good agreement with the observations of cold electrons at 67P from Rosetta. Electron-neutral collisions, in combination with the electric and magnetic fields, can generate a cold electron population, even at low outgassing rates.

Chapter Summary

- I have demonstrated that trapping of electrons in an ambipolar potential well can drive electron cooling even at very low outgassing rates.
- I have shown that a substantial cold electron population is sustained in the inner coma for outgassing rates as low as $Q = 10^{26} \text{ s}^{-1}$.
- The impact of electron dynamics on the electron depth, and collisionality of electrons has been assessed and compared to the previously assumed case of radial outflow.
- I have proposed a new electron cooling exobase, which includes the substantial impact of the electric and magnetic fields on collisional processes. This is in good agreement with the cold electron observations at comet 67P, over the modelled range of outgassing rates.

Chapter 4

Multi-instrument analysis of electron-induced far ultraviolet emissions from comet 67P

In this chapter, I present a multi-instrument analysis of far ultraviolet emissions in the southern hemisphere of comet 67P at large heliocentric distances. This is an extension of the methodology presented by [Galand et al. \(2020\)](#), which examines dissociative excitation by electron impact in the northern hemisphere. CO₂ was much more prevalent within the southern hemisphere coma, leading to significant atomic carbon line emissions. The model structure and input datasets from various instruments are outlined in Section [4.1](#). Additional processing of the electron data and far-ultraviolet (FUV) spectra are discussed in Sections [4.2](#) and [4.3](#), respectively.

The multi-instrument analysis is applied in two main configurations. The first case comprises nadir viewing over a shadowed nucleus under quiet solar wind conditions. These well constrained cases are used to confirm the source of FUV emissions is dissociative excitation by electron impact (see Section [4.4](#)). The second configuration took place during Corotating Interaction Regions (CIRs), which reached comet 67P throughout the summer of 2016. In these cases, the temporal variation of the electron-impact excitation frequency and FUV emission brightnesses are compared, demonstrating that the variation of the electron population is occurring globally rather than on small scales (see Section [4.5](#)).

4.1 Description of the multi-instrument analysis

The multi-instrument analysis used in this chapter considers FUV emissions driven by dissociative excitation through electron-impact ($e + M$ for a species M). The emissions from the coma are

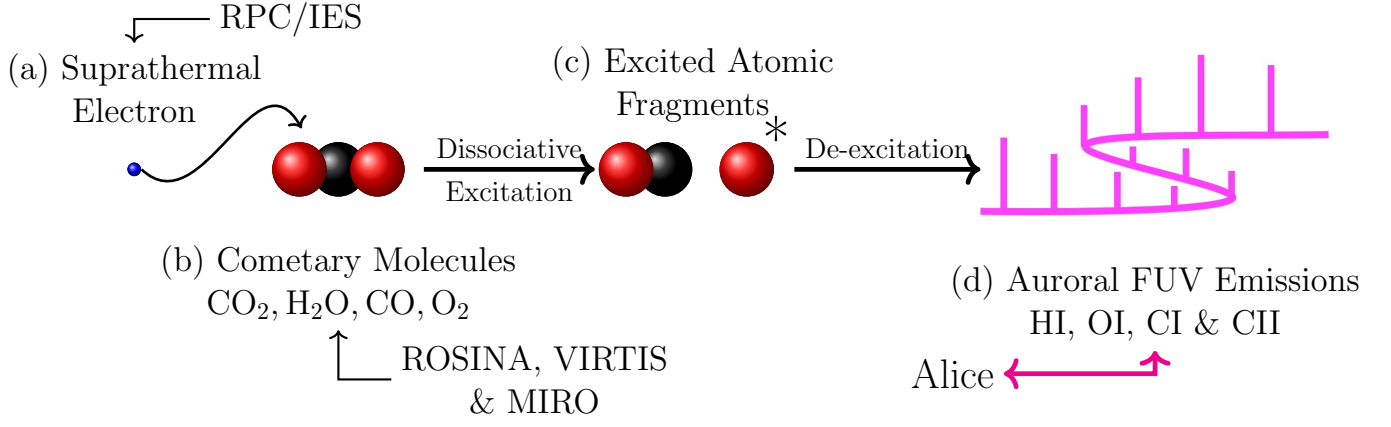


Figure 4.1: Schematic of dissociative excitation by electron impact leading to a line emission in the FUV from an oxygen, carbon or hydrogen atom. The instruments used for each component of the multi-instrument analysis are highlighted. (a) An energetic population of electrons is present within the coma, which was measured by RPC/IES (see Section 4.1.3). The electrons have enough energy to dissociate and excite the neutral gas molecules. (b) The neutral gas coma. The four major species in the southern hemisphere of 67P were: CO_2 , H_2O , CO , and O_2 (see Section 4.1.2). (c) Neutral molecules dissociate when impacted by an energetic electron. The atomic fragment is produced in an excited state. (d) The atomic fragment de-excites, releasing an FUV photon. These photons can be detected using the Alice FUV imaging spectrograph (see Section 4.1.1). Credit: Stephenson et al. (2021).

modelled using a simple physics based approach, which assimilates various datasets from different instruments on board the Rosetta spacecraft. The process of dissociative excitation and the instruments used in the analysis are outlined in Figure 4.1. The observed brightnesses of FUV emission lines are extracted from the Alice FUV imaging spectrograph (see Section 4.1.1) and then directly compared to the modelled line brightnesses (B^X for a line X). The modelled brightness is calculated using

$$B^X = 10^{-6} \sum_l N_l \int_{E_{Th,l}}^{E_{Max}} \sigma_l^X(E) J(E) dE = 10^{-6} \sum_l N_l \nu_l^X. \quad (4.1)$$

N_l is the column density along the line of sight of the FUV imaging spectrograph for each neutral species l . The model includes the four major neutral species in the coma: H_2O , CO_2 , CO and O_2 . The calculation of the neutral column density is discussed in Section 4.1.2. $J(E)$ is the electron particle flux at an energy, E , at the position of Rosetta, which is computed from measurements by RPC/IES (see Sections 4.1.3 and 4.2). The electron flux is combined with the emission cross section, $\sigma_l^X(E)$, from dissociative excitation by electron-impact of each neutral species, l , and leading to the emission of the line, X (see Section 4.1.3). The integral over energy extends from the threshold energy, $E_{Th,l}$, for each line, l , and species, X , up to a maximum energy, $E_{Max} = 300$ eV, above which the electron flux is small. The integral is equivalent to the emission frequency, ν_l^X , of the electron-impact excitation process. In addition to the emissions from electron-impact

excitations, there are also non-electron induced emissions from the neutral gas coma, which have been assessed in Section 4.1.4. The differences in the methodology between the nadir observations in quiet conditions and the CIR observations during in 2016 are highlighted in the Sections 4.1.1, 4.1.2, 4.4.1 and 4.5.

4.1.1 Observed brightness of FUV emission lines

The brightnesses of the FUV emission lines are derived from the Alice FUV imaging spectrograph (see Section 1.1.3; Stern et al., 2007), which operated at wavelengths between 700 and 2050 Å. The Alice slit comprised 32 rows and had a dogbone-like shape. The rows at either end of the slit had a width of 0.10° while central rows only subtend an angle of 0.05° . Two rows (12 and 19) act as a transition between the two widths and have been excluded from the analysis.

The Alice scans last between 5 and 10 minutes, although multiple consecutive scans can be co-added to improve the signal-to-noise ratio. As well as co-adding scans, adjacent rows can be combined to improve the signal-to-noise ratio. In this case, even numbers of rows are used to mitigate the effect of an odd-even oscillation in brightness that was present between rows.

The observations used in this study are split into two types: quiet period observations in the nadir direction and observations during CIRs. For nadir viewing, the comet was fairly stationary in the field of view of the Alice slit, so only a small region of the coma is probed. As the nucleus moves little during the selected nadir observations, consecutive Alice scans are combined without significantly changing the probed region of the coma.

The nadir cases are selected from times when the surface of the nucleus was shadowed, to minimise any contamination of the emission spectra from reflected solar flux. Only one region of the Alice slit is considered for these observations, which corresponds to the nadir viewing geometry. Figure 4.2 shows an example of the nadir viewing geometry which is employed and the corresponding emission spectra in the case of a shadowed nucleus. The emission line brightnesses used for the nadir cases were provided by Feldman et al. (2018) and Feldman (2019).

During the CIR observations, the temporal variation of the emissions is highly relevant. Therefore, consecutive Alice observations have not been co-added, but the brightness is calculated in several regions of the Alice slit to account for some spatial variability. In addition, there are few periods when the CIR was observed at 67P during the summer of 2016 so it was not possible to only choose observations when looking in the nadir over a shadowed nucleus. The Alice observations during the CIRs are across a range of viewing geometries, with both limb and off-nadir views of the nucleus, including times with an illuminated nucleus. The emission line brightnesses were

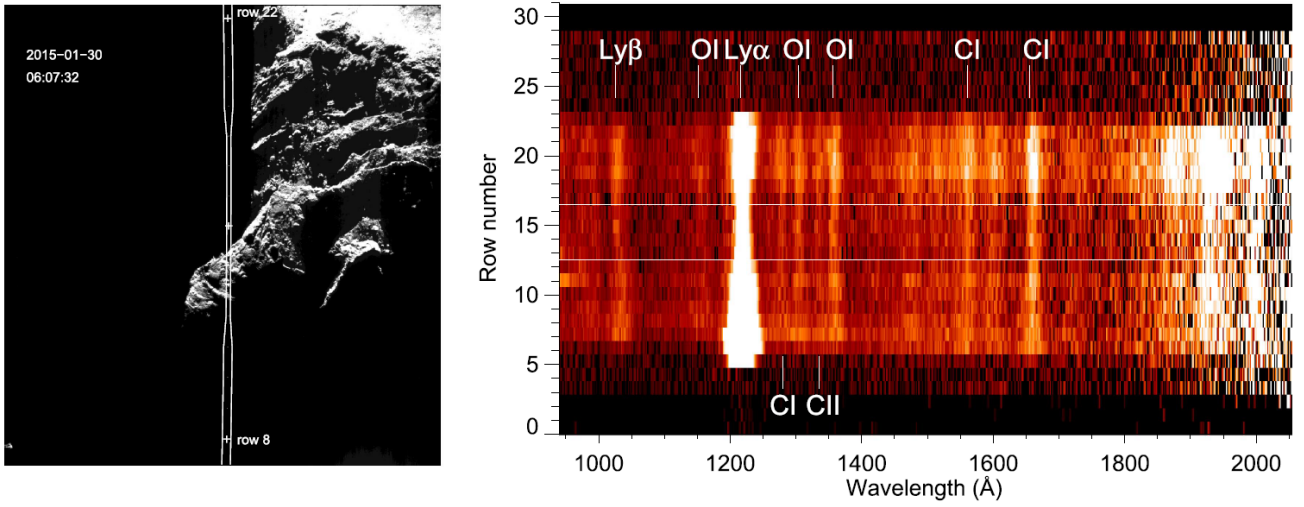


Figure 4.2: (a) NAVCAM image of the viewing geometry of an observation over the shadowed nucleus on 30 Jan 2015. The Alice slit is superimposed in white. (b) Alice FUV emission spectra from the southern hemisphere of 67P, when observing the shadowed nucleus in the nadir. Credit: [Feldman et al. \(2018\)](#)

computed from the Alice Level 4 dataset (comprising photon flux measurements) as outlined in Section 4.3, including the removal of scattered solar flux.

I consider five lines and multiplets in the FUV: Lyman- β , OI1304, OI1356, CI1657 and CII1335, which are atomic emissions from components of the four major neutral species within the coma. Previous work by [Galand et al. \(2020\)](#) did not consider carbon line emissions, or the contribution from carbon-containing species, as it focused on the northern hemisphere where they were not significant. The five atomic lines considered are highlighted in Figure 4.3 for two cases with a large (blue) and small (orange) electron flux. Throughout, I have discounted Lyman- α from the analysis despite it being the brightest emission line from the coma. During the Rosetta mission, the detector degraded over the wavelength range of Lyman- α , which made calibration of this line very difficult. Additionally, solar flux and the interplanetary medium (IPM) have very strong contributions to Lyman- α , at 1216 Å, which make it increasingly challenging to discern the emissions that originate from the coma. The IPM also contributes to the Lyman- β brightness producing background emissions of 2 R. However, Lyman- α emissions by the IPM are 300 times larger ([Feldman et al., 2015](#)).

As well as atomic emission lines, there are several other emission features from molecular transitions that contribute in the FUV. The CO Fourth Positive Group (CO4PG) emits in the range 1400-1800 Å, with several bands close to the CI emission at 1657 Å ([Beegle et al., 1999](#)). The strongest bands close to the 1657 Å multiplet are (3,4) at 1648 Å, (0,2) at 1653 Å and (1,3) at

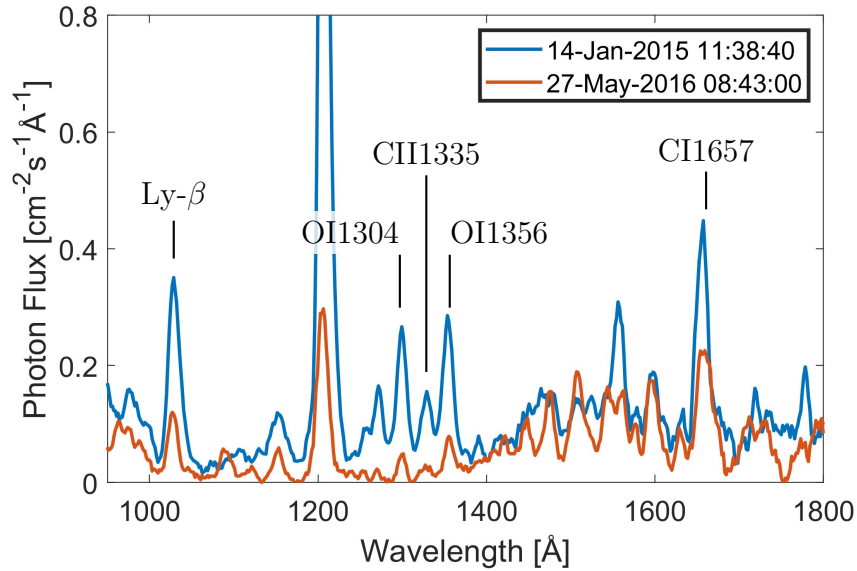


Figure 4.3: FUV emission spectra from Alice for nadir viewing over the southern hemisphere during two intervals in quiet observation periods. The photon fluxes have been co-added over four rows in the Alice slit and a five-point moving average has been applied over wavelength to reduce the noise in the spectra. The conditions for the two observation periods are listed in Table 4.2. The emission lines considered in the multi-instrument analysis have been highlighted. Credit: [Stephenson et al. \(2021\)](#).

1670 Å ([Beegle et al., 1999](#), see Section 4.1.4).

4.1.2 Neutral Column Density

The brightness of the emissions is highly dependent on the column density of neutral gas along the line of sight of the FUV spectrograph. The approach and instrumentation used are quite different between the nadir cases (in Section 4.4) and the cases analysed during CIRs (see Section 4.5). This is due to the distinct viewing geometries and the applicability of the instruments in each scenario.

In nadir viewing, the neutral gas is moving radially away from the surface, which is approximately along the line of sight of Alice. As a result, the neutral gas at different points throughout the column originates from a similar region of the nucleus surface. The neutral gas sublimates from near-surface ices, with no evidence of a significant extended source for the major neutral species ([Hässig et al., 2015](#); [Bieler et al., 2015a](#)). As a result, the column of neutral gas that is expected to have a homogeneous composition throughout. Consequently, the composition of the column is reliably determined from in situ measurements by the mass spectrometer, ROSINA/DFMS (see Section 1.1.2). The lack of significant extended neutral source also ensures that the neutral number density follows a $1/r^2$ dependence. Assuming the FUV spectrograph is looking in the

nadir, the total column density along the line of sight is:

$$N_{Tot} = n(r_{Rosetta})r_{Rosetta}\left(\frac{r_{Rosetta}}{r_{67P}} - 1\right), \quad (4.2)$$

where $r_{Rosetta}$ is the cometocentric distance of the spacecraft and r_{67P} is the radius of the nucleus at the base of the gas column. The neutral density, $n(r_{Rosetta})$ is measured at the spacecraft by ROSINA/COPS, with a correction for the neutral composition (see Section 1.1.2; Gasc et al., 2017b). The total column density is divided into the four neutral species using $N_l = x_l N_{Tot}$ for $l = \text{H}_2\text{O}, \text{CO}_2, \text{CO}, \text{O}_2$, where x_l is the volume mixing ratio measured by ROSINA/DFMS.

The extrapolation of the column density from in situ measurements is highly dependent on the cometoradius at the foot of the gas column, r_{67P} . This varies significantly across the surface of the nucleus because of its bilobal shape (Jorda et al., 2016). An average radius of $r_{67P} = 1.7$ km is used throughout this study, with a standard deviation of $0.26 \times r_{67P}$ (Gaskell et al., 2017). The uncertainty in the cometoradius leads to uncertainty of 30% in the total column density, which increases to 35% when the spacecraft is close to the nucleus (~ 10 km).

In addition to uncertainty in the cometoradius, the outflow velocity of the neutral gas introduces error into the column density. Equation 4.2 relies on the assumption of a constant outflow velocity. However, the neutral gas accelerated away from the nucleus in a region close to the surface (Heritier et al., 2017a; Bykov and Zakharov, 2020), which would enhance the neutral density in that near-nucleus region. Therefore, assuming a constant outflow leads to an underestimate of the neutral column density.

In geometries other than nadir, the properties of the neutral gas may vary substantially along the line of sight. Thus, it is not reliable to extrapolate from in situ measurements. Remote sensing instruments onboard Rosetta also probed several of the major neutral species. VIRTIS (see Section 1.1.3; Coradini et al., 2007) measured the presence of H_2O and CO_2 through the ν_3 vibrational bands of each species, which appear in the infrared at $2.67 \mu\text{m}$ and $4.27 \mu\text{m}$ (Bockelée-Morvan et al., 2015). The derivation of the column densities from VIRTIS was done in line with Bockelée-Morvan et al. (2015). VIRTIS could also measure the presence of CO through the ν (1-0) band, although this is a much weaker transition than the ν_3 bands. The weak band coupled with the low mixing ratio of CO, led to a low signal-to-noise ratio for the CO column when at large heliocentric distances. Only VIRTIS-H has been used for this analysis, as VIRTIS-M ceased operation in May 2015 (Bockelée-Morvan et al., 2016) and the analysed CIR events occurred in summer 2016.

MIRO (see Section 1.1.3; Gulkis et al., 2007) measured the presence of H_2O and CO in the sub-mm range, using the (110-101) rotational line of H_2O (H_2^{18}O) at 557 GHz (548 GHz) and the

CO (5-4) rotational line at 576 GHz. Emission spectra were taken in limb viewing, whereas for nadir viewing absorption spectra were preferred (Biver et al., 2015, 2019). Similarly to VIRTIS, the CO(5-4) line is intrinsically weaker than the H₂O lines. The weak line and low CO abundance make it difficult to retrieve CO column density estimates.

Both the infrared and sub-mm spectrometers were roughly aligned with the line of sight of the centre of the Alice slit (see Fig. 1.8). Therefore, the columns of gas probed by MIRO, VIRTIS and Rows 14 and 15 of Alice should be approximately the same. These observations are preferable when looking at the comet limb, as much less is known about the profile of the neutral gas due to spatially varying composition and outgassing rate. The remote observations are not used for the nadir cases. MIRO observes a substantial background emission from the surface, which reduces the contrast with emissions from the coma. This makes it very challenging to retrieve nadir column densities from MIRO, when at large heliocentric distances. It is possible to use nadir VIRTIS observations, but measurements in this configuration were infrequent throughout the mission and did not occur around the same times as the Alice observations.

4.1.3 Emission Frequency of dissociative excitation by electron-impact

The emission frequency of dissociative excitation by electron-impact is given by:

$$\nu_l^X = \int_{E_{Th,l}}^{E_{Max}} \sigma_l^X(E) J(E) dE. \quad (4.3)$$

This is calculated from electron-impact emission cross sections, $\sigma_l^X(E)$, and the electron particle flux, $J(E)$, derived from RPC/IES measurements during each Alice observation period as outlined below.

Dissociative excitation cross sections

The dissociative excitation cross sections, and relevant threshold energies, used in this analysis are outlined in Table 4.1 and shown in Figure 4.4. Unfortunately, it is common for the excitation cross sections to be known only at one or two energies for each emission process, which leaves uncertainty in the energy dependence of the cross sections. As such, a number of assumptions have been made about the shapes of the cross sections, which are also specified in Table 4.1.

Several of the emission cross sections were updated by Ajello et al. (2019), including the emission of OI1356 from electron impact on CO₂. However, the updated OI1356 cross section has not been used in this study. The new cross section of OI1356 from e + CO₂ is an order of

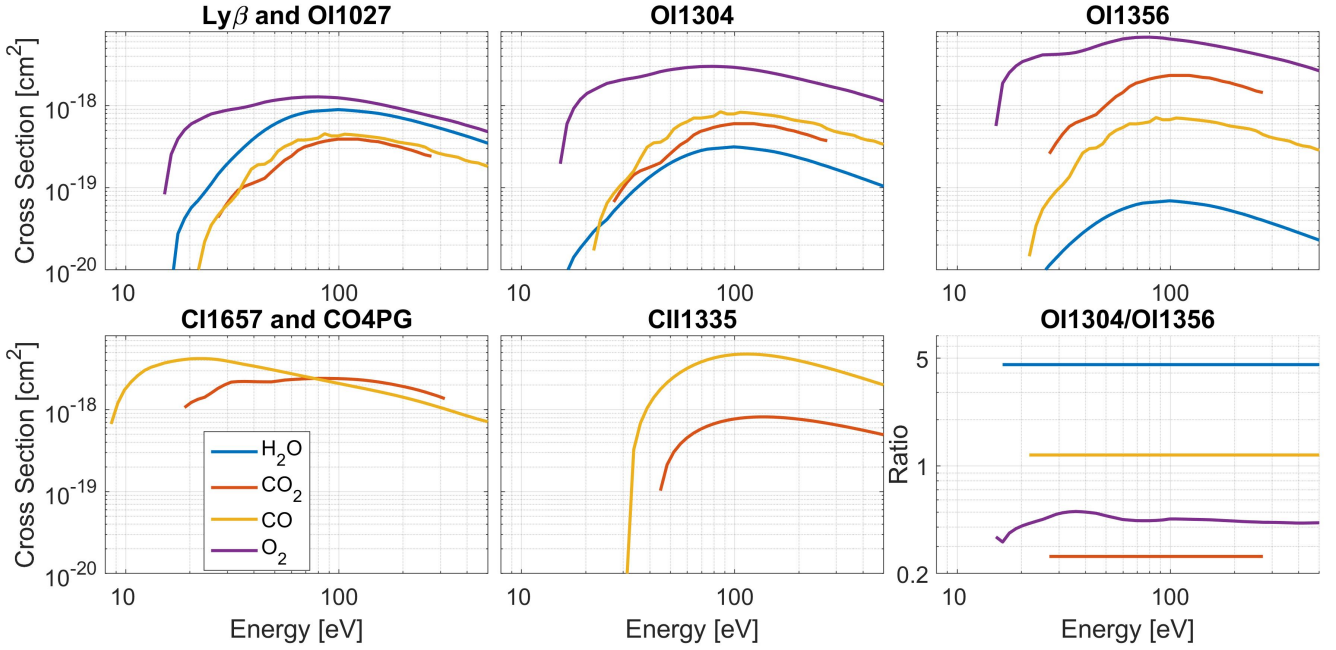


Figure 4.4: Emission cross sections of dissociative excitation by electron impact for the emission features considered in this study: (a) Lyman- β and OI1027; (b) OI1304; (c) OI1356; (d) CI1657 and the CO Fourth Positive Group; and (e) CII1335. (f) The ratio between OI1304 and OI1356 cross sections. The cross sections, and ratio, are shown for the four major neutral species in the coma: H_2O , CO_2 , CO and O_2 . The relevant references and assumptions are outlined in Table 4.1.

magnitude smaller than previous estimates (Wells et al., 1972; Wells and Zipf, 1974), and gives a OI1304/OI1356 line ratio of ~ 3.2 from electron impact on CO_2 . This line ratio is inconsistent with observations from Rosetta when electron impact on CO_2 was the dominant emission process (Section 4.4; Feldman et al., 2018) and an emission ratio < 1 was observed.

OI1356 emission is associated with a forbidden-transition, so the upper ^5S state has a long radiative lifetime ($180 \mu\text{s}$; Wells and Zipf, 1974). In a sufficiently dense gas, the long-lived state can be quenched through collisions, which prevents the emission of OI1356. Previously, the estimated cross sections were derived from separate measurements of the production and lifetime of the ^5S state (Wells et al., 1972; Wells and Zipf, 1974) and were therefore not as susceptible to quenching of the intermediate state. Ajello et al. (2019) used emission spectra of CO_2 in a relatively dense neutral gas background ($\sim 3 \times 10^{11} \text{ molecules cm}^{-3}$). This is 3-4 orders of magnitude denser than the neutral gas coma at Rosetta for large heliocentric distances. Therefore, the measurements by Ajello et al. (2019) may have been more susceptible to quenching and consequently underestimated the OI1356 cross section.

Suprathermal electron flux

The suprathermal electron flux is derived from measurements by RPC/IES and corrected using the spacecraft potential, as measured by RPC/LAP (see Section 1.1.1). The calculation of the

Table 4.1: Emission cross-sections for the dissociative excitation of cometary molecules by electron impact. ¹ Mumma et al. (1972). ² McConkey et al. (2008).

Emission Line	Species	Threshold Energy [eV]	Reference and Assumptions
Ly- β & OI1027	H ₂ O	17.21	Makarov et al. (2004). Assume the same shape as Ly- α with ratio 7/55 at 200 eV. Includes coincident OI line.
	CO ₂	21 ± 2 ¹	Kanik et al. (1993) Assume the same shape as OI1304. Use ratio at 200 eV.
	CO	23.17	James et al. (1992).
	O ₂	20.6	Wilhelmi and Schartner (2000). Absolute value given at 200 eV. Assume same shape as OI1304.
OI1304	H ₂ O	15.2	Makarov et al. (2004).
	CO ₂	21 ± 2	Mumma et al. (1972). Reduced by a factor of 0.59 due to updated measurements of H ₂ Ly- α (McConkey et al., 2008).
	CO	20.6	Ajello (1971a). Some uncertainty at energies > 100 eV.
	O ₂	14.6 ²	Kanik et al. (2003). Scaled up by factor 2.93/2.90 in line with the recommendation by McConkey et al. (2008).
OI1356	H ₂ O	15.2	Makarov et al. (2004). Assume same threshold and shape as OI1304.
	CO ₂	20.6 ²	Feldman et al. (2015). Excitation rate of OI1356 is 33 times larger for CO ₂ than H ₂ O (Wells et al., 1972), after revision of the lifetime of the ⁵ S° state (Wells and Zipf, 1974). Assume the same shape as OI1304.
	CO	20.6	Ajello (1971a). Ratio given at 100 eV (Wells and Zipf, 1974; Wells et al., 1972). Assume the same shape as OI1304.
	O ₂	14.6	Kanik et al. (2003). Scaled up by factor 6.47/6.40 in line with recommendation by McConkey et al. (2008).
CI1657	CO ₂	25 ± 2	Mumma et al. (1972). Difficult to measure cross-section due to the strong overlapping CO4PG band. No contribution from dissociative excitation of CO considered for CI1657.
	CO		
CO4PG	CO ₂	25 ± 2	Contribution of (0,2) bands included in CI1657 cross-section of Mumma et al. (1972). Beegle et al. (1999). Absolute values for bands given at 100 eV. Shape of (0,1) band given. Scaled down by factor 0.925 due to remeasurement of calibrating NI line (Ajello et al., 2019).
	CO	8	
CII1335	CO ₂	44	Mumma et al. (1972). Ajello (1971a).
	CO	33	

electron particle flux from Level 2 count data for each RPC/IES scan is outlined in Section 4.2, including the correction for the spacecraft potential.

As the spacecraft potential was typically negative at $V_{S/C} \approx -10$ V, RPC/IES could only detect electrons with energies in excess of $E_{\min} = 4.32 \text{ eV} - V_{S/C} [\text{V}]$. The threshold energies of many of the emission processes (see Table 4.1) were below the minimum detection energy of the instrument during many scans, which, if neglected, would lead to an underestimate of the emission frequency. To remedy this, the electron fluxes have been extrapolated to low energies. Extrapolation was tested using a constant value and using a power law based on the shape of the electron flux near the minimum-energy detection limit. However, it was found that there was little difference between the two extrapolation methods as the cross section decreases sharply with decreasing energy close to the threshold energy (see Figure 4.4). Consequently, I have extrapolated using a constant value of the flux down to low energies (dashed lines, Figure 4.5).

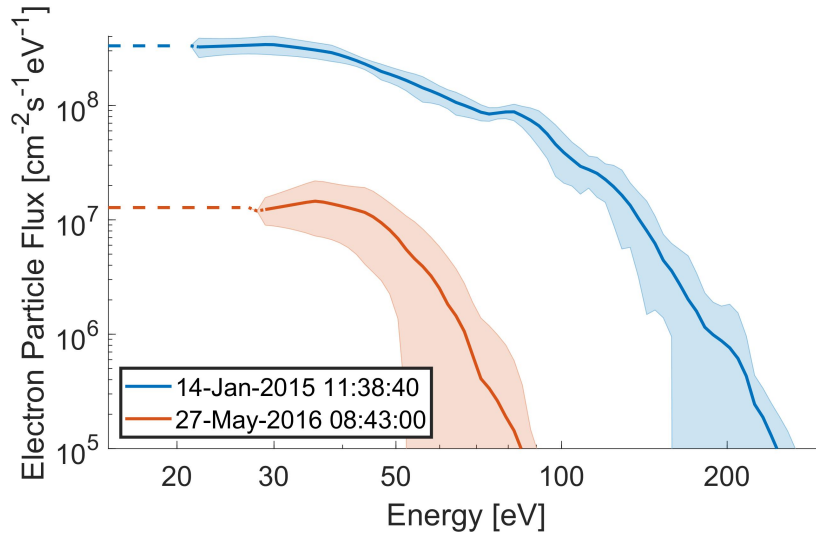


Figure 4.5: Suprathermal electron particle flux during two nadir observations by the Alice FUV spectrograph. The solid line shows the average electron flux at each energy throughout the observation period of the FUV spectrograph, with the shaded region indicating the standard deviation during that time. The spacecraft potential often restricted measurement of low energy electrons, so the flux has been extrapolated in this region. Extrapolated values of the electron flux are plotted with a dashed line. Credit: [Stephenson et al. \(2021\)](#).

The suprathermal electron fluxes are calculated for the quiet nadir cases and the CIR analysis in slightly distinct manners. In the nadir cases, the FUV observations are accumulated in a stationary geometry over an extended period (> 30 mins). The electron flux is time-averaged over the Alice observation time period, once the scans have been individually corrected for the spacecraft potential. Figure 4.5 displays two examples of electron fluxes during high (blue) and low (orange) levels of electron activity. The shaded regions correspond to the temporal variation of the electron flux at a given energy, during the Alice scan. The extrapolation to low energies is

applied after the electron fluxes have been combined.

When considering the CIRs in the summer of 2016, it is more relevant to compare the temporal variation of the FUV emissions and electron flux. Therefore, the electron flux is calculated for each individual RPC/IES scan at the temporal resolution of the electron spectrometer.

The electron flux is determined in situ, but the electron induced emissions occur throughout the neutral column along the line of sight. The electron flux is assumed to be constant throughout the column along the line of sight, which is consistent with work by [Chaufray et al. \(2017\)](#). To examine this assumption further, I consider the electron depth:

$$\tau^{e-} = \sum_l \sigma_l^{e-,inel} N_l, \quad (4.4)$$

where $\sigma_l^{e-,inel}$ is the total inelastic collision cross section of electrons with neutral species, l . Cross sections for both water and CO₂ are taken at 30 eV. The electron depth is analogous to optical depth, so for $\tau^{e-} \gg 1$ electrons are expected to undergo many collisions and become cold whereas for $\tau^{e-} \ll 1$ electrons are not expected to collide inelastically, that is, to be degraded in energy. For all the cases used in this analysis $\tau^{e-} < 0.35$, so electrons are unlikely to undergo inelastic collisions. Therefore, there is not expected to be substantial electron cooling along the observed column of gas and the assumption of constant electron flux is reasonable.

4.1.4 Non-auroral emission sources

In addition to the electron induced emissions from the coma, there are several other sources of FUV photons that need to be accounted for. Firstly, there is the background source of Lyman series photons from the IPM, rather than from the coma. This background is only visible when not obstructed by the nucleus, and so is subtracted from the Alice observations when observing the limb. For this study, only the contribution towards Lyman- β needs to be taken into account, which is roughly 2 R.

As for emissions from the coma, prompt-photodissociation of water and resonance fluorescence of CO are included in the multi-instrument analysis. The photodissociation of water contributes to Lyman- β emissions, whereas fluorescence leads to CO4PG emissions. Both of these processes are induced by solar photons which are incident on the observed column of neutral gas. The brightness of each emission process, $B_l^{X,h\nu}$, is given by:

$$B_l^{X,h\nu} = 10^{-6} N_l \int_{\lambda_{min}}^{\lambda_{Th}} \sigma_l^{X,h\nu}(\lambda) I(\lambda) d\lambda, \quad (4.5)$$

where $\sigma_l^{X,h\nu}(\lambda)$ is the emission cross section. The photon flux, $I(\lambda)$, is taken from measurements by TIMED/SEE (Woods et al., 2005). This is extrapolated from 1 au to the position of Rosetta using a $1/r_h^2$ dependence and correcting for the change in the solar phase. The CO fluorescence is based on the model of Lupu et al. (2007) and the prompt-photodissociation emission cross section is taken from Hans et al. (2015).

The modelled brightness of the non-auroral emissions is likely to be an upper bound, as it is assumed that the whole column of neutral gas is fully illuminated by the Sun. Realistically, it is likely that some of the gas column will be shadowed by the nucleus, especially as Rosetta typically orbited in the terminator plane. This would reduce the modelled brightness of the photon induced emissions.

4.2 Calculation of electron flux and emission frequency from RPC/IES

The electron particle flux at Rosetta is calculated from Level 2 data from RPC/IES (see Section 1.1.1), comprising counts for each azimuthal, elevation and energy bin. The conversion from counts to fluxes is also outlined by Heritier (2018). Firstly, the background particle counts (C_{L3BG} given in the Level 3 data on the PSA) are removed from each of the bins. However, it is necessary to correct the background particle count to give:

$$C_{BG} = C_{L3BG} + \sqrt{5}C_{L3BG} \quad (4.6)$$

RPC/IES resolved a maximum of $16 \times 16 \times 128$ bins in azimuth, elevation and energy, but it was not feasible to use so many bins at all times due to constraints on telemetry. In many cases, neighbouring bins are combined in both the spatial and energy dimensions. In the Level 2 dataset, any combination of the azimuthal bins has been separated back onto the original grid, but combinations of elevation and energy have not. The conversion to a particle flux requires separation of the bins through:

$$C'(\theta_0, \phi_0, E_0, t) = \frac{C(\theta_b, \phi_b, E_b, t) - C_{BG}(t)}{N_{Bins}}, \quad (4.7)$$

assuming counts are distributed evenly between combined bins. $C'(\theta_0, \phi_0, E_0, t)$ is the corrected particle counts for each elevation (θ), azimuth (ϕ) and energy (E). The subscript 0 indicates that it is calculated on the underlying instrument grid, as opposed to the combined binned grids (b).

N_{Bins} is the total number of bins combined, including both elevation and energy.

In addition to removing the background electrons and separating bins, the instrument field of view was partially obstructed as a result of its location on the Rosetta spacecraft. The various other instruments restricted the field of view of RPC/IES more severely for some bins (Clark et al., 2015), and needs to be corrected using a geometric factor (Broiles et al., 2016b). The geometric factor, $G(\theta_0, \phi_0, E_0)$, is given for the intrinsic instrument grid, justifying the need to separate any combined bins. The differential energy flux, $g'(\theta_0, \phi_0, E_0, t)$, is calculated from the corrected counts using:

$$g'(\theta_0, \phi_0, E_0, t) = \frac{C'(\theta_0, \phi_0, E_0, t)}{\Delta t \times G(\theta_0, \phi_0, E_0)}, \quad (4.8)$$

where Δt is the integration time of the RPC/IES scans. Once the differential energy flux is derived, it is re-binned to the energy space of the instrument mode. This is achieved by averaging the flux over the combined bins. The flux is then corrected for the efficiency of the Micro-Channel plates (MCP) in the detector, which is dependent on the energy of the incident electron. This efficiency of the MCP, $0 < \epsilon < 1$, is given by (Kurz, 1979):

$$\begin{aligned} \epsilon(E) = 0.52 \exp \left(- [\log(E + 37) - 2.3]^2 / 0.82 \right) + 0.071 \\ + 0.16 \log(E + 37) - 0.028 \log(E + 37)^2, \end{aligned} \quad (4.9)$$

where the impacting electron energy, E , is given in eV. The differential particle flux is calculated by dividing by the average electron energy within each bin of the detector, E_b :

$$j(\theta_0, \phi_0, E_b, t) = \frac{\sum_{\text{Comb. Energies}} g'(\theta_0, \phi_0, E_0, t)}{N_{\text{Comb. Energies}} \times \epsilon(E_b) \times E_b}. \quad (4.10)$$

As there were issues with many of the azimuthal bins in the detector (see Section 1.1.1), there is little useful information about the angular distribution of electrons. For the purposes here, the angular distribution is also not required, so the electron flux is integrated over the field of view of the instrument. In regions not observed by RPC/IES, it is assumed that the electron flux is isotropic. The electron particle flux, $J(E)$, is:

$$J(E_b) = \frac{4\pi}{2\pi \sin 48^\circ} \int_{\theta_0=-48^\circ}^{48^\circ} \int_{\phi_0=0^\circ}^{180^\circ} \cos \theta_0 \times j(\theta_0, \phi_0, E_b) d\phi_0 d\theta_0 \quad (4.11)$$

where the integrals are over the field of view of the spectrometer and the numerical factor outside the integral corrects to a 4π solid angle. Half of the azimuthal instrument bins degraded during

the mission, which limits the azimuthal range to only 180° .

While this gives the electron particle flux measured at the detector, it is not reflective of the electron flux in the cometary plasma. The potential well around the spacecraft changes the energy of the detected electrons before they reach the sensor. Typically, the spacecraft potential was in the range $[-15, -5]$ V throughout the mission (Odelstad et al., 2017), repelling electrons away from the detector. The electron flux is therefore corrected for the spacecraft potential using Liouville’s theorem:

$$\frac{J(E)}{E} = \frac{J_{IES}}{E_{IES}} \quad \text{where} \quad E [\text{eV}] = E_{IES} [\text{eV}] - V_{S/C} [\text{V}], \quad (4.12)$$

where the subscript *IES* indicates the values measured at the detector. This correction is applied to each RPC/IES scan individually, as the spacecraft potential varied substantially over time.

4.3 Further processing of the Alice dataset

The observations by the Alice FUV imaging spectrograph during the CIRs were under illuminated conditions. During the July observations, the surface of the comet nucleus was illuminated and during the August observations there was still a substantial contribution from scattered solar photons. As the study is focused on emissions from the coma, it is desirable to remove scattered flux from the spectra before calculating the brightness of emission lines.

The Alice Level 4 dataset (available on the PSA) gives the photon flux in spatial and wavelength bins along the slit. For the comparison to the modelled emission lines, the spectral flux is converted to a line brightness, during which the flux is integrated over the wavelength range of the emission feature. As the signal-to-noise ratio is small for a single spatial bin and to mitigate odd-even oscillations (see Section 1.1.3) four neighbouring spatial bins along the slit are averaged.

The scattered solar flux is particularly strong at the long end of the Alice wavelength range (Feldman et al., 2018) and has a significant component in several emission lines, especially CII1335. For the 9-10 July observations, the shape of the solar spectrum is derived from TIMED/SEE (Woods et al., 2005) measurements on 16 July 2016, which occurred at the same Carrington longitude. At the large heliocentric distances considered, the neutral coma was optically thin, so there was little absorption of the solar flux (Heritier et al., 2018b). To estimate the magnitude of solar flux observed by Alice, I compared the long wavelength end of the Alice spectra with the TIMED/SEE solar flux. For each set of co-added rows, the photon fluxes are compared between 1500 and 1800 Å (see Figure 4.6), although regions around emission features at 1561 and 1657 Å are excluded from the fitting. The linear fit is used to scale the solar background for each region of

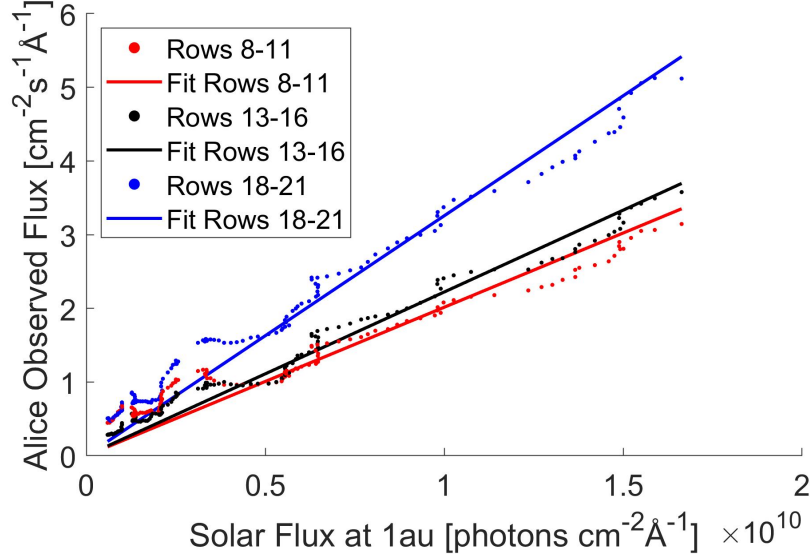


Figure 4.6: Comparison of photon flux measured by the Alice FUV spectrograph at 15:58 UT 9 July 2016 with the solar photon flux, measured by TIMED/SEE. The TIMED/SEE flux is averaged over the wavelength bins of the Alice instrument. The flux is compared at long wavelengths (1500 Å - 1800 Å), excluding regions with atomic emission features. The flux is separately compared for the three distinct regions of the Alice slit: Rows 8-11 [red], Rows 13-16 [black] and Rows 18-21 [blue]. The linear fits (solid lines) are to scale the magnitude of the solar flux, so it can be subtracted from the observed Alice emission spectra. Credit: [Stephenson et al. \(2021\)](#).

the slit (green, Figure 4.7). The scattered solar flux is subtracted from the Alice observations (dark blue) to give the residual emissions from the coma (light blue). The peaks in the TIMED/SEE dataset are much narrower than those observed in the Alice dataset, which may be driven by the lower spectral resolution of the Alice instrument. Also, the peak in emission from the coma at 1657 Å incorporates the atomic CI line in addition to several bands of the CO4PG, which further widens the peak. Before removing the scaled solar flux from the observed spectra, the TIMED/SEE data is smoothed using a 10 Å sliding window to broaden the peaks and be consistent with the spectral resolution of Alice.

The emission features in the residual spectra are fitted with a linear combination of two Gaussian distributions. The combination of two Gaussians gives the best fits to the emission spectra, as the peaks in the solar spectrum are still narrower than those in the Alice data. For the brightness to be included in the dataset, the adjusted goodness of fit must exceed 0.65. The brightness of the emission line, X , is given by:

$$B^X = (A_1 + A_2) \times 4 \arcsin \left[\sin \left(\frac{\alpha}{2} \right) \sin \left(\frac{\beta}{2} \right) \right] \times \frac{10^6}{4\pi} \quad (4.13)$$

where $A_{1,2}$ are the amplitudes of the Gaussian distributions. α, β are the angles subtended by the co-added rows in the Alice slit, e.g., 0.05° and $4 \times 0.3^\circ$ for four co-added rows in the central region

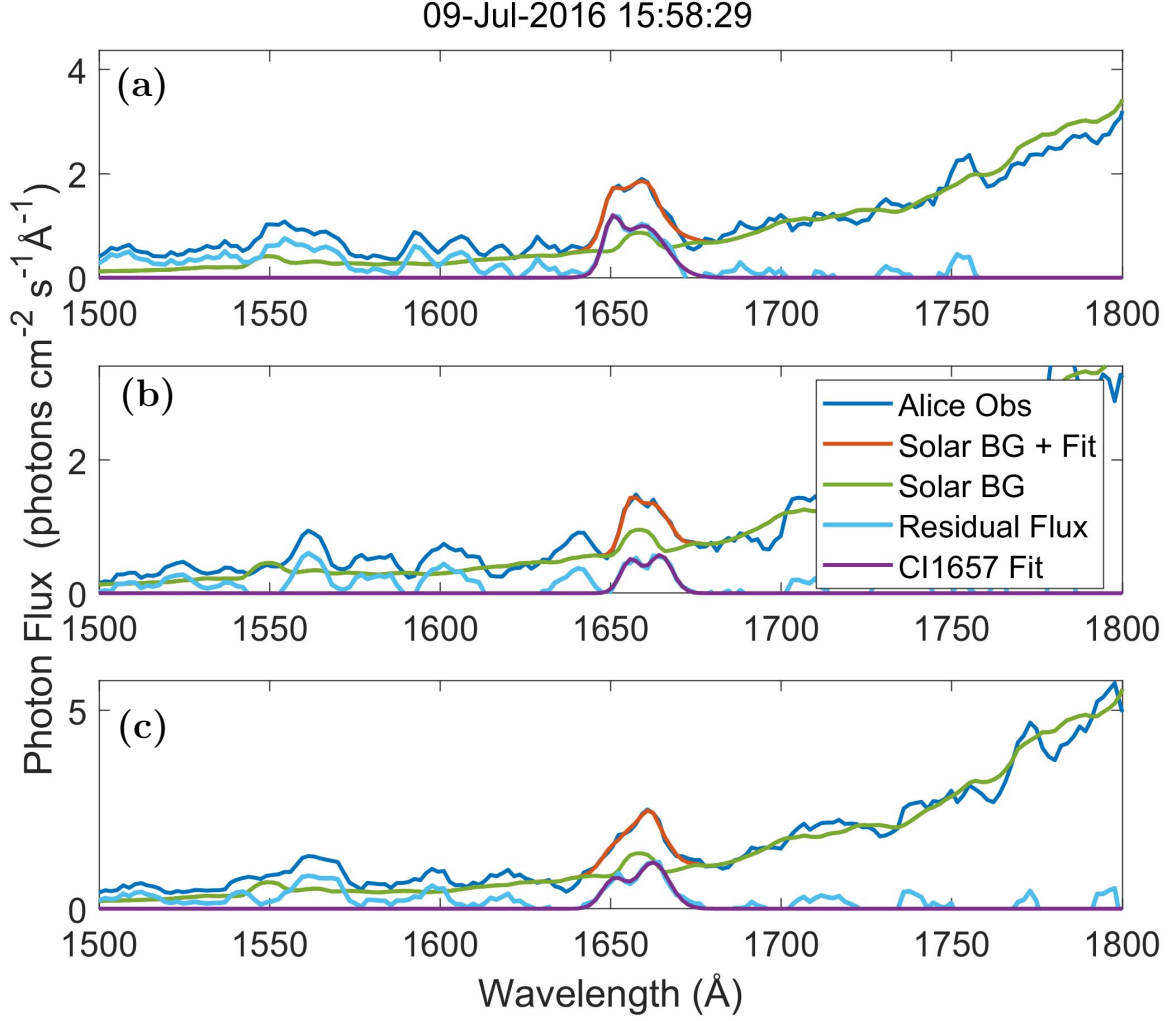


Figure 4.7: Fitting procedure used to retrieve the brightness of the CI1657 and CO4PG emissions from spectra contaminated with solar flux. The photon fluxes from Alice (dark blue) are plotted for three regions of the Alice slit (a) Rows 8 – 11, (b) Rows 13 – 16 and (c) Rows 18 – 21. The scaled background solar flux from TIMED/SEE (green) is subtracted from the observed flux to give the residual flux, which was emitted from the coma (light blue). The residual flux is fitted using a combination of two normal distributions (purple). The combination of the fitted emission with the solar background is shown in orange. Credit: [Stephenson et al. \(2021\)](#).

of the slit. The numerical factor, $10^6/4\pi$, originates from the definition of Rayleighs. This has been applied to all four of the emission lines considered for the analysis of emission during the CIRs (see Section 4.5).

4.4 Nadir analysis during quiet periods

In this section, the multi-instrument analysis is applied to cases looking in the nadir over a shadowed nucleus. The aim of this section is to determine the source of the FUV emissions from the coma, using well constrained conditions. The nadir viewing provides the best possible conditions to determine the composition throughout the neutral gas column for all four of the major neutral species (see Section 4.1.2). In addition, observing the shadowed nucleus minimizes any contamination of the spectra from reflected solar flux (see Section 4.1.1), ensuring all the observed emissions should originate from the neutral coma.

4.4.1 Selected cases

Thirteen cases of nadir viewing over the shadowed nucleus have been selected, which occurred over the southern hemisphere at large heliocentric distances. Only thirteen cases are selected as there were few times during the mission which satisfy the required viewing conditions, whilst also having measurements by all the required instruments over the time period. The properties of the cases are outlined in Table 4.2, which have been separated into two parts. The first set occurred at times when there was a large flux of suprathermal electrons detected by RPC/IES, whereas during the second set of observations few energetic electrons were present. The average electron flux is given in Table 4.3 over two energy ranges: 20 – 60 eV and 60 – 120 eV. There is a notable difference in the electron flux between the two sets of nadir cases, but this is particularly pronounced over the higher energy range.

An example of the electron flux associated with the high flux cases (1-8) is shown in Figure 4.5 (blue), with the low flux equivalent (for cases 9-13) in orange. Corresponding examples of the FUV spectra during the same intervals are shown in Figure 4.2. Figure 4.8 displays the emission frequencies of all the considered processes for each FUV line and for each of the nadir cases (see Section 4.1.3). The neutral column densities, which are used to compute the modelled line brightness (see Section 4.1.2), are given in Figure 4.9. These datasets are used to interpret the modelled FUV brightnesses and the observations made with the FUV spectrograph.

The distinction between the high and low electron flux cases is also evidenced by the lower emission frequencies from electron impact processes in cases 9-13, compared with cases 1-8.

Table 4.2: Properties of nadir observation periods in the southern hemisphere of 67P at large heliocentric distances. High flux cases (1-8) are separated from low flux cases (9-13).

Case	Date	Start time [UT]	Integration time [s]	Cometocentric distance [km]	Heliocentric distance [au]	Spacecraft latitude [°]	Spacecraft longitude [°]	Total column density [10^{15} cm^{-2}]
1	14/01/2015	11:38:40	3629	28.4	2.55	-23.4	-82.9	0.58
2	29/01/2015	18:40:49	6048	27.8	2.44	-63.8	5.4	0.27
3	30/01/2015	04:25:44	2419	27.8	2.43	-64.6	56.6	0.22
4	30/01/2015	06:34:42	2419	27.8	2.43	-64.2	-11.4	0.51
5	30/01/2015	07:17:41	1763	27.8	2.43	-64.0	-34.0	0.48
6	30/01/2015	11:32:18	2419	27.9	2.43	-62.5	-167.4	0.18
7	30/01/2015	15:25:50	2419	27.9	2.43	-60.5	71.35	0.28
8	26/04/2016	06:06:12	4452	21.2	2.9	-33.1	-107	1.88
9	29/01/2015	07:51:27	3629	27.8	2.44	-58.4	-17.1	0.75
10	21/04/2016	23:01:00	3398	30.9	2.85	-24.6	-57.7	1.24
11	21/03/2016	00:05:00	2603	12.2	2.62	-24.2	-36.8	1.43
12	14/05/2016	14:39:34	4613	9.8	3.0	-53.1	-111.7	1.13
13	27/05/2016	08:43:00	5592	7.0	3.09	-56.2	-42.3	1.32

Table 4.3: Average electron flux for each nadir observation period (see Table 4.2). The average electron flux is calculated over two energy ranges: 20 – 60 eV and 60 – 120 eV. The distinction between the high (cases 1 – 8) and low (cases 9 – 13) electron flux observations is clear in both energy ranges.

Case	Ave. Electron Flux for 20 – 60 eV [$10^7 \text{ cm}^{-2} \text{ s}^{-1} \text{ eV}^{-1}$]	Ave. Electron Flux for 60 – 120 eV [$10^7 \text{ cm}^{-2} \text{ s}^{-1} \text{ eV}^{-1}$]
1	23.2 ± 1.2	6.33 ± 0.85
2	30.4 ± 1.9	5.68 ± 1.34
3	27.7 ± 3.6	5.10 ± 2.62
4	20.5 ± 1.3	4.82 ± 0.95
5	16.9 ± 0.9	4.36 ± 0.65
6	22.2 ± 0.8	5.88 ± 0.56
7	10.5 ± 1.4	2.47 ± 1.01
8	6.42 ± 0.51	2.60 ± 0.37
9	3.51 ± 0.84	0.05 ± 0.61
10	1.18 ± 0.05	0.22 ± 0.04
11	1.40 ± 0.12	0.06 ± 0.09
12	0.51 ± 0.09	0.01 ± 0.07
13	1.03 ± 0.11	0.03 ± 0.08

4.4.2 Nadir cases 1-8: large electron flux

As discussed in Section 4.1.2, the column density of the neutral gas can be extrapolated from in situ measurements. However, this is quite uncertain due to the variable cometoradius and the expansion of the neutral gas near the surface. Alternatively, the OI1356 brightness can be used to set the total column density along the line of sight. The OI1356 emission line is associated with a spin-forbidden transition of the oxygen atom ($^5\text{S} - ^3\text{P}$), so has very few potential sources. For example, photon induced processes, such as resonance scattering and fluorescence, are negligible at this wavelength. All the observed OI1356 emissions are attributed to electron impact. Therefore, the neutral column density is set such that the modelled OI1356 brightness is equal to the observed line brightness, while retaining the composition measured by ROSINA/DFMS (see Section 4.1.2 and Figure 4.9). With this neutral column applied to all five emission lines, there is excellent agreement between the observed and modelled line brightnesses for all lines in cases 1-8 (see Figure 4.10). Therefore, the multi-instrument analysis captures all the important FUV emission processes, when there is a substantial energetic electron flux. The FUV emissions are dominated by dissociative excitation by electron impact for all of the emission lines.

The OI1356 emissions (Figure 4.10a) were dominated by electron impact on CO_2 (red) when there was a large electron flux. The major neutral species in cases 1-8 were water (blue, Figure 4.9) and CO_2 (red) with water generally slightly more prevalent in the coma. The majority of

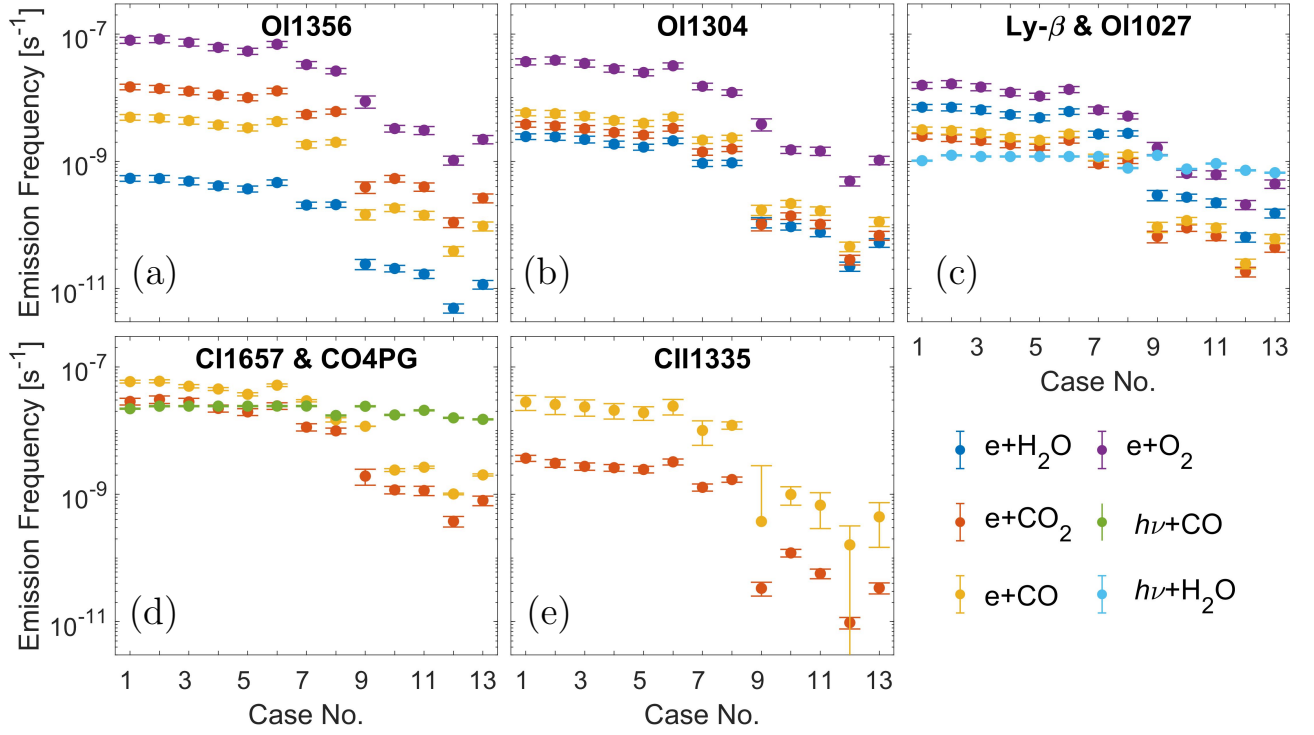


Figure 4.8: Emission frequency, v_l^X (Eq. 4.3), of each process, l , and emission line, X : (a) OI1356, (b) OI1304, (c) Ly- β and OI1027, (d) CI1657 and CO4PG, and (e) CII1335. The processes included are electron impact ($e + M$) on CO_2 (red), H_2O (dark blue), CO (orange), and O_2 (purple, see Section 4.1.3), as well as photon-induced emissions ($h\nu + M$). $h\nu + \text{CO}$ refers to fluorescence of CO (green), while $h\nu + \text{H}_2\text{O}$ is the prompt-photodissociation of water (light blue), which produces Lyman- β (see Section 4.1.4). Credit: Stephenson et al. (2021).

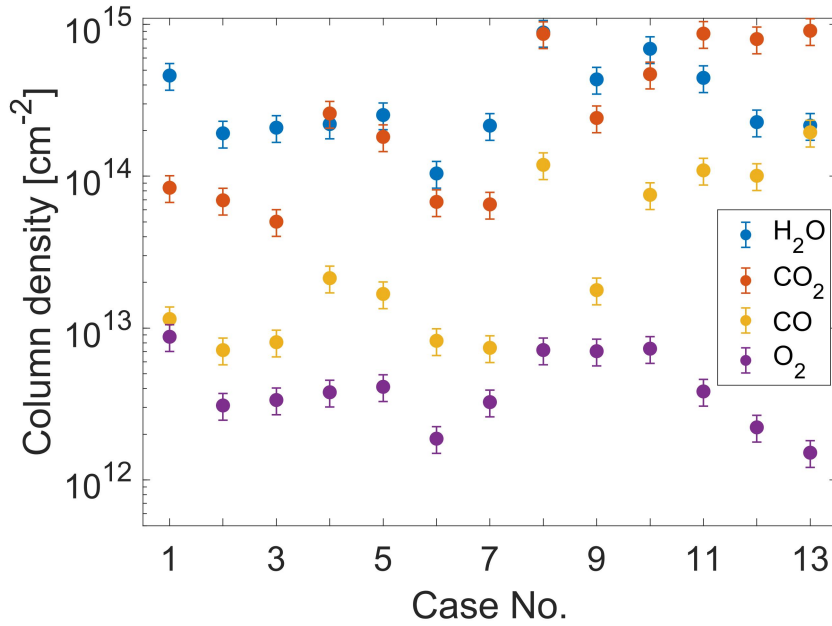


Figure 4.9: Column density of the major neutral species within the coma for each of the FUV spectrograph scans. The volume mixing ratios are derived from ROSINA/DFMS measurements (see Section 4.1.2). Credit: Stephenson et al. (2021)

these cases (1-7) occurred early in the Rosetta mission, when water was still the major species in the southern hemisphere (Läuter et al., 2018). However, case 8 occurred post-perihelion, when the outgassing of CO₂ was significantly boosted (Gasc et al., 2017a), so the water and CO₂ columns were approximately equal (Figure 4.9). The dominance of electron impact on CO₂ arises from the difference in scale of the emission frequency (Figure 4.8a). Electron impact on CO₂ is 25 times more efficient at emitting OI1356 ($1.08 \times 10^{-8} \text{ s}^{-1}$) than electron impact on H₂O ($4.0 \times 10^{-10} \text{ s}^{-1}$). Therefore, the OI1356 brightness had a negligible contribution from excitation of water (dark blue, Figure 4.10) and is not sensitive to the water column density.

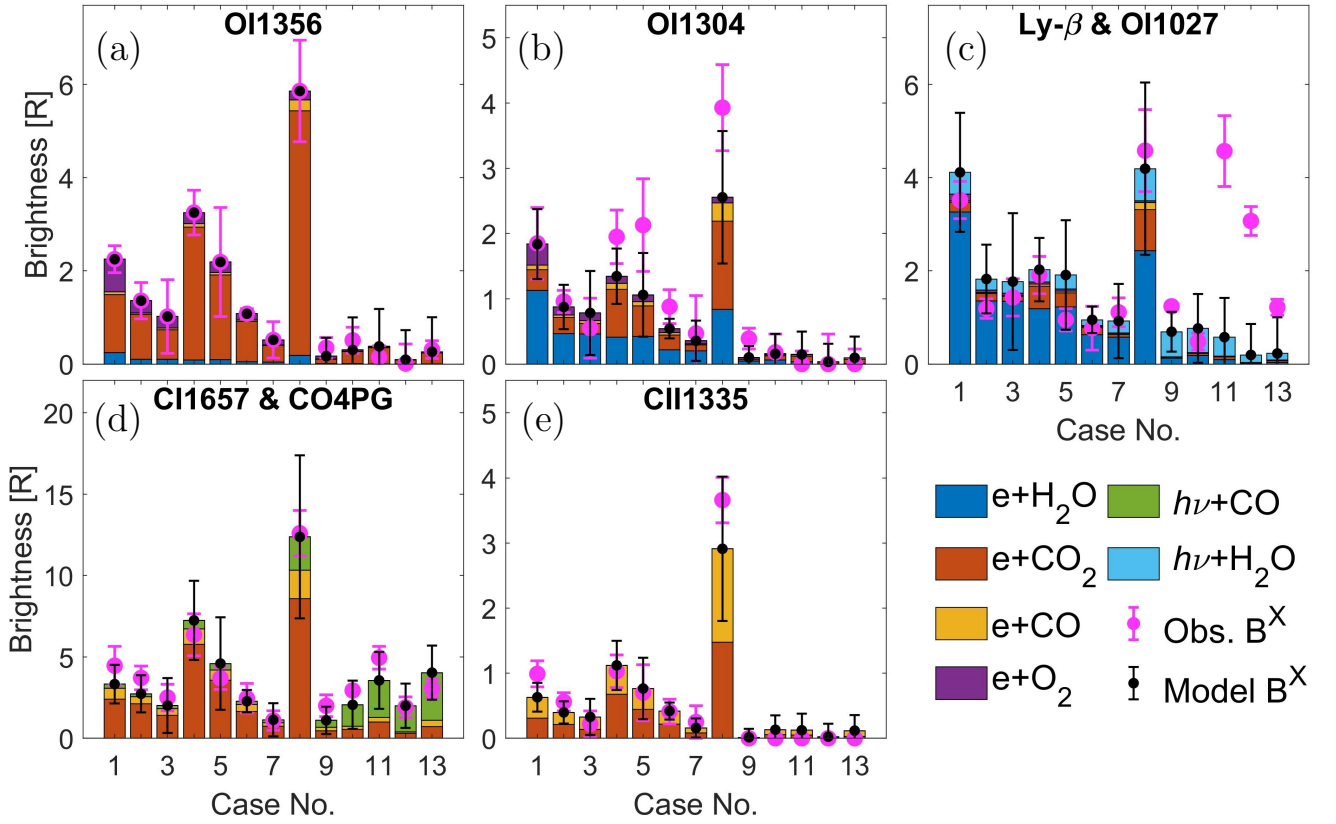


Figure 4.10: Modelled (black) and observed (pink) brightnesses, B^X , of each emission line. The stacked bars show the contribution of each emission process to the total brightness. The colour code is the same as used in Figure 4.8. The error on the observed brightness is derived from the integration of the FUV photon flux. The error on the modelled brightness is from the temporal variation of the electron flux and column density, as well as a 20% uncertainty in the neutral composition. The observed OI1356 brightness is used to fit the total neutral column density in cases 1-8 (see Section 4.4.2), and the error on the modelled OI1356 brightness is included in the error of the other modelled emission brightnesses. Credit: Stephenson et al. (2021).

Conversely, electron impact on O₂ is the most efficient process with an average emission frequency of $5.98 \times 10^{-8} \text{ s}^{-1}$ across cases 1-8, but it is only a minor species in the neutral column. The small column density of O₂ relative to CO₂ ensures that it is not a large contributor to the total brightness. However, in case 1, the O₂ column density ($8.9 \times 10^{12} \text{ cm}^{-2}$, Fig. 4.9) is

approximately three times larger than in cases 2-8 ($3.1 \pm 0.9 \times 10^{12} \text{ cm}^{-2}$). As a result, electron impact on O_2 is a significant emitter of OI1356 with a brightness of 0.69 R, compared to 0.1 to 0.2 R in the subsequent cases. The larger mixing ratio of O_2 seen in case 1 is attributed to the more northerly latitude (-23.8° , see Table 4.2) of the measurement compared to cases 2-7 ($\sim -60^\circ$), as O_2 was more prevalent in the northern hemisphere early in the mission. Cases 1 and 8 occurred at similar latitudes, but case 8 was post-perihelion and beyond 2.6 au where the outgassing of O_2 dropped off significantly (Läuter et al., 2018).

OI1304 emissions were mostly driven by electron impact on CO_2 (red) and H_2O (blue, see Fig. 4.10b). Whereas for OI1356 , electron impact on CO_2 was 27 times more efficient than water, it is only 1.5 times for emission of OI1304 (see Figure 4.8b). The similar column densities for the two major species allows each source to have a substantial contribution to the total brightness. Electron impact on both of the minor species (O_2 , CO) was more efficient than impact on CO_2 by a factor of 1.5 for CO and 10 for O_2 . However, the small mixing ratios ($\text{O}_2/\text{CO}_2 = 0.04$; $\text{CO}/\text{CO}_2 = 0.11$; Fig. 4.9) of each species ensure the contributions to the total brightness remain small. Nevertheless, at times when the mixing ratio of either minor species increases, such as case 1 for O_2 and case 8 for CO , the contribution to the emissions from the minor species can be important (see Fig. 4.10b).

The emission feature at $1027 \text{ \AA}$ includes both Lyman- β and OI1027 emissions. Throughout cases 1-8, the emissions are dominated by Lyman- β , which is produced by electron impact on water (dark blue, Figure 4.10). As was the case for OI1356 and OI1304 , the most efficient emission process at $1027 \text{ \AA}$ was electron impact on O_2 ($1.17 \times 10^{-8} \text{ s}^{-1}$, Figure 4.8). However, this is only twice the emission frequency of electron impact on water ($5.3 \times 10^{-9} \text{ s}^{-1}$). As O_2 was only a few percent relative to water, the contribution of electron impact on O_2 to the emissions at $1027 \text{ \AA}$ is very minor. There was a substantial contribution of OI1027 from electron impact on CO_2 ($< 0.9 \text{ R}$) emissions, which was not present in the northern hemisphere (Galand et al., 2020). This is particularly significant for the post-perihelion case 8, as the CO_2 column is large ($8.66 \times 10^{14} \text{ cm}^{-2}$, see Fig. 4.9). As well as the electron-induced emissions, prompt-photodissociation of H_2O (light blue, Figure 4.10) also contributes to the Lyman- β brightness. However, in the high electron flux cases the emission frequency is 5 times smaller from prompt-photodissociation than from electron impact on water. Electron impact on water is the main source of the emissions at $1027 \text{ \AA}$ when the electron flux is large, but electron impact on CO_2 and photodissociation of water should not be neglected.

At $1657 \text{ \AA}$, the emissions from the coma are dominated by CI1657 emission from electron impact on CO_2 (red, Figure 4.10d). There is an additional contribution from electron impact

on CO (orange), which primarily drives emission in bands of the CO4PG (see Section 4.1.1). The emission frequency of the overlapping CO4PG bands is $4.58 \times 10^{-8} \text{ s}^{-1}$ across the high flux cases, twice that of electron impact on CO₂. When there is a large population of suprathermal electrons, fluorescence of CO (green) has a similar emission frequency to electron impact on CO₂ (see Figure 4.8). However, in cases 1-7 the column of CO is small, so emissions from both electron impact and fluorescence of CO are minor. In case 8, the CO column density ($1.19 \times 10^{14} \text{ cm}^{-2}$) is larger than in cases 1-7 and emissions from CO cannot be neglected.

CII1335 is driven by electron impact on both CO and CO₂ with roughly equal contributions from each species (see Figure 4.10e). The emission frequency of electron impact on CO ($2.04 \times 10^{-8} \text{ s}^{-1}$) is eight times that of electron impact on CO₂ (Figure 4.8e). However, the volume mixing ratio of CO/CO₂ = 0.11 offsets the difference in emission frequencies. The threshold energies of CII1335 emissions from e + CO (33 eV) and e + CO₂ (44eV, Table 4.1) are much higher than for the other emission lines (typically $\sim 15 \text{ eV}$, see Table 4.1). Consequently, the CII1335 emissions are driven by higher energy electrons than the other emission lines, mostly in the 60 – 120 eV range. The average flux across this range varies little across the high flux cases (see Table 4.3), which leads to the roughly constant emission frequencies across the cases (see Figure 4.8e). As the emission frequencies are similar, the differences in the emission brightness are driven by changes in the CO and CO₂ column densities. The emission frequency from CO is much greater than from CO₂, the CII1335 brightness is most sensitive to the changes in the CO column density. The volume mixing ratio of CO is derived from ROSINA/DFMS (see Section 1.1.2). This requires a significant correction as CO₂ may fragment inside the mass spectrometer, leading to detection of CO. The close agreement between the observed and modelled CII1335 brightnesses indicates that the correction for CO₂ fragmentation works well, and the mass spectrometer accurately captures the mixing ratio of CO.

4.4.3 Nadir cases 9-13: small electron flux

In cases 9 -13, the suprathermal electron flux was very low compared to cases 1-8 in both the 20 – 60 eV and 60 – 120 eV energy ranges. Between 20 and 60 eV, the electron flux was smaller by a factor 11.8 compared to the high flux cases. The difference was more pronounced from 60 to 120 eV, where the flux was a factor of 60 smaller than seen in cases 1-8. Most of the emission lines depend more heavily on the 20 – 60 eV electrons. This results from the large portion of electron flux over this energy range (e.g., Figure 4.5) in combination with the high cross sections between 20 and 60 eV (see Figures 4.4a-d). Consequently, the emission frequencies of electron-induced

emissions are reduced by a factor of ~ 20 in cases 9-13 (e.g. factor 26.6 for Ly- β from $e + \text{H}_2\text{O}$; dark blue, Fig. 4.8c). However, CII1335 is more dependent on the higher energy electrons because of the high energy of the emission thresholds (see Table 4.1) and peak cross sections (see Figure 4.4e). Therefore, the CII1335 emission frequencies are ~ 50 times smaller than in the high flux cases, which is more in line with the electron flux ratio from 60 – 120 eV.

In the low flux cases, Alice captures no substantial emission of OI1356 from the coma (pink, Figure 4.10a). Therefore, it is not possible to determine the total column density using the OI1356 brightness. Instead, the radial column density is derived using Eq. 4.2 and measurements from the pressure sensor (see Section 4.1.2). Using the radial column density, the modelled emissions of OI1356 are also very small (black) due to the low emission frequency of the electron impact processes (see Figure 4.8a). This agrees very well with the observed OI1356 brightnesses.

As seen for OI1356, OI1304 has negligible emissions in the low flux cases (see Figure 4.10b), which is well reproduced in the model. The column densities are similar in cases 9 -13 to those in the high flux cases (Figure 4.9), so the lack of oxygen multiplet emissions is due to the lack of suprathermal electrons. CII1335 emissions present a similar picture, with negligible emissions arising from the lack of highly energetic electrons from 60-120 eV (see Table 4.3). The lack of observed emissions from the OI and CII lines confirms that there are no other substantial sources of emission from the coma other than dissociative excitation by electron impact for these lines. Across all three lines, the modelled brightnesses agree well with the observed emissions.

There were still substantial emissions at 1657 Å when the population of energetic electrons was small (Figure 4.10 d). The emission frequency was small from electron impact on both CO ($3.96 \times 10^{-9} \text{ s}^{-1}$) and CO₂ ($1.07 \times 10^{-9} \text{ s}^{-1}$), because of the lack of energetic electrons. However, fluorescence of CO, which emits in the CO4PG, was much more efficient ($1.86 \times 10^{-8} \text{ s}^{-1}$, see Figure 4.8) than electron impact on either species. As a result, fluorescence of CO was the dominant source of emissions at 1657 Å in the low flux cases. Cases 10-13 have similar columns and mixing ratios ($\text{CO}/\text{CO}_2 = 0.14 \pm 0.05$) to case 8 (see Figure 4.9), as they all occurred post-perihelion (see Table 4.2). The only major difference between cases 10-13 and case 8 is the electron flux, and the significantly decreased efficiency of the electron-induced emissions (see Figure 4.8d). In the pre-perihelion cases, the CO column was a factor 3 smaller than post-perihelion, so the contribution from fluorescence to the 1657 Å brightness was small (0.27 R).

There is still some uncertainty in the origin of the emissions at 1657 Å in the low flux cases. The Cameron bands, which are seen at the long wavelength end of the Alice spectra, have widths that indicate they are induced by electron impact. In order to excite the Cameron bands without generating substantial OI1356 emissions, a substantial population of electrons at ~ 10 eV would

be required. The electron spectrometer was not able to detect these electrons within the coma due to the very negative spacecraft potential during the low flux Alice observations (-23 to -17 eV, as measured by RPC/LAP). These low energy electrons, if present, could have induced some CO4PG emissions from CO, as the threshold energy is only 8 eV (see Table 4.1). Other emission processes would be unaffected by the low energy electrons, as they have higher threshold energies (>15 eV). Although there is some uncertainty regarding a low energy electron population, the CI1657 and CO4PG modelled brightnesses, which were deduced from extrapolated electron fluxes (see Figure 4.5), agree very well with the observed emissions. When there is not a large population of energetic electrons in the coma, dissociative excitation by electron impact is not a major source of emissions at 1657 Å and the relative contribution of fluorescence by CO to the emission at 1657 Å may become significant.

When the population of suprathermal electrons was small, the emission frequencies of Lyman- β and OI1027 from electron impact were less than from prompt-photodissociation of H₂O ($8.6 \times 10^{-10} \text{ s}^{-1}$, Fig. 4.8c). Emissions at 1027 Å from H₂O were dominated by prompt-photodissociation, which had four times the emission frequency of electron impact on water ($1.97 \times 10^{-10} \text{ s}^{-1}$). Electron impact on O₂ was comparable in emission frequency to the prompt-photodissociation but the low volume mixing ratio, O₂/H₂O < 0.02 resulted in only a minor contribution of O₂.

The observed and modelled brightnesses at 1027 Å agree well for cases 9 and 10, but in cases 11-13 the observed brightness is significantly underestimated. The unexplained, intense Lyman- β emissions are not likely to be driven by impacts of suprathermal electrons. An energetic electron population would also drive substantial emissions in other lines. For example, electron impact on water would generate OI1304 emissions at a factor 2.9 smaller than the Lyman- β brightness, which was not observed (see Figure 4.10b).

Despite issues with the Lyman- α calibration (see Section 4.1.1), the Lyman- α /Lyman- β ratio is a useful indicator of the emission processes. A spectrum of only electron impact on water should generate a line ratio of Lyman- α /Lyman- β = 8 (Makarov et al., 2004). Galand et al. (2020) analysed a spectrum of pure electron impact on water from 29 Nov 2014 over the northern hemisphere of 67P, which had a ratio of Lyman- α /Lyman- β = 4.4. The lower line ratio here may result from the calibration issues with the Lyman- α line (see Sections 1.1.3 and 4.1.1), or differences in the shapes of the Lyman series cross sections. Additionally, some discrepancy in the cascade emissions could also contribute to the lower-than-expected line ratio. Case 8 is another example with substantial emissions from electron impact on water, but with an observed line ratio of 2.56. However, the emissions at 1027 Å in case 8 also had a substantial OI1027 contribution from electron impact on CO₂ (see Figure 4.10c). This is also consistent with the brightness in

other lines, such as OI1356 (see Figure 4.10a). Taking only the Lyman- β emissions from electron impact on water, the line ratio with Lyman- α is 4.4 for case 8, which is consistent with the finding in Nov 2014.

The FUV observations in cases 11-13 had line ratios of $\text{Ly-}\alpha/\text{Ly-}\beta = 2.6, 3.2$ and 3.3 , respectively. As they are smaller than the expected ratio from electron impact, the emissions must be induced by a process with a small $\text{Ly-}\alpha/\text{Ly-}\beta$ ratio. Electron impact on other species (generating OI1027) cannot be responsible for the emissions as emissions of the other atomic lines would also be generated, and this was not observed (see Figure 4.10c). Resonance scattering of solar flux on atomic hydrogen within the coma would give a ratio of $\text{Ly-}\alpha/\text{Ly-}\beta = 300$ (Feldman et al., 2015), greatly increasing the observed line ratio. Additionally, atomic hydrogen is minimal close to the nucleus, as the timescale for dissociation of water ($> 10^5$ s; Huebner and Mukherjee, 2015; Galand et al., 2016) is much greater than the timescale to transport it away from the nucleus (order of seconds; Galand et al., 2016). Prompt-photodissociation of water does satisfy the low line ratio with $\text{Ly-}\alpha/\text{Ly-}\beta = 1.4$ (Hans et al., 2015), and does not generate substantial oxygen line emissions, as both OI1304 and OI1356 are forbidden in this process (Wu and Judge, 1988). However, if prompt-photodissociation were so greatly underestimated, there should be a substantial discrepancy in the other cases as well.

Finally, a poorly estimated column density could be responsible for the underestimation of Lyman- β emissions. It is not possible to increase the column density of all the neutral species while maintaining the composition, as this would greatly increase the emissions of the CO4PG beyond what was observed (see Figure 4.10). Increasing the column of water only by a factor of 8, 15 and 5, respectively, would bring the modelled emissions into agreement for cases 11-13. The other emission lines would not be significantly impacted by this change, as the emission frequencies from electron impact are so low. However, the increased water density gives neutral columns that are composed of 80% water in cases 11 and 12 (50% in case 13). This is contrary to the mass spectrometer measurements, which occurred over the same period (see Figure 4.9). It also disagrees with the wider trends in the outgassing over the mission. Cases 11-13 all occur towards the end of mission in the southern hemisphere of 67P, where outgassing of CO_2 was more prevalent than H_2O (Gasc et al., 2017a; Läuter et al., 2018). Therefore, the source of the observed Lyman- β emissions in cases 11-13 remains unclear.

4.5 FUV emissions during corotating interaction regions

4.5.1 Selection of cases

Under well-constrained conditions and with nadir viewing, dissociative excitation by electron impact has been confirmed as the major source of FUV emissions in the southern hemisphere of 67P far from perihelion. In this section, I examine the temporal variation of the FUV emissions and suprathermal electron population during several CIRs in the summer of 2016. The CIRs were observed at comet 67P over four solar rotations from June to September. Two appearances of the CIR are considered here, which occurred on the 9-10th July and 4th August. Higher levels of FUV emissions were also observed from the coma during early and late September, but the FUV observations were infrequent during both events. As such, it was not possible to examine the temporal variation during either period.

In the July and August events, the electron flux varied by a factor of 100 within several hours (see Tables 4.4 and 4.5, Fig. 4.12). Over the same time periods, the brightness of the FUV emission lines also varied, but only by a factor of 10. Variations in brightness of this magnitude at 67P have also been observed in other solar events in October 2014 (Galand et al., 2020) and during a CME in summer 2015 (Noonan et al., 2018). In the multi-instrument analysis, I have used the highest

Table 4.4: Properties of the four intervals on 4 Aug 2016 at 3.5 au. The first period has been split into peaks and troughs in the electron flux, which can be seen in Fig. 4.13. These are the same periods as shown in Fig. 4.12 in dark blue (peaks) and light blue (troughs). ¹ From VIRTIS-H. ² From MIRO. ³ 3σ upper limits from MIRO.

Period	Start Time [UT]	End Time [UT]	CO ₂ Column Density ¹ [10 ¹⁴ cm ⁻²]	H ₂ O Column Density ² [10 ¹⁴ cm ⁻²]	CO Column Density ³ [10 ¹⁴ cm ⁻²]	Ave. Electron Flux for 20 - 60 eV [10 ⁷ cm ⁻² s ⁻¹ eV ⁻¹]
1 - Peaks						15.5 - 44.9
1 - Troughs	01:38:59	05:42:30	6.21 ± 0.16	0.5 ± 0.03	<1.1	0.56 - 10.1
2	07:25:24	10:59:15	2.65 ± 0.17	2.24 ± 0.09	–	0.77 - 23.3
3	11:51:51	15:56:18	8.43 ± 0.14	0.36 ± 0.02	<1.3	3.16 - 20.4
4	17:38:16	21:12:03	7.93 ± 0.23	0.31 ± 0.02	–	3.48 - 7.95

temporal resolution possible for both the FUV (see Section 4.1.1) and electron flux (Section 4.1.3) datasets. This best captures the variability of both the emissions from the coma and the electron population during the events.

The observed line brightnesses from Alice are derived from single scans in three regions of the slit. The brightnesses for rows 8 – 11, 13 – 16, and 18 – 21 are given by the red, black, and blue crosses in Figures 4.13 and 4.15. Brightnesses calculated from the same scan of the FUV spectrograph are linked by vertical black lines. In cases where not all the regions of the slit are

plotted, measurements were discarded due to poor fitting (see Section 4.3). In the analysis of both the July and August events, scattered solar flux is subtracted from the FUV spectra to minimise contamination of the emission spectra (see Section 4.3).

During both the July and August observations, the nucleus moved slowly in the field of view of the remote instruments for extended periods, which were separated by manoeuvres of the spacecraft. These manoeuvres correlate with the blank regions (no data shown) in Figures 4.13 and 4.15. The modelled brightnesses for each period are distinguished with coloured lines. The neutral gas column is set as constant within each period, so the variation in the modelled brightnesses is only driven by the fluctuation in the energetic electron population. The average electron fluxes during each period are shown in Figures 4.12 and 4.14. The first period in the August event has been split into the peaks (dark blue) and troughs (light blue) to highlight the variability of the electron population during that interval.

For the modelled brightnesses, the emission frequencies of each line and species are calculated for each scan of the electron spectrometer and the associated electron fluxes, which have been individually corrected for the spacecraft potential (Section 4.1.3). The column densities used in Eq. 4.1 cannot be derived from in situ ROSINA measurements, as the FUV spectrograph in the July and August cases is not looking nadir (see Section 4.1.2). On 4 August, Alice was observing the limb of the comet (see Figure 4.11). In the July event, Alice was imaging the nucleus, but was pointed off-nadir. In both scenarios, different parts of the neutral gas column originate from varying regions of the nucleus surface. As both the composition and outgassing rate vary substantially across the nucleus surface (Hässig et al., 2015; Gasc et al., 2017a; Läuter et al., 2018), it is not reasonable to extrapolate from localised measurements.

For the limb observations in August, remote observations by VIRTIS-H and MIRO can be used to derive the column densities of CO₂ and H₂O (see Section 4.1.2), and somewhat constrain the column of CO. The column densities are specified for four periods during the August event in Table 4.4.

In July, the FUV observations occurred when the nucleus surface was illuminated by the Sun, which prevented reliable extraction of column densities from either VIRTIS-H or MIRO. Instead, the column density of CO₂ is set such that the magnitude of the observed and modelled OI1356 brightnesses are in agreement (see Table 4.5). This is consistent with the approach and findings of Section 4.4.

4.5.2 4 August 2016

Overview

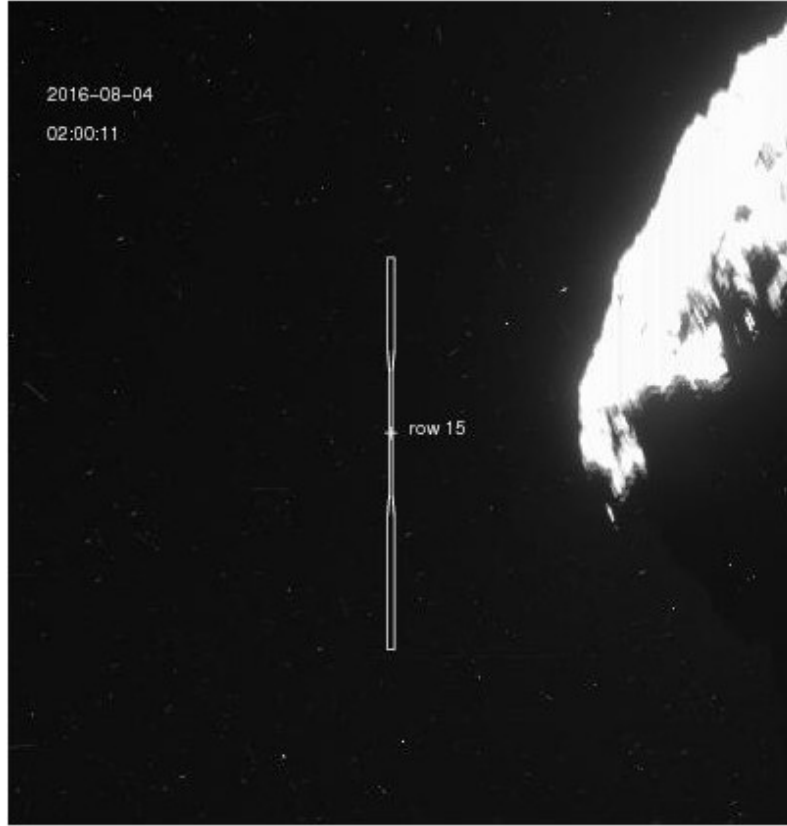


Figure 4.11: OSIRIS WAC image (Keller et al., 2007b) from 4 Aug 2016 02:00 UT during period 1 (see Section 4.5.2) with the Alice viewing slit shown in white. The line of sight passes within ~ 500 m of the comet nucleus.

Observations during the 4th August CIR were taken in limb viewing (see Figure 4.11). The event is split into four periods, separated by manoeuvres. The column densities during each of the periods, which are derived from VIRTIS-H and MIRO (see Section 4.1.2), are outlined in Table 4.4.

The CIR occurred close to the end of the Rosetta mission at 3.5 au. In each of the neutral gas columns CO_2 was dominant over H_2O , which is consistent with the ratio in outgassing ($\text{H}_2\text{O}/\text{CO}_2 \sim 0.05$) in the southern hemisphere at the time (Läuter et al., 2018). During the second observation period, the line of sight of the spectrograph passed over the neck of the comet. This region was associated with an increased abundance and density of water in the coma (Migliorini et al., 2016), which is reflected in the large observed water column from MIRO.

There was no detection of CO in any of the observed neutral columns by MIRO, but the 3σ upper limit of the CO column has been included in Table 4.4. The FUV emission spectra do include some weak molecular CO emissions, suggesting there is some CO present. However, when computing the FUV modelled brightnesses I have assumed there is no CO present as we do not

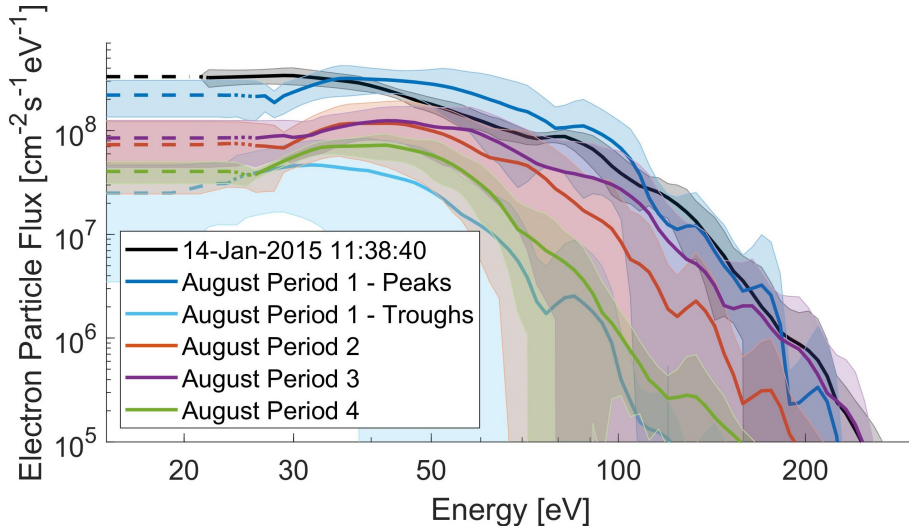


Figure 4.12: Average electron particle flux during the three periods listed in Table 4.4, with the standard deviation of the flux shown by the shaded regions. The colour of each period is the same as in Fig. 4.13. The first period has been split into the peaks (dark blue) and troughs (light blue) in the electron flux to highlight the variability in this period. The dotted lines indicate energies which could not be probed by some of the RPC/IES measurements during the period, due to a very negative spacecraft potential (see Section 4.1.3). The dashed lines denote energies that could not be probed by any of the RPC/IES scans during the period. The electron flux from Case 1 in the nadir study (see Section 4.4 and Fig. 4.5) is plotted for comparison (black). Credit: Stephenson et al. (2021).

have a good constraint on the CO column density or mixing ratio.

Neither the sub-mm nor the IR spectrometers could measure the presence of O₂ within the neutral column, so we have neglected any emissions from O₂. The volume mixing ratio O₂/CO₂ was small (< 1%) towards the end of mission (Läuter et al., 2018) and O₂ was less prevalent at lower latitudes (Hässig et al., 2015). Therefore, we do not expect any significant emissions from electron impact on O₂. Including a few percent of O₂ relative to H₂O does not significantly impact the brightness of the modelled emissions. The emissions of atomic oxygen lines are dominated by dissociative excitation from CO₂ over this period.

Periods 2-4

Throughout periods 2-4, the modelled brightness of OI1356 closely replicates the magnitude and variations of the observed emissions (see Figure 4.13a). The OI1356 emissions are dominated by electron impact on CO₂, which makes up 98% of the total brightness. This agrees well with the dominance of CO₂ as the source of the emissions, as seen in the nadir cases (see Section 4.4.2). The close agreement in magnitude confirms that there are no other major sources of OI1356 emissions during these periods.

The relatively low brightnesses seen in period 2 arise from the smaller column of CO₂ (see

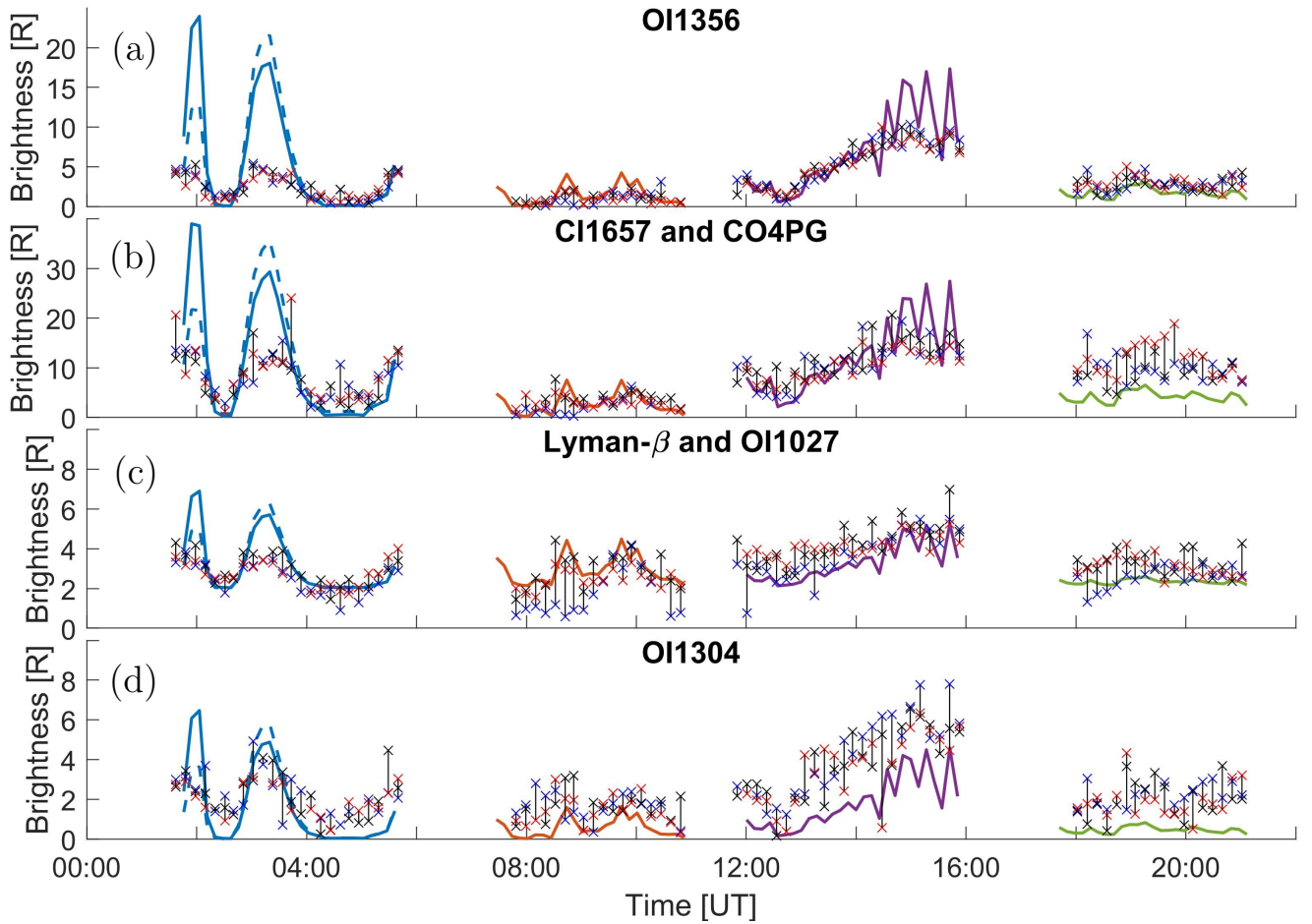


Figure 4.13: Comparison of the observed (crosses) and modelled (coloured lines) brightness of four emission features, (a) OI1356, (b) CI1657 and CO4PG, (c) Lyman- β and OI1027 and (d) OI1304, during four time periods, during which a CIR was observed at comet 67P, on 4 Aug 2016 (see Table 4.4). The observed brightnesses are from three regions of the FUV spectrograph slit (Rows 8-11 [red], 13-16 [black] and 18-21 [blue]). Vertical black lines link simultaneous measurements of the brightness. Credit: [Stephenson et al. \(2021\)](#).

Table 4.4), compared to the later periods. The OI1356 emission frequency from $e + \text{CO}_2$ increases throughout period 3 from $7.1 \times 10^{-10} \text{ s}^{-1}$ at 12:35 UT to $2.1 \times 10^{-8} \text{ s}^{-1}$ at 15:42 UT, which is closely traced by the increase in the observed OI1356 brightness. In the final period, there are few emissions of OI1356 as the suprathermal electron flux is small (green, Figure 4.12 and Table 4.4). This results in a small OI1356 emission frequency from $e + \text{CO}_2$ in period 4, which peaks at $3.9 \times 10^{-9} \text{ s}^{-1}$. This is five times smaller than the peak emission frequency in period 3.

During the nadir observations with a large electron flux, the emission feature at $1657 \text{ \AA}$ was dominated by electron impact on CO_2 , with only a small contribution from fluorescence of CO (dark green, Fig. 4.10d). As CO has been neglected here, the modelled CI1657 emissions are purely from electron impact on CO_2 . The observed brightness is well reproduced in both periods 2 and 3 (Fig. 4.13b), which suggests there was no substantial CO column within either period ($\text{CO}/\text{CO}_2 < 0.05$). A significant contribution from fluorescence of CO is unlikely, as electron impact is the more efficient process when there is a large suprathermal electron population (see Fig. 4.8d).

In period 4, the emissions at $1657 \text{ \AA}$ are underestimated in the model, which may result from the exclusion of CO, when computing the modelled brightnesses. As the electron flux was small during this period, fluorescence of CO may have had a more significant contribution to the total brightness (e.g. cases 9-13, Figure 4.10). Adding a column of CO with $\text{CO}/\text{CO}_2 = 0.2$ would resolve the disparity between the modelled and observed brightnesses. This is slightly larger than the ratio in outgassing ($\text{CO}/\text{CO}_2 = 0.1$) in the southern hemisphere of 67P over the same period (Läuter et al., 2018).

When viewing the comet limb, it is necessary to include a 2 R contribution from the IPM towards the Lyman- β brightness. This was not required for the nadir observations, as it was blocked by the nucleus. The same variation is seen in the Lyman- β brightness as is exhibited by the electron flux (see Figure 4.13c). This confirms that dissociative excitation is a major source of the emission line. As the magnitude of the observed brightness is also well reproduced, there are no other significant sources of Lyman- β throughout periods 2-4.

The modelled contribution from prompt-photodissociation of H_2O is negligible throughout the CIR. There could feasibly be additional resonance scattering of Lyman- β from atomic hydrogen in the extended coma. The atomic hydrogen population is generated by dissociation of water as it is transported away from the nucleus. However, it is difficult to constrain the column density of hydrogen as there are no constraints from remote instruments on Rosetta. Nevertheless, the good agreement between the modelled electron-impact emissions and the observed brightnesses suggests that resonance scattering was not significant.

The OI1304 observed brightness mirrors the variations in the electron flux throughout periods 2-4. Therefore, electron impact was the major driver of the emissions. When looking nadir, electron impact on CO₂ and H₂O were the major sources of emission (see Fig. 4.10 b) and no emissions were observed when the suprathermal electron population was small. However, when viewing the limb, there were still emissions of ~ 3 R when the electron flux from 20 – 60 eV was less than $10^7 \text{ cm}^{-2}\text{s}^{-1}\text{eV}^{-1}$ (see Table 4.4). The underestimation of the modelled brightness by the observed emissions is roughly constant throughout periods 2-4. Therefore, the unexplained emissions cannot be electron induced, as the electron flux varied substantially over the same time frame. The emissions could result from resonance scattering of atomic oxygen in the extended coma, but it is difficult to constrain the contribution from this source. There were no remote measurements of the atomic oxygen population, so I cannot determine whether this would be sufficient to explain the remaining brightness.

Period 1

In the first period on 4 August, the variations in the observed brightnesses also mirrored the changes in the electron flux, as was the case in periods 2-4. For all four of the emission lines, there were two peaks in the brightness at 01:45-02:20 UT and 02:40-03:40 UT (Figure 4.13). The electron flux also peaked in these intervals, with the average electron flux shown in Figure 4.12 (dark blue). In the intervening troughs in brightness, the electron flux was also at a minimum (light blue, 4.12). Following the two peaks in the flux, the energetic population was small from 03:40 UT until 05:20 UT, and no substantial emissions were observed in any of the atomic lines. The remaining 2 R of Lyman- β emission are background emissions from the IPM. From 05:20 UT, the electron flux increases towards the end of the period, which is joined by an increase in the observed FUV brightness.

However, despite the highly correlated variations, the magnitudes of the emissions do not agree well. The modelled peaks greatly exceed those observed with Alice. The difference in scale could be caused by a poor estimation of either the column density or the electron flux along the line of sight.

The dominant emission source during period 1 was electron impact on CO₂. A reduction of the CO₂ column density by a factor of 0.4 would give a close agreement for all four emissions lines throughout the first period, although OI1304 brightness would be slightly underestimated. This underestimation is consistent with the later periods of the CIR, and could be rectified by resonance scattering of atomic oxygen.

As there was some movement of the nucleus within the field of view, the CO₂ column density

may have varied during the period. To examine this, the column density derived from VIRTIS during period 1 was split into four shorter intervals. With higher temporal resolution, the column density was found to be lower during the first peak ($3.37 \times 10^{14} \text{ cm}^{-2}$, 01:40-02:40 UT), but increased during the second peak ($7.4 \times 10^{14} \text{ cm}^{-2}$, 02:40-03:40 UT). The resulting modelled brightness is plotted with dashed blue lines in Figure 4.13. The first peak has much better agreement between the observed and modelled brightnesses, but in the second peak the disparity is greater.

Alternatively, the assumption of a constant electron flux along the line of sight may not be valid in period 1. The electron flux is measured at 12 km from the nucleus, but the line of sight of Alice passes within roughly 500 m of the surface at the closest point (see Figure 4.11). Using the higher time resolution column density from VIRTIS, the electron flux would need to be reduced by factor 0.6 during the first peak and by 0.3 in the second, in order to give a good agreement in brightness across all the emission lines. However, if the assumption of constant electron flux was invalid, periods 2-4 should give similar discrepancies in brightness, which was not seen. Differences cannot be primarily attributed to substantially different viewing geometries, as all four periods have a line of sight passing within 1 km of the nucleus.

Despite the difference in magnitude between the observed and modelled brightnesses, the temporal variations agree very well throughout period 1. Therefore, the emissions must be driven by electron-impact on cometary neutrals. It is not clear why the magnitude of the brightnesses are overestimated in the model.

4.5.3 9-10 July 2016

During the CIR on 9-10th July, the FUV spectrograph was viewing the illuminated surface of the nucleus at an off-nadir angle. Reflection of solar flux heavily contaminated the FUV spectra, particularly at long wavelengths ($> 1500 \text{ Å}$). To retrieve the brightness of emissions from the coma, the reflected solar flux is subtracted from the observed FUV spectra (see Section 4.3).

Table 4.5: Properties of the three intervals on 9-10 July.

Period	Start Time [After 9 July 2016 00:00 UT]	End Time [After 9 July 2016 00:00 UT]	CO ₂ Column Density [10^{14} cm^{-2}]	Total Radial Column Density [10^{14} cm^{-2}]	Ave. Electron Flux for 20 - 60 eV [$10^7 \text{ cm}^{-2} \text{ s}^{-1} \text{ eV}^{-1}$]
1	15:00:00	23:30:00	6.0	3.83	0.16 - 15.3
2	29:52:00	34:30:00	2.0	2.25	2.46 - 25.0
3	35:10:00	48:00:00	1.2	0.76	1.97 - 36.2

The illuminated surface also prevented the retrieval of reliable column densities from either

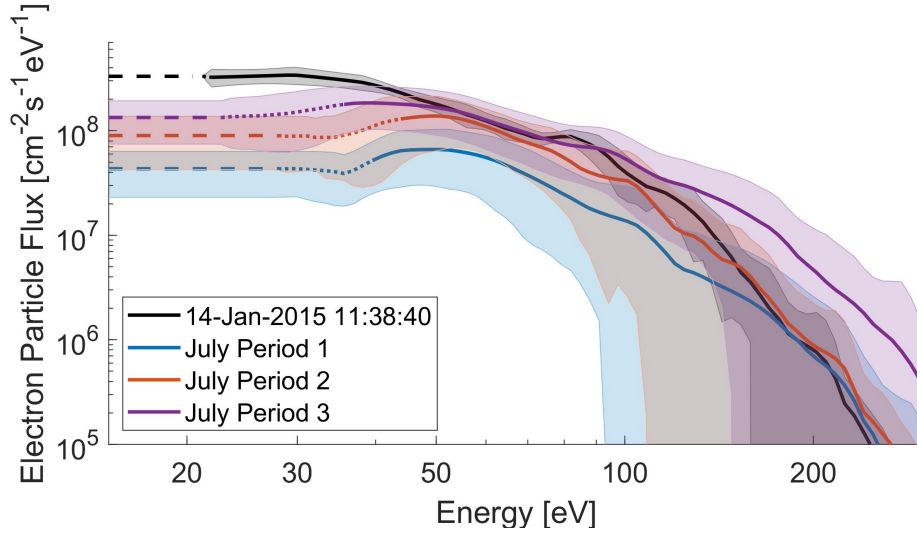


Figure 4.14: Average electron particle flux during the three periods listed in Table 4.5, with the standard deviation of the flux shown by the shaded regions. The colour of each period is the same as in Fig. 4.15. The format of the plot is the same as outlined in Figure 4.12. Credit: Stephenson et al. (2021).

VIRTIS or MIRO (see Section 4.1.2). It is not possible to extrapolate from the ROSINA in-situ composition and density measurements, because of the off-nadir angle. Despite these drawbacks, this is still a worthwhile event to examine, as there were few periods with numerous Alice observations during a CIR.

The column density is determined using the OI1356 emissions during each observation period, which is consistent with the approach in Section 4.4.2. The neutral column is purely made up of CO₂, which dominated the OI1356 emissions in the southern hemisphere (see Sections 4.4.2 and 4.5.2). Therefore, the modelled emissions in this event are only driven by electron impact on CO₂. Assuming the coma is purely CO₂, the densities derived from the OI1356 observations are similar to those derived from in-situ pressure observations combined with the Haser model. The columns are between 0.88 and 1.6 times the radial column density (see Table 4.5), which is a good agreement given the uncertainty from spatially varying outgassing and the cometary radius. The radial column density is derived from ROSINA/COPS pressure gauge measurements (see Section 4.1.2). The inferred total number density has been corrected assuming the neutral gas is pure CO₂ (Gasc et al., 2017a).

There is not a good way to constrain the neutral columns of the other species within the coma, so these have been neglected. As a result, I only consider the emission lines OI1356 and CI1657 which are primarily driven by electron impact on CO₂, without other major sources (see Section 4.4). The OI1304 and Lyman- β lines also have substantial contributions from the solar flux, whereas OI1356 is not affected by this contamination.

The observed OI1356 brightness closely follows the variations in the electron flux throughout

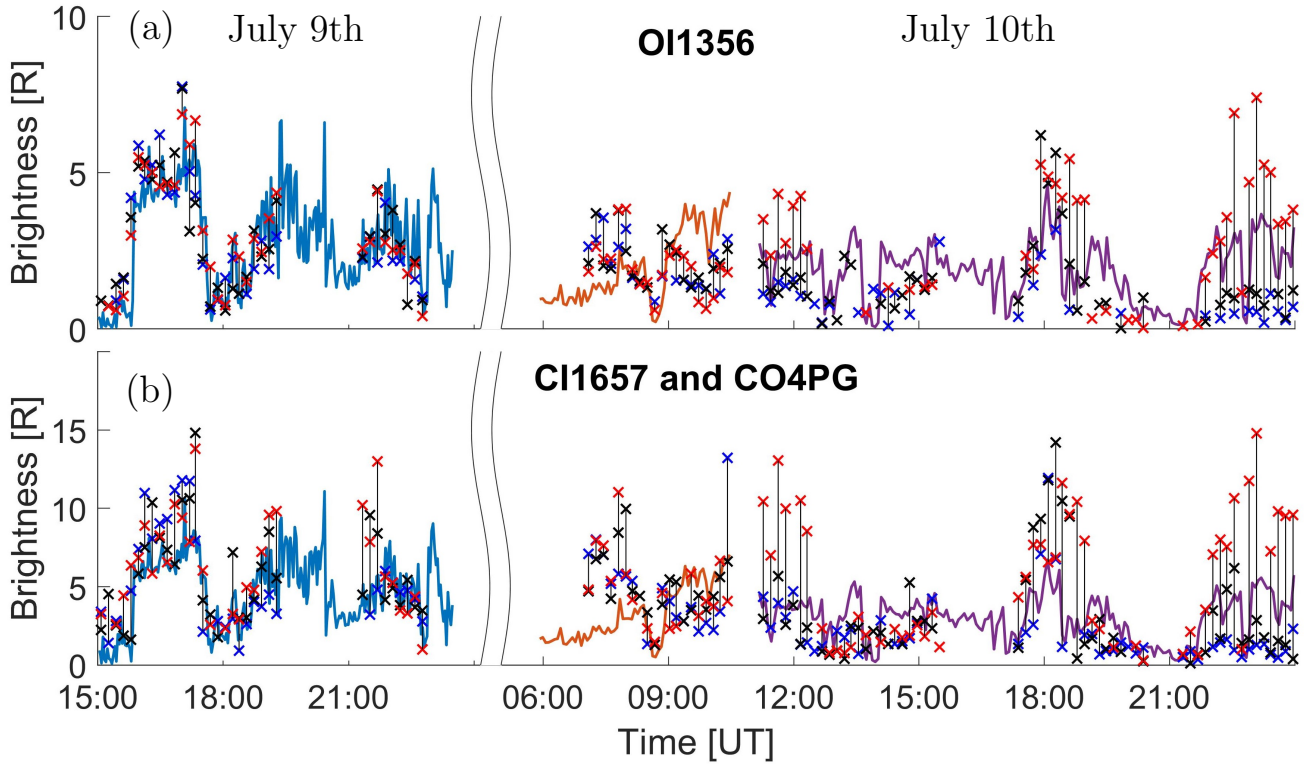


Figure 4.15: Comparison of the observed and modelled brightness of the (a) OI1356 and (b) CI1657 emission lines from 9 July 15:00 UT to 11 July 00:00 UT 2016. The plots follow the same format as outlined in Figure 4.13. The modelled brightnesses shown here are only driven by electron impact on CO₂. Credit: [Stephenson et al. \(2021\)](#).

the solar event, such as the peak in the electron flux between 16:00 and 18:00 UT on 9 July. The emission frequency of electron impact on CO₂ increased from 10^{-9} s^{-1} at 15:45 UT to $9 \times 10^{-9} \text{ s}^{-1}$. The emission frequency plateaued until 17:30 UT, at which point the electron flux dropped significantly and the emission frequency decreased to $4 \times 10^{-10} \text{ s}^{-1}$ at 17:45 UT. Between 07:30 and 09:30 UT on 10 July, the observed brightness and electron flux also show the same temporal variation. The emission frequency of OI1356 from $e + \text{CO}_2$ increased to a maximum of $1.3 \times 10^{-8} \text{ s}^{-1}$ at 08:00 UT, before reaching a minimum of $1.1 \times 10^{-9} \text{ s}^{-1}$ at 08:40 UT. Shortly after this, both the emission frequency and observed brightness increased rapidly at 08:50 UT, to $2.0 \times 10^{-8} \text{ s}^{-1}$ and 3.2 R, respectively.

The same temporal structures as seen for OI1356 are also present in the CI1657 observed and modelled brightnesses (e.g. between 16:00 and 18:00 UT on 9 July; Fig. 4.15b), which agree very well in both magnitude and variability. A peak in the observed brightness was seen at 18:00 UT on 10 July and was mirrored by a peak in the emission frequency from electron impact on CO₂ at $5.59 \times 10^{-8} \text{ s}^{-1}$. Following the peak, both the emission frequency and observed brightness decreased until 21:00 UT. At this point, there were few suprathermal electrons present, and nearly no observed emissions at 1657 Å from the coma. Therefore, there were no other major sources of

emissions at 1657 Å from the coma during this event.

4.5.4 Origin of the suprathermal electrons

An excellent temporal correlation was seen between the observed and modelled FUV emission lines in both the July and August solar events (see Figures 4.13 and 4.15). The viewing geometries of the FUV spectrograph were limb and off-nadir in the two events. In these scenarios, the electrons which induce the FUV emissions are spatially distanced from the electrons which are measured at the spacecraft. As emissions originate from the neutral gas, the emissions are most heavily weighted towards the densest region of the coma along the line of sight. When viewing the limb or off-nadir, the dense region of the coma is far from the spacecraft and may be under very different neutral and plasma conditions.

The electrons which induce emissions must also be accelerated before they can generate emissions. Both solar wind and newly-born cometary electrons are typically produced at 10 eV (Cravens, 1987; Galand et al., 2016), which is less than the threshold energy for most of the FUV emissions (see Table 4.1). If the acceleration was driven by local heating, distant electrons which induce the emissions would not correlate well with the electron population measured in-situ. The simultaneous variations in the measured electron flux and observed emission brightnesses, indicate that local heating cannot be the source of acceleration for the suprathermal electrons. Additionally, when there were few energetic electrons measured locally at Rosetta, no substantial FUV emissions were observed along the extended line of sight. This shows that there was not significant heating along the observed column, when there was not a large population of suprathermal electrons at the spacecraft. In addition to the observations in the northern hemisphere (Galand et al., 2020), this confirms that local heating is not the major source of energetic electrons in the coma.

Instead, the electrons must be accelerated by a large scale process, with temporal variations occurring approximately simultaneously throughout the coma. The likely candidate for this process is an ambipolar field around the weakly outgassing comet (Deca et al., 2017, 2019; Divin et al., 2020). This forms a potential well around the inner coma, into which the solar wind electrons can fall and gain energy. As the emissions are induced by accelerated charged particles from outside the cometary environment, the FUV emissions can be categorized as aurorae (Galand and Chakrabarti, 2002). The close correlation between the observed FUV auroral brightness, particularly the OI1356 emissions, and the electron flux means that FUV spectroscopy may be used as a remote probe of the solar wind conditions, and to observe larger solar wind structures.

The cometary aurorae examined here are quite distinct from auroral emissions at Earth, Jupiter

or Ganymede, where the intrinsic magnetic fields give structure to the aurorae. The lack of intrinsic magnetic field at 67P ([Heinisch et al., 2019](#)) allows the solar wind electrons to reach all parts of the coma and generate a ‘diffuse’ aurora. This is similar to auroral emissions in regions of Mars, without remnant crustal fields ([Schneider et al., 2015](#)). In both the cometary and Martian cases, accelerated solar wind electrons enter the atmosphere along open draped field lines as shown here for 67P and by [Schneider et al. \(2015\)](#) for Mars. Diffuse aurorae at Mars were only observed during extreme solar events, whereas they were persistent at comet 67P during quiet solar wind conditions (see Section 4.4). The mechanism and location of the acceleration is distinct between the two scenarios. The diffuse Martian aurorae are generated by electrons accelerated at the Sun ([Schneider et al., 2015](#)), whereas the auroral electrons at 67P undergo acceleration in the cometary system.

Chapter Summary

- I have completed the first forward modelling of FUV emissions in the southern hemisphere of comet 67P. This included the modelling of carbon line emissions, which are much more prevalent in the southern hemisphere, due to the asymmetric outgassing of CO₂. The considered emission lines are: Lyman- β , OI1304, OI1356, CI1657 and CII1335.
- Dissociative excitation of cometary neutrals, especially CO₂, by electron impact is confirmed as the major source of FUV emissions in the southern hemisphere at large heliocentric distances. Nadir observations of the shadowed nucleus are used to minimize contamination of FUV spectra.
- Modelled and observed brightnesses agree very well for all lines in cases with large electron flux and for most lines when the suprathermal electron flux was small, during nadir observations. The source of some unexplained Lyman- β emissions remains unclear when the electron flux was small.
- FUV emissions are modelled during two CIR events in the summer of 2016: 9-10 July and 4 August. Observed FUV emissions showed the same temporal variation as the measured electron population throughout both events. The magnitude of the modelled brightnesses agreed well with the observations in all periods, except the first period on 4 Aug.
- Correlation between the observed and modelled brightnesses during limb and off-nadir viewing, suggests that electrons are accelerated on large scales. This is likely driven by an ambipolar electric field ([Deca et al., 2017](#)).

Chapter 5

The source of cometary electrons

Although the source of cometary electrons has been examined for several cases throughout the Rosetta mission (Vigren et al., 2015; Galand et al., 2016; Heritier et al., 2018b), there has not been a mission wide examination of the origin of electrons within the coma. The relative importance of photoionization and electron-impact ionization has not been systematically addressed throughout the escort phase. The source of the energetic electrons within the coma is also not well known. Electrons produced within the coma and those that are transported into the coma from the solar wind are indistinguishable to the instruments of Rosetta. As well as the uncertain source of electrons, the conditions required to drive substantial electron-impact ionization have not been established.

In this chapter, I examine the origin of electrons within the coma and the ionization processes which generate cometary electrons at a comet. This is approached in two ways, the first being a statistical overview of the electron-impact ionization (EII) frequency throughout the Rosetta mission in Section 5.1. This is used to determine whether electron-impact is the major ionization process during the Rosetta mission, and the origin of the energetic electrons which cause ionization. In Section 5.2, the test particle model that was presented in Chapter 2 is further exploited and used to disentangle the importance of the different electron populations. In Section 5.3, I discuss the recent measurements of accelerated cometary ions ($> 10 \text{ km s}^{-1}$) close to the nucleus ($\sim 30 \text{ km}$) and how these relate to the electron-impact ionization frequency throughout the coma.

5.1 Ionization frequency throughout the Rosetta mission

5.1.1 Determining the ionization frequency

The electron particle flux, $J(E)$, is calculated in 15-minute intervals throughout the Rosetta mission using the same methodology as discussed in Sections 4.1.3 and 4.2. The electron-impact ionization frequency of water, $\nu_{e,\text{H}_2\text{O}}^{\text{ioni}}$, is given by:

$$\nu_{e,\text{H}_2\text{O}}^{\text{ioni}} = \sum_X \int_{E_{Th,X}}^{E_{Max}} \sigma_{e,\text{H}_2\text{O}}^{\text{ioni},X}(E) J(E) dE, \quad (5.1)$$

where $\sigma_{e,\text{H}_2\text{O}}^{\text{ioni},X}(E)$ is the ionization cross section for an ion product, X , at the electron energy, E (see Figure 2.5). The integral goes from the threshold energy of each process, E_{Th} , to a maximum energy of $E_{Max} = 300$ eV, beyond which the electron flux is small. The electron-impact ionization cross sections are given by Itikawa and Mason (2005) and shown in Figure 2.5. Figure 5.1a shows the electron-impact ionization frequency (blue) in 15-minute intervals throughout the Rosetta mission.

In addition to electron-impact ionization, I have also calculated the photoionization frequency of water, $\nu_{h\nu,\text{H}_2\text{O}}^{\text{ioni}}$ (see Figure 5.1a, orange), which is given by:

$$\nu_{h\nu,\text{H}_2\text{O}}^{\text{ioni}} = \int_{\lambda_{min}}^{\lambda_{th}} \sigma_{h\nu,\text{H}_2\text{O}}^{\text{ioni}}(\lambda) I(\lambda) d\lambda. \quad (5.2)$$

The photon flux, $I(\lambda)$, is extrapolated from TIMED/SEE measurements at Earth to the position of Rosetta, as outlined in Section 4.1.4, and the photoionization cross section of water, $\sigma_{h\nu,\text{H}_2\text{O}}^{\text{ioni}}(\lambda)$, is taken from Vigren and Galand (2013). The photon flux used in the calculation has not been corrected for any optical depth of the coma, so it may be overestimated in regions close to the nucleus around perihelion as photoabsorption becomes significant. The coma is optically thin down to the surface of the nucleus for outgassing rates below $Q = 10^{27} \text{ s}^{-1}$ (Heritier, 2018). Absorption of solar flux is only significant at high outgassing rates, which occurred at low heliocentric distances ($r_h < 2$ au; L  uter et al., 2018; Biver et al., 2019).

Simon Wedlund et al. (2019a) derived the frequencies of cometary ion production from solar wind ion processes throughout the Rosetta mission, using RPC/ICA ion measurements (see Section 1.1.1; Nilsson et al., 2007). The solar wind ion frequencies are calculated at the frequency of the ICA measurements, which are typically at 3 minute intervals. The two key processes are

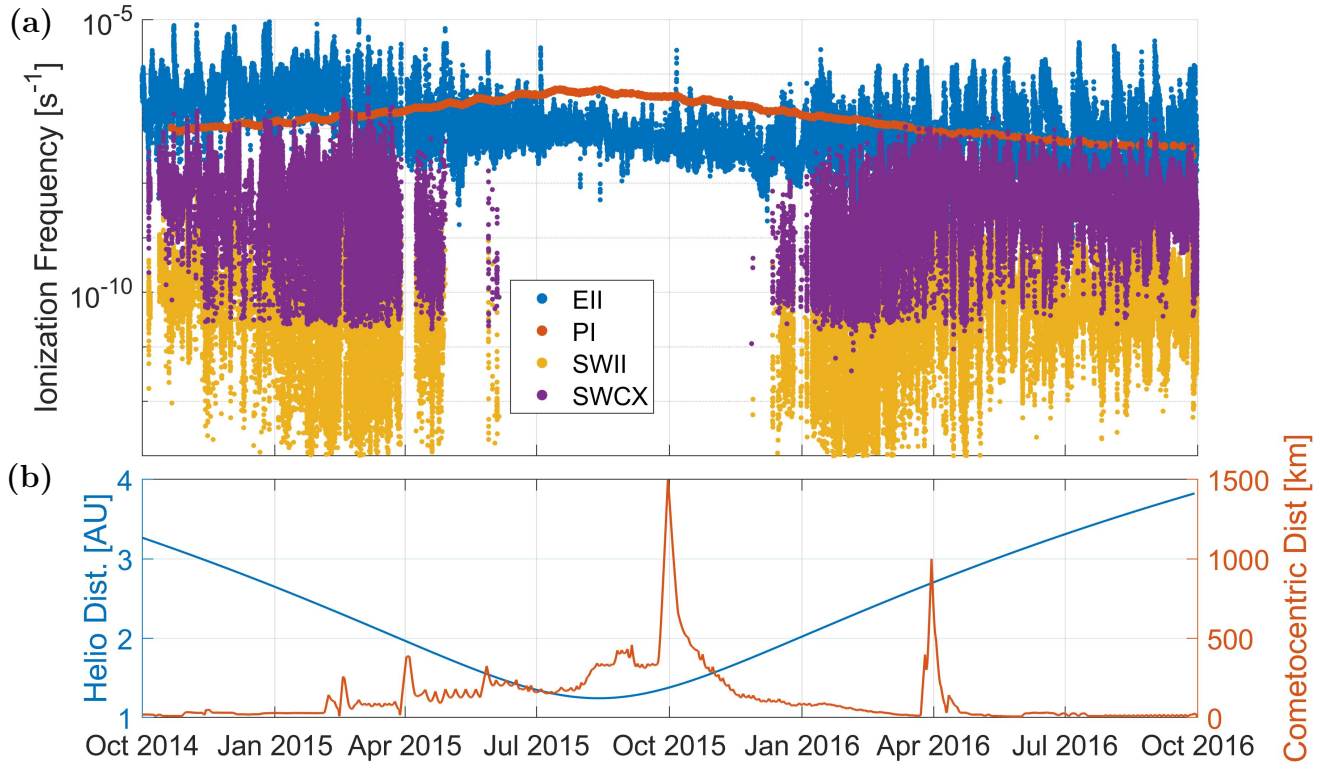
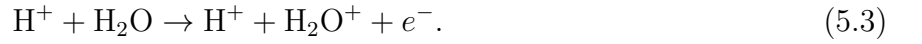


Figure 5.1: (a) Ionization processes throughout the Rosetta mission. Electron-impact ionization (EII, blue) is derived from RPC/IES measurements and averaged over 15-minute intervals. Photoionization (red) is calculated in daily intervals with measurements from TIMED/SEE at Earth and extrapolated to comet 67P (photoabsorption neglected). The solar wind ion impact (SWII) ionization frequency and solar wind charge exchange (SWCX) frequency (Simon Wedlund et al., 2019a) are given at the time resolution of the RPC/ICA measurements, which are typically every 3 minutes. (b) Heliocentric distance (blue) and cometocentric distance (orange) throughout the Rosetta mission.

Table 5.1: Datasets from the Rosetta mission, retrieved from the PSA, which are compared to the electron-impact ionization frequency. The relevant symbols and instruments for each dataset are provided and have been outlined in Section 1.1. ¹ Balsiger et al. (2007). ² Trotignon et al. (2007). ³ Eriksson et al. (2007). ⁴ Glassmeier et al. (2007b). ⁵ Nilsson et al. (2007)

Name	Equation/Symbol	Units	Instrument
Heliocentric distance	r_h	au	
Cometocentric Distance	r_{Ros}	km	
Spacecraft Latitude		°	
Spacecraft Longitude		°	
Neutral Density	n_{H_2O}	cm ⁻³	ROSINA ¹
Outgassing Proxy	$n_{H_2O} \times r_{Ros}^2$	cm ⁻¹	ROSINA ¹
Electron Density	n_e	cm ⁻³	RPC/MIP ² & LAP ³
Spacecraft Potential	$V_{S/C}$	V	RPC/LAP ³
Magnetic Field Strength	B	nT	RPC/MAG ⁴
Clock Angle	$\arctan(B_y/B_z)$	°	RPC/MAG ⁴
Cone Angle	$\arctan(\sqrt{B_y^2 + B_z^2}/B_x)$	°	RPC/MAG ⁴
H ₂ O ⁺ Density (< 60 eV)		cm ⁻³	RPC/ICA ⁵
H ⁺ Density		cm ⁻³	RPC/ICA ⁵
H ⁺ z velocity		ms ⁻¹	RPC/ICA ⁵

solar wind ion-impact ionization and solar wind charge exchange (SWCX). Solar wind ion impact (SWII, yellow, Figure 5.1) on cometary neutrals can ionize the molecules, generating new cometary electrons and ions , e.g.



Solar wind charge exchange (SWCX, purple, Figure 5.1) is the transfer of a charge between an energetic solar wind ion and a neutral atom, e.g.



The products of such an interaction are a low energy cometary ion and an energetic particle that was initially a solar wind ion. This may be a less charged ion, as seen in reaction 5.4 or an energetic neutral atom (ENA, in reaction 5.5). As this process only involves the transfer of charge, there is no net increase in the plasma (or electron) density as a result of charge exchange.

As well as the ionization processes, many other datasets from the Rosetta mission have been compiled into 15-minute averages across the escort phase, which can then be compared with the electron-impact and photo-ionization frequencies. Table 5.1 outlines the datasets used and the instruments from which they are derived.

The electron-impact ionization frequencies are compared to the numerous datasets using

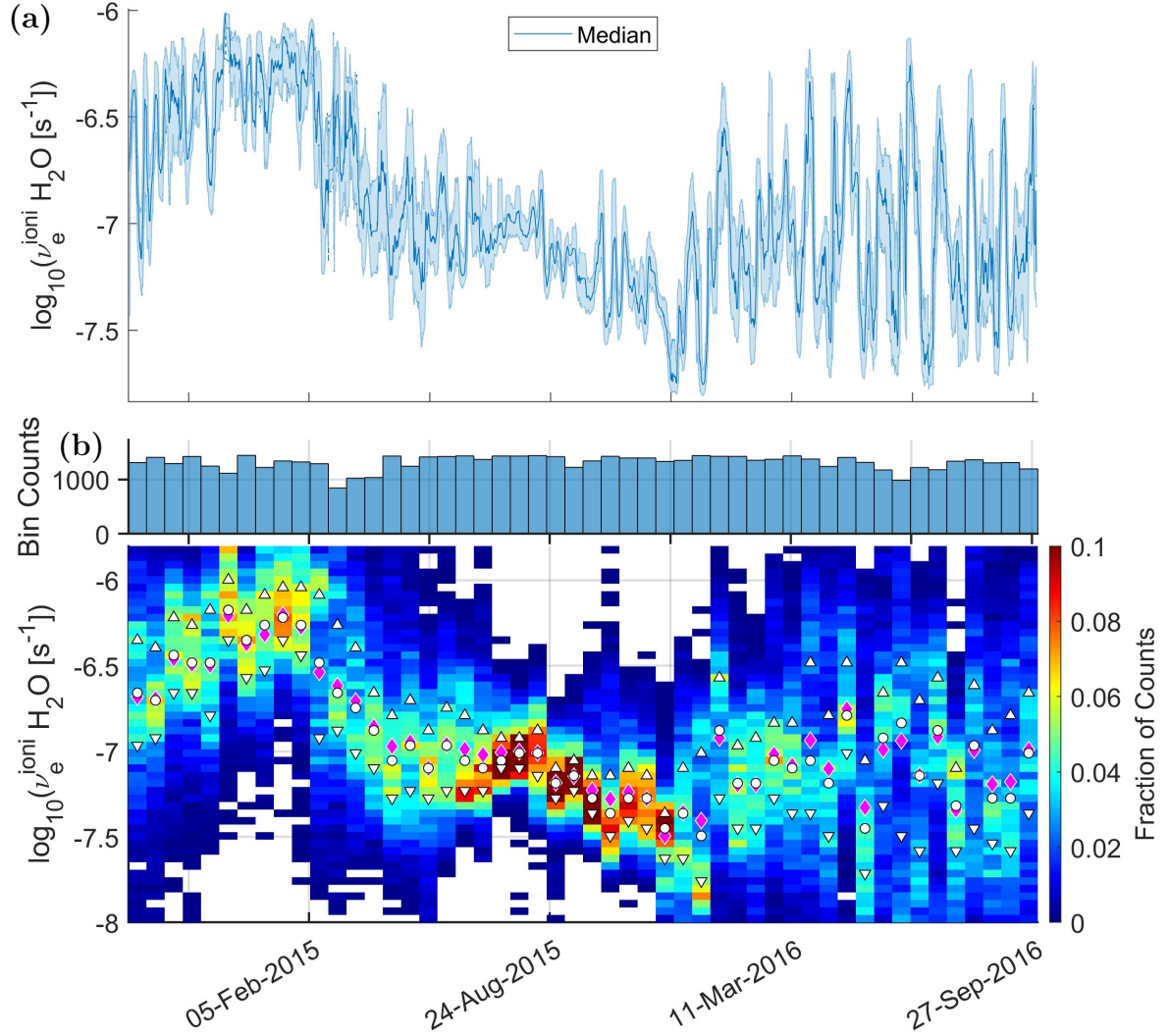


Figure 5.2: (a) Electron-impact ionization frequency, derived from RPC/IES, throughout the Rosetta mission. The solid line is the 48 hr median values, while the shaded region is the interquartile range. (b) Histogram of the electron-impact ionization frequency over the Rosetta mission. The mission is split in 50 bins in time and ionization frequency. The counts in each bin along the x -axis are normalized to 1.

Table 5.2: Time periods considered during the mission.

Period	Start Date	End Date	Heliocentric Distance [au]
Early Mission	08-Sep-2014	05-Feb-2015	2.4 - 3.4
Around perihelion	10-May-2015	02-Dec-2015	1.24 - 1.8
Late Mission	01-Apr-2016	30-Sep-2016	2.7 - 3.8
Pre-perihelion	08-Sep-2014	11-Aug-2015	3.4 - 1.24
Post-perihelion	11-Aug-2015	30-Sep-2016	1.24 - 3.8

histograms as shown in Figure 5.2b. The data points for each 15-minute interval are discretized into larger bins in both the x and y axes. In this case, the data are separated by time and ionization frequency. However, simply using the raw counts in the histograms ignores potential biases in the trajectory of the comet or in the conditions at the spacecraft. To mitigate the impact of these biases, I have normalized the counts in each column to 1. The mean (pink diamond), median (white circle) and quartiles (white triangles) are also plotted for each bin along the x -axis. While the normalization may not be as important when considering temporal variation, it is crucial when looking at trends with magnetic field conditions or cometocentric distance, for example. Figure 5.2a shows the time series of the 2-day moving average of the electron-impact ionization frequency at Rosetta (blue line), with the 15-minute data then forming the histogram in Figure 5.2b. It is useful to split the mission into several periods as the coma underwent significant changes moving closer to the Sun and also as it passed perihelion. Generally, I have split the mission into three periods: the early mission, a period around perihelion and the late mission. The conditions and time periods are outlined in Table 5.2.

5.1.2 Comparison of ionization sources

Figure 5.1 shows the four major ionization processes throughout the Rosetta mission. Photoionization (PI, red) is the steadiest process throughout the mission, although this does not include any correction for the optical depth of the neutral coma (Heritier et al., 2018b; Beth et al., 2019a). The photoionization frequency is 10^{-7} s^{-1} at the start of the mission, increasing to $5.2 \times 10^{-7} \text{ s}^{-1}$ on 17th July 2015 near perihelion. As the comet moves away from perihelion, the photoionization frequency decreases to $4.74 \times 10^{-8} \text{ s}^{-1}$ at the end of mission. The long term variation of the photoionization frequency is primarily due to the change in heliocentric distance (blue, Figure 5.1b), alongside a decrease in the solar activity over the duration of the mission. The oscillations seen on shorter timescales are associated with the ~ 28 day rotation period of the Sun.

The electron-impact ionization frequency (EII, blue) is much more variable than the photoionization frequency, fluctuating by nearly three orders of magnitude in a short period towards the

end of mission. Similar levels of variability (two orders of magnitude) are seen at large heliocentric distances pre-perihelion. The electron population, and consequently the EII frequency, is much more stable when close to perihelion than seen at large heliocentric distances, with fluctuations only of a single order of magnitude.

Around perihelion (from June 2015 to Jan 2016), the contribution from electron-impact to ionization was consistently weaker than photoionization at the spacecraft. At larger heliocentric distances, it became more prevalent than photoionization. Towards the end of mission (from Jan 2016), electron-impact ionization fluctuated between being the dominant ionization process (up to $1.4 \times 10^{-7} \text{ s}^{-1}$) and being much weaker than photoionization (at $\nu_{\text{H}_2\text{O}}^{\text{ioni}} \sim 5 \times 10^{-8} \text{ s}^{-1}$). This agrees well with the intermittent dominance of electron-impact ionization that was observed over several case studies by [Heritier et al. \(2018b\)](#), near the end of the Rosetta mission. Near the start of the mission, the electron-impact ionization frequency was generally higher than near the end of mission. Between Sep 2014 and Feb 2015, the minima in the electron-impact ionization frequency were generally comparable or greater than the photoionization frequency ($\sim 1.2 \times 10^{-7} \text{ s}^{-1}$) over the same period. As such, electron-impact ionization was the primary source of cometary electrons early in the mission.

Solar wind ion-impact ionization and charge exchange ([Simon Wedlund et al., 2019a](#)) overall were consistently weaker than both electron-impact and photo-ionization throughout the Rosetta mission (with some exceptions on short timescales). Around perihelion, the Rosetta spacecraft spent an extended period of time in the solar wind ion cavity ([Nilsson et al., 2017](#)). As solar wind ions could not reach Rosetta within the cavity, solar wind charge exchange and ion-impact ionization were not occurring around perihelion at the spacecraft. In addition, charge exchange was not a source of electrons within the coma and ion-impact was always orders of magnitude weaker than either photoionization or electron-impact ionization. Therefore, collisions involving solar wind ions did not represent a significant source of electrons within the coma across the whole mission and are not discussed in the rest of Chapter 5.

Electron-impact ionization vs. electron density

At times during the mission, electron-impact ionization was the strongest ionization process in the coma (see Figure 5.1a). The electron density, assuming loss is only through transport, varies with the ionization frequency and cometocentric distance (Eq. 2.38). To remove the dependence on cometocentric distance, the electron density is corrected, assuming it follows a $(r - r_{67P})/r^2$ dependence ([Galand et al., 2016](#); [Heritier et al., 2017b](#)), with $r_{67P} = 1.7 \text{ km}$ ([Jorda et al., 2016](#)). There is not a significant difference in the correlations for the raw or corrected electron densities

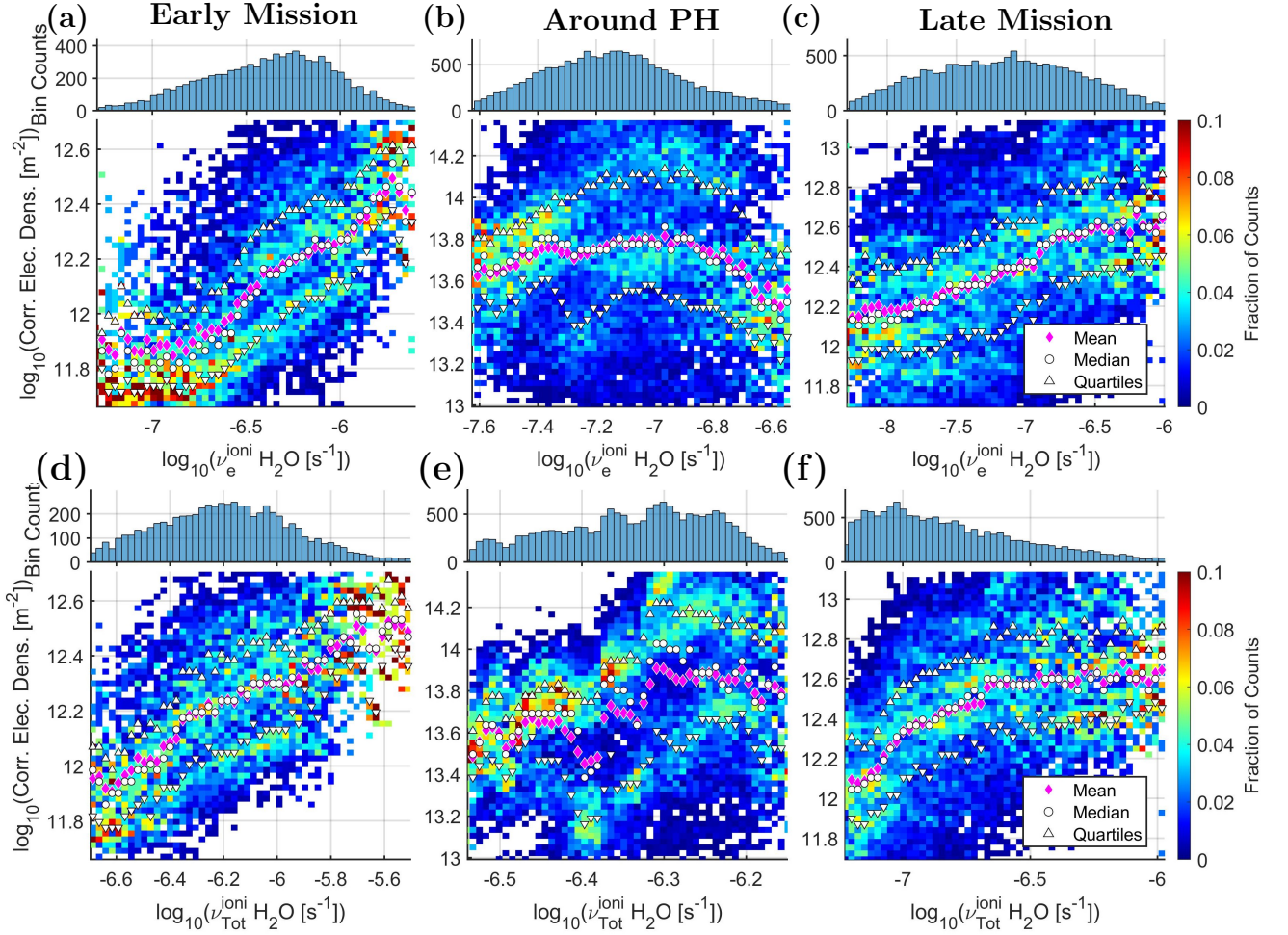


Figure 5.3: (a-c) Histogram of the cross-calibrated electron density measured at Rosetta by RPC/MIP and LAP (see Section 1.1.1), corrected for cometocentric distance (assuming $n_e \propto 1/r$, Heritier et al., 2017b), against electron-impact ionization frequency. Mean (pink), median (white circle) and quartile values (white triangles) are plotted for each bin along x . (d-f) Same as (a-c) but against the total ionization frequency (photoionization and electron-impact).

in the early mission period as the range of cometocentric distances is fairly small (10-30 km). However, late in the mission and around perihelion, the range of cometocentric distances is much larger (2 km to 400 km, Figure 5.1) and so the required corrections are much more significant.

Figures 5.3 a-c show the relation between the EII frequency and the corrected density of electrons in the coma, during the different periods of the mission. Early and late in the mission (Figures 5.3a and c), there was a clear positive correlation between the EII frequency and the corrected density of electrons within the coma. The median values show a clear positive correlation both early (correlation coefficient, $R = 0.976$ for $\nu_{e,H_2O}^{\text{ioni}} > 10^{-7}\text{s}^{-1}$) and late in the mission, when the EII frequency was not small.

Far from perihelion, the gradient becomes much shallower when EII was weak ($< 1.5 \times 10^{-7}\text{s}^{-1}$ early in mission or $< 3 \times 10^{-8}\text{s}^{-1}$, late in mission). Photoionization becomes relatively more important within the coma at these times, with few energetic electrons and a low EII frequency. If the electron density is directly compared to the total ionization frequency (including both electron-impact and photoionization, Figures 5.3d-f), the positive correlation extends to all ionization frequencies both early and late into the mission, although over a smaller range.

Close to perihelion, the correlation between the EII frequency at Rosetta and the corrected electron density is much weaker (see Figure 5.3). There is not an obvious relationship between the EII frequency and the electron density, as the dominant ionization process close to perihelion is photoionization (see Figure 5.1). The corrected electron density is also not well organised by the total ionization frequency (Figure 5.3e). As photoionization is a very steady process (except during extreme solar events such as flares), the range of ionization frequencies is small near perihelion (see Figure 5.1). This means the main source of variation in the electron density around perihelion was not fluctuations in the ionization frequency, but instead variation of the outgassing rate and neutral density.

As the electron density is very well correlated to the EII frequency, electron-impact ionization is the major source of electrons when at large heliocentric distance. Far from perihelion, the cometary electrons are not photoelectrons, but instead originate mostly from electron-impact ionization. Close to the Sun, EII was less important and cometary electrons are largely be photoelectrons.

The EII frequency is also highly correlated to the spacecraft potential both early and late in the mission, as seen in Figure 5.4. When far from perihelion, a more negative spacecraft potential is well correlated with higher EII frequencies. This is a reflection of the link between the EII frequency and the electron density within the coma during these periods (see Figure 5.3). The Rosetta spacecraft potential is dependent on the electron population in the coma and is used in determining the electron density from RPC/LAP measurements (Odelstad et al., 2015; Johansson

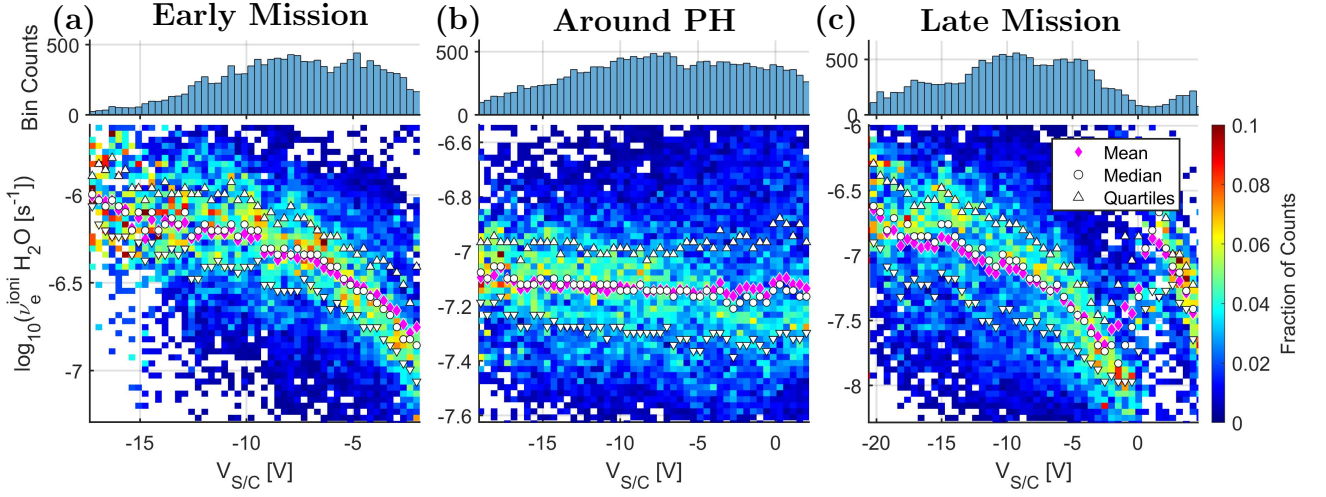


Figure 5.4: Electron-impact ionization frequency against spacecraft potential (measured by RPC/LAP, 1.1.1) (a) early in the mission (b) around perihelion and (c) late in the mission.

et al., 2021). Higher EII frequencies generate more electrons within the coma. The high electron densities then lead to more negative spacecraft potentials. The spacecraft potential is also linked to the temperature of the electron population, though the electron density varies over a larger range than T_e and is the strongest driver of the spacecraft potential. That said, if the electron temperature increases and more energetic electrons are present ($T_e > 12$ eV) in the coma, high electron-impact ionization frequencies and very negative spacecraft potentials would result. A dense and energetic electron population would drive a high electron-impact ionization frequency, as well as a very negative spacecraft potential.

Around perihelion, there was no significant dependence of the electron-impact ionization frequency on the spacecraft potential. This further suggests that electron-impact ionization was not the major source of electrons near perihelion, as was seen in Figure 5.1. When the comet is near the Sun, photoelectrons were more prevalent within the coma and drove the variations in the spacecraft potential.

Electron-impact ionization vs. low-energy cometary ions

Another measure of the plasma density within the coma is the density of low energy water ions. Taking the moments of order 0 of ion distributions (over the relevant energy range), measured by RPC/ICA, gives the number density of low energy (< 60 eV) water ions at the spacecraft. The dataset from ICA used to derive ion densities has not been corrected for the effects of the spacecraft potential. The negative potential pulls ions towards the spacecraft and can significantly perturb the ion velocity, especially for the low energy ions (Bergman et al., 2020). However, this drawback is mitigated somewhat as the moments are only used in a high level, statistical approach.

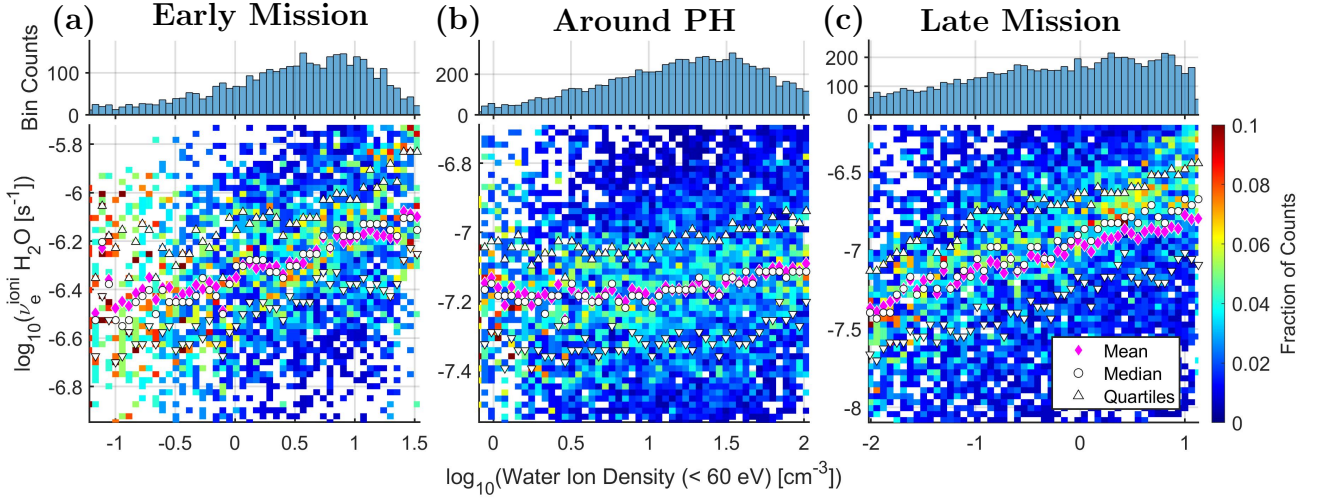


Figure 5.5: Electron-impact ionization frequency against low-energy cometary water ion density (a) early in the mission (b) around perihelion and (c) late in the mission.

The low energy water ion density is positively correlated with the ionization frequency during all three periods considered (see Figure 5.5). The gradient is more positive during the early and late periods of the mission, while quite shallow around perihelion. Once again, this supports the hypothesis that electron-impact ionization is the primary ionization process when at large heliocentric distances. When close to perihelion, electron-impact ionization was still a source of water ions in the coma, but the smaller gradient indicates that other ionization processes were more significant (namely photoionization, see Figure 5.1).

5.1.3 Origin of ionizing electrons

Having established that electron-impact ionization was overall the major source of cometary plasma at large heliocentric distances, it is useful to examine the origin of the ionizing electrons within the coma. This is again achieved by comparing the electron-impact ionization frequency with a number of other datasets measured by instrumentation onboard Rosetta.

Electron-impact ionization vs. heliocentric distance

Figure 5.6 shows the EII frequency as a function of the heliocentric distance, r_h , of comet 67P during the (a) pre-perihelion and (b) post-perihelion phases of the mission. From the arrival of Rosetta at 67P, the EII frequency increased from less than 10^{-7} s^{-1} beyond 3.3 au to 10^{-6} s^{-1} at 2.5 au. As the comet moved closer to the Sun (up to 2 au), the median electron-impact ionization frequency decreased to $\sim 10^{-7} \text{ s}^{-1}$. As the comet continued from 2 au towards perihelion at 1.24 au, the electron-impact ionization frequency was fairly steady at $\sim 10^{-7} \text{ s}^{-1}$.

After perihelion, the EII frequency decreased to $1.6 \times 10^{-8} \text{ s}^{-1}$ at 2 au. As the comet moved

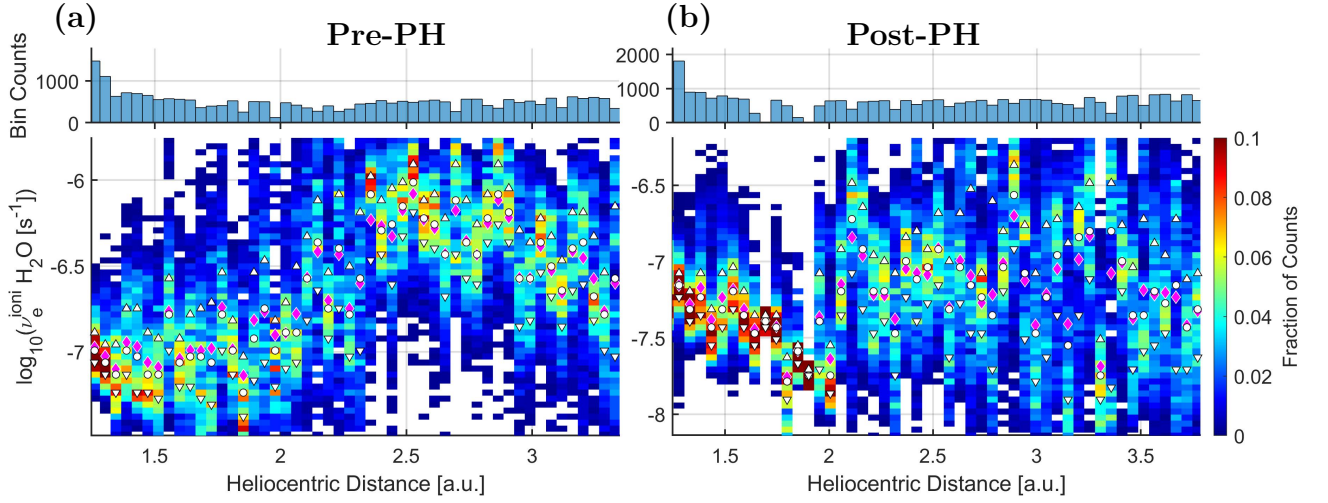


Figure 5.6: Electron-impact ionization frequency against heliocentric distance for (a) the pre-perihelion and (b) post-perihelion phases of the escort phase.

beyond 2 au, the mean and median electron-impact ionization frequencies increased and remained larger between 2 and 3 au. However, the EII frequency is not as well-organized by heliocentric distance post-perihelion, compared to the pre-perihelion measurements.

While Figure 5.6 shows the dependence of ionization frequency with heliocentric distance, many other temporal variations are also caught up in this relation. For example, the excursion to 1500 km that occurs shortly after perihelion (see Figure 5.1b, orange) may be responsible for the reduction in the electron-impact ionization frequency. At this time, there was also a step increase in the outgassing of molecules from the nucleus (Biver et al., 2019; Läuter et al., 2018), particularly over the southern hemisphere.

The relation between the EII frequency and heliocentric distance is consistent with an energetic electron population that largely originated in the solar wind. Under this hypothesis, the EII frequency would depend on the upstream solar wind conditions and the ambipolar potential well around the comet. The potential well is formed by the bulk of the cometary electron population (see Section 1.2.2). This is further supported by the comparisons to other datasets in Section 5.1.2) and with the test particle simulations (see Section 5.1.3) at large heliocentric distances.

Far from perihelion, the population of cometary electrons was quite small due to both low ionization frequencies and weaker neutral outgassing. This limited the strength of the ambipolar field around the comet nucleus and led to relatively little acceleration or funnelling of the solar wind electrons (e.g. Figure 2.17). In addition to the small population of cometary electrons, the solar wind density is roughly proportional to $1/r_h^2$ (Cravens, 1997b). The combination of few solar wind electrons and little acceleration may result in the small electron-impact ionization frequency. As the comet and Rosetta moved closer to the Sun, the cometary electron population increased

and the density of the solar wind trended upwards. The strength of the potential well would rise with the growing cometary electron population, which then feeds back into the acceleration and funnelling of the solar wind electrons into the inner coma. This may be the driving process at heliocentric distances down to 2.5 au.

Between 2.5 au and 2 au, the outgassing rate of the comet continued to increase with decreasing distance to the Sun. The higher outgassing rate led to more electron-neutral collisions in the coma. The energy degradation processes oppose increases in the ambipolar potential, such as seen in Figure 2.23. As the electron-neutral collisions become more dominant in the inner coma, fewer electrons are strongly accelerated into this region. The negative feedback between electron-neutral collisions and the potential well is seen in the test particle simulation in Section 2.6.3.

Inwards of 2 au, the cometary electrons are primarily photoelectrons rather than produced by electron-impact. Here electron-neutral collisions are prevalent within the coma, and boundaries, such as the diamagnetic cavity, form within the coma. These further complicate the structure of any potential well around the comet nucleus. As few energetic electrons were observed within the cavity (Nemeth et al., 2016; Madanian et al., 2020), most electrons within this region are photoelectrons. If the majority of the energetic electrons are photoelectrons, then the electron-impact ionization frequency may be expected to remain fairly steady around perihelion, as seen in Figure 5.1a.

Electron-impact ionization vs. neutral coma

Figure 5.7 shows the relation between the electron-impact ionization frequency and the neutral outgassing conditions. To remove the dependence of the neutral density on cometocentric distance, I use $n \times r^2$ as a proxy measurement of the local outgassing rate (Hässig et al., 2015; Hansen et al., 2016). This does neglect any acceleration of the neutral gas as it moves away from the nucleus, but this typically occurs within the first few kilometres of the nucleus (Heritier et al., 2017a). This may have some impact in the late mission period, but the spacecraft was not often this close to the nucleus early in the mission or around perihelion (see Figure 5.1b). The relationships between the outgassing rate and ionization frequencies are very similar to the correlations with neutral density throughout the mission.

Early and late in the mission, the electron-impact ionization frequency is positively correlated with the outgassing rate (see Figures 5.7a and b). The positive dependence on outgassing rate is seen at low outgassing rates ($n \times r^2 < 3 \times 10^{10} \text{ cm}^{-1}$) for both the pre-perihelion and post-perihelion phases of the journey. The drop in ionization frequency at higher outgassing (corresponding to smaller heliocentric distances) reflects the variation with heliocentric distance in Figure 5.6. This is consistent with energetic electrons originating in the solar wind, and undergoing acceleration in

an ambipolar potential well. At the low outgassing rates, an increase in outgassing may lead to a stronger potential well, which generates more energetic electrons within the inner coma. Above $n \times r^2 = 3 \times 10^{10} \text{ cm}^{-1}$, higher outgassing rates begin to introduce more electron-neutral collisions and therefore moderates the potential well. At even higher outgassing rates ($n \times r^2 = 3 \times 10^{11} \text{ cm}^{-1}$), the comet was close to perihelion and electron-impact was not the major ionization process.

The extent to which EII was important is shown in Figure 5.7c and d, which compares the total ionization frequency (photoionization and EII) with the outgassing rate proxy. Close to the Sun, the total ionization frequency was dominated by photoionization (see Figure 5.1). Therefore, any potential well, if it persists in the highly collisional coma, would be sustained by the photoionization, which is much steadier than electron-impact ionization. The disparity between the correlations early and late in the mission may be caused by the relative strength of photoionization vs electron-impact during these times. Early in the mission, electron-impact was clearly the dominant ionization process in the coma (blue vs. orange, Fig. 5.1), whereas late in the mission the two processes are much more comparable in strength. Early in the mission, an increase in the strength of a potential well would have a stronger positive feedback than if photo-ionization were also a significant source of electrons.

During the early and late mission periods, the electron-impact ionization frequency varies slightly with the latitude of the Rosetta spacecraft (see Fig 5.8). Early in the mission, electron-impact ionization frequencies are larger at higher latitudes, whereas the reverse is true late in the mission. This is likely caused by the dependence of the local outgassing rate on the latitude and season. Early in the mission, outgassing is stronger in the northern hemisphere, whereas late in the mission the southern hemisphere has a higher outgassing rate (Biver et al., 2019; Läuter et al., 2018).

Electron-impact ionization vs. magnetic field

Figure 5.9 shows the relation between the magnetic field strength and electron-impact ionization frequency throughout the mission. Early in the mission (see Figure 5.9a) the electron-impact ionization frequency and magnetic field strength are very well correlated. The electron-impact ionization frequency increases with magnetic field strength. Late in the mission (see Figure 5.9c), a positive, but weaker, correlation is also seen between the ionization frequency and magnetic field strength. The correlation holds very well at low field strengths ($< 12 \text{ nT}$), but beyond this the mean and median ionization frequencies plateau at $\nu_{e,\text{H}_2\text{O}}^{\text{ioni}} = 10^{-7} \text{ s}^{-1}$. At the higher field strengths, the number of data points is quite small (≤ 100 per bin above 16 nT), so the correlation can be easily disturbed by infrequent events. Around perihelion, the electron-impact ionization

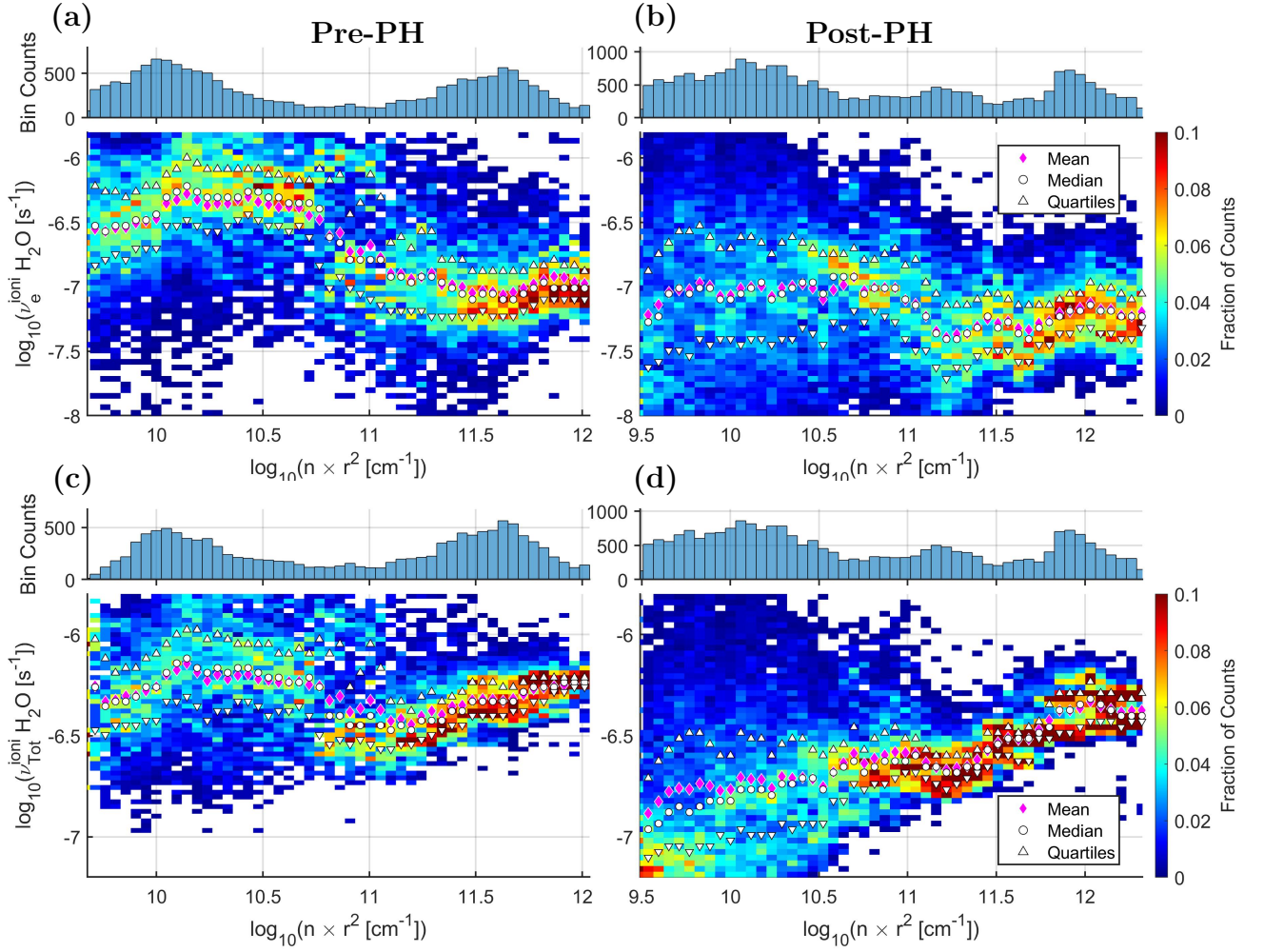


Figure 5.7: Electron-impact ionization frequency against a proxy measurement of the outgassing rate ($n \times r^2$, where n is from ROSINA) for the (a) pre-perihelion and (b) post-perihelion phases. Total ionization frequency of water (photoionization and electron-impact ionization) against outgassing rate for (a) pre-perihelion and (b) post-perihelion.

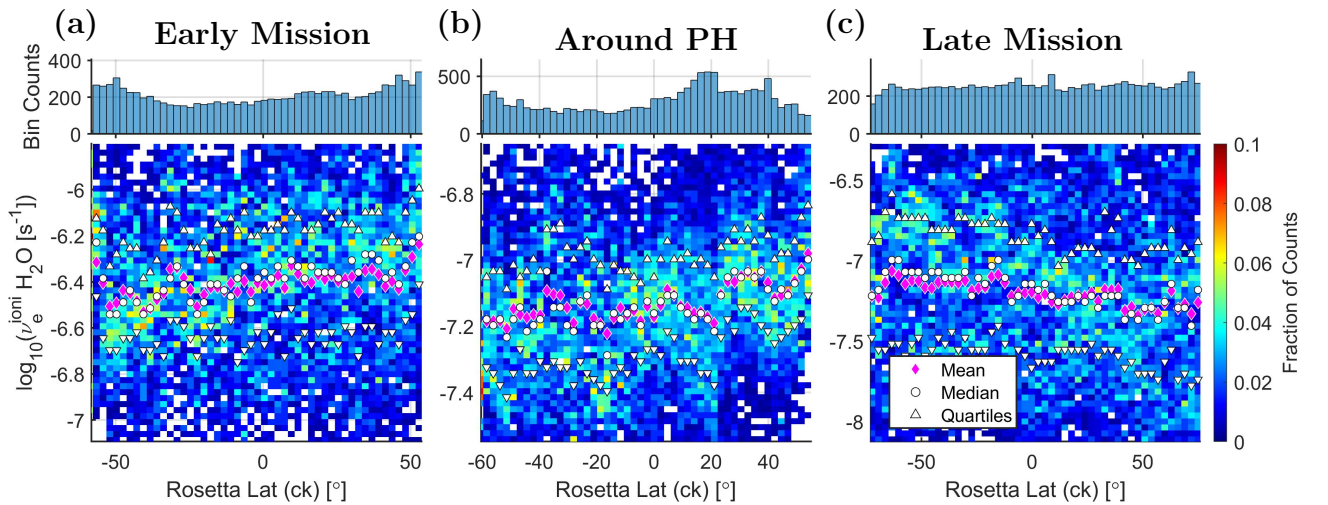


Figure 5.8: Electron-impact ionization frequency vs. spacecraft latitude during the Rosetta mission.

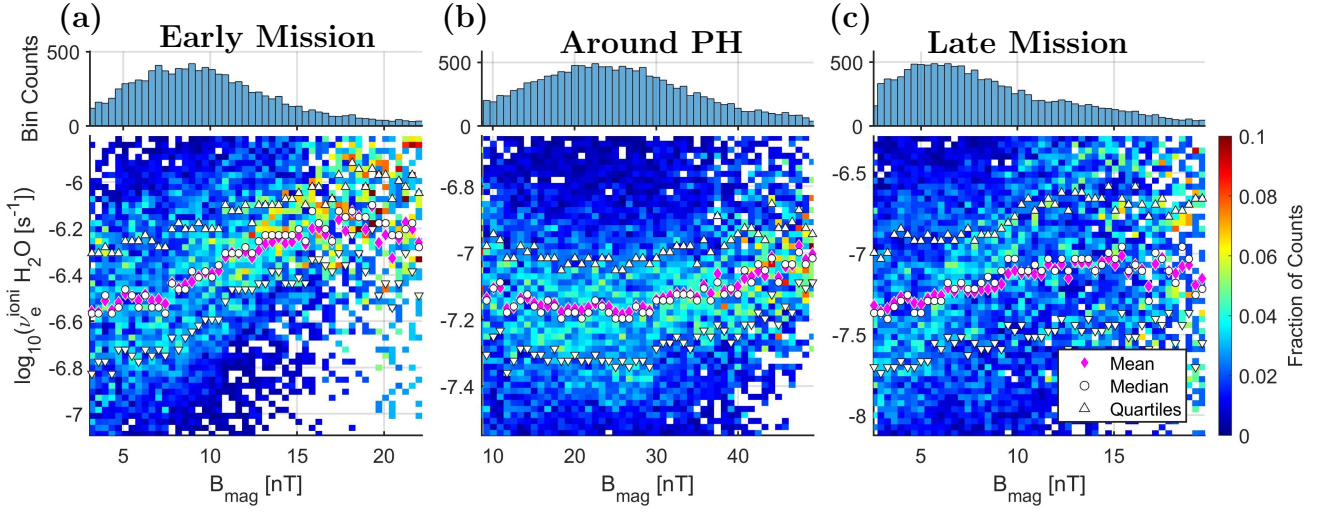


Figure 5.9: Electron-impact ionization frequency vs. magnetic field magnitude (a) early in the mission, (b) around perihelion and (c) late in the mission.

frequency is not linearly correlated with the magnetic field (see Figure 5.9b). For low magnetic field strengths (< 25 nT), the electron-impact ionization frequency decreases slightly, or is flat, with an increase in magnetic field strength. However, beyond 25 nT, the electron-impact ionization frequency and field strength are positively correlated.

I also examined the relationship between the electron-impact ionization frequency and the clock and cone angles of the magnetic field with respect to the Sun-comet line. In comparison with both angles, there was clear non-linear structure in the histograms. However, the same structure and behaviour were apparent in the comparison of the angles with the magnetic field strength. Therefore, the observed relationships are likely to just be a reflection of the correlation with magnetic field strength that is seen in Figures 5.9a and c.

The positive correlation with magnetic field strength may indicate that electron-impact ionization is strongest in regions of magnetic pile up. When the solar wind magnetic field is obstructed by the cometary ionosphere, mass loading causes the solar wind to slow and compresses the magnetic field. It is also associated with an increase in the density of solar wind ions and electrons in the coma. This pile up region is likely to be situated deeper into the coma and inside the ambipolar potential well. The good correlation between the EII frequency and magnetic field strength suggests that it is solar wind electrons that are being accelerated in the ambipolar potential well and piling-up. The correlation with field strength may also partially arise from magnetic mirroring of the electrons as they pass through the coma (see Figure 2.2). Under adiabatic conditions, the perpendicular energy of an electron is proportional to the magnetic field strength as the magnetic moment must be conserved. While the conditions here are not adiabatic (due to the presence of a potential well), this process does provide some additional acceleration of electrons in the pile up

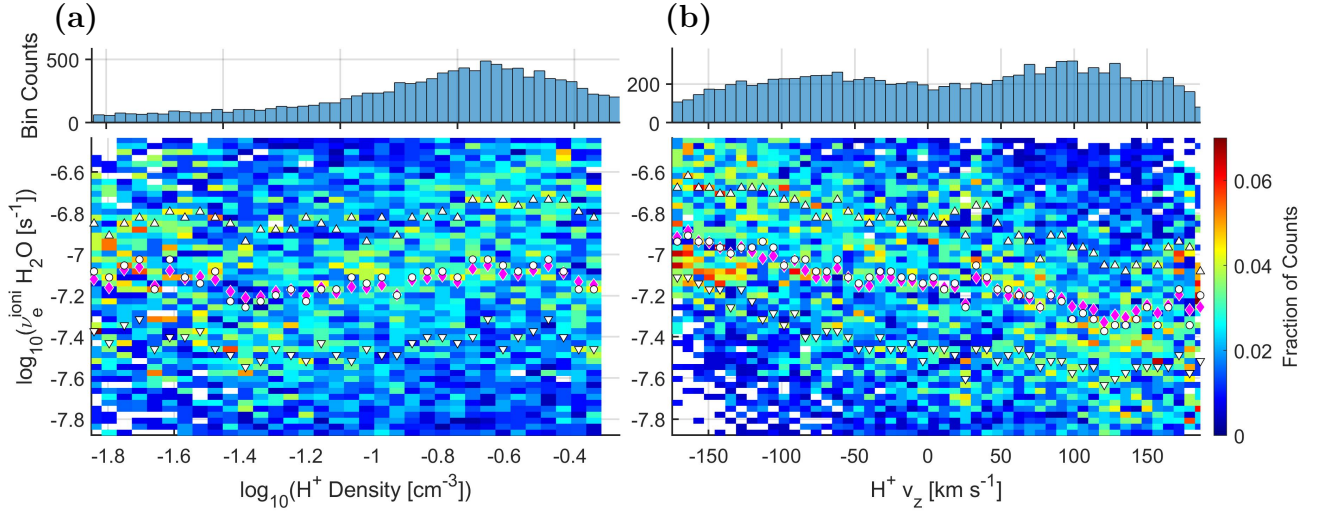


Figure 5.10: Electron-impact ionization frequency vs. proton density from ICA and proton z velocity late in the Rosetta mission (1st Apr to 30th Sep 2016).

region.

Electron-impact ionization vs. solar wind ions

Figure 5.10 shows the dependence of the electron-impact ionization frequency on the properties of the solar wind protons late in the Rosetta mission. There were far fewer measurements of the solar wind ions by ICA early in the mission compared to the late mission, so it is not possible to observe any reasonable correlation during the early part of the mission

Late in the mission, the electron-impact ionization frequency increases slightly with the density of the solar wind protons (see Figure 5.10a) for $n_p > 0.05 \text{ cm}^{-3}$. There is also a clear correlation between the ionization frequency and proton velocity. For negative z velocities (in CSEQ), the ionization frequency clearly increases as the z velocity becomes increasingly negative. For positive velocities, the relation to the ionization frequency flattens and there is no strong relation to the solar wind velocity.

The correlations with the solar wind is consistent with the comparison of the ionization frequency with the magnetic field strength; it may again indicate that electron-impact ionization is strongest in regions where there is substantial pile-up of the solar wind. Pile up results in an increase in the ion density and a deflection of the solar wind velocity. As the solar wind initially travels along x in CSEQ, the deflection will be to either $\pm z$ as seen in simulations (e.g. Deca et al., 2019).

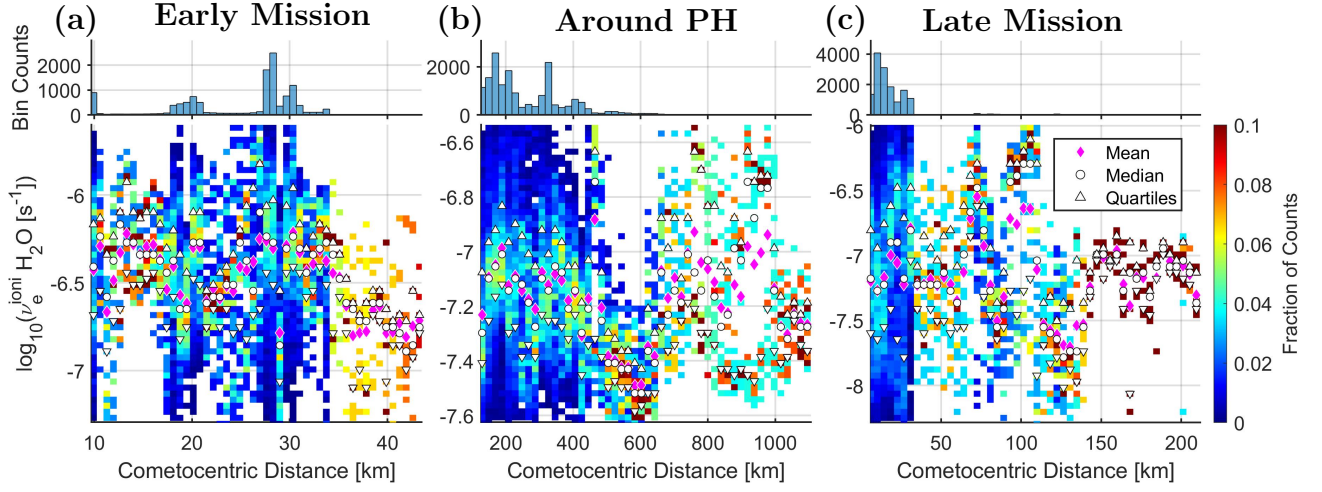


Figure 5.11: Electron-impact ionization frequency vs. cometocentric distance (a) early in the mission (b) around perihelion and (c) late in the mission.

5.1.4 Dependence of ionization frequency on cometocentric distance

Finally, I consider the dependence of the electron-impact ionization frequency on the cometocentric distance. The same approach used in Sections 5.1.2 and 5.1.3 cannot be applied here. The trajectory of the spacecraft around the comet was often confined to quasi-orbits of the nucleus at a fairly steady cometocentric distance. Early and late in the escort phase, the majority of the data was taken in a few bands of cometocentric distance, with very little data at intermediate distances (see Figures 5.11a and c). Therefore, it is not possible to observe any reliable correlation between cometocentric distance and ionization frequency early and late in the mission. Around perihelion, the cometocentric distance did vary over a much larger range (100 - 1500 km) but very little time was spent at these higher distances and therefore the histogram is not well populated. Despite this, around perihelion and far from the comet (200 km - 600 km), the electron-impact ionization frequency does seem to decrease with cometocentric distance.

As no useful conclusions can be drawn from the histograms away from perihelion, I then consider several shorter periods in which the cometocentric distance of the spacecraft changed substantially. The first period is over Feb and Mar 2015 (see Figure 5.12). At the beginning of Feb 2015, Rosetta was at a cometocentric distance of 28 km, where it remained until 4 Feb 2015. Rosetta then moved to a higher cometocentric distance over the following three days to 140 km on 7 Feb. As the cometocentric distance increases, there is no substantial change in the electron-impact ionization frequency. There is a slight increase from 5×10^{-7} to 10^{-6} s^{-1} from 28 km to 140 km, but this is minor compared to the temporal variations within the period. On shorter timescales of a few hours, the fluctuations in the electron-impact ionization frequency seem to be anti-correlated with the fluctuations in the neutral density. The variation may also be driven

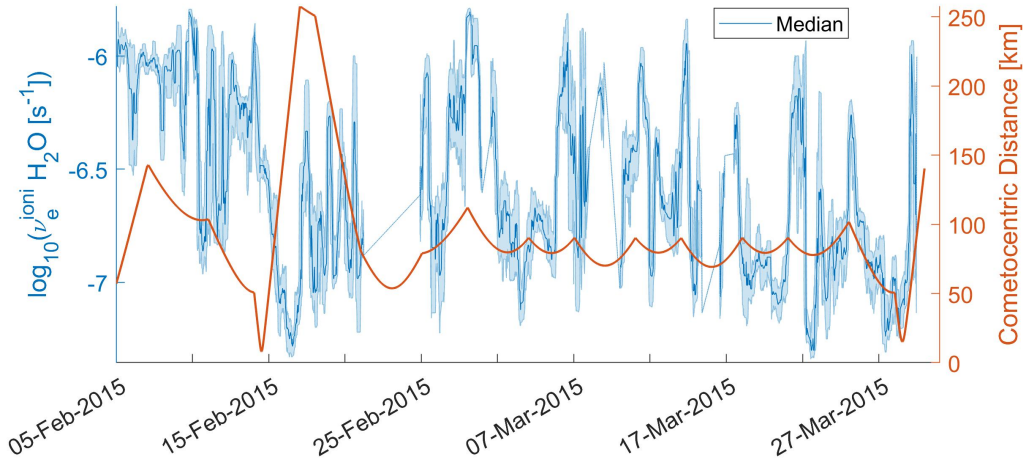


Figure 5.12: Electron-impact ionization frequency (blue) and cometocentric distance (orange) in February and March 2015. The solid lines give the 8-hour median values, while the shaded region regions give the upper and lower quartiles.

by changing solar wind conditions. Rosetta drops to a cometocentric distance of 40 km on 15 Feb 2015. Over this descent, the EII frequency fluctuates between 10^{-7} and $3.15 \times 10^{-6} \text{ s}^{-1}$, but there is no significant change in the average value of the ionization frequency.

This is shortly followed by an increase in the cometocentric distance to 260 km by the start of 17 Feb. This increase in distance is accompanied by a decrease in electron-impact ionization from 3.15×10^{-7} to $4 \times 10^{-8} \text{ s}^{-1}$. The decrease in the ionization frequency follows closely the trend in the neutral density over the same period, but the shorter term fluctuations appear anti-correlated with the ionization frequency. However, when the spacecraft is at a distance of ~ 250 km, there is a peak in the electron-impact ionization frequency at 10^{-6} s^{-1} . As the spacecraft returns from 260 km to a more stable cometocentric distance between 80 and 100 km, there are substantial fluctuations in the ionization frequency (from 3.15×10^{-8} to 10^{-6} s^{-1}) but no overall change in the population of energetic electrons.

From 25 to 28 March, Rosetta descends from 100 km to only 30 km from the nucleus. Alongside this, the electron-impact ionization frequency also decreases from $6.3 \times 10^{-7} \text{ s}^{-1}$ to $6.3 \times 10^{-8} \text{ s}^{-1}$. As the cometocentric distance falls, the neutral density at Rosetta increases. However, in contrast to earlier periods, the short period fluctuations in the neutral density are positively correlated with the short term changes in the electron-impact ionization frequency.

Throughout February and March 2015 there is no consistent relation between the electron-impact ionization frequency and the cometocentric distance of the spacecraft. Therefore, it is not reasonable to draw any conclusions on whether the energetic electron population is heavily dependent on cometocentric distance from this dataset.

In November 2014 and Mar 2016, large changes in cometocentric distance elicited mixed

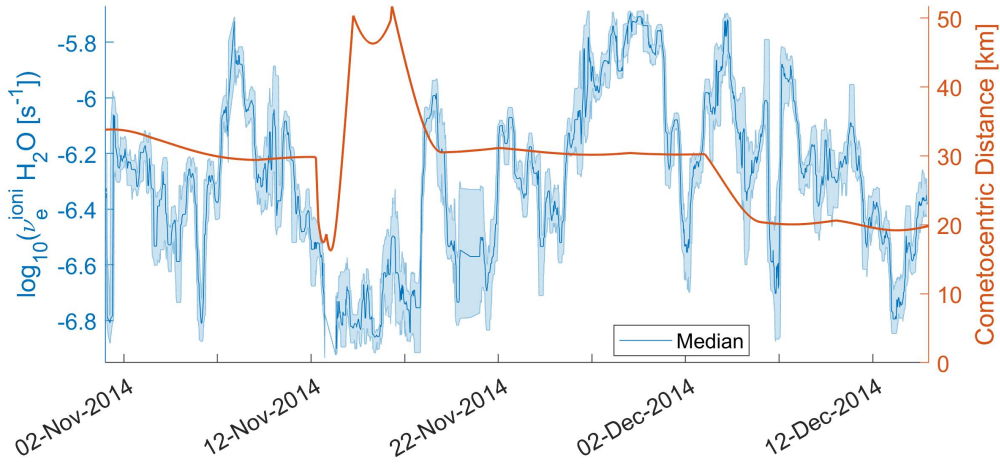


Figure 5.13: Electron-impact ionization frequency (blue) and cometocentric distance (orange) in Nov 2014. The solid lines give the 8-hour median values, while the shaded region regions give the upper and lower quartiles.

responses in the electron-impact ionization frequency (see Figures 5.13 and 5.14). From 12 to 18 November 2014, the cometocentric distance varied from 30 km, down to 18 km and up to 50 km (orange, Fig 5.13), which is met with only a slight initial decrease in the electron-impact ionization frequency ($3.2 \times 10^{-7} \text{ s}^{-1}$ to 10^{-7} s^{-1}) and no noticeable change following the initial decrease.

An inconsistent picture is also drawn during the excursion of Rosetta to 1000 km (see Figure 5.14) in Mar and Apr 2016 (see Figure 5.14). The increases in cometocentric distance from 30 to 400 km and from 300 to 1000 km were paired with decreases in the electron-impact ionization frequency (from $2 \times 10^{-6} \text{ s}^{-1}$ to 10^{-8} s^{-1} and 10^{-6} s^{-1} to 10^{-7} s^{-1}). However, as the spacecraft returned from 1000 km, the electron-impact ionization frequency did not increase substantially ($6.3 \times 10^{-8} \text{ s}^{-1}$ to $1.5 \times 10^{-7} \text{ s}^{-1}$). The overall change in EII frequency during the descent was small compared to the fluctuations in over the same period, and much smaller than the change during the ascent.

Having examined the mission wide dataset and several case studies from Rosetta, there is no clear correlation between the cometocentric distance and the electron-impact ionization frequency. There may be a decrease in the electron-impact ionization frequency with cometocentric distance when close to perihelion from 200 to 600 km. At large heliocentric distances, there is not a systematic relationship between the cometocentric distance and energetic electron population.

5.2 Origin of cometary electrons with test particle simulations

In this section, I present the results of collisional test particle simulations (see Chapter 2) under two sets of outgassing conditions. The two simulations occur at outgassing rates of $Q = 10^{26} \text{ s}^{-1}$ and

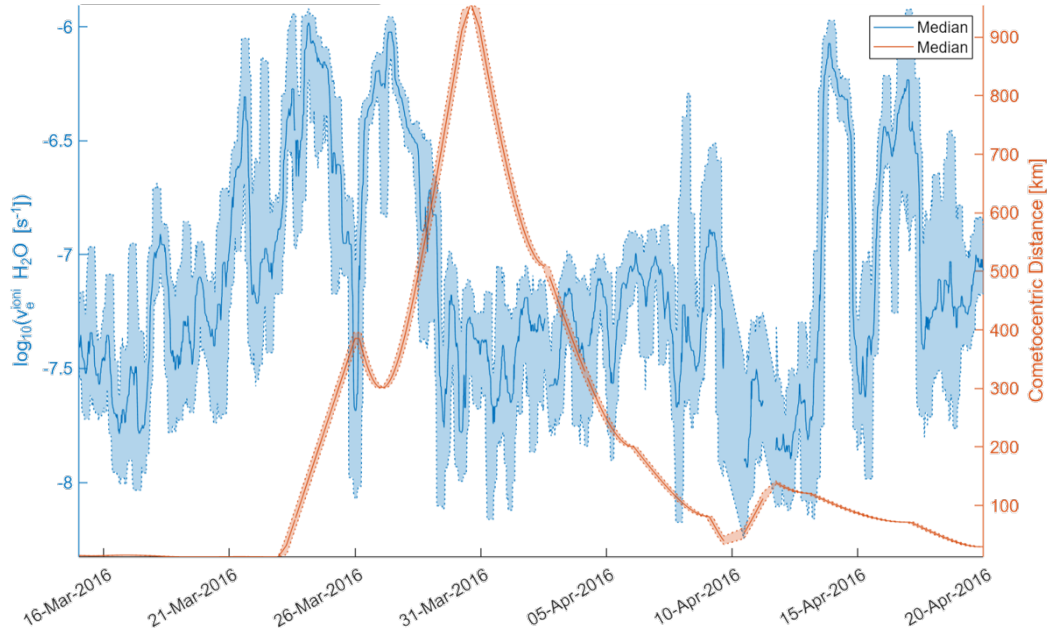


Figure 5.14: Electron-impact ionization frequency (blue) and cometocentric distance (orange) during an excursion in March and April 2016. The solid lines give the 8-hour median values, while the shaded region regions give the upper and lower quartiles.

$Q = 1.5 \times 10^{27} \text{ s}^{-1}$, applying spherically symmetric outgassing conditions. The lower outgassing case gives a weakly collisional coma, and the more strongly outgassing conditions result in a coma where collisional processes are becoming more significant. The electric and magnetic fields for both simulations are calculated using a collisionless Particle-in-Cell (PiC) model as discussed in Section 2.5.3, and the full set of conditions for each simulation (1 and 3) is outlined in Table 2.4. The spatial resolution used in the PiC simulation was 7.66 km for the lower outgassing case, and 10 km for the higher outgassing case.

5.2.1 Comparison of electron population sources

One of the benefits of the test particle model is the ability to distinguish between the various sources of electrons, which is not possible with measurements at Rosetta. Figure 5.15 shows the electron density within the coma from (a & d) photoelectrons, (b & e) solar wind electrons and (c & f) secondary electrons.

In the low outgassing case, photoelectrons (Figure 5.15a) are confined to a fairly small region of the inner coma. The dense region of the photoelectrons ($> 10 \text{ cm}^{-3}$) extends only 50 km from the nucleus in both the xz and xy (not shown) planes. A narrow high density region extends tailward ($+x$) and towards $+z$, where the electrons are transported from the inner coma. The photoionization frequency is uniform throughout the coma, as the coma is optically thin to EUV solar radiation for these outgassing conditions (Heritier et al., 2017a; Heritier, 2018). However, the

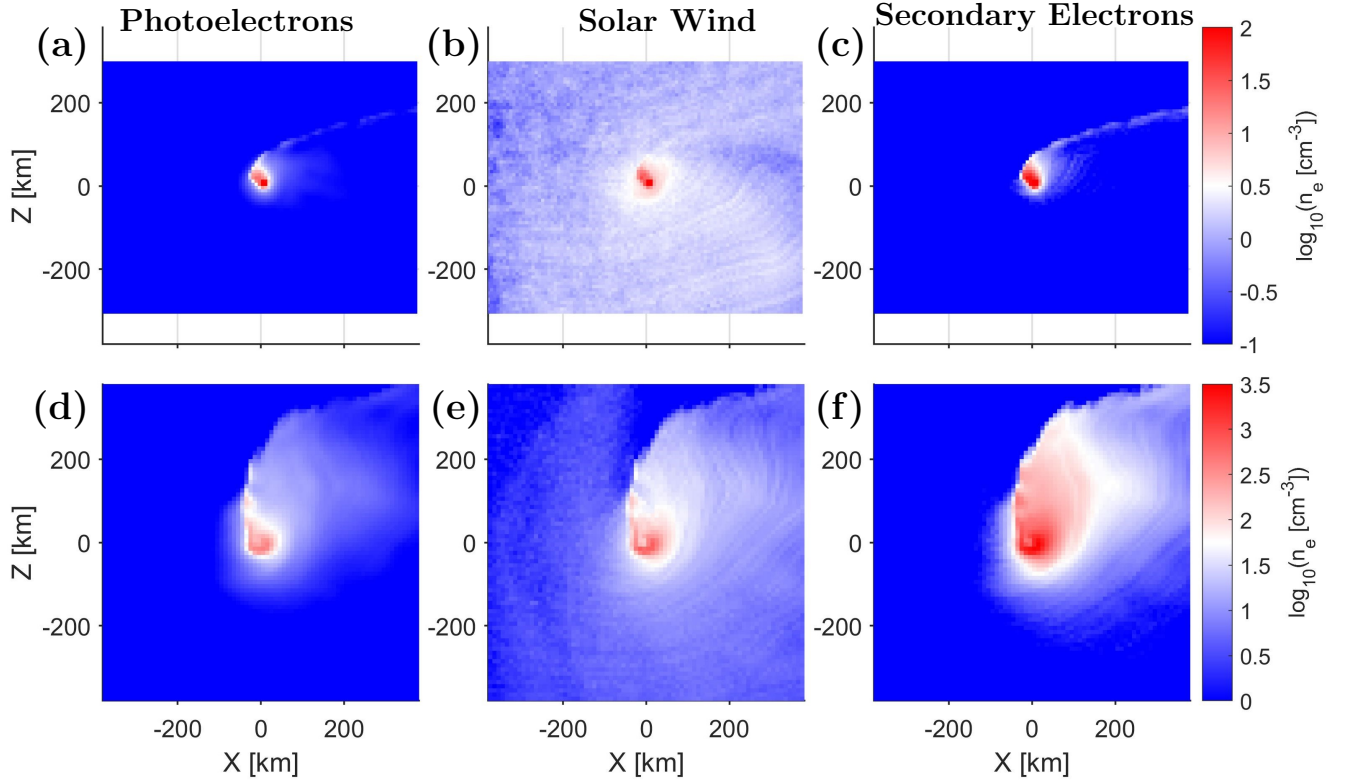


Figure 5.15: Electron density of (a & d) photoelectrons, (b & e) solar wind electrons and (c & f) secondary electrons for outgassing rates of (a-c) $Q = 10^{26} \text{ s}^{-1}$ and (d-f) $Q = 1.5 \times 10^{27} \text{ s}^{-1}$. The densities are plotted in the xz plane. The colour bars are over different ranges for the two outgassing cases.

production rate of photoelectrons is still weighted towards the near nucleus region, as the neutral density follows a $1/r^2$ dependence.

The solar wind electrons (Figure 5.15b) are much more prevalent throughout the wider cometary environment. Upstream, the undisturbed solar wind has a density of 1 cm^{-3} , but this increases close to the nucleus to 8 cm^{-3} . Within the inner coma ($< 40 \text{ km}$), the photoelectrons and solar wind electrons have similar densities (within a factor of 2). The high density region is driven by the funnelling and trapping of solar wind electrons by the ambipolar field, which also accelerates them as they enter the inner coma (see Figure 2.19).

Additionally, there is a substantial population of secondary electrons (Figure 5.15 c) in the weakly outgassing coma. The secondary electron density is comparable to the total density of primary electrons (photoelectrons and solar wind) in the densest regions of the coma and within 30 km of the nucleus. However, the density decreases more rapidly with cometocentric distance, than seen for photoelectrons. Beyond 50 km of the nucleus, the photoelectron density exceeds the secondary electrons. At 100 km from the nucleus, the electrons are almost entirely solar wind electrons, except in regions connected to the inner coma through transport (i.e. the tailward region).

At the higher outgassing case ($Q = 1.5 \times 10^{27} \text{ s}^{-1}$), there is also a substantial population of photoelectrons (see Figure 5.15d). The photoionization frequency is identical to the lower outgassing case (see Table 2.4), so the photoelectron production rate is a factor 15 larger (driven by the ratio in neutral density). The ratio in the photoelectron densities is similar to this factor (between 10 and 20) in the high-density, inner coma region ($r \leq 50 \text{ km}$) of the $Q = 10^{26} \text{ s}^{-1}$ simulation. However, the differences in the electric and magnetic fields between the two simulations result in a much larger photoelectron cloud at $Q = 1.5 \times 10^{27} \text{ s}^{-1}$, with a region of substantial electron density ($\sim 30 \text{ cm}^{-3}$) extending over 300 km downstream (at $z = 100 \text{ km}$). The beginning of a narrow tailward region can be seen in the top right of Figure 5.15d, like that seen in the lower outgassing simulation.

The solar wind conditions at the upstream boundary are the same as in the lower outgassing case (see Table 2.4). The difference in the densities between the two solar wind simulations (Figures 5.15b and e) are therefore driven by the fields, which are taken from the collisionless PiC simulations, and the disparity in the strength of collisional processes with stronger outgassing. The density of solar wind electrons is enhanced for the higher outgassing rate of $Q = 1.5 \times 10^{27} \text{ s}^{-1}$, reaching 300 cm^{-3} close to the nucleus. The solar wind electrons are more efficiently funnelled into the ambipolar potential well, and subsequently trapped in this region. As the neutral density is larger by a factor 15, electron neutral collisions cool the solar wind electrons more efficiently in the region close to the nucleus. Once the accelerated electrons are cooled in the inner coma, they cannot easily escape the potential well and are trapped for longer.

For $Q = 1.5 \times 10^{27} \text{ s}^{-1}$, the solar wind and photoelectron densities are comparable throughout the dense region of the photoelectron cloud ($n_{e,h\nu} > 5 \text{ cm}^{-3}$, Figure 5.15d and e). The solar wind electron density is generally larger by a factor of up to 3 in this region, but the solar wind to photoelectron density ratio is smallest (~ 1) where the photoelectron density peaks. The cloud of solar wind electrons also extends well beyond the dense region of photoelectrons, but there is a particularly low density region that extends from $(-100, 0, 100) \text{ km}$ towards $+z$ and slightly downstream.

The density of secondary electrons (see Figure 5.15f) has a similar shape to the photoelectron cloud, but has a larger density throughout the coma. In this case, the secondary electron density actually exceeds that from both photoelectrons and solar wind electrons, reaching $\sim 1400 \text{ cm}^{-3}$ in the inner coma. The high density of secondary electrons in the collisional simulation does not invalidate the fields from the collisionless PiC simulation. In the non-collisional simulation, the photoelectron densities are actually much larger than for the collisional simulation, with densities up to 1200 cm^{-3} in the inner coma. The introduction of collisions allows photoelectrons to be

more efficiently transported out of the potential well, through elastic collisions with the neutral gas (see Section 2.3). Although the bulk of the electrons are from differing populations in the collisional and non-collisional simulations, the total electron density and resulting fields are similar (see Figure 2.24). Under the higher outgassing conditions, many secondary electrons are produced in the inner coma, by collisions of the solar wind electrons, and are then efficiently trapped and cooled in the potential well. The secondary electrons also have a substantial contribution from the third and fourth generation of electrons, whereas in the lower outgassing case, these further generations were fairly insubstantial. The substantial presence of secondary electrons in both outgassing conditions agrees well with the findings in Section 5.1, which suggested electron-impact was a key source of ionization at large heliocentric distances.

5.2.2 Origin of ionizing electrons

Electron-impact ionization frequency from all three populations

Having established that secondary electrons are the major population of cometary electrons using the test particle model in Section 5.2.1, it is now useful to examine the origin of the ionizing electrons. Similarly to simulations used in Section 5.2.1, it is possible to distinguish the secondary electrons by their parent species i.e. a photoelectron, solar wind electron or another secondary electron. As the electron density was split by population in Figure 5.15, the electron-impact ionization frequency can be similarly separated (see Figure 5.16). The electron-impact ionization frequency, $\nu_e^{\text{ioni}}(\mathbf{x})$, is calculated from the energy distribution function, $f(\mathbf{x}, E)$, using:

$$\nu_e^{\text{ioni}}(\mathbf{x}) = \sum_X \int_{E_{Th,X}}^{E_{Max}} \sigma_e^{\text{ioni},X}(E) \times f(\mathbf{x}, E) \times \sqrt{\frac{2E}{m_e}} dE \quad (5.6)$$

where $\sigma_{\text{ioni},e}^X(E)$ is the electron-impact ionization cross section for production of an ion, X , (see Figure 2.5b) at an incident electron energy, E . The calculation of the energy distribution function is outlined in Section 2.4. Properties of secondary electrons in the test particle code are not calculated using the energy distribution function, but are instead produced stochastically through collisions of macroparticles (see Section 2.3.2). Using the edf gives a smoother estimate of the electron-impact ionization frequency for this comparison, rather than deriving it from the electron-impact collisions. Far from the nucleus, electron-impact ionization is quite infrequent and few secondary electron macroparticles are generated, which can lead to low statistics. In regions where the electron-impact ionization frequency is high, the two approaches give the same result. Figure 5.16 shows the electron-impact ionization frequency generated by (a & d) photoelectrons,

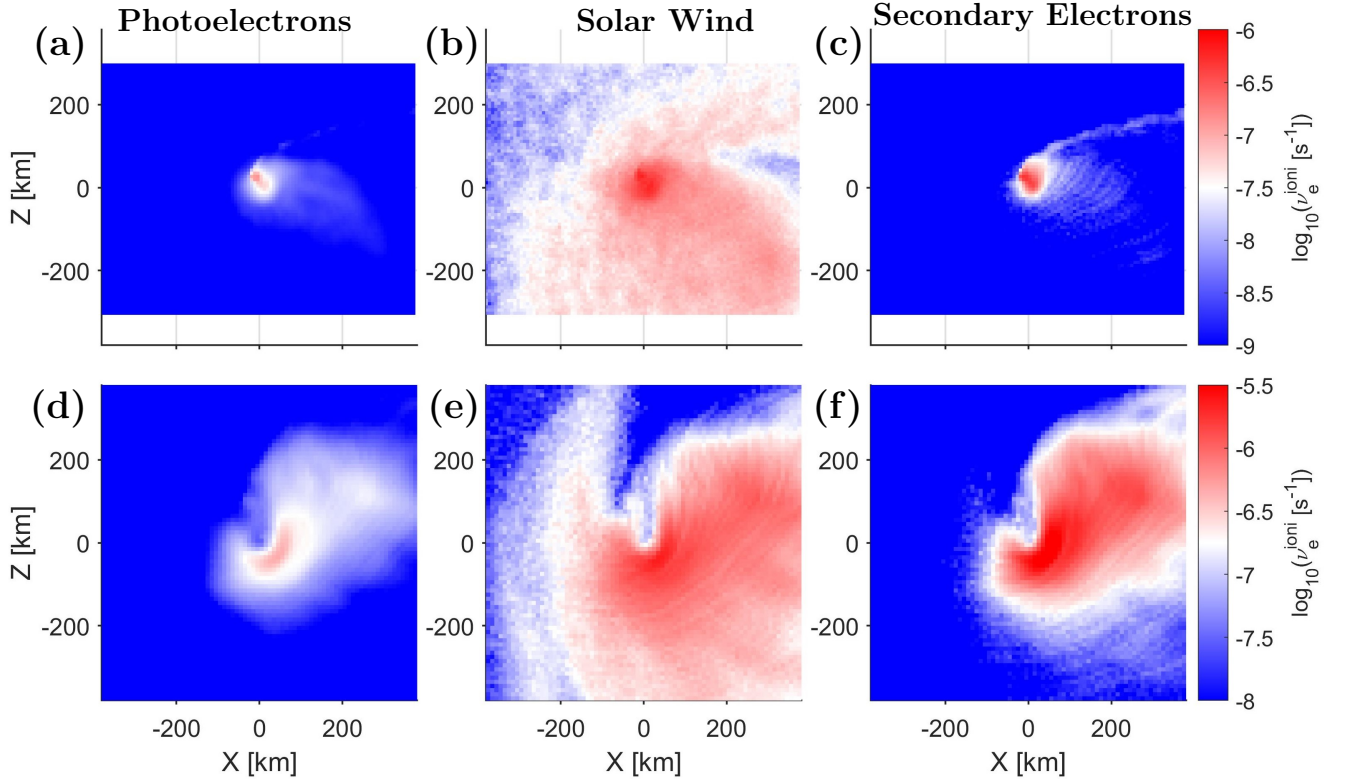


Figure 5.16: Electron-impact ionization frequency from collisions by (a,d) photoelectrons, (b,e) solar wind electrons and (c,f) secondary electrons for outgassing rates of (a-c) $Q = 10^{26} \text{ s}^{-1}$ and (d-f) $Q = 1.5 \times 10^{27} \text{ s}^{-1}$.

(b & e) solar wind and (c & f) secondary electrons at outgassing rates of (a-c) $Q = 10^{26} \text{ s}^{-1}$ and (d-f) $Q = 1.5 \times 10^{27} \text{ s}^{-1}$.

At $Q = 10^{26} \text{ s}^{-1}$, the electron-impact ionization frequency from photoelectrons is at its highest in the inner coma, reaching a maximum of $6 \times 10^{-8} \text{ s}^{-1}$ (see Figure 5.16a). The ionization frequency driven by impacts of photoelectrons drops off quickly with distance from the comet, falling to 10^{-8} s^{-1} at a cometocentric distance of 50 km, and continues to decrease farther from the comet. This results from the decrease in the number density of photoelectrons (see Figure 5.15 a) and the climbing of the potential well. Electron-impact ionization from collisions of photoelectrons is weaker throughout the coma than photoionization ($1.32 \times 10^{-7} \text{ s}^{-1}$), as expected in an optically thin coma.

The electron-impact ionization frequency from solar wind electrons (see Figure 5.16b) exceeds the electron-impact ionization frequency from photoelectrons across the whole domain. In the innermost coma ($< 40 \text{ km}$), electron-impact ionization peaks at $6 \times 10^{-7} \text{ s}^{-1}$, four times that of the photoionization frequency. The electron-impact ionization frequency of solar wind electrons is comparable to, or larger than, the photoionization frequency up to 200 km from the nucleus, downstream of the nucleus and in $-z$. Solar wind electron-impact ionization is a major source of electrons in the wider coma, and solar wind electrons are the dominant driver of electron-impact

ionization in the coma.

Secondary electrons can also generate further electrons through electron-impact ionization in the coma (see Figure 5.16c). This source of electrons is confined to only the inner coma, as the density of the secondary electrons falls quickly outside this region (see Fig. 5.15c) and the electrons are less energetic in the boundaries of the potential well. In the inner coma, secondary electrons are more ionizing than photoelectrons. The two populations have similar densities, but the secondary population is more energetic. The second generation of electrons are mostly generated through collisions of solar wind electrons rather than photoelectrons (see Figure 5.16a vs. b), as the solar wind electrons are much more energetic (energies up to 250 eV after falling into the potential well, see Fig. 2.19). Therefore, the secondary electrons inherit a substantial amount of energy from the ‘parent’ electron, and can drive further ionization within the coma.

In the higher outgassing case (see Figures 5.16d-f), electron-impact ionization is a strong process over a much wider region of the coma for all three electron populations, extending from 100 km upstream to 380 km downstream of the nucleus. The maximum electron-impact ionization frequencies are all offset from the innermost coma, where the neutral density is highest. The peaks are actually found at (-50, 0, -50) km for all three populations. Although the electron density is maximal near the nucleus, the electrons are efficiently cooled in this part of the coma by collisions with the neutral gas (see Chapter 3). Farther from the nucleus, the potential well is deep enough to generate energetic electrons (> 150 eV), while cooling processes are much less efficient.

Similarly to the lower outgassing case, solar wind electrons are more ionizing than photoelectrons throughout the coma (see Figs. 5.16 d and e). However, in contrast to the lower outgassing rate, the secondary electrons are a stronger source of ionization than solar wind electrons in the inner coma. Solar wind electron-impact ionization produces secondary electrons that are also energetic. These electrons are more efficiently trapped in the potential well than the solar wind electrons and are more likely to undergo numerous collisions with the neutral coma. As a result, the second generation of electrons are strongly ionizing. Further generations also cause ionization throughout the coma, but they become progressively weaker as the energy is divided between more electrons and dissipated through other inelastic processes (e.g., excitation). Although secondary electrons are an important source of ionization, these descend originally from solar wind electrons rather than photoelectrons.

Electron-impact ionization frequency vs. magnetic field

The methodology applied in Section 5.1.3 can be similarly applied to the outputs of the test particle simulations. The cell values from a test particle simulation are organized into a 2D histogram, with

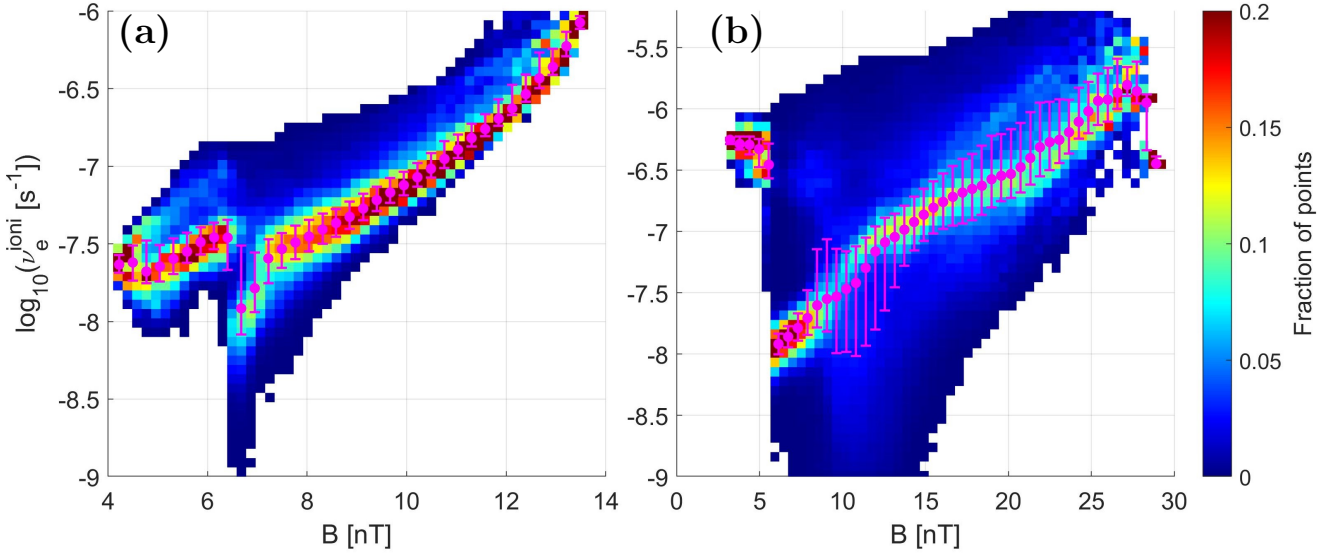


Figure 5.17: Electron-impact ionization frequency against magnetic field strength throughout the coma for outgassing rates of (a) $Q = 10^{26} \text{ s}^{-1}$ and (b) $Q = 1.5 \times 10^{27} \text{ s}^{-1}$. The pink points give the median and quartile values for each bin.

the median and quartile values for the bins along x are given by the pink points and error bars (e.g. Fig. 5.17). Using data from Rosetta, the histogram is populated by a single measurement point that moves through an evolving coma, whereas test particle model outputs encompass a 3-dimensional picture of the coma under a single set of conditions and at a steady state.

Firstly, in Figure 5.17 I have compared the electron-impact ionization frequencies in the coma to the magnitude of the magnetic field. Under both sets of outgassing conditions, the electron-impact ionization frequency is positively correlated with the magnetic field magnitude, as was seen with the measurements from Rosetta (see Figure 5.9). For the low outgassing case at $Q = 10^{26} \text{ s}^{-1}$:

- the ionization frequency increases from $3.2 \times 10^{-8} \text{ s}^{-1}$ at 8 nT to 10^{-6} s^{-1} at 13 nT. The magnetic field strength in the coma increases closer to the nucleus, as a result of the increasing pile up of the solar wind magnetic field and acceleration in the ambipolar potential well.
- the regions with very low magnetic field ($B < 6 \text{ nT}$) are found downstream of the comet, in the wake of the cometary ionosphere. These regions are quite weakly populated with solar wind electrons and are in a region where the potential well is quite weak. As the solar wind electron density and temperatures are low, there are few energetic electrons to induce ionization.
- the discontinuity in the ionization frequency, at 6.5 nT, is caused by the solar wind upstream of the comet nucleus. The interplanetary magnetic field is 6.5 nT near the upstream boundary of the test particle grid. Here, the electron density is primarily solar wind electrons,

which have not yet fallen into the ambipolar potential well. The electron temperature at $x = -380$ km is unchanged from the quiet solar wind condition at ~ 10 eV, meaning few of the electrons (only the high-energy tail) have enough energy to ionize the cometary neutrals. As such, the ionization frequencies are small $\sim 10^{-9} \text{ s}^{-1}$ near the upstream boundary and reduce the median ionization frequency values at and just above the 6.5 nT threshold.

At the higher outgassing rate ($Q = 1.5 \times 10^{27} \text{ s}^{-1}$, Fig. 5.17b):

- the median ionization frequency increases from 10^{-8} s^{-1} at 6 nT, to $1.6 \times 10^{-6} \text{ s}^{-1}$ at 25 nT (pink). This agrees well with the hypothesis of increased pile up and trapping of solar wind electrons in the regions of large magnetic field strength.
- there is a discontinuity in the median electron-impact ionization frequency around 5.6 nT, as seen in the lower outgassing case. The minimum magnetic field strengths ($B < 5$ nT) are found over 300 km downstream of the nucleus between $y = \pm 30$ km.
- the lowest median values of the ionization frequency (at $1.2 \times 10^{-8} \text{ s}^{-1}$) also correspond to the upstream boundary regions, where the solar wind has not been substantially accelerated.
- the smallest values of ionization frequency in the domain, reaching as low as 10^{-9} s^{-1} , have magnetic field strengths of 10 to 12 nT. These values originate in an electron depleted region, seen at (-50, 0, 200) km in Figure 5.15e. This area is a maximum in the parallel (ambipolar) potential well, at a potential 50 V higher than the solar wind. The potential barrier opposes electrons entering the region, and decelerates any that do overcome the ambipolar field.
- in contrast to the lower outgassing conditions, the electron-impact ionization frequency decreases above 26 nT. Magnetic field strengths exceeding 26 nT are only found very close to the nucleus, where the neutral density peaks. The high density of neutrals makes this region of the coma very collisional. Electrons close to the nucleus are efficiently cooled, whether they begin in the solar wind or are of cometary origin. Consequently, there is a reduction in the number of energetic electrons close to the nucleus, despite being deeper in the ambipolar potential well.

The relationship between the fields and ionization frequency is subject to the caveat that there is no feedback from collisional processes onto the electric and magnetic fields in the test particle simulation. Particularly in the higher outgassing case, the substantial cooling of electrons in the inner coma may result in a weaker ambipolar field in the collisional region. This would reduce the strength of the potential well (see Section 2.6.3) and weaken the electron trapping. Any resulting

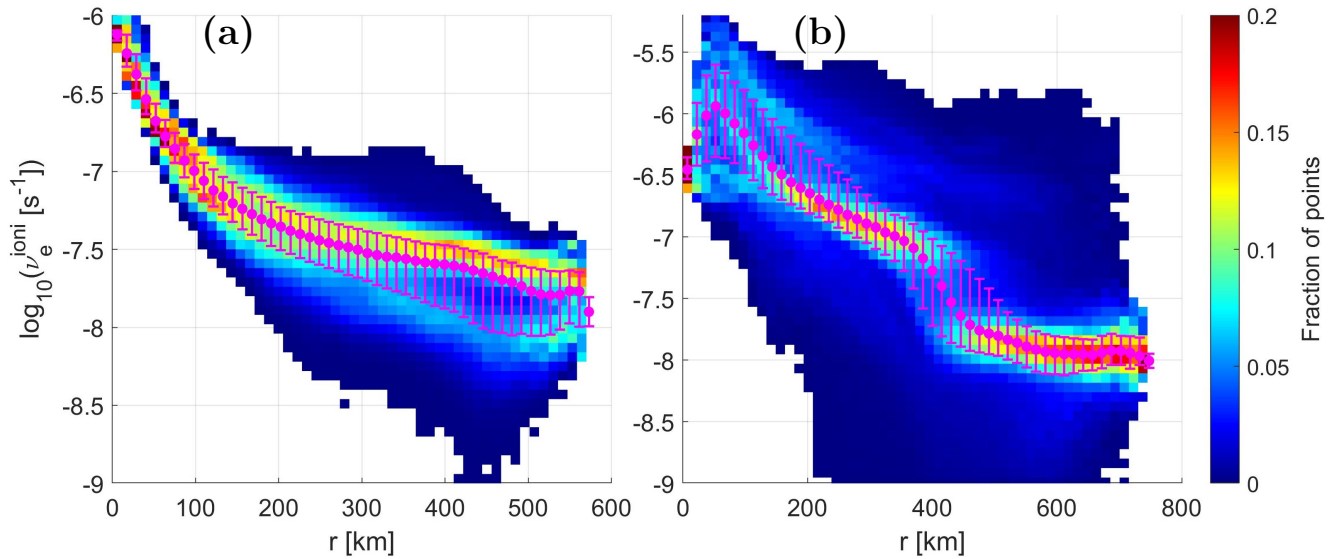


Figure 5.18: Total electron-impact ionization frequency against cometocentric distance throughout the coma from test particle simulations at outgassing rates of (a) $Q = 10^{26} \text{ s}^{-1}$ and (b) $Q = 1.5 \times 10^{27} \text{ s}^{-1}$. The pink points give the median and quartile values for each bin.

changes to the magnetic field strength are unlikely to be very substantial, as the field quickly saturates during solar wind pile up. Feedback from collisional processes would likely result in dampening of ionization frequencies in the inner coma, where the magnetic field strength is largest.

5.2.3 Dependence of ionization frequency on cometocentric distance

The relationship between cometocentric distance and the electron-impact ionization frequency is shown in Figure 5.18 for the two sets of outgassing conditions. In both cases, the electron-impact ionization frequency is seen to increase moving closer to the nucleus. In the low outgassing case (see Figure 5.18a), the ionization frequency is fairly constant far from the nucleus ($> 300 \text{ km}$). In this region, the plasma is mostly solar wind that is largely undisturbed and has not been substantially accelerated by the ambipolar field. Closer to the nucleus, the ionization frequency starts to increase, with the strongest gradient seen within 100 km of the comet surface. The electron-impact ionization frequency increases by an order of magnitude from 10^{-7} s^{-1} at 100 km to 10^{-6} s^{-1} at the comet surface. Close to the nucleus, the ionization frequency is almost entirely driven by collisions of accelerated solar wind electrons (or their secondaries, see Figure 5.16). As the potential well is deepest in the inner coma, the solar wind electrons are at their densest and most energetic in this region. At $Q = 10^{26} \text{ s}^{-1}$, the neutral coma is not dense enough to efficiently cool a large portion of the solar wind electron population, so the EII frequency is large.

In the higher outgassing case (see Figure 5.18), the behaviour is very similar beyond 50 km from the nucleus. At large distances, the undisturbed, un-accelerated solar wind electrons produce

Table 5.3: Set of test cases to examine ion acceleration in the coma. Rosetta has been set at a cometocentric distance of 30 km.

Case	Ion bulk velocity	Electron-impact freq
1	Constant at 0.6 km s^{-1}	Constant at $3 \times 10^{-7} \text{ s}^{-1}$
2	Constant at 5 km s^{-1}	Constant at $3 \times 10^{-7} \text{ s}^{-1}$
3	Linear increase: $u_i(r_{67P}) = 0.6 \text{ km s}^{-1}$, $u_i(r_{Ros}) = 5 \text{ km s}^{-1}$.	Constant at $3 \times 10^{-7} \text{ s}^{-1}$
4	Linear increase: $u_i(r_{67P}) = 0.6 \text{ km s}^{-1}$, $u_i(r_{Ros}) = 5 \text{ km s}^{-1}$.	$\propto 1/r$. $3 \times 10^{-7} \text{ s}^{-1}$ at Rosetta

a constant ionization frequency at 10^{-8} s^{-1} . Moving closer to the nucleus, solar wind electrons and energetic cometary electrons contribute increasingly to the ionization frequency, as the potential well becomes deeper.

The median ionization frequency peaks at 10^{-6} s^{-1} 50 km from the nucleus. Within the first 50 km of the surface, the electron-impact ionization frequency decreases with lower cometocentric distances. This is the most collisional region of the coma, and the accelerated solar wind electrons are effectively quenched by collisions with the neutral gas (see Figure 5.16e). As the solar wind electrons are strongly accelerated before being degraded in energy, the ionization collisions generate many energetic secondary electrons that can also cause electron-impact ionization.

In the inner coma, the inelastic collisions are efficient enough to cause substantial cooling of both cometary and solar wind electrons, when paired with trapping by the potential well.

For both sets of outgassing conditions, the feedback from collisions on the fields has been neglected in the test particle model. At lower outgassing rates, the impact of collisions is minor, but may result in a flattening of the potential well in the inner coma (see Section 2.6.3). In Figure 5.18, the reduced acceleration and wider potential well would appear as a flattening of the electron-impact ionization frequency at low r . In the higher outgassing case, the ambipolar potential well would also be expected to decrease in depth.

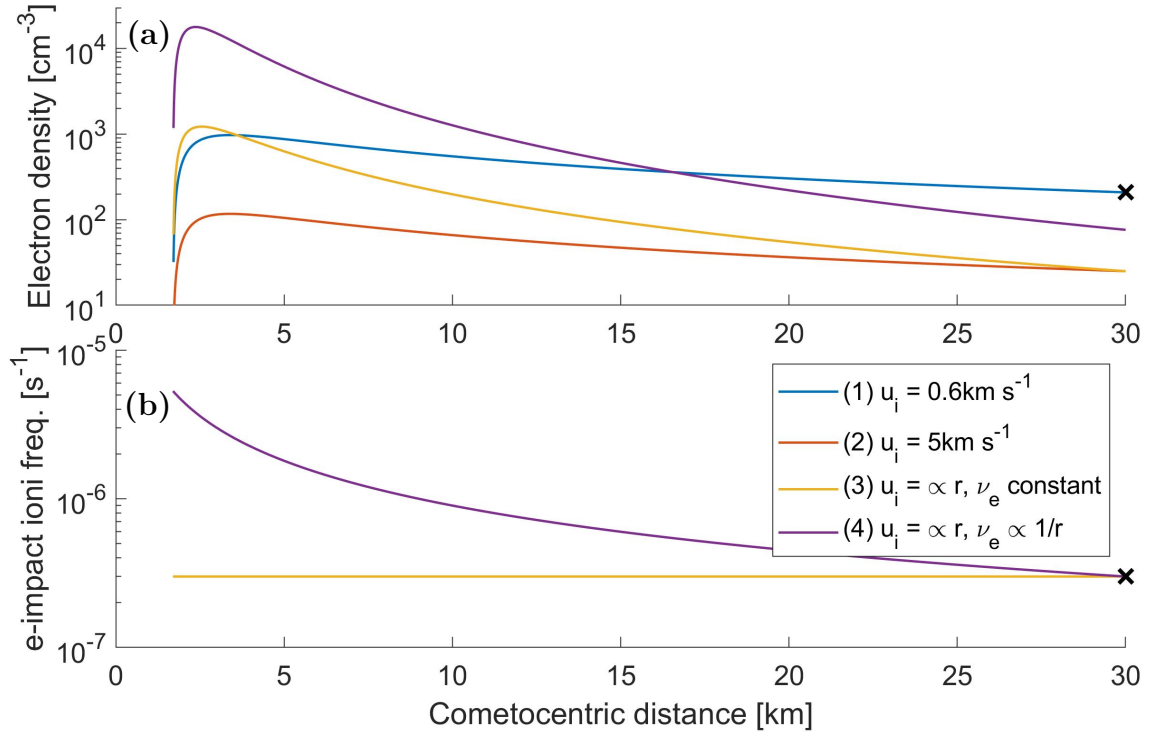


Figure 5.19: (a) Electron density and (b) electron-impact ionization frequency as a function of cometocentric distance for the four test cases (1) - (4) outlined in Table 5.3. The black crosses give the electron density and ionization frequency measured at Rosetta (at 30 km).

5.3 Electron-impact ionization throughout the coma: a discussion

Recent measurements of the ion flow speeds in the coma by Johansson et al. (2021) and Nilsson et al. (2020), using RPC/ICA and LAP (see Section 1.1.1), have highlighted a key area of discussion: the spatial dependence of the electron-impact ionization frequency (and energetic electron population) in the cometary environment at large heliocentric distances. These studies have estimated ion flow speeds, $u_i(r_{Ros})$, at Rosetta in excess of 10 km s^{-1} within 30 km of the nucleus. To achieve such radial speeds, the ions must undergo substantial acceleration between the nucleus surface and Rosetta, as the newly-born ions move with the neutral gas flow speed ($0.4 - 1 \text{ km s}^{-1}$ Marshall et al., 2017). The high ion velocities at Rosetta challenge assumptions made in the multi-instrument analyses (namely $u_i = u_{gas}$). This assumption has been effective in explaining the observed electron densities over a large range of cometocentric distances (0-80 km) and conditions at large heliocentric distances ($r_h > 2 \text{ au}$; Galand et al., 2016; Heritier et al., 2017b, 2018b). Incorporating higher ion and plasma outflow speeds at the location of Rosetta into the multi-instrument model would require a significant increase in the electron-impact ionization frequency between Rosetta and the nucleus, to reconcile the modelled and observed electron densities.

Multi-instrument analyses of electron density and FUV emissions from the coma have shown good agreement with both in situ and remote observations, when assuming a constant energetic electron-impact ionization and dissociative excitation frequency with cometocentric distance (see Section 4, [Galand et al., 2016, 2020](#); [Heritier et al., 2017b, 2018b](#); [Stephenson et al., 2021](#)). Both processes are driven by electrons over similar energy ranges (12-25 eV). These studies use the in situ measurements of the energetic electron population to derive ionization and excitation frequencies (see Sections 1.1.1 and 2.3.2) within the coma over the periods of interest. These analyses accurately reproduce electron densities at large heliocentric distances ([Galand et al., 2016](#); [Heritier et al., 2017b, 2018b](#)) at a variety of times throughout the mission, when assuming the electron-impact ionization frequency is constant with cometocentric distance between Rosetta and the nucleus. Similarly, modelling of FUV emissions, using a constant ionization frequency, closely matches independent and remote measurements of the emission brightness ([Galand et al., 2020](#); [Stephenson et al., 2021](#)).

If it is true that the ions are undergoing a substantial acceleration between the surface and Rosetta, what impact would this have on the results of the multi-instrument studies? I examine four test cases to interpret the implications of accelerating ions, which are outlined in Table 5.3.

In the first two cases, the ion speeds, u_i , and electron-impact ionization frequency, ν_e^{ioni} , are assumed constant with cometocentric distance, r , from the nucleus. These are limiting cases with (case 1) ions always at the gas velocity $u_i(r) = u_{gas}$ or (case 2) ions always at the maximum accelerated velocity, $u_i(r) = u_i(r_{Ros})$. The gas velocity is set at 600 m s^{-1} , which is a typical value at large heliocentric distances ([Marshall et al., 2017](#); [Biver et al., 2019](#)). The radial ion velocity at Rosetta is fixed at 5 km s^{-1} ([Johansson et al., 2021](#)). The ion velocity profiles are paired with a constant electron-impact ionization frequency of $\nu_e^{ioni} = 3 \times 10^{-7} \text{ s}^{-1}$, which was a typical value far from perihelion (see Fig. 5.1). For simplicity, I have neglected photoionization throughout these cases, but electron-impact was found to be the dominant source of electrons in the coma at large heliocentric distances (see Section 5.1.2). For cases 1 and 2, the electron densities at a cometocentric distance, r , are given by:

$$n_e(r) = \frac{Q\nu_e^{ioni}}{4\pi u_{gas} \times u_i(r)} \times \frac{r - r_{67P}}{r^2} \quad (5.7)$$

The multi-instrument studies by [Galand et al. \(2016\)](#) and [Heritier et al. \(2017b, 2018b\)](#), which are based on Eq. 5.7 (except with the inclusion of photoionization), have shown that case 1 (blue, Figure 5.19a) is a good model of the plasma density in the coma. If the ions flow radially outward

at 5 km s^{-1} , the plasma density would be much lower at Rosetta than was observed (red vs. blue, Figure 5.19a) and the multi-instrument model of electron density would show substantial discrepancy with the observations.

This conclusion is also drawn from test case 3 (see Table 5.3). In this scenario, the ions accelerate linearly from the gas velocity at the surface to an ion velocity of 5 km s^{-1} at Rosetta, in line with the results of Johansson et al. (2021). The electron-impact ionization frequency is still set as constant with distance from the nucleus (yellow, Fig. 5.19b). The plasma density at a distance r (in Eq. 5.7) is independent of the ion velocity at other radii, assuming radial outflow. Consequently, the plasma density measured at Rosetta would be identical in cases 2 and 3, given that the speeds are set equal at Rosetta. As before, the electron density (yellow, Fig. 5.19a) is greatly underestimated compared to the measured electron densities at Rosetta and the model that can accurately reproduce them (blue). To compensate for this higher ion velocity at Rosetta, more electrons must be produced between Rosetta and the comet surface, requiring an increased electron-impact ionization frequency.

Case 4 incorporates an electron-impact ionization frequency that is proportional to $1/r$ (see Table 5.3). This dependence of electron-impact ionization frequency with distance has been previously used in models of FUV emissions (Feldman et al., 2015), assuming that energetic electrons behave similarly to the bulk of the plasma. The ionization frequency is constrained by the RPC/IES measurements at Rosetta (purple, Figure 5.19b), so this value is fixed. If the ions undergo linear acceleration and the electron-impact ionization frequency varies as $\nu_e^{\text{ioni}}(r) \propto \frac{1}{r^n}$, the plasma density is given by:

$$n_e(r) = \frac{Q\nu_e^{\text{ioni}}(r)}{4\pi u_{\text{gas}} \times u_i(r) \times r} \times \begin{cases} \log\left(\frac{r}{r_{67P}}\right) & \text{if } n = 1 \\ \frac{1}{n-1} \left(\frac{r}{r_{67P}}^{n-1} - 1\right) & \text{otherwise;} \end{cases} \quad (5.8)$$

Assuming $\nu_e^{\text{ioni}}(r) \propto \frac{1}{r}$ (Feldman et al., 2015), the electron density is approximately reproduced for Rosetta at 30 km from the nucleus (purple, Fig. 5.19a), and the electron-impact ionization frequency is greatly enhanced near the nucleus (Fig. 5.19a). An index of $n = 1.89$ would exactly reproduce the electron density at Rosetta in this scenario, but this would further boost the electron density and ionization frequency near the nucleus, compared to the $1/r$ case.

For a large ion bulk velocity at Rosetta, artificially boosting the energetic electron population can reconcile the electron density measurements and the multi-instrument analysis. However, this neglects the impact of the electron population on the FUV emissions. The FUV emissions are much more susceptible to the conditions near the nucleus, where the coma is densest. The

electron density is built up over a greater distance, as each shell of equal depth dr contributes proportionally to $\nu_e^{ioni}(r)$. When generating FUV emissions, each shell of depth dr contributes to the total brightness proportionally to $\nu_e^{em}(r)/r^2$ (where $\nu_e^{em}(r)$ is the emission frequency), meaning layers near the surface are much more important. If the energetic electron population does vary with $1/r$, the layers near the nucleus should be 10-15 times as ionizing, and exciting as the layer measured by RPC/IES at Rosetta. This would greatly inflate the emissions from the coma by an order of magnitude. While there are uncertainties in the multi-instrument modelling of FUV emissions, an order of magnitude difference between the observed and modelled line brightnesses would be evident in the studies by [Galand et al. \(2020\)](#) and [Stephenson et al. \(2021\)](#).

To summarize, a substantial acceleration of ions between the surface and Rosetta would have significant effects on the electron density and FUV emissions. If electron densities are reconciled by increasing the energetic electron population near the surface, the modelled FUV emissions would no longer be consistent with the remote observations. These distinct sets of measurements are not consistent with each other, and require further examination.

In light of this inconsistency, it is useful to review whether a substantial variation in the electron-impact ionization frequency with cometocentric distance is observed in other datasets or modelling. When analysing FUV emissions from the coma, [Feldman et al. \(2015\)](#) assumed the energetic electron population varied in the same way as the bulk population (i.e., $\propto 1/r$). This was used to estimate the mean electron density along the line of sight. However, the bulk and suprathermal populations of electrons are distinct populations and have very different origins, so do not have to exhibit the same spatial variations. [Chaufray et al. \(2017\)](#) found that the variation in brightness of Lyman- β emissions was consistent with a constant electron-impact excitation frequency.

Analysis of the electron-impact ionization frequency, as derived from RPC/IES measurements, throughout the Rosetta mission does not show a significant dependence with the cometocentric distance (see Section 5.1.4). Around perihelion, electron-impact ionization frequency does appear to decrease with distance from the nucleus over large scales (200 - 600 km, see Figure 5.11 b). However, during the early and late mission periods, the spacecraft trajectory limited any substantive conclusions over long periods. Several cases with large variation in the cometocentric distance over short timescales were also inconclusive (see Section 5.1.4). At times, electron-impact ionization frequency appears correlated with cometocentric distance, but the opposite conclusion can equally be drawn from neighbouring periods. Multi-instrument analysis during the final descent of Rosetta on 30 Sep 2016 showed that electron densities were consistent with a constant electron-impact ionization frequency, all the way to the surface ([Heritier et al., 2017b](#)).

The collisional test particle simulations do indicate that the electron-impact ionization frequency increases closer to the nucleus (see Sections 5.2.2 and 5.2.3). This is caused by the acceleration and trapping of solar wind electrons, by the ambipolar potential well around the comet nucleus. In the higher outgassing case ($Q = 1.5 \times 10^{27} \text{ s}^{-1}$), electron-impact ionization frequency decreases with decreasing r within 50 km of the nucleus as the energetic electrons are cooled by collisions with the neutral coma. There are several notable caveats to the test particle model results. Firstly, the resolution of the electric and magnetic fields is poor close to the nucleus, with the highest resolutions used here at 7.66 km (see Table 2.4). This limits the interpretation of features that appear very close to the nucleus.

There also is no feedback from the electron-neutral collisions on the electric and magnetic fields in the test particle model. In Section 2.6.3, I estimate the impact that the electron collisions would have on the electric field in the inner coma. The cooling of electrons close to the nucleus reduces the electron pressure, and consequently the ambipolar field strength. The outcome of this is a weaker potential well that has a wider, flatter bottom in the inner coma. While the test particle models do suggest that electron-impact ionization increases with decreasing cometocentric distance, this feedback process may result in a more constant ionization frequency in the inner coma. To assess this more thoroughly, it would be ideal to incorporate some form of electron-neutral collisions into the Particle-in-Cell model.

Over large scales ($>100 \text{ km}$), there is likely to be a decrease in the energetic electron population with increasing r when far from perihelion, as the limits of the ambipolar potential well are reached. However, closer to the nucleus the shape of the ambipolar potential well is not as well known, due to potential feedbacks from collisions onto the electric field. A substantial acceleration of ions between the surface and Rosetta cannot simply be rectified by boosting the electron-impact ionization frequency near the nucleus. This leads to a major discrepancy with the observation and modelling of electron-induced FUV emissions. Direct measurements of the electron-impact ionization frequency do not show a clear decrease in energetic electrons with increasing cometocentric distance, including measurements down to the surface at the end of mission (Heritier et al., 2017b). It is as yet unclear how the measurements of accelerated ions at Rosetta can be reconciled with the observations and modelling of electron density, electron-impact ionization frequency and FUV emissions.

Chapter Summary

- I have created a new dataset of the electron-impact ionization (EII) frequency throughout the Rosetta mission. Electron-impact ionization was the major ionization source at large heliocentric distances and was highly variable. Close to perihelion, photoionization was more prevalent than electron-impact ionization.
- I compared the electron-impact ionization frequency to a number of datasets from the Rosetta mission. At large heliocentric distances, electron and cometary ion density were well correlated to the EII frequency
- I have examined the source of the ionizing electrons detected at Rosetta. The EII frequency is structured by heliocentric distance and outgassing, which may result from the evolution of the ambipolar potential well throughout the Rosetta mission. The correlations of the EII frequency with magnetic field and solar wind proton properties suggests that the ionizing electrons originate in the solar wind.
- I have examined electron-impact ionization using test particle simulations. Secondary electrons are the major component of cometary electrons at low outgassing rates, most of which are generated by energetic solar wind or secondary electrons.
- I discussed the relationship between cometocentric distance and EII frequency at 67P. The data from Rosetta show no obvious correlation with cometocentric distance, although the test particle simulations suggest that EII is stronger close to the nucleus. The variation of the EII frequency with cometocentric distance remains unclear.
- I have discussed the impact of ion acceleration in the context of multi-instrument analyses of electron density. The EII frequency must be artificially increased close to the nucleus to resolve the discrepancy in inner coma, that is created if the ions undergo acceleration. If the energetic electron population is much larger close to the nucleus, a substantial discrepancy with FUV emissions would result. It is not clear how these measurements can be reconciled.

Chapter 6

Conclusions

Since the end of the Rosetta mission in September 2016, there has been a significant effort to process and consolidate the returned data and derive new data products. These were made publicly available on the ESA Planetary Science Archive in 2019. There is still much to be exploited from the Rosetta datasets, and much that is still not fully understood in the cometary environment. The future of cometary ionospheric science looks promising, with a new multi-spacecraft mission, ESA/Comet Interceptor, slated to launch with the exoplanetary mission, ESA/Ariel, in 2028 with the aim to fly by a dynamically new comet (Tinetti et al., 2018; Snodgrass and Jones, 2019). This would provide the first multipoint measurements in a cometary environment and provide the first opportunity to get a 3D picture of the coma, the plasma boundaries, and energy transfer through different plasma regions.

Section 6.1 summarizes the work in this thesis, assessing the role of electron-neutral collisions at comet 67P through data analysis and modelling. The key electron processes at a weakly outgassing comet are summarised in Figure 6.1. In section 6.2, I discuss remaining challenges that are left in the wake of Rosetta, and areas of cometary plasma science that should be explored in the future.

6.1 Summary

My thesis assesses the role of electrons in the cometary environment through two main approaches: the development and exploitation of a new collisional test particle model of cometary electrons and the analysis of data from the Rosetta mission.

A collisional model of electrons at a comet I have developed the first collisional three-dimensional model of electrons at a comet (see Chapter 2). The model incorporates a stationary model of the neutral coma, and a stationary set of electric and magnetic fields (see Section 2.5),

obtained from a kinetic, collisionless model of plasma at a weakly outgassing comet. The electron test particle model is the first to capture both the collisional processes (Section 2.3) and the three-dimensional dynamics of electrons in the coma.

The outputs of the model include particle trajectories (e.g., Figures 2.13 and 2.15), plasma density, bulk velocity, electron temperature and the energy distribution of electrons in the coma (Section 2.4). These can be separately calculated for the different electron populations within the coma: photoelectrons, solar wind electrons and secondary electrons from electron-impact ionization. Further products, such as the electron-impact ionization frequency, can be derived either directly from the stochastic collisions in the simulation or from the energy distribution of the electrons (see Section 5.2.2).

Differences between the test particle and collisionless PiC simulations are discussed in Chapter 2, particularly in relation to the ion-electron mass ratio, which is reduced in the PiC simulation ($m_p/m_e = 100$, Section 2.6.2). The electron mass directly impacts the gyroradius, and consequently the energy range of the electron in a single gyration. The difference in mass has particular impact on the solar wind flow into the domain, and the solar wind electron energies in the inner coma.

Cometary electrons are trapped in the inner coma by the ambipolar electric field, while solar wind electrons are substantially accelerated by it. The test particle model allows electron-neutral collisions to be modelled in combination with both the acceleration and trapping processes. Substantial energy degradation of electrons is seen in the coma of even a weakly outgassing comet (see Section 2.6.3 and Chapter 3).

Electron-neutral collisions feedback on the electric field within the coma (Section 2.6.3). Electron cooling close to the nucleus weakens the electron pressure gradient compared to the collisionless case, and weakens the ambipolar electric field in the inner coma. However, the total depth of the potential well is not significantly reduced, as the ambipolar field acts over a large region. This feedback may act to flatten the potential well close to the nucleus.

Cooling of electrons at a weakly outgassing comet A cold electron population can be formed from electron trapping and electron-neutral collisions for even a weakly outgassing comet ($Q = 10^{26} \text{ s}^{-1}$, Section 3.2). Cold electrons are generated by trapping, mostly cometary, electrons in a dense region of the coma by the ambipolar field. The trapping by the field causes the electron to travel much further through the densest region of the coma and makes them much more likely to undergo multiple collisions. When cooled, the electrons are transported out of the inner coma and into the tail by an $\mathbf{E} \times \mathbf{B}$ drift.

The cold population grows in density and as a fraction of the total electron density, as the

outgassing rate increases. The cold electrons are primarily generated close to the nucleus, with some asymmetry due to the transport of electrons away from the inner coma. Transport of the cold electrons also gives a region of increased density that extends tailwards.

The collisionality of the electrons in the inner coma is not well captured by radial outflow (Section 3.3). When using realistic electric and magnetic fields, the trapping of electrons in the ambipolar potential well and the gyration around the magnetic field boosts the electron depth by a factor of ~ 100 compared to the case of radial outflow. Consequently, electrons produced within the coma are much more likely to undergo collisions and to be degraded than previously thought. With this in mind, I derived a new estimate of electron exobase location for outgassing rates of $Q = 10^{26} - 1.5 \times 10^{27} \text{ s}^{-1}$ (Section 3.4). The new exobase estimate fits well with the cold electron observations from RPC/MIP and RPC/LAP. The previously unexplained cold electron observations throughout the Rosetta mission can be explained when collisional processes are combined with realistic fields in the coma.

Multi-instrument analysis of electron-induced far ultraviolet emissions from comet 67P

I applied a multi-instrument approach to model atomic FUV emissions (Lyman- β , OI1304, OI1356, CI1657 and CII1335) in the southern hemisphere of comet 67P (see Chapter 4), where strong carbon emissions were prevalent. Dissociative excitation of cometary neutrals, especially CO₂, by electron-impact is the major source of FUV emissions over the southern hemisphere away from perihelion. This is confirmed with nadir observations of the shadowed nucleus (Section 4.4), which minimized contamination of the spectra from reflected solar flux in the FUV.

The magnitude and temporal variations of emissions from the coma during impact of a CIR on 9-10th July and 4th August 2016 are well captured by the multi-instrument analysis (Section 4.5). In the limb and off-nadir viewings, the FUV line brightness is mostly driven by energetic electrons in the densest region of the coma, which was usually distant from the spacecraft. The electrons which drove the FUV emissions (probed remotely through the emission spectra) are well correlated with the electrons measured in situ at Rosetta by RPC/IES, suggesting a global acceleration process (Section 4.5.4). This correlation is consistent with acceleration of solar wind electrons in an ambipolar potential well. The close agreement between the observed and modelled emissions allows OI1356 to be used as a probe of the solar wind conditions at a weakly outgassing comet.

The source of cometary electrons A new database of the electron-impact ionization frequency throughout the Rosetta mission has been produced (Section 5.1). Electron-impact ionization frequency was highly variable during the Rosetta mission. It was the major source of cometary

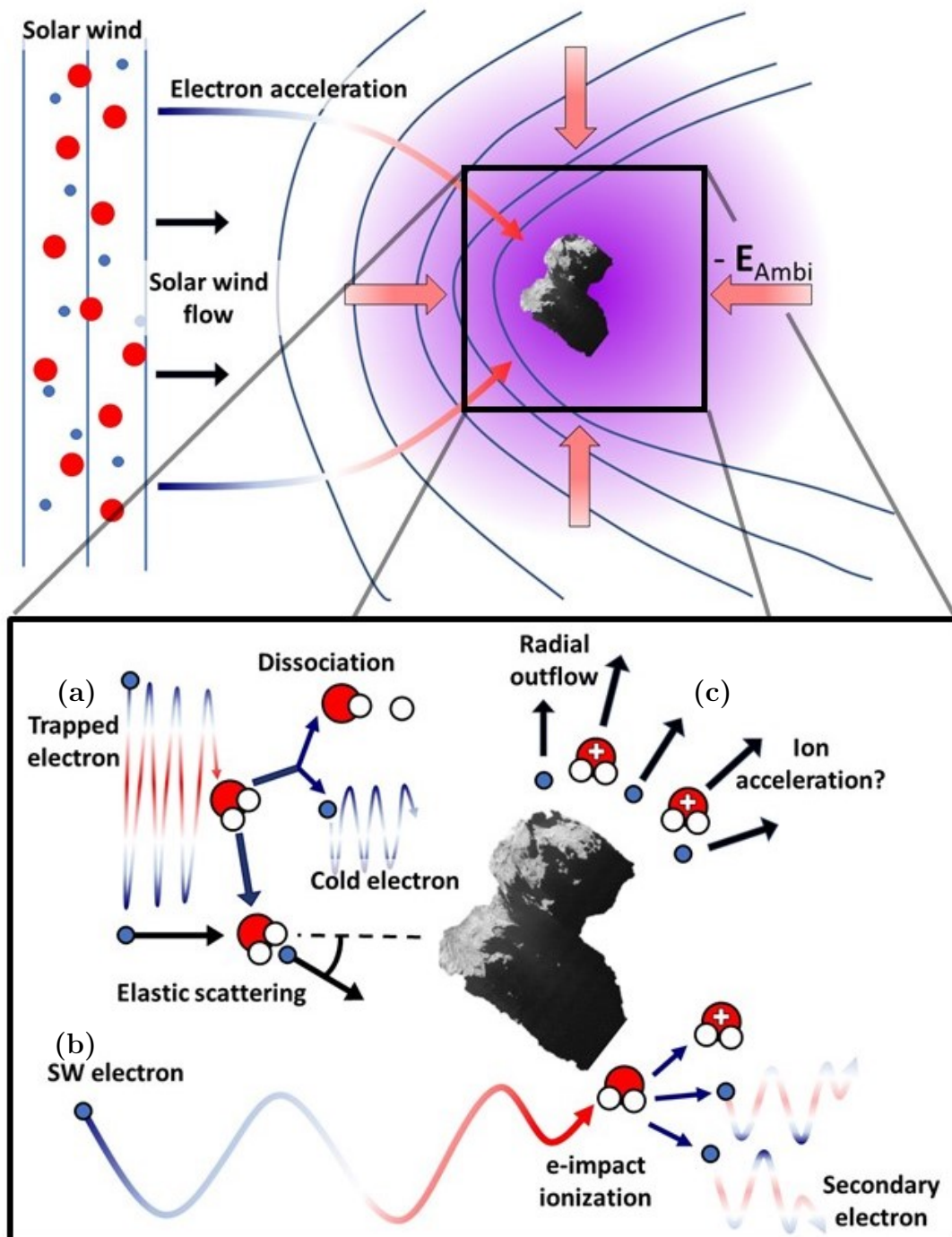


Figure 6.1: A schematic of a weakly outgassing comet. **Top** - The interaction of the solar wind with the cometary environment. The solar wind flows through the cometary environment, where it is slowed by mass loading. The solar wind magnetic field (blue lines) drapes around the cometary ionosphere (pink cloud), and piles up in the coma. An ambipolar field is set up around the nucleus (red arrows) by the warm cometary electrons. The field accelerates solar wind electrons into the inner coma. **Bottom** - Collisional electrons in the coma. (a) A cometary electron is generated by ionization in the coma (either photoionization or electron impact) and is trapped by the ambipolar potential well. It undergoes collisions with the neutral coma, being degraded in energy or elastically scattered. After enough collisions, the cometary electron becomes cold. (b) An accelerated solar wind electron ionizes a neutral molecule, generating a secondary electron in the coma. (c) Ions flow away from the nucleus in the inner coma and may undergo some acceleration.

electrons at large heliocentric distances (Section 5.1.2). Closer to perihelion, electron-impact ionization frequency was weaker than photoionization and was much less variable than seen at large heliocentric distances. The total electron density was driven by electron-impact ionization far from perihelion. Correlation was also found between the electron-impact ionization frequency and the spacecraft potential.

Test particle simulations corroborate that electron-impact ionization, rather than photoionization, is the major source of cometary electrons for a weakly outgassing comet (Section 5.2.1). Solar wind electrons were found to have comparable densities to photoelectrons within the coma, although only one set of solar wind conditions have been tested.

Electron-impact ionization was dependent on the outgassing rate throughout the Rosetta mission, but the relationship was non-linear. This may be caused by the increasing depth of the ambipolar potential well, as the outgassing rate increases, which is then mitigated as electron-neutral collisions become frequent (Section 5.1.3).

Magnetic field strength was highly correlated with electron-impact ionization, suggesting the electrons are denser and more energetic in regions of increased pile-up and may be of solar wind origin. The relationship between magnetic field strength and electron-impact ionization frequency was also observed in the test particle simulations (Section 5.2.2).

The simulations show that the ionizing electrons, seen in the coma, originate in the solar wind for low outgassing rates, and are accelerated by the ambipolar potential well. Photoelectrons have only a minor contribution to the electron-impact ionization frequency. The correlation of the ionization frequency with properties of the solar wind protons at Rosetta, supports this conclusion (Section 5.1.3).

The variation of the electron-impact ionization frequency with cometocentric distance is unclear (Section 5.3). Data from Rosetta does not show a clear correlation between ionization frequency and cometocentric distance, except at large distances, $r > 200$ km, around perihelion. The response of the electron-impact ionization frequency to sharp changes in cometocentric distance was found to be variable, with both positive and negative correlations observed. The test particle simulations indicate that the ionization frequency increases closer to the nucleus. However, the feedback of collisional processes on the field may weaken the relationship close to the comet.

High electron-impact ionization frequencies close to the nucleus have been proposed in order to reconcile recent measurements of accelerated cometary ions with the measured electron densities. Arbitrarily increasing electron-impact ionization would greatly impact the brightness of FUV emissions in the coma, which are well captured through a multi-instrument approach. Therefore, it is unlikely that the energetic electron population is greatly enhanced in the inner coma.

6.2 Future Work

There are many outstanding questions that remain to be answered in the wake of Rosetta, many of which relate to the collisionality of electrons. Thus, further development of the collisional electron models have great potential towards improving our understanding of the cometary environment.

Firstly, the test particle model could better represent the environment of 67P, that was probed by Rosetta. This includes improving the model of the neutral coma, introducing day-night and/or north-south asymmetries. Additionally, more species (CO_2 , CO , O_2) could be included as an input to the model. With better refinement of the coma model, products such as the FUV atomic emission line brightnesses could be computed and compared with observations from Rosetta. Other cooling processes, such as Coulomb collisions, could also be included.

Secondly, electron-neutral collisions could be incorporated into the fully-kinetic PiC model. This would allow electron-neutral collisions to feedback on the fields in the cometary environment. The complexity of the collisional processes that can be implemented is likely to be limited due to computational constraints. However, any limitations of the implemented collisional approach could be assessed using a test particle model, such as the one developed here (see Chapter 2). With fields calculated self-consistently in a collisional PiC model, higher outgassing rates could be simulated.

The diamagnetic cavity is poorly understood at 67P. It is unclear what the key forces at the boundary are and what is in balance. At Rosetta, the cavity boundary was seen to be correlated with the electron exobase (Henri et al., 2017), suggesting electrons play a substantial role in its formation. A 3D collisional electron model at high outgassing rates may help to shine light on the key processes taking place at the cavity boundary.

Finally, there are many avenues of future work in analysing the FUV emissions from the coma of 67P. The electron-induced emissions from the coma of 67P have yet to be modelled where the coma is collisional. In this scenario, the energetic electron population is variable along the line of sight of the FUV spectrograph and any long-lived states are subject to quenching. Once the electron flux is better constrained throughout the highly-outgassing coma, FUV emissions can be modelled through a multi-instrument approach. At lower outgassing rates, other emission features, such as $\text{OI}6300$, may be driven by electron-impact ionization, but this has not yet been modelled using the electron population measured at Rosetta.

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